LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099513.D
Acq On : 15 Oct 2017 14:57
Operator : SJ/JU
Sample : I5752-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-118-7(0-5)

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-BF092317.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	5.069	504	507	524	rBV	311759	453352	17.86%	1.717%
2	5.469	571	575	591	rBV	2199842	2426859	95.58%	9.190%
3	6.487	742	748	766	rBV	2095171	2539074	100.00%	9.615%
4	6.616	766	770	773	rBV	2608336	2475271	97.49%	9.374%
5	6.845	805	809	816	rBV	708614	609005	23.99%	2.306%
6	6.998	831	835	839	rBV	2117547	1884690	74.23%	7.137%
7	7.410	900	905	908	rBV	1607590	1512654	59.58%	5.728%
8	8.122	1023	1026	1030	rBV	856740	817613	32.20%	3.096%
9	8.681	1117	1121	1131	rBV	327627	250202	9.85%	0.947%
10	9.198	1204	1209	1212	rBV	2781022	2526710	99.51%	9.568%
11	9.592	1273	1276	1279	rBV	817074	619545	24.40%	2.346%
12	9.880	1321	1325	1328	rBV	958285	791508	31.17%	2.997%
13	9.910	1328	1330	1336	rVB	58697	48100	1.89%	0.182%
14	10.086	1356	1360	1363	rVB	41426	38098	1.50%	0.144%
15	10.428	1414	1418	1423	rVB	57598	49409	1.95%	0.187%
16	10.592	1442	1446	1450	rVB	1094474	902023	35.53%	3.416%
17	10.675	1456	1460	1463	rBV	1271403	1210588	47.68%	4.584%
18	10.922	1499	1502	1506	rBV	54012	50221	1.98%	0.190%
19	10.975	1506	1511	1514	rBV	223173	218751	8.62%	0.828%
20	11.004	1514	1516	1517	rVV	36330	32303	1.27%	0.122%
21	11.022	1517	1519	1523	rVB	36240	30687	1.21%	0.116%
22	11.269	1558	1561	1564	rVB2	50338	42325	1.67%	0.160%
23	11.369	1574	1578	1580	rBV	807855	664760	26.18%	2.517%
24	11.392	1580	1582	1586	rVV	457587	343965	13.55%	1.303%
25	11.445	1586	1591	1595	rVV	100898	85946	3.38%	0.325%
26	11.604	1612	1618	1622	rBV	29684	36279	1.43%	0.137%
27	11.869	1658	1663	1666	rBV2	46723	54797	2.16%	0.208%
28	11.898	1666	1668	1673	rVB2	61860	56289	2.22%	0.213%
29	11.980	1679	1682	1685	rBV	51648	55818	2.20%	0.211%
30	12.404	1751	1754	1755	rBV2	23328	26715	1.05%	0.101%
31	12.580	1781	1784	1790	rBV	341229	304073	11.98%	1.151%
32	12.810	1817	1823	1829	rBV	275813	312470	12.31%	1.183%
33	12.951	1843	1847	1850	rVB	1735921	1504775	59.26%	5.698%
34	13.139	1872	1879	1882	rBV2	33621	53066	2.09%	0.201%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099513.D
Acq On : 15 Oct 2017 14:57
Operator : SJ/JU
Sample : I5752-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-118-7(0-5)

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.833	1992	1997	2001	rBV4	79680	104965	4.13%	0.397%
36	14.010	2022	2027	2030	rBV2	669517	701219	27.62%	2.655%
37	14.039	2030	2032	2039	rVB	129024	122634	4.83%	0.464%
38	14.898	2175	2178	2181	rVB4	24754	28328	1.12%	0.107%
39	15.051	2200	2204	2208	rBV	116919	189723	7.47%	0.718%
40	15.163	2221	2223	2227	rVB	27607	32272	1.27%	0.122%
41	15.357	2252	2256	2262	rVB	79514	108149	4.26%	0.410%
42	15.421	2263	2267	2271	rBV	113322	140371	5.53%	0.532%
43	15.480	2271	2277	2282	rBV	508175	737438	29.04%	2.793%
44	15.898	2344	2348	2355	rVB	126325	183851	7.24%	0.696%
45	16.398	2428	2433	2448	rVB	149064	293848	11.57%	1.113%
46	16.980	2524	2532	2540	rBV4	126292	317517	12.51%	1.202%
47	17.415	2602	2606	2613	rVB	38412	75302	2.97%	0.285%
48	17.674	2643	2650	2664	rVB4	88804	226597	8.92%	0.858%
49	18.503	2784	2791	2801	rVB3	41824	116695	4.60%	0.442%

Sum of corrected areas: 26406850

LSC Report - Integrated Chromatogram

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Data File : BF099513.D
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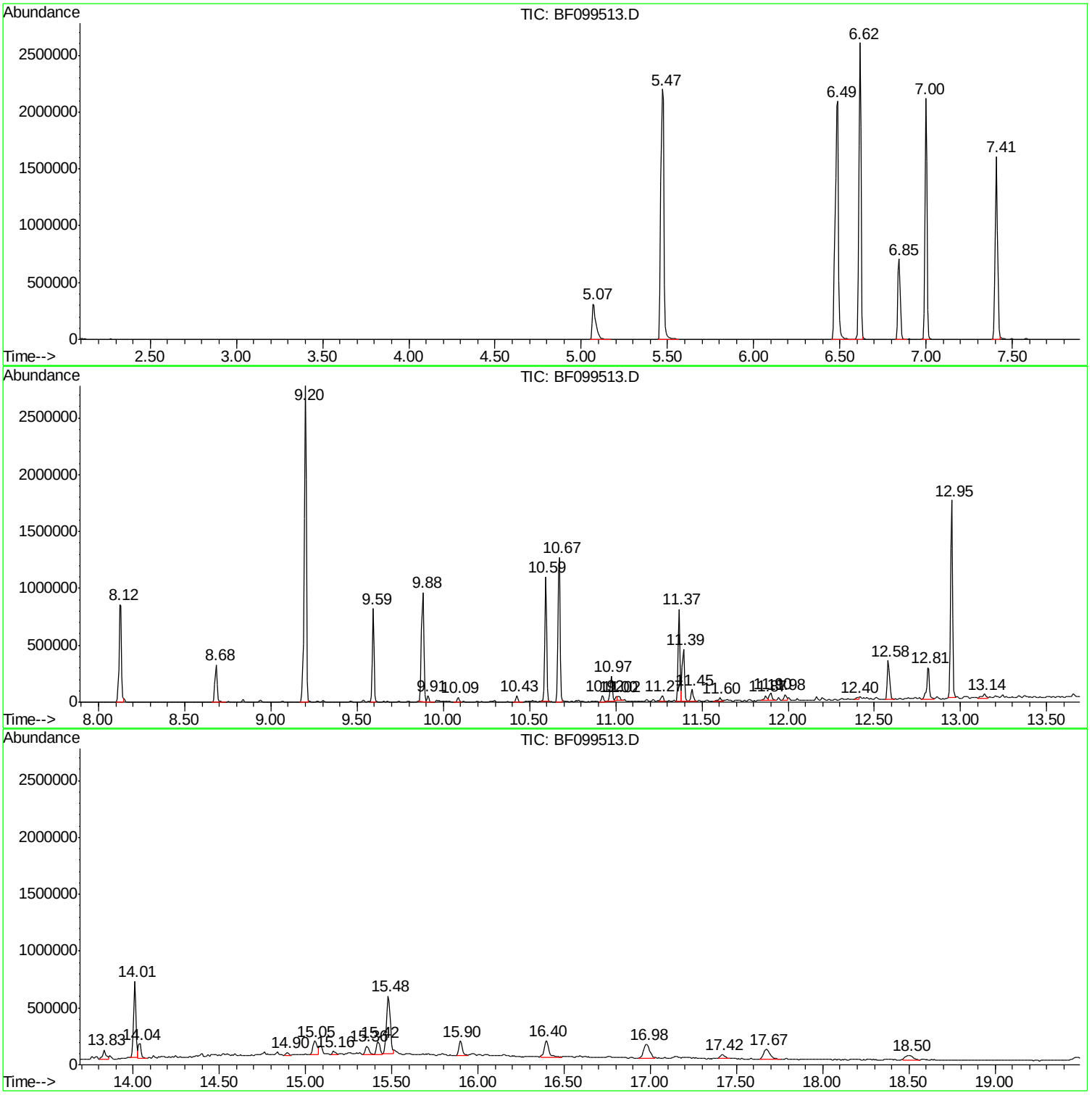
Operator : SJ/JU
Sample : I5752-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-118-7(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099513.D
Acq On : 15 Oct 2017 14:57
Operator : SJ/JU
Sample : I5752-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-118-7(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

