LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
Data File : BF101217.D
Acq On : 7 Dec 2017 20:40
Operator : SJ/JU
Sample : I6615-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-2-OW(0-10)

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-BF113017.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	516	rBV	47724	62865	5.60%	0.566%
2	5.469	571	575	595	rBV	986878	1033707	92.11%	9.305%
3	6.487	743	748	766	rBV	984399	1072380	95.56%	9.653%
4	6.616	766	770	773	rBV	1256041	1070722	95.41%	9.638%
5	6.839	805	808	812	rBV	319060	252174	22.47%	2.270%
6	6.998	831	835	838	rBV	1023467	840026	74.85%	7.562%
7	7.251	875	878	882	rVB	23338	19420	1.73%	0.175%
8	7.410	897	905	908	rBV	644155	613102	54.63%	5.519%
9	8.122	1023	1026	1030	rBV	344139	299605	26.70%	2.697%
10	9.198	1205	1209	1212	rBV	1306065	1122250	100.00%	10.102%
11	9.592	1273	1276	1279	rBV	53158	41632	3.71%	0.375%
12	9.798	1307	1311	1316	rBV	21434	19580	1.74%	0.176%
13	9.880	1321	1325	1329	rVV2	348890	288654	25.72%	2.598%
14	10.298	1393	1396	1399	rVB	26825	22677	2.02%	0.204%
15	10.675	1456	1460	1463	rBV	657860	548172	48.85%	4.935%
16	10.775	1474	1477	1482	rBV	28456	31958	2.85%	0.288%
17	11.222	1550	1553	1556	rBV2	31803	26714	2.38%	0.240%
18	11.374	1575	1579	1581	rBV	309331	279088	24.87%	2.512%
19	11.398	1581	1583	1586	rVV	106995	87606	7.81%	0.789%
20	11.445	1589	1591	1594	rBV	20754	17130	1.53%	0.154%
21	11.539	1603	1607	1611	rBV3	7582	13266	1.18%	0.119%
22	11.892	1661	1667	1675	rBV3	68507	93011	8.29%	0.837%
23	11.986	1680	1683	1686	rBV2	20019	23485	2.09%	0.211%
24	12.057	1692	1695	1700	rBV2	14893	12941	1.15%	0.116%
25	12.427	1752	1758	1759	rBV3	12346	16200	1.44%	0.146%
26	12.592	1782	1786	1789	rBV	175603	158800	14.15%	1.429%
27	12.680	1798	1801	1806	rVB5	19318	18750	1.67%	0.169%
28	12.774	1814	1817	1819	rBV	27735	21355	1.90%	0.192%
29	12.821	1822	1825	1828	rVB	167537	138865	12.37%	1.250%
30	12.963	1844	1849	1852	rBV	969911	908864	80.99%	8.181%
31	13.039	1858	1862	1866	rBV5	11567	18399	1.64%	0.166%
32	13.127	1873	1877	1879	rBV5	12922	17627	1.57%	0.159%
33	13.151	1879	1881	1883	rVV2	21507	18272	1.63%	0.164%
34	13.204	1887	1890	1894	rVB4	16416	20499	1.83%	0.185%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
Data File : BF101217.D
Acq On : 7 Dec 2017 20:40
Operator : SJ/JU
Sample : I6615-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-2-OW(0-10)

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-BF113017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.251	1894	1898	1901	rBV2	28158	30369	2.71%	0.273%
36	13.380	1916	1920	1921	rBV3	14652	15236	1.36%	0.137%
37	13.433	1924	1929	1934	rBV	355294	412255	36.73%	3.711%
38	13.510	1939	1942	1946	rVV2	23518	33506	2.99%	0.302%
39	13.633	1960	1963	1965	rBV3	10792	14168	1.26%	0.128%
40	13.663	1965	1968	1972	rVB	19824	21830	1.95%	0.197%
41	13.821	1993	1995	1996	rBV2	15662	15165	1.35%	0.137%
42	13.845	1996	1999	2002	rVB	130831	131707	11.74%	1.186%
43	14.021	2025	2029	2032	rBV2	310641	336270	29.96%	3.027%
44	14.045	2032	2033	2036	rVB	64349	51922	4.63%	0.467%
45	14.115	2043	2045	2047	rBV2	16096	16005	1.43%	0.144%
46	14.180	2054	2056	2060	rVB	29286	25005	2.23%	0.225%
47	14.268	2069	2071	2075	rVB2	28733	34195	3.05%	0.308%
48	14.463	2101	2104	2110	rVB5	37537	60037	5.35%	0.540%
49	14.627	2128	2132	2139	rBV2	59433	97051	8.65%	0.874%
50	15.068	2204	2207	2211	rBV	48522	71199	6.34%	0.641%
51	15.374	2256	2259	2266	rVB2	44233	61168	5.45%	0.551%
52	15.439	2266	2270	2275	rVB	50549	71451	6.37%	0.643%
53	15.504	2275	2281	2285	rBV	167094	236728	21.09%	2.131%
54	16.609	2467	2469	2476	rVB6	19837	31621	2.82%	0.285%
55	16.992	2529	2534	2543	rVB7	30227	79513	7.09%	0.716%
56	17.445	2608	2611	2618	rVB	18424	32736	2.92%	0.295%