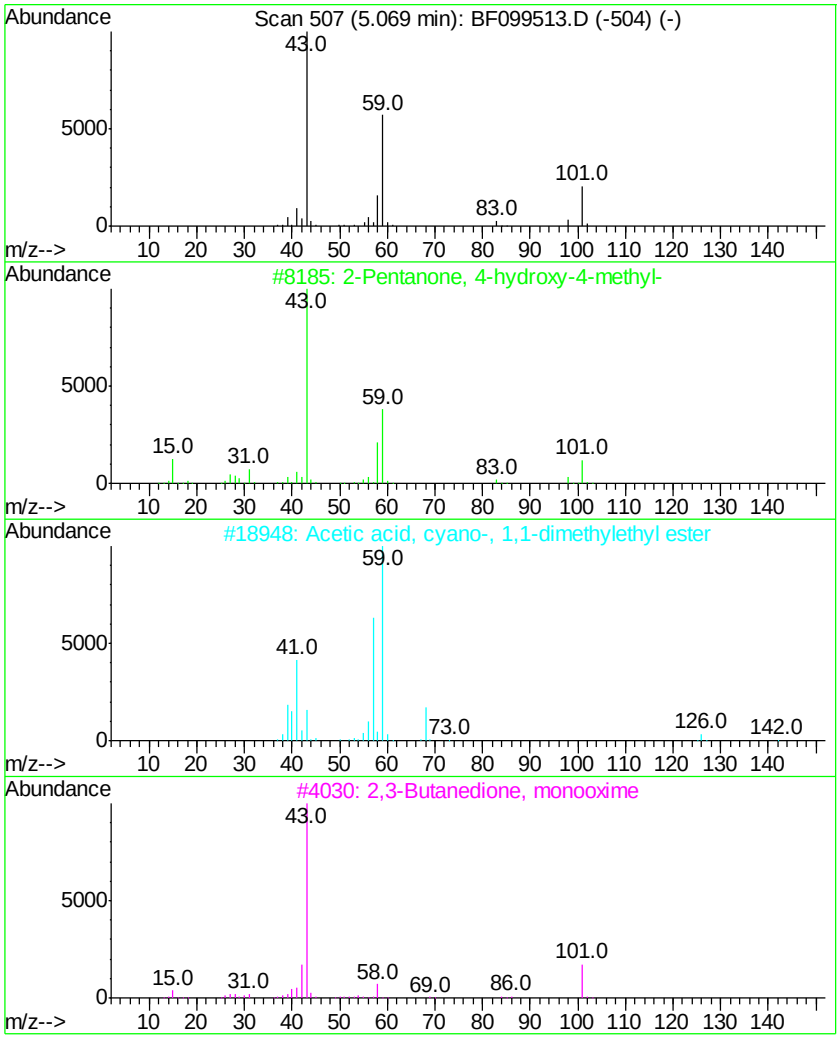
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

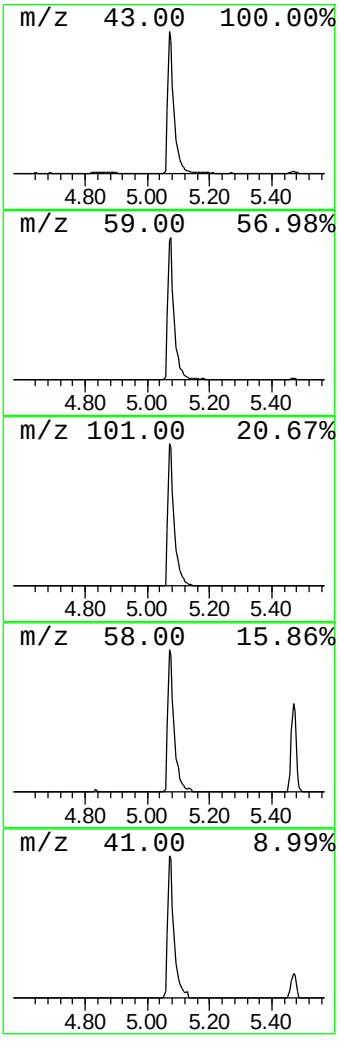
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	14.89 ng	453352	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9





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Operator : SJ/JU
Sample : I5752-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-118-7(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