Sum of corrected areas: 11108933

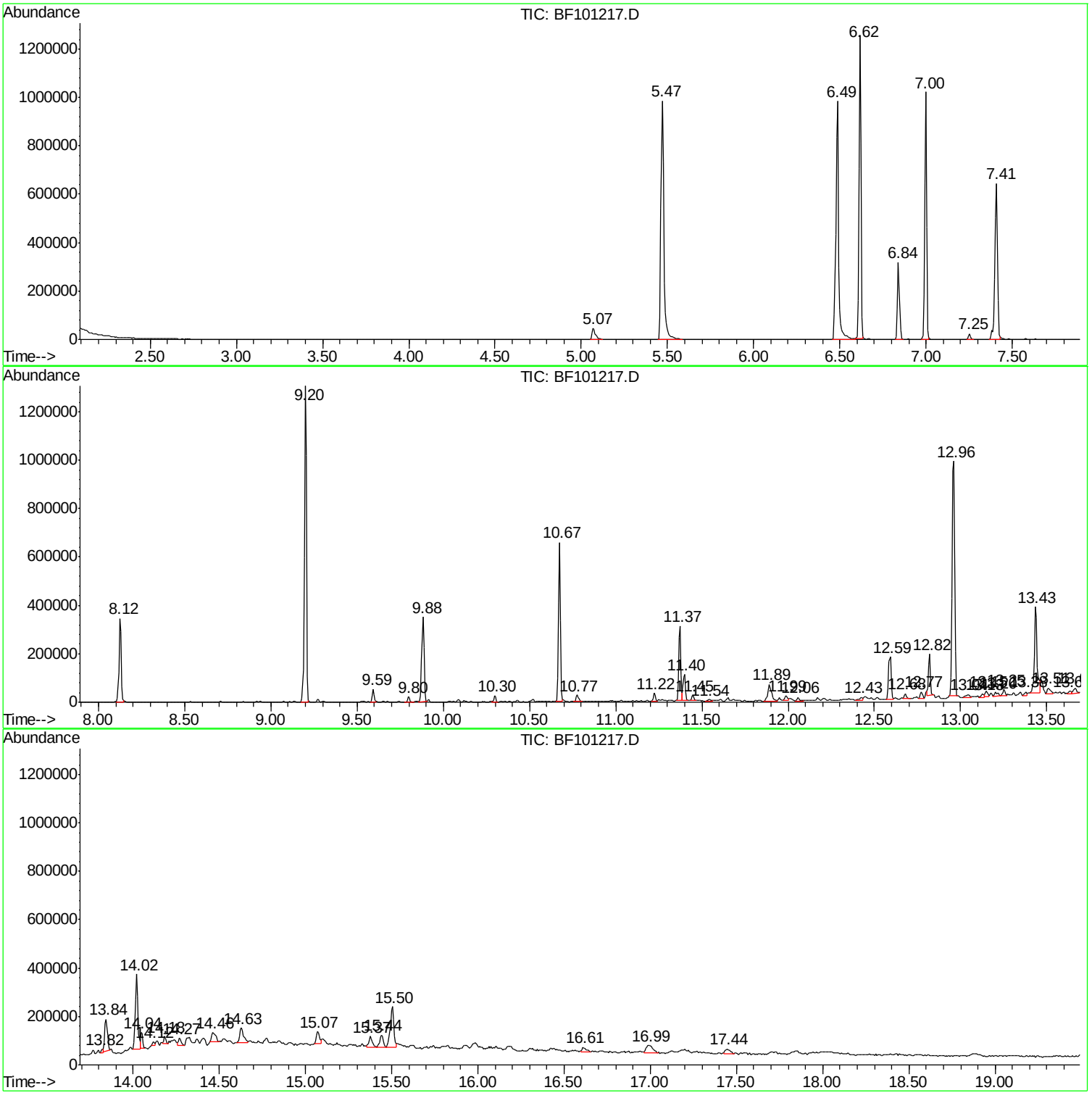
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
Data File : BF101217.D
Acq On : 7 Dec 2017 20:40
Operator : SJ/JU
Sample : I6615-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB-2-OW(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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\BF120717\
Data File : BF101217.D
Acq On : 7 Dec 2017 20:40
Operator : SJ/JU
Sample : I6615-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-2-OW(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

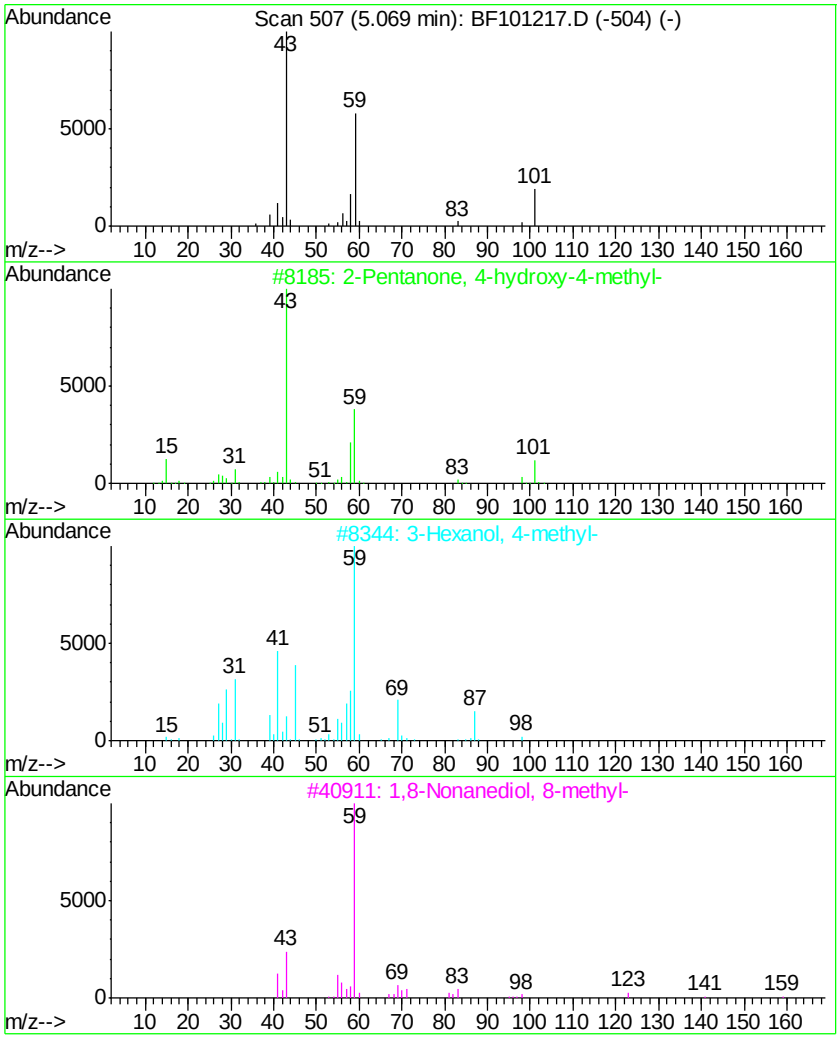
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

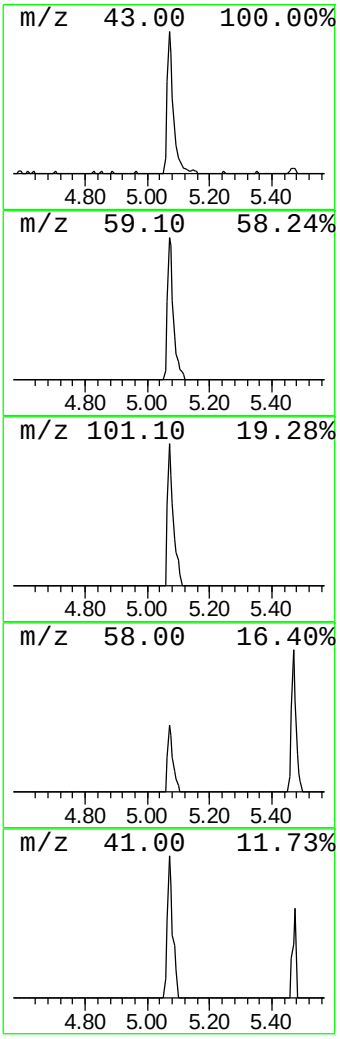
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	4.99 ng	62865	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
Data File : BF101217.D
Acq On : 7 Dec 2017 20:40
Operator : SJ/JU
Sample : I6615-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-2-OW(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