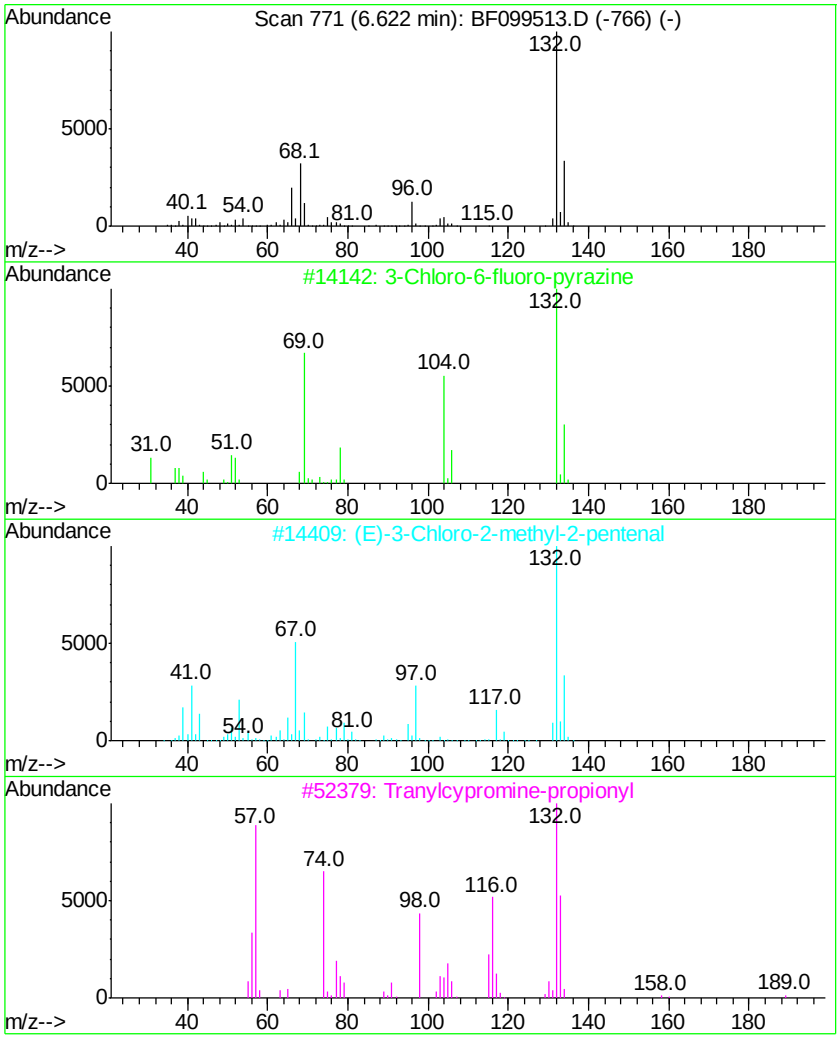
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

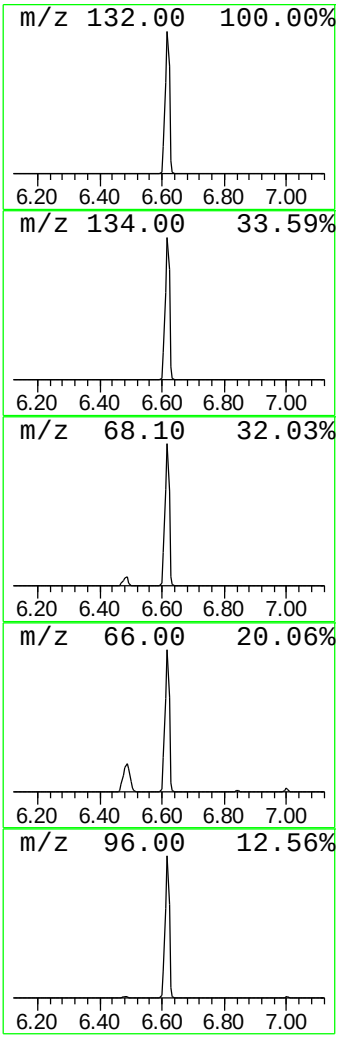
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	81.29 ng	2475270	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099513.D
Acq On : 15 Oct 2017 14:57
Operator : SJ/JU
Sample : I5752-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-118-7(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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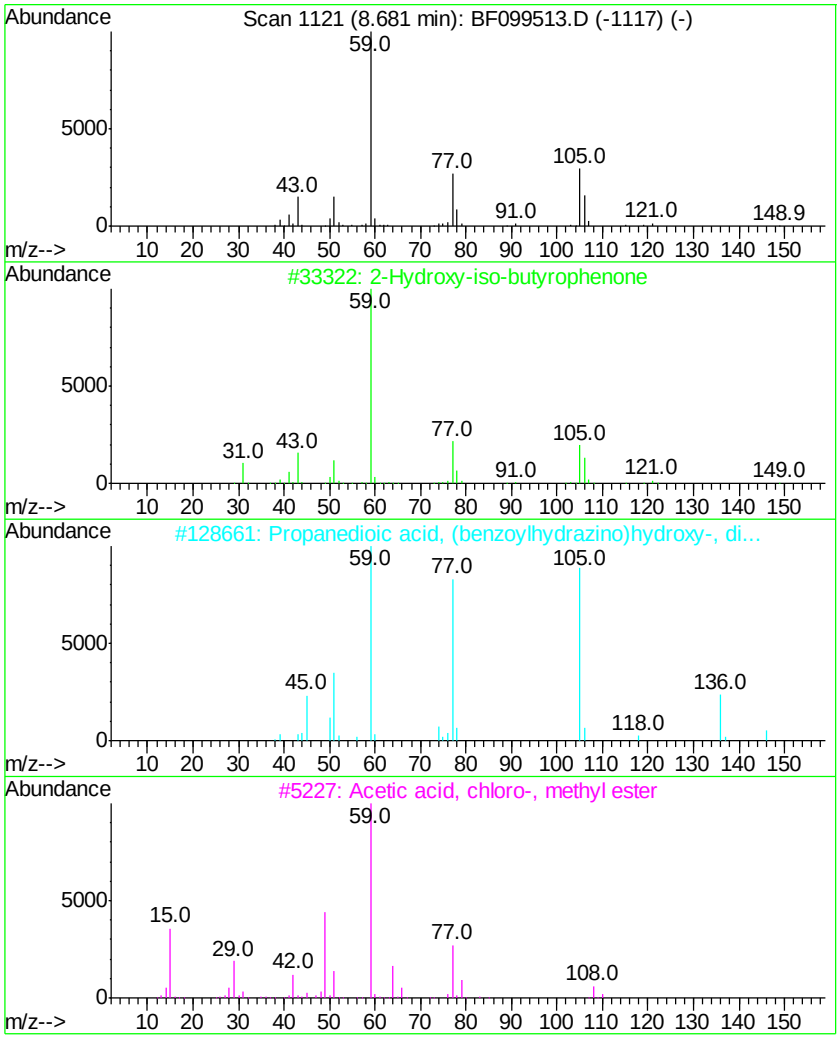
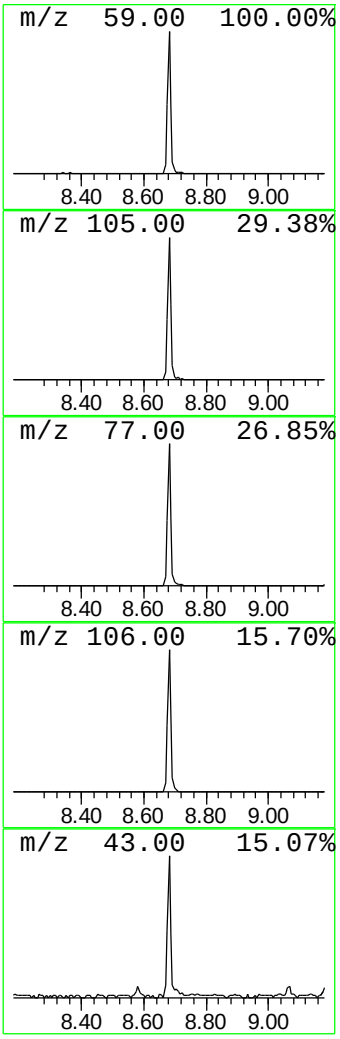
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.68	6.12 ng	250202	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Propanedioic acid, (benzoylhydra...	282	C12H14N2O6	1000142-99-9	23
3	Acetic acid, chloro-, methyl ester	108	C3H5ClO2	000096-34-4	9
4	Ethanone, 2-amino-1-phenyl-	135	C8H9NO	000613-89-8	9
5	Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	9





Library Search Compound Report

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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-118-7(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

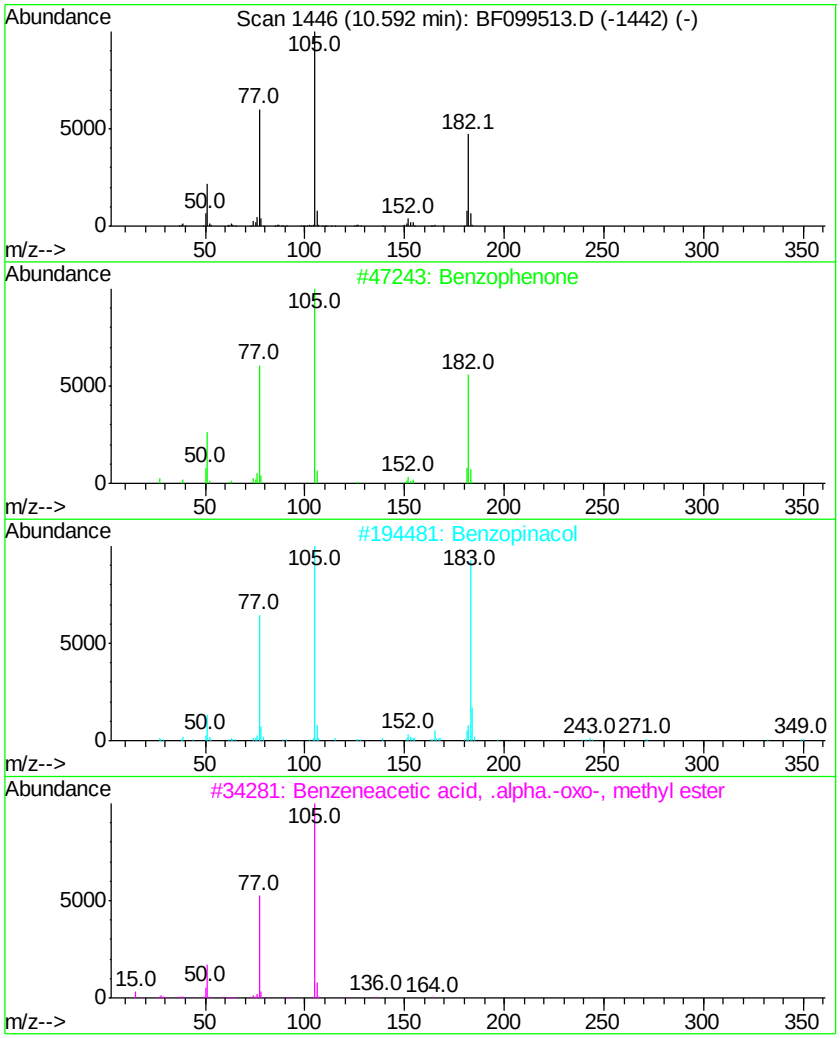
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

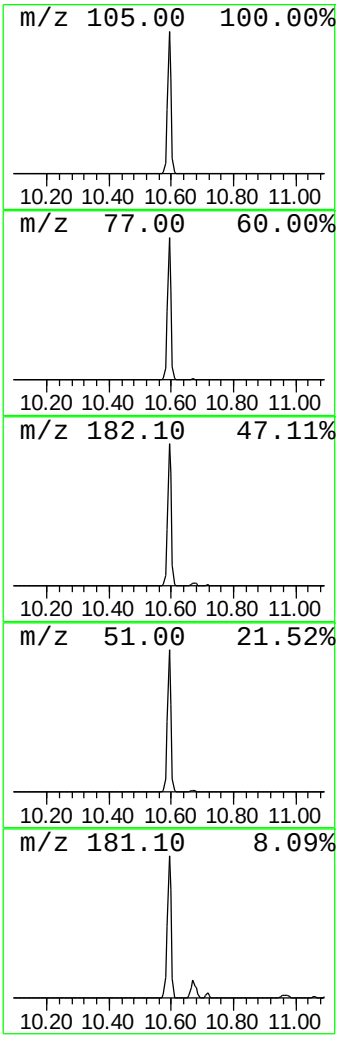
****

Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	22.79 ng	902023	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzopinacol	366	C26H22O2	000464-72-2	47
3	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
4	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47





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Misc :
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Instrument : BNA_F
ClientSampleId : ENV-118-7(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