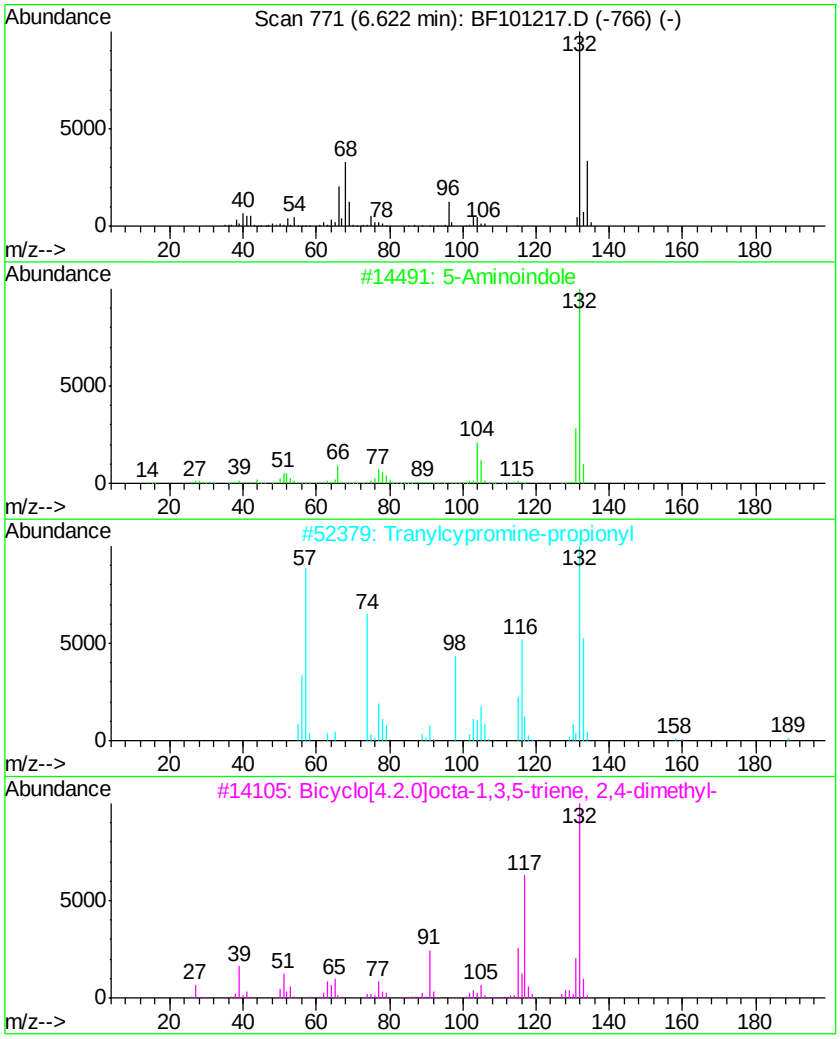
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

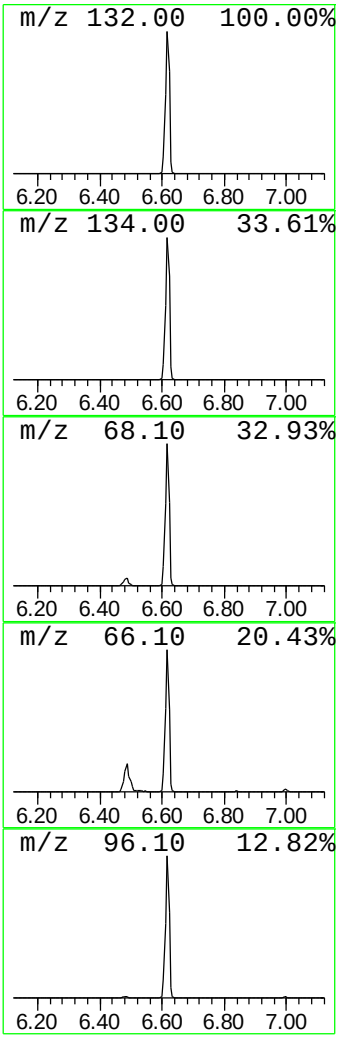
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	84.92 ng	1070720	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
Data File : BF101217.D
Acq On : 7 Dec 2017 20:40
Operator : SJ/JU
Sample : I6615-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-2-OW(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

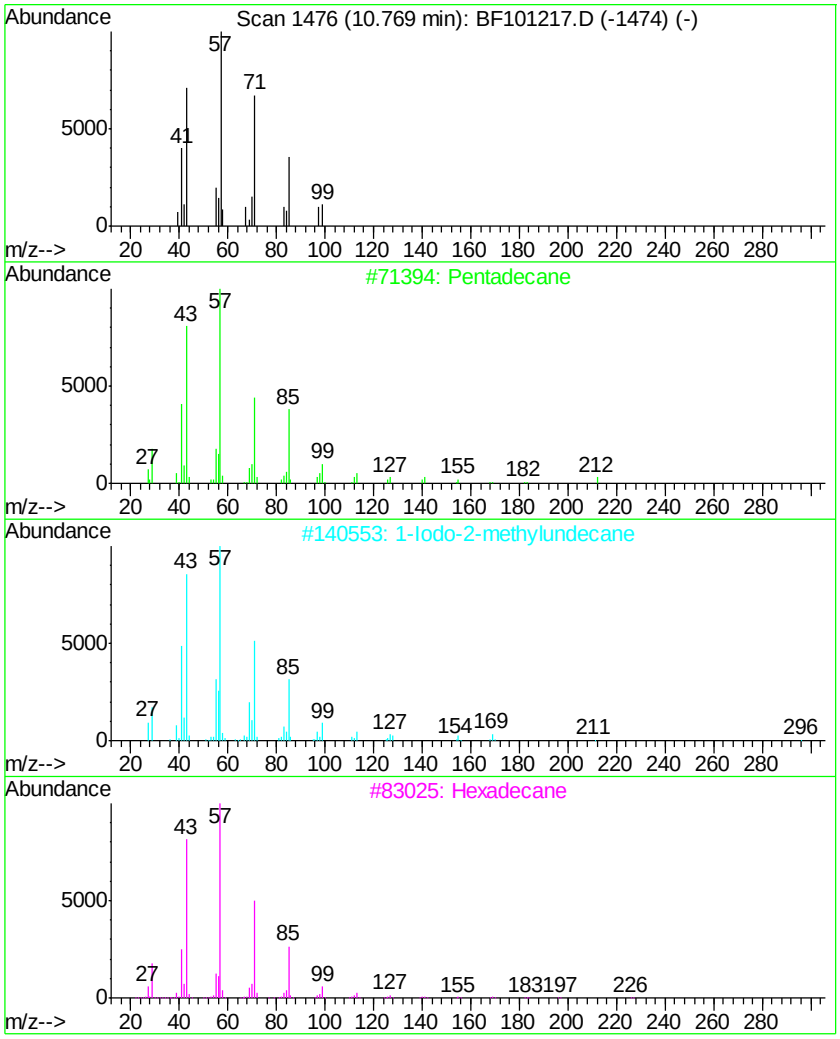
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

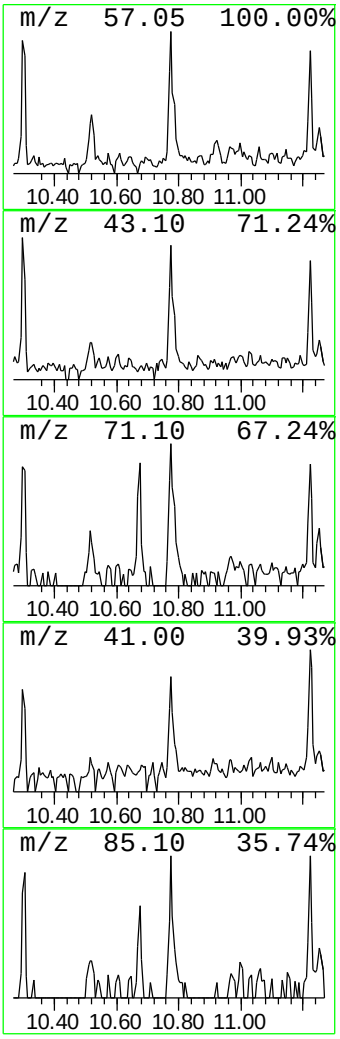
****

Peak Number 4 Pentadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	2.29 ng	31958	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	83
2	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	83
3	Hexadecane	226	C16H34	000544-76-3	78
4	Tridecane	184	C13H28	000629-50-5	78
5	Tetradecane	198	C14H30	000629-59-4	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
Data File : BF101217.D
Acq On : 7 Dec 2017 20:40
Operator : SJ/JU
Sample : I6615-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-2-OW(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

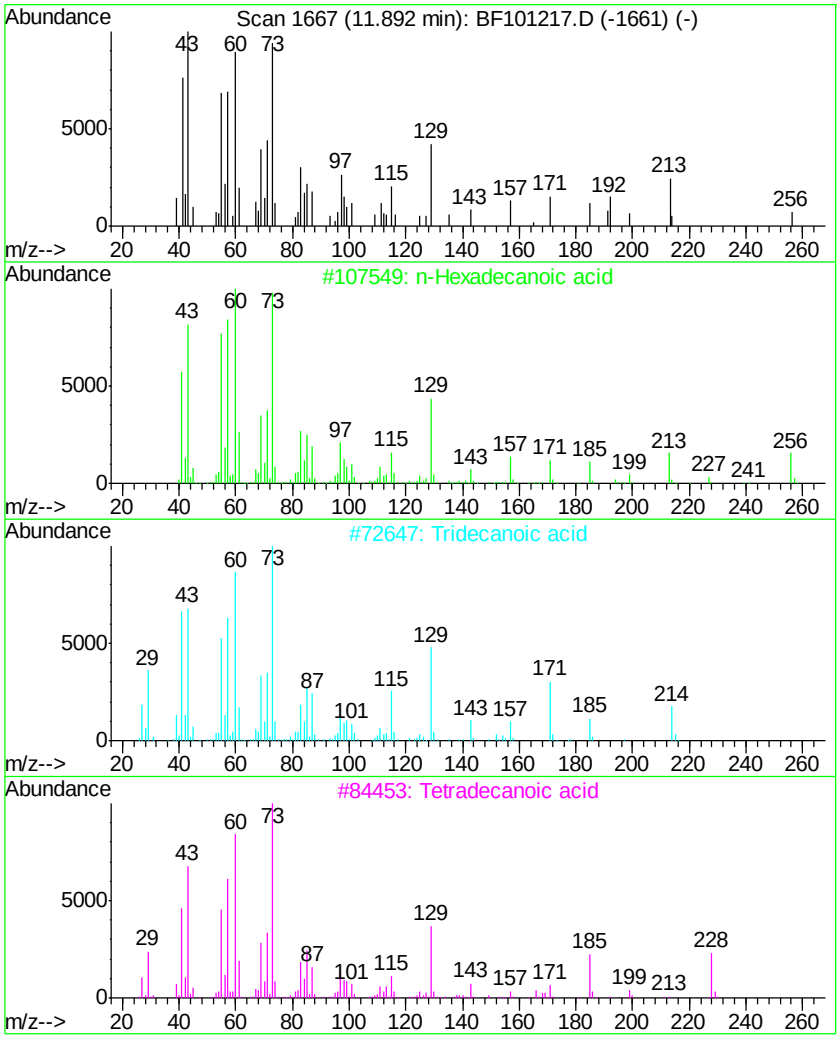
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

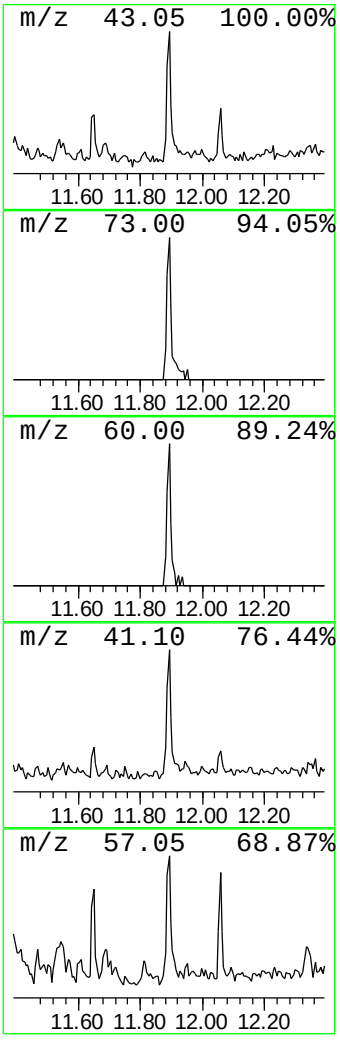
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	6.67 ng	93011	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
Data File : BF101217.D
Acq On : 7 Dec 2017 20:40
Operator : SJ/JU
Sample : I6615-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-2-OW(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

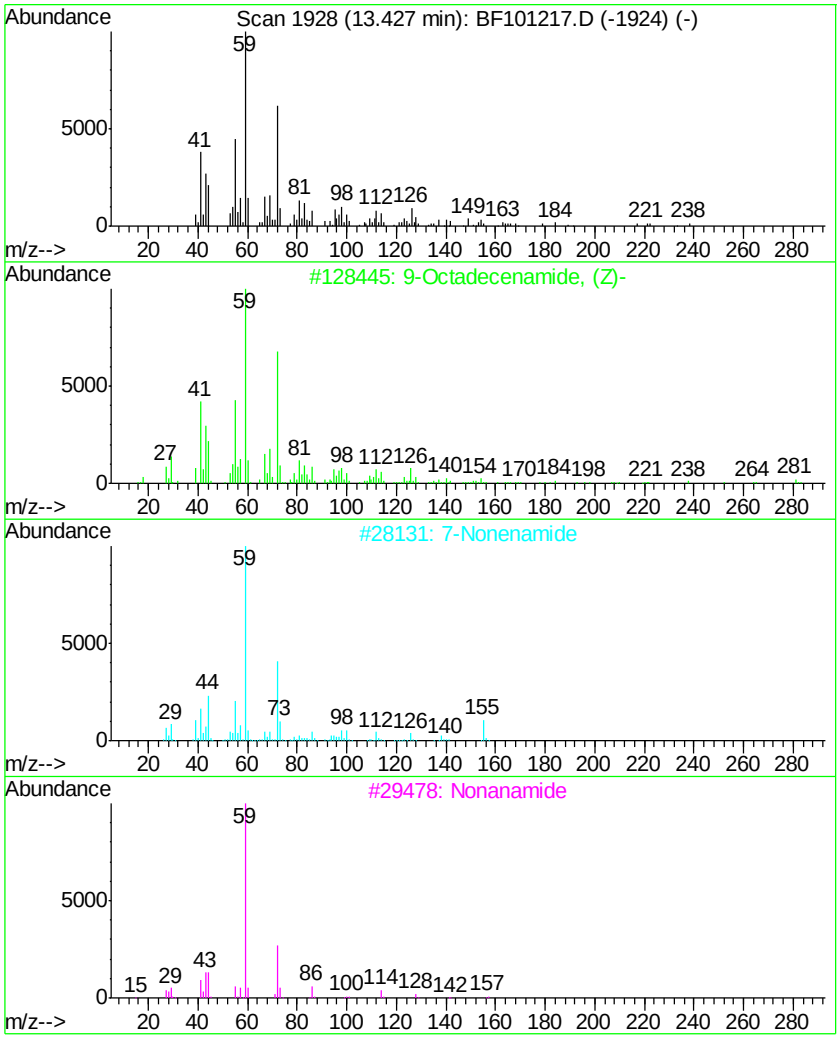
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