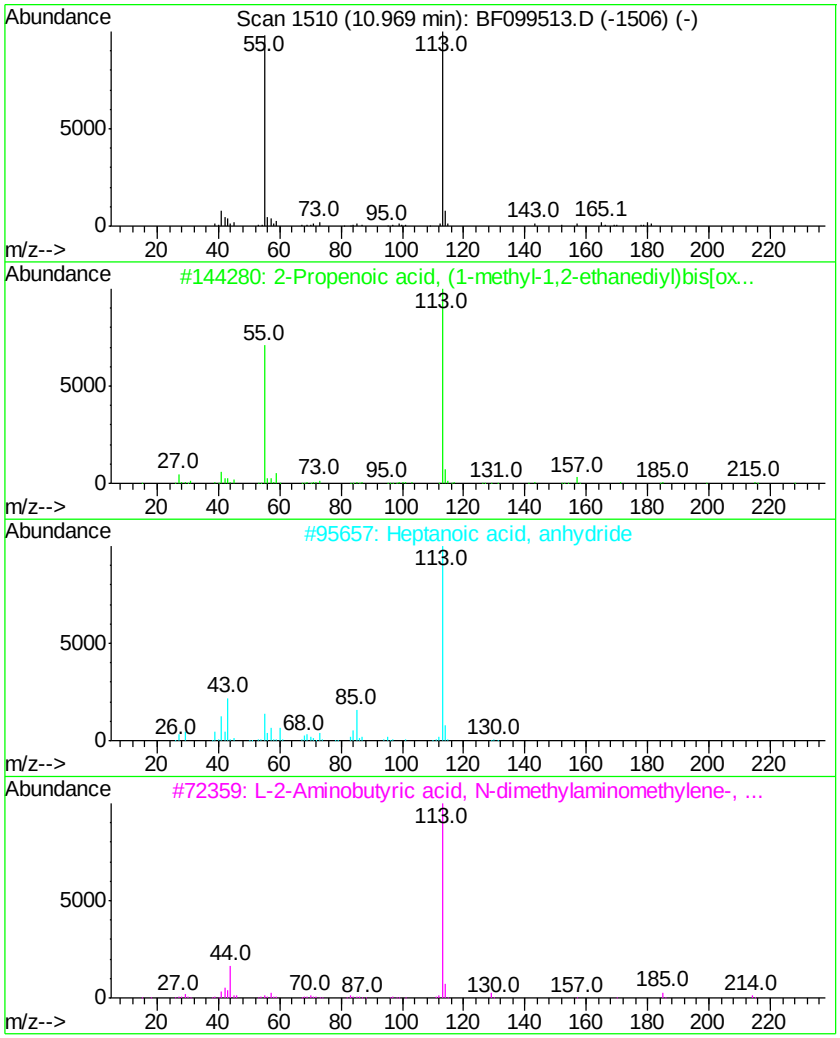
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

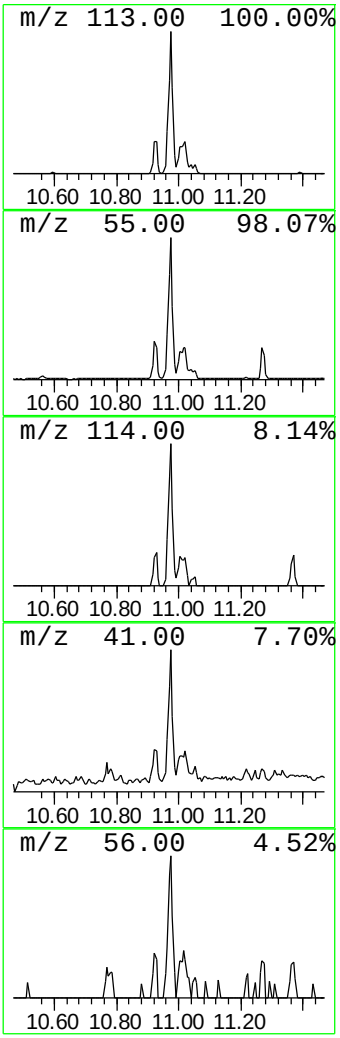
****

Peak Number 6 2-Propenoic acid, (1-methyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.97	6.58 ng	218751	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, (1-methyl-1,2-...	300	C15H24O6	042978-66-5	78
2	Heptanoic acid, anhydride	242	C14H26O3	000626-27-7	36
3	L-2-Aminobutyric acid, N-dimethy...	214	C11H22N2O2	1000375-52-5	33
4	Propanedioic acid, 2-propenyl-, ...	172	C8H12O4	040637-56-7	9
5	Vardenafil	488	C23H32N6O4S	224785-90-4	9





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Acq On : 15 Oct 2017 14:57
Operator : SJ/JU
Sample : I5752-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-118-7(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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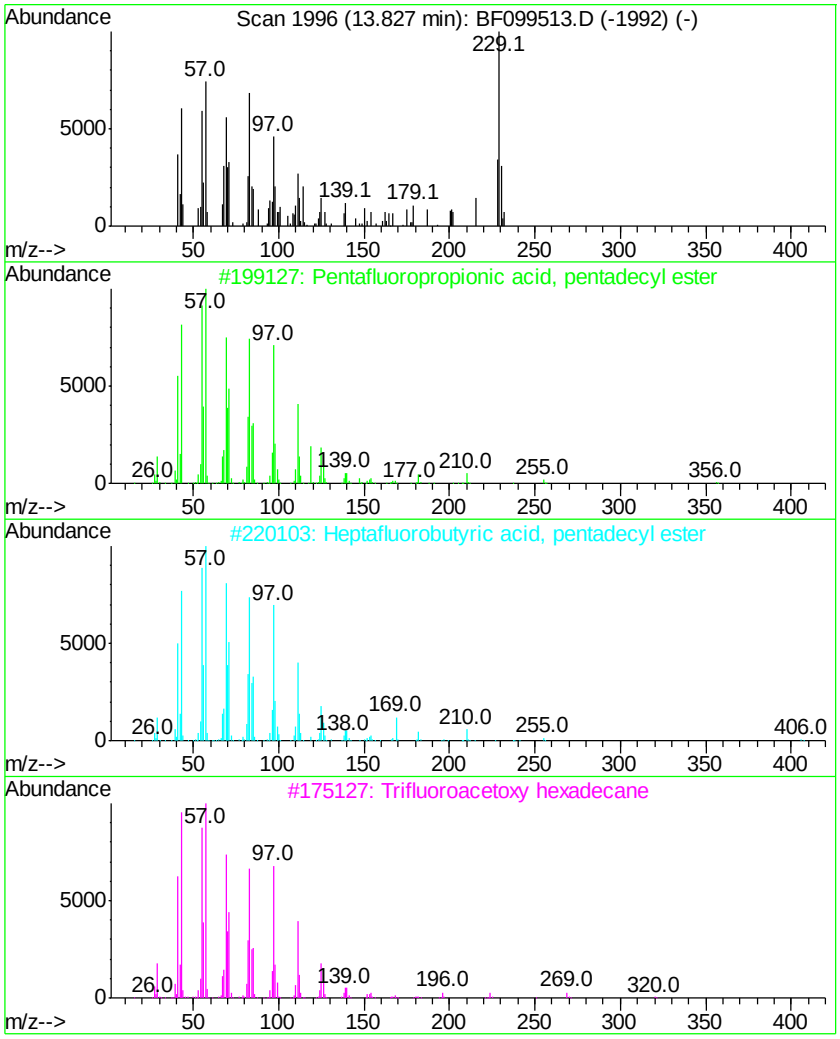
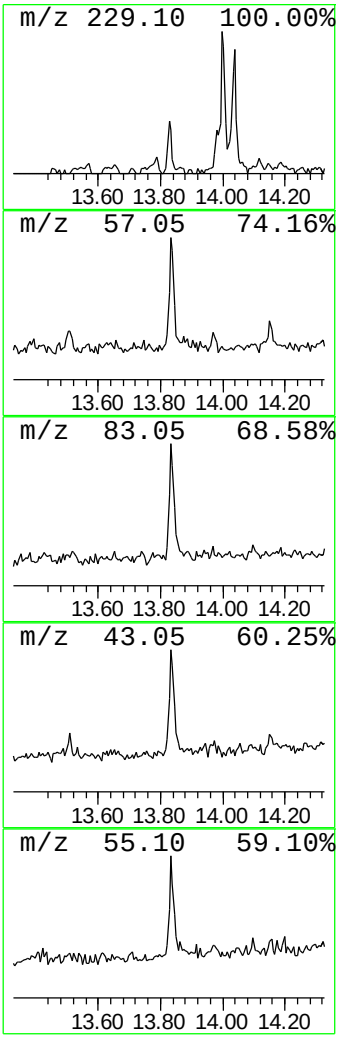
Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.99 ng	104965	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4	1-Heptacosanol	396	C27H56O	002004-39-9	93
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93





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Sample : I5752-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-118-7(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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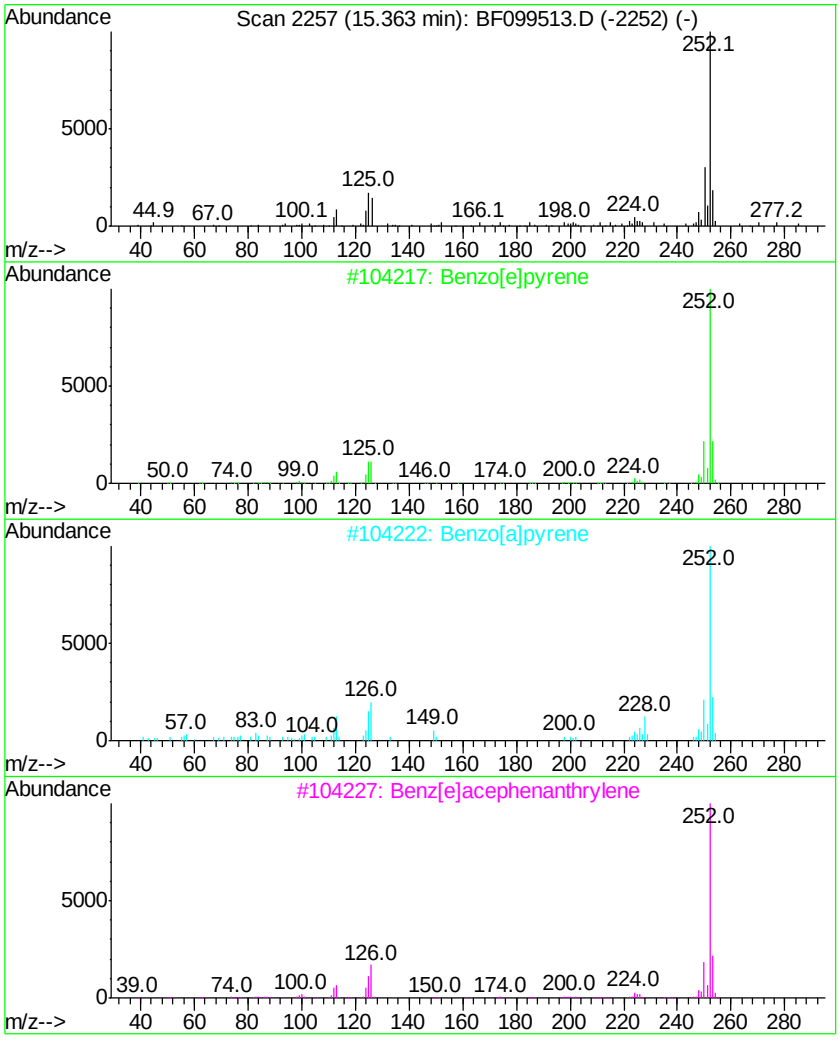
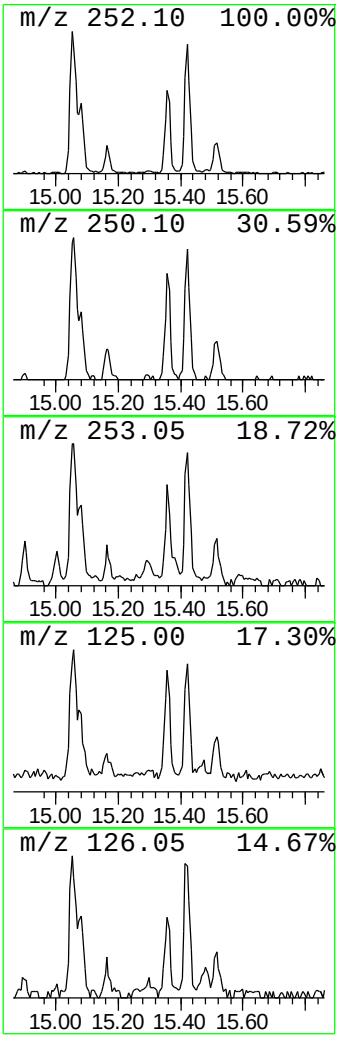
Peak Number 8 Benzo[e]pyrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	2.93 ng	108149	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[a]pyrene	252	C20H12	000050-32-8	94
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5	Perylene	252	C20H12	000198-55-0	90