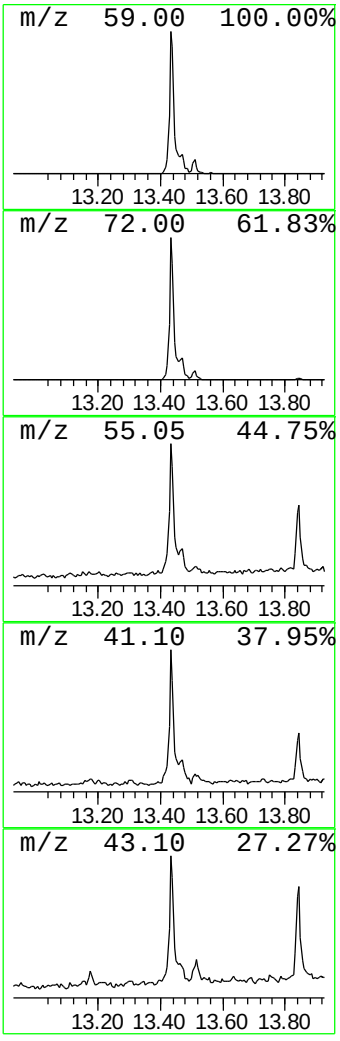
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	24.52 ng	412255	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	7-Nonenamide	155	C9H17NO	090949-53-4	72
3	Nonanamide	157	C9H19NO	001120-07-6	53
4	Octanamide	143	C8H17NO	000629-01-6	53
5	Dodecanamide	199	C12H25NO	001120-16-7	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
Data File : BF101217.D
Acq On : 7 Dec 2017 20:40
Operator : SJ/JU
Sample : I6615-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-2-OW(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

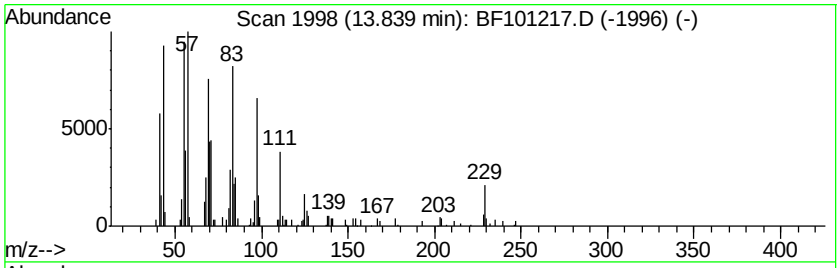
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

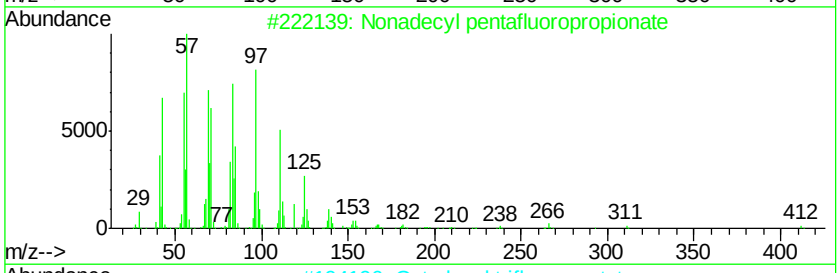
****

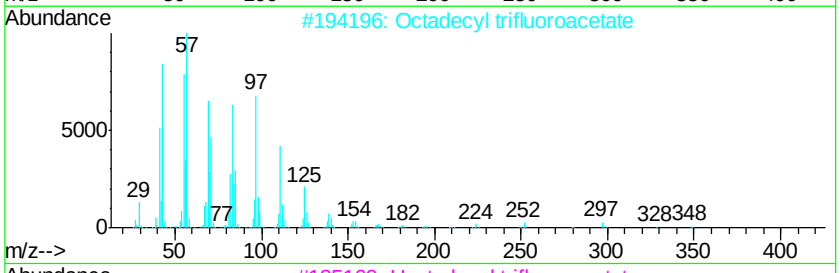
Peak Number 7 Nonadecyl pentafluoropropio... Concentration Rank 4

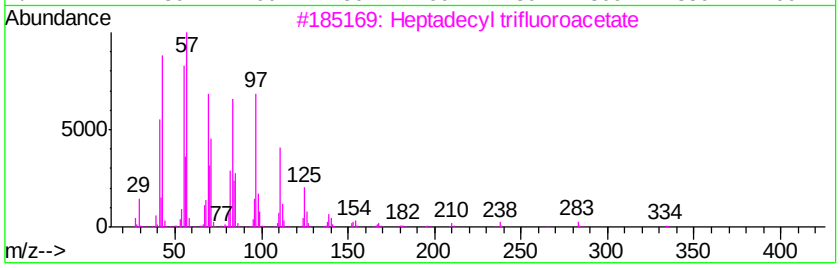
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	7.83 ng	131707	Chrysene-d12	14.02

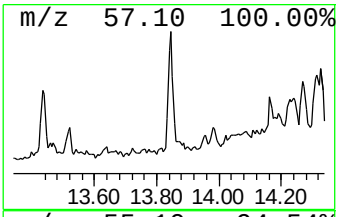
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	94
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94