Library Search Compound Report

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Data File : BF099513.D
Acq On : 15 Oct 2017 14:57
Operator : SJ/JU
Sample : I5752-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-118-7(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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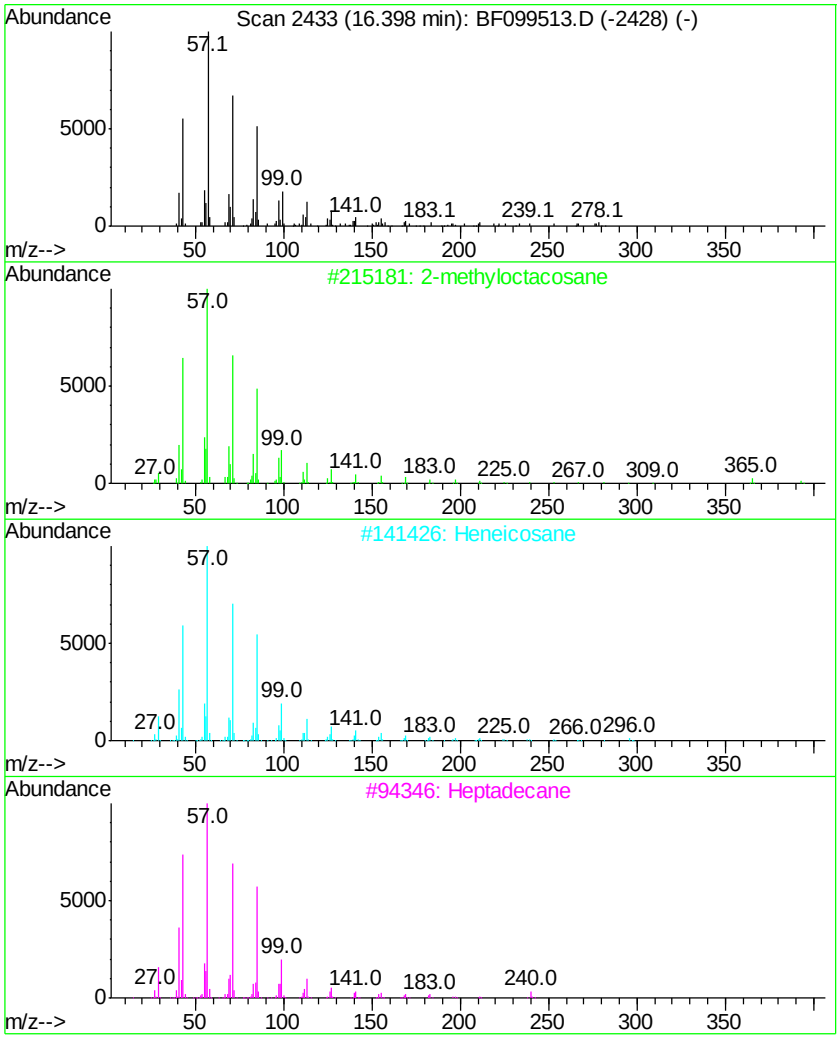
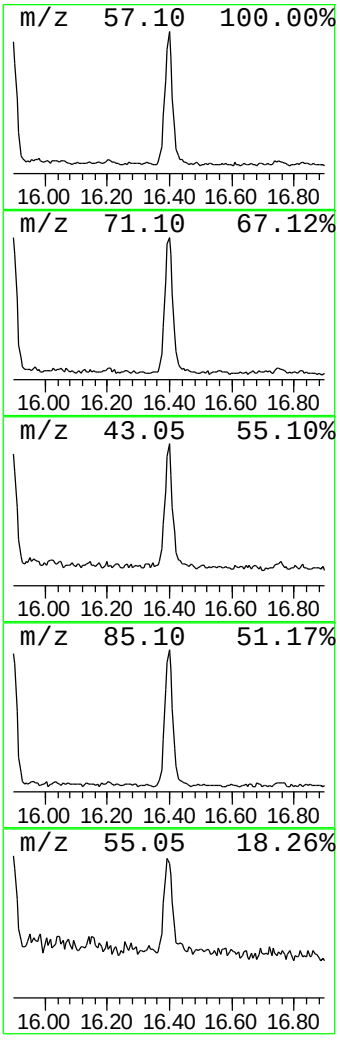
Peak Number 10 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	7.97 ng	293848	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Heptadecane	240	C17H36	000629-78-7	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Octacosane	394	C28H58	000630-02-4	90





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Operator : SJ/JU
Sample : I5752-03
Misc :
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Instrument : BNA_F
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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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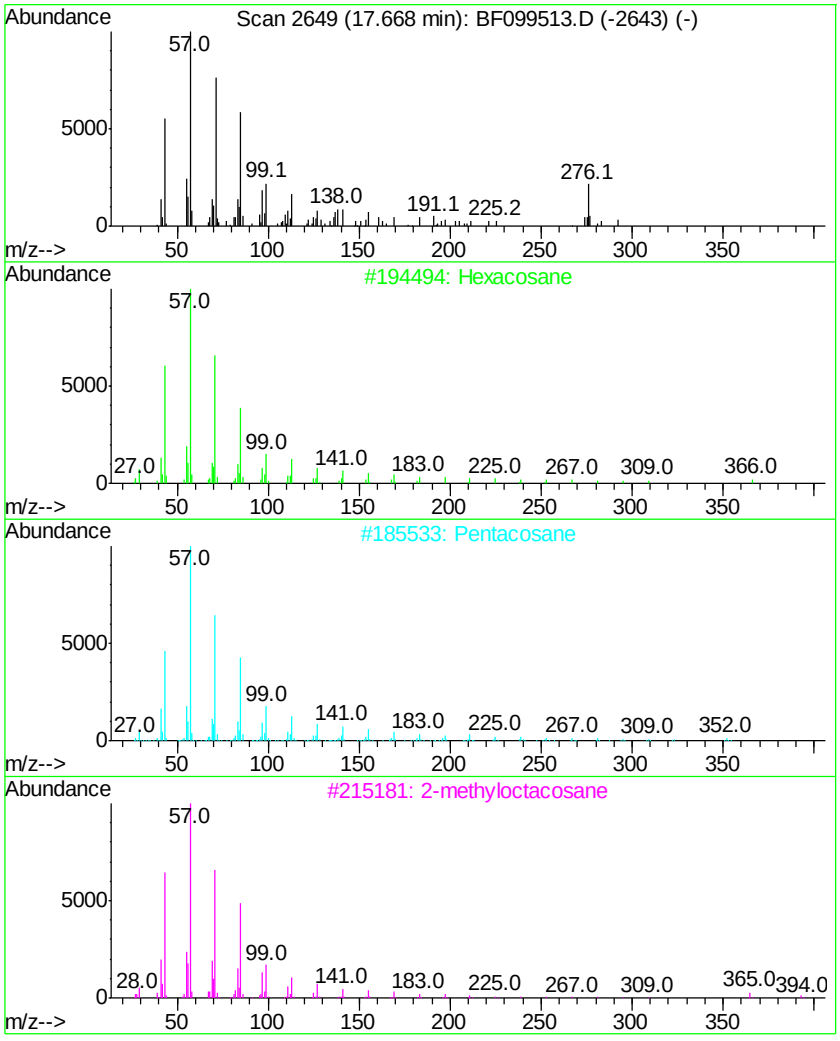
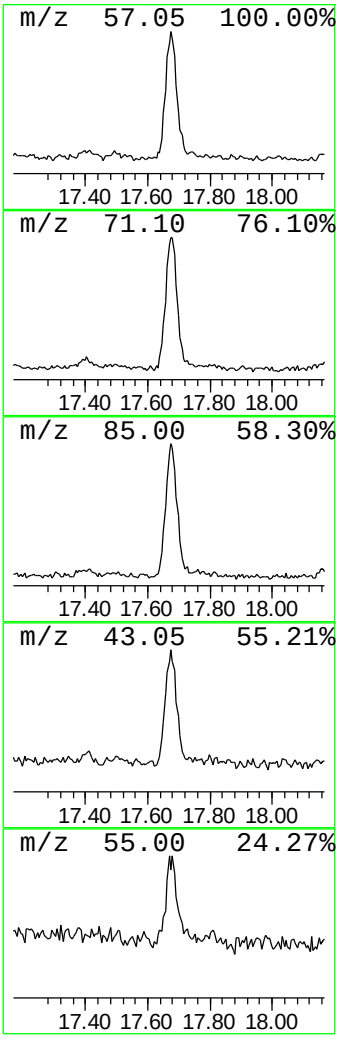
Peak Number 11 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.67	6.15 ng	226597	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	76
2	Pentacosane	352	C25H52	000629-99-2	76
3	2-methyloctacosane	408	C29H60	1000376-72-8	76
4	Heneicosane	296	C21H44	000629-94-7	70
5	Triacontane	422	C30H62	000638-68-6	68