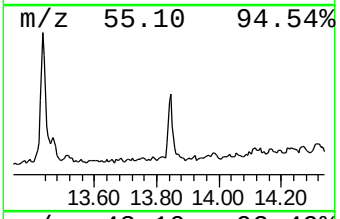


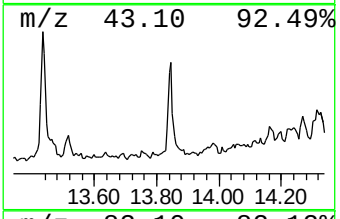


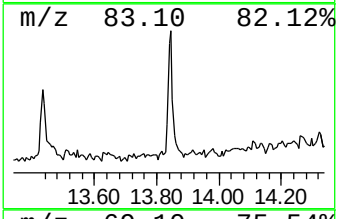


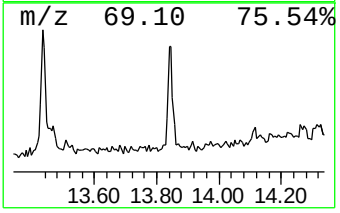












Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
Data File : BF101217.D
Acq On : 7 Dec 2017 20:40
Operator : SJ/JU
Sample : I6615-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-2-OW(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

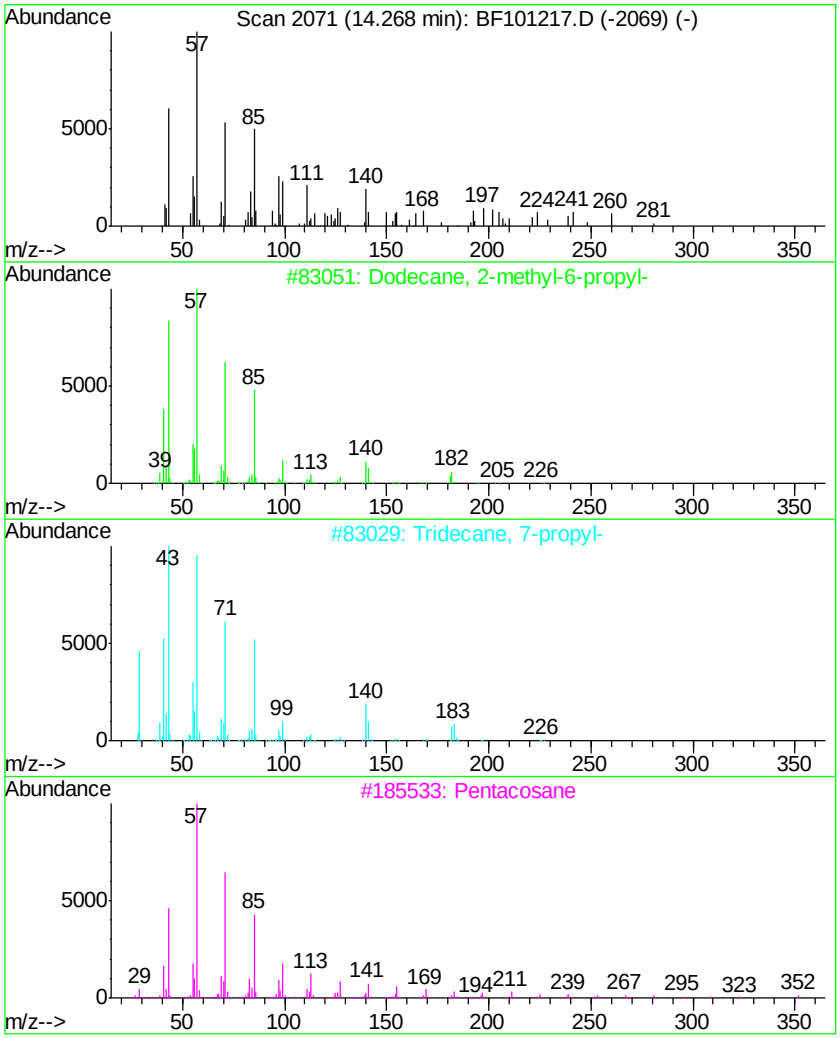
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

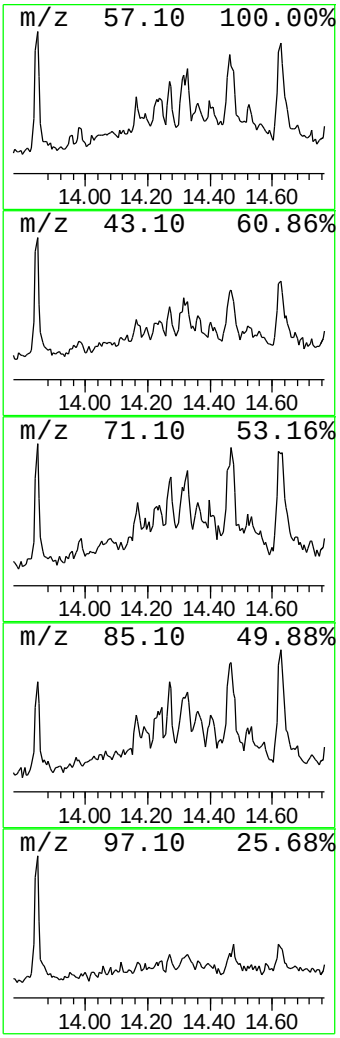
****

Peak Number 8 unknown14.27 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.27	2.03 ng	34195	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	47
2	Tridecane, 7-propyl-	226	C16H34	055045-09-5	43
3	Pentacosane	352	C25H52	000629-99-2	43
4	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	43
5	Oxalic acid, decyl propyl ester	272	C15H28O4	1000309-26-3	43





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Data File : BF101217.D
Acq On : 7 Dec 2017 20:40
Operator : SJ/JU
Sample : I6615-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-2-OW(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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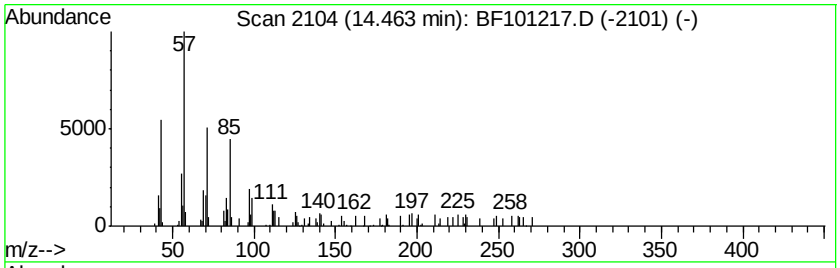
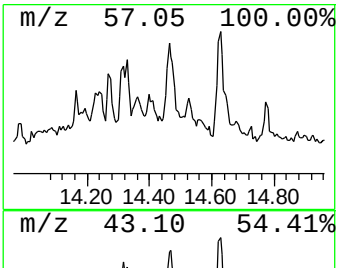
Peak Number 9 Sulfurous acid, butyl hepta... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	3.57 ng	60037	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	64
2	Hentriacontane	437	C31H64	000630-04-6	64
3	Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	64
4	Pentatriacontane	493	C35H72	000630-07-9	59
5	Tetratetracontane	619	C44H90	007098-22-8	52





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Sample : I6615-01
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Instrument : BNA_F
ClientSampleId : PB-2-OW(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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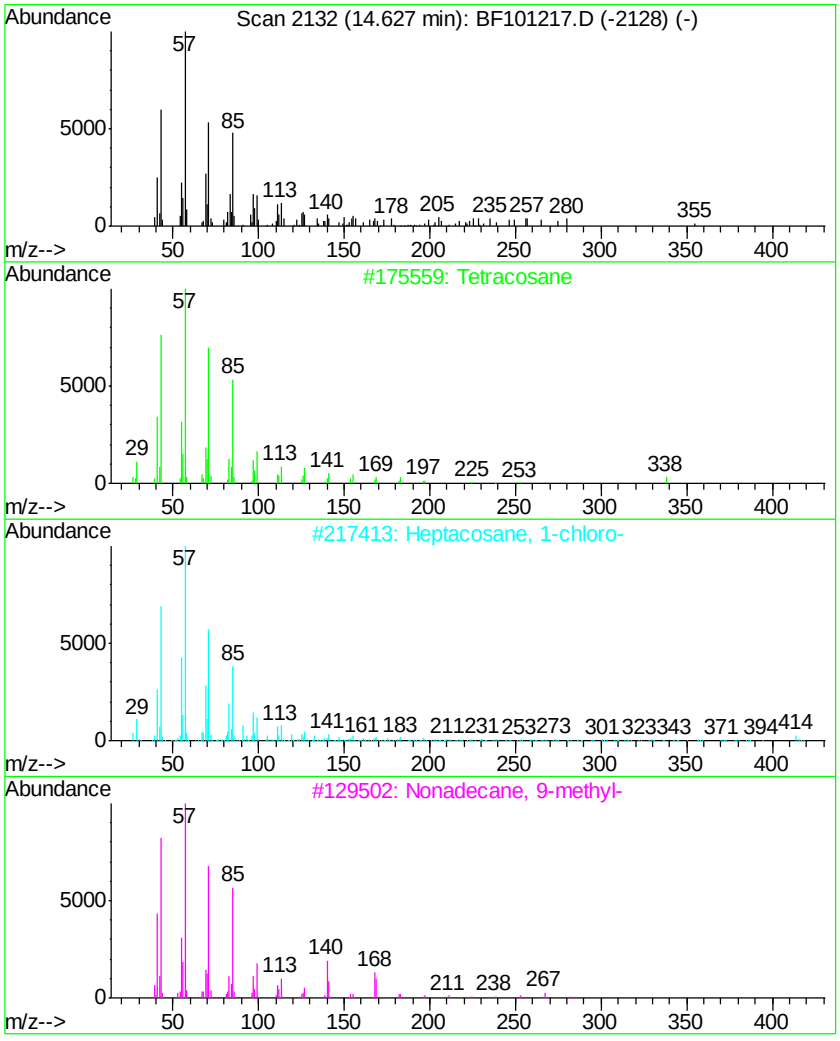
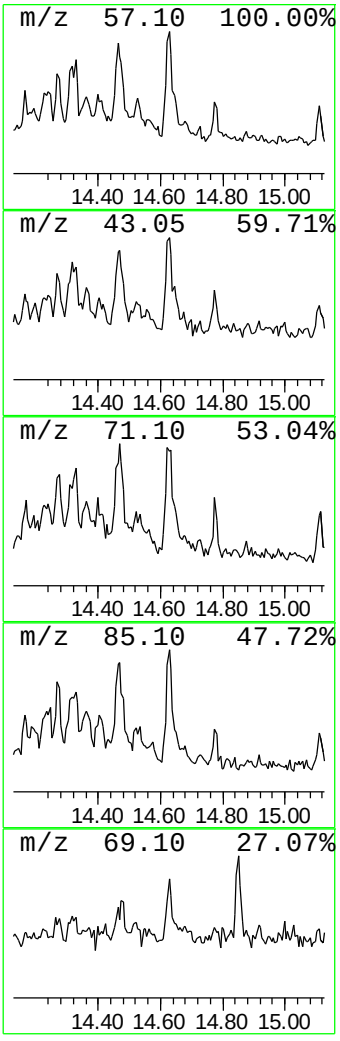
Peak Number 10 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	5.77 ng	97051	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	87
2	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	86
3	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	86
4	Heptadecane	240	C17H36	000629-78-7	83
5	Tritetracontane	605	C43H88	007098-21-7	83





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Acq On : 7 Dec 2017 20:40
Operator : SJ/JU
Sample : I6615-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-2-OW(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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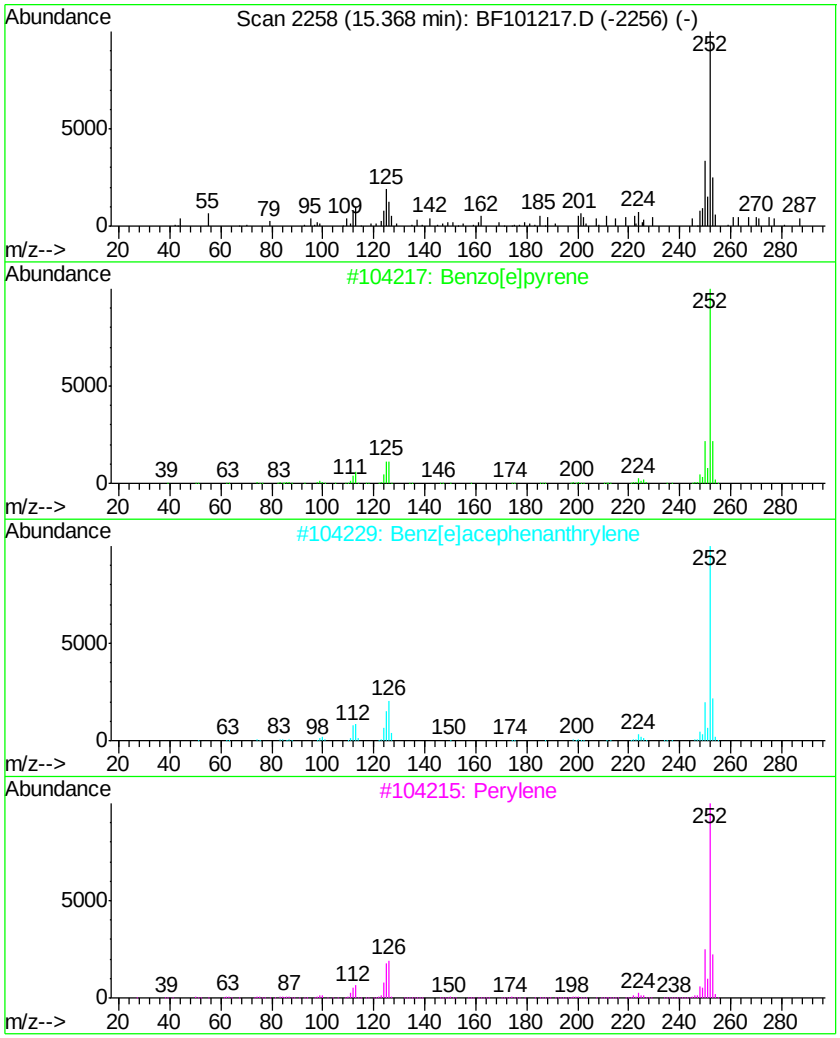
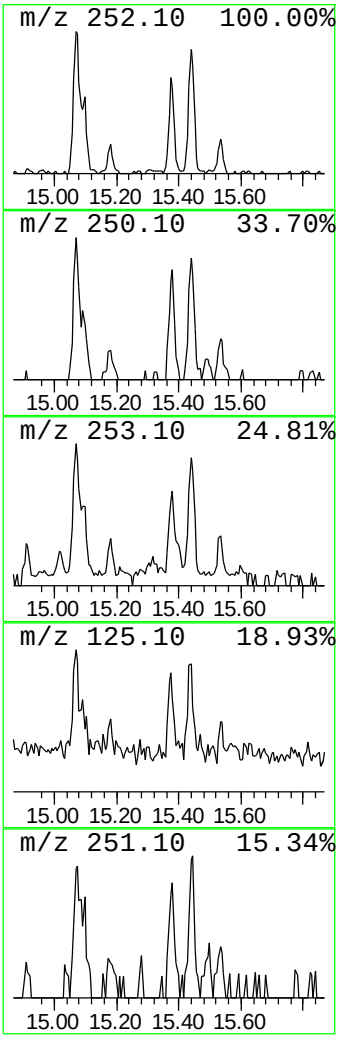
Peak Number 11 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	5.17 ng	61168	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	81
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	81
3	Perylene	252	C20H12	000198-55-0	76
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	76
5	(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	72