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Acq On : 15 Oct 2017 14:57
Operator : SJ/JU
Sample : I5752-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-118-7(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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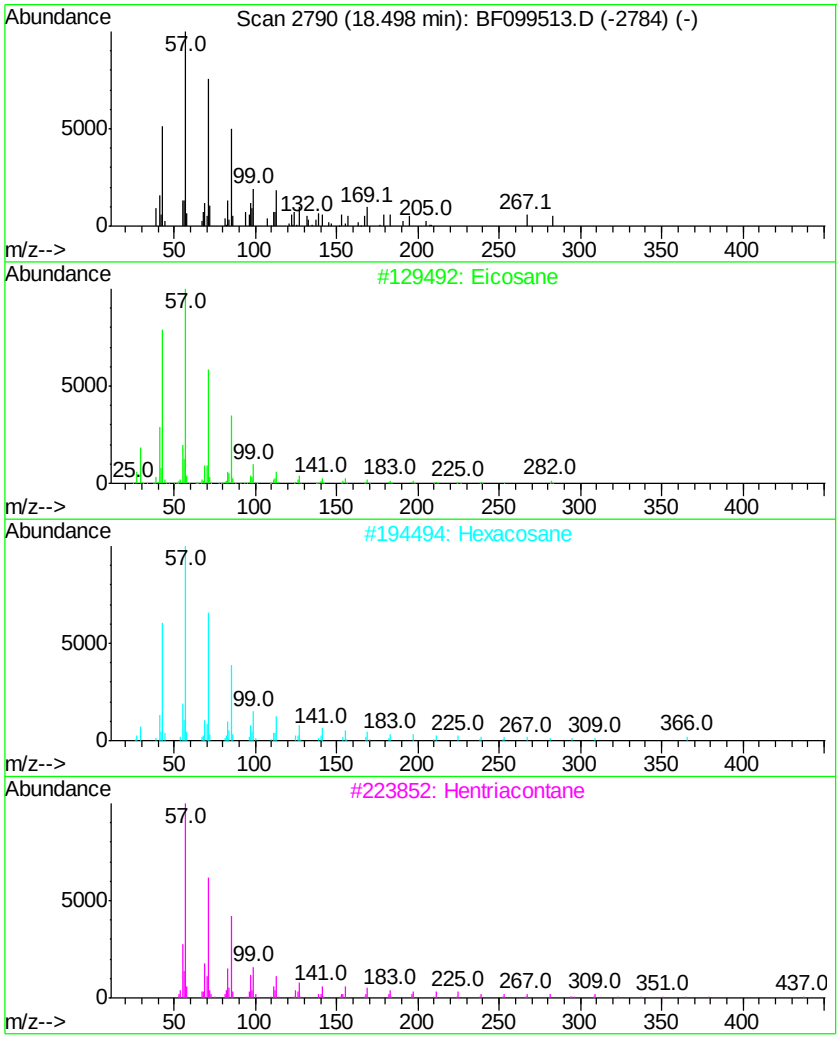
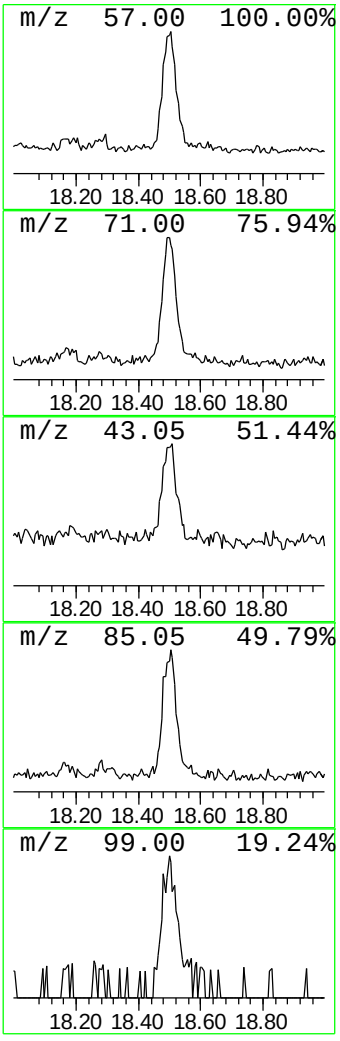
Peak Number 12 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.50	3.16 ng	116695	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Hexacosane	366	C26H54	000630-01-3	87
3	Hentriacontane	437	C31H64	000630-04-6	83
4	Pentacosane	352	C25H52	000629-99-2	83
5	Nonacosane	408	C29H60	000630-03-5	80





Tentatively Identified Compound (LSC) summary

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Data File : BF099513.D
Acq On : 15 Oct 2017 14:57
Operator : SJ/JU
Sample : I5752-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-118-7(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	5.07	14.9	ng	453352	1	6.85	609005	20.0
unknown6.62	6.62	81.3	ng	2475270	1	6.85	609005	20.0
2-Hydroxy-iso-but...	8.68	6.1	ng	250202	2	8.13	817613	20.0
Benzophenone	10.59	22.8	ng	902023	3	9.88	791508	20.0
2-Propenoic acid,...	10.97	6.6	ng	218751	4	11.37	664760	20.0
Pentafluoropropio...	13.83	3.0	ng	104965	5	14.01	701219	20.0
Benzo[e]pyrene	15.36	2.9	ng	108149	6	15.49	737438	20.0
2-methyloctacosane	16.40	8.0	ng	293848	6	15.49	737438	20.0
Hexacosane	17.67	6.2	ng	226597	6	15.49	737438	20.0
Eicosane	18.50	3.2	ng	116695	6	15.49	737438	20.0