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Sample : I6615-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-2-OW(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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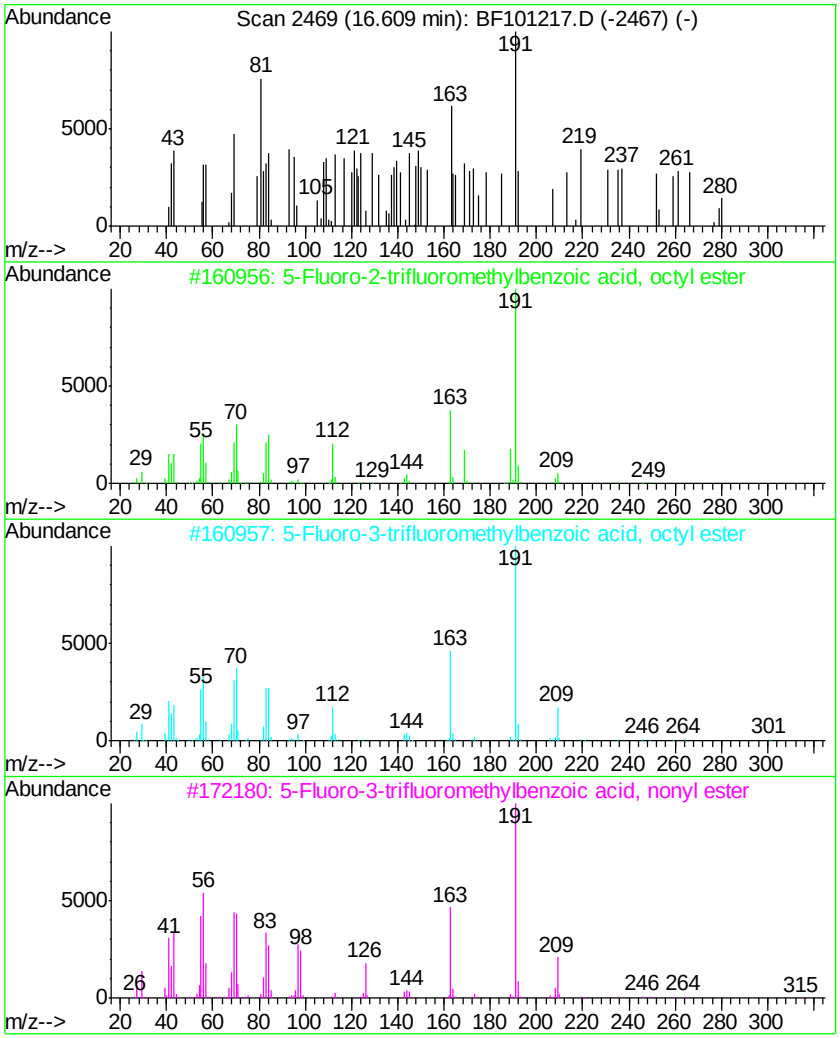
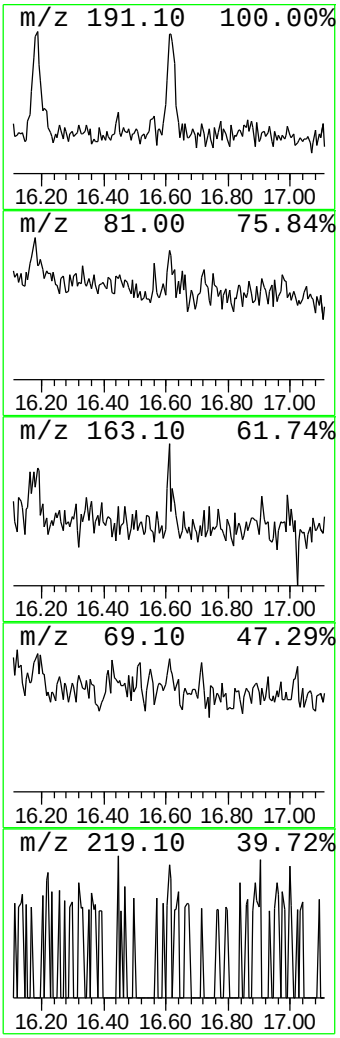
Peak Number 12 unknown16.61 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.61	2.67 ng	31621	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-trifluoromethylbenzoi...	320	C16H20F4O2	1000338-74-4	27
2	5-Fluoro-3-trifluoromethylbenzoi...	320	C16H20F4O2	1000338-90-0	27
3	5-Fluoro-3-trifluoromethylbenzoi...	334	C17H22F4O2	1000338-90-1	16
4	Oxazole, 4-ethyl-4,5-dihydro-2-(...	191	C11H13NO2	1000142-01-8	14
5	Phenol, 2,6-diisopropyl-4-(morph...	277	C17H27NO2	1000304-55-0	12





Tentatively Identified Compound (LSC) summary

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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	5.0	ng	62865	1	6.84	252174	20.0
unknown6.62	6.62	84.9	ng	1070720	1	6.84	252174	20.0
Pentadecane	10.77	2.3	ng	31958	4	11.37	279088	20.0
n-Hexadecanoic acid	11.89	6.7	ng	93011	4	11.37	279088	20.0
9-Octadecenamide,...	13.43	24.5	ng	412255	5	14.02	336270	20.0
Nonadecyl pentafl...	13.84	7.8	ng	131707	5	14.02	336270	20.0
unknown14.27	14.27	2.0	ng	34195	5	14.02	336270	20.0
Sulfurous acid, b...	14.46	3.6	ng	60037	5	14.02	336270	20.0
Tetracosane	14.63	5.8	ng	97051	5	14.02	336270	20.0
Benzo[e]pyrene	15.37	5.2	ng	61168	6	15.50	236728	20.0
unknown16.61	16.61	2.7	ng	31621	6	15.50	236728	20.0