LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090817\
Data File : BF098359.D
Acq On : 8 Sep 2017 19:15
Operator : SJ/JU
Sample : I5071-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-0-2.5

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-BF081517.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	4.198	356	359	365	rBV	28753	36854	2.83%	0.270%
2	4.851	467	470	479	rBV	243084	276475	21.25%	2.025%
3	5.287	540	544	558	rBV	1034186	1046824	80.45%	7.667%
4	6.322	716	720	731	rBV	1287597	1196765	91.97%	8.766%
5	6.451	738	742	745	rBV	1292189	1121383	86.18%	8.214%
6	6.681	777	781	784	rBV	758491	596951	45.88%	4.372%
7	6.834	803	807	811	rBV	1127510	993848	76.38%	7.279%
8	7.245	873	877	880	rBV	904892	760158	58.42%	5.568%
9	7.963	995	999	1002	rBV	888936	739006	56.79%	5.413%
10	8.675	1118	1120	1124	rBV	23037	18463	1.42%	0.135%
11	8.775	1134	1137	1141	rVB	21374	16406	1.26%	0.120%
12	9.039	1178	1182	1185	rBV	1603416	1301222	100.00%	9.531%
13	9.433	1245	1249	1253	rBV	161122	150846	11.59%	1.105%
14	9.575	1271	1273	1277	rBV	16234	15313	1.18%	0.112%
15	9.716	1293	1297	1301	rBV	775726	650910	50.02%	4.768%
16	9.822	1312	1315	1319	rVB	33850	29619	2.28%	0.217%
17	10.263	1387	1390	1394	rVB	17621	18243	1.40%	0.134%
18	10.504	1427	1431	1441	rVB	351424	340582	26.17%	2.495%
19	10.633	1448	1453	1456	rBV3	52218	70947	5.45%	0.520%
20	10.686	1459	1462	1465	rBV	84857	72761	5.59%	0.533%
21	10.722	1465	1468	1471	rVV2	80217	91926	7.06%	0.673%
22	10.751	1471	1473	1476	rVV2	67148	70493	5.42%	0.516%
23	10.780	1476	1478	1480	rVV	42932	35181	2.70%	0.258%
24	10.822	1480	1485	1486	rVV2	27333	44637	3.43%	0.327%
25	10.833	1486	1487	1489	rVV	32818	23879	1.84%	0.175%
26	10.863	1489	1492	1496	rVV3	57781	71642	5.51%	0.525%
27	10.904	1496	1499	1501	rVV	81285	69034	5.31%	0.506%
28	10.945	1504	1506	1512	rVB	48260	43584	3.35%	0.319%
29	11.069	1525	1527	1530	rBV2	25244	21671	1.67%	0.159%
30	11.098	1530	1532	1536	rVB2	21155	20372	1.57%	0.149%
31	11.198	1545	1549	1551	rBV	671032	563489	43.30%	4.127%
32	11.222	1551	1553	1557	rVV	138440	109955	8.45%	0.805%
33	11.274	1557	1562	1565	rVB	47892	50162	3.85%	0.367%
34	11.498	1597	1600	1603	rVB2	19985	15943	1.23%	0.117%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090817\
Data File : BF098359.D
Acq On : 8 Sep 2017 19:15
Operator : SJ/JU
Sample : I5071-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-0-2.5

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-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.698	1631	1634	1637	rBV	32585	27445	2.11%	0.201%
36	11.727	1637	1639	1643	rVB	38439	30614	2.35%	0.224%
37	11.774	1643	1647	1650	rBV2	20133	23684	1.82%	0.173%
38	11.810	1650	1653	1655	rVV	44269	49019	3.77%	0.359%
39	11.833	1655	1657	1662	rVB	21327	21395	1.64%	0.157%
40	11.992	1681	1684	1687	rBV2	24044	26022	2.00%	0.191%
41	12.174	1712	1715	1717	rBV4	19161	20724	1.59%	0.152%
42	12.245	1724	1727	1730	rBV	29727	32902	2.53%	0.241%
43	12.333	1739	1742	1746	rBV3	21633	29354	2.26%	0.215%
44	12.404	1751	1754	1758	rVV	166923	163080	12.53%	1.194%
45	12.633	1788	1793	1796	rBV	196818	198581	15.26%	1.455%
46	12.669	1796	1799	1802	rVV2	48244	47731	3.67%	0.350%
47	12.780	1815	1818	1822	rBV	1104103	942241	72.41%	6.901%
48	13.268	1898	1901	1905	rVB	170770	151449	11.64%	1.109%
49	13.833	1993	1997	2000	rBV2	671040	698695	53.70%	5.118%
50	15.251	2234	2238	2245	rVB	378090	504292	38.76%	3.694%

Sum of corrected areas: 13652772

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Misc :
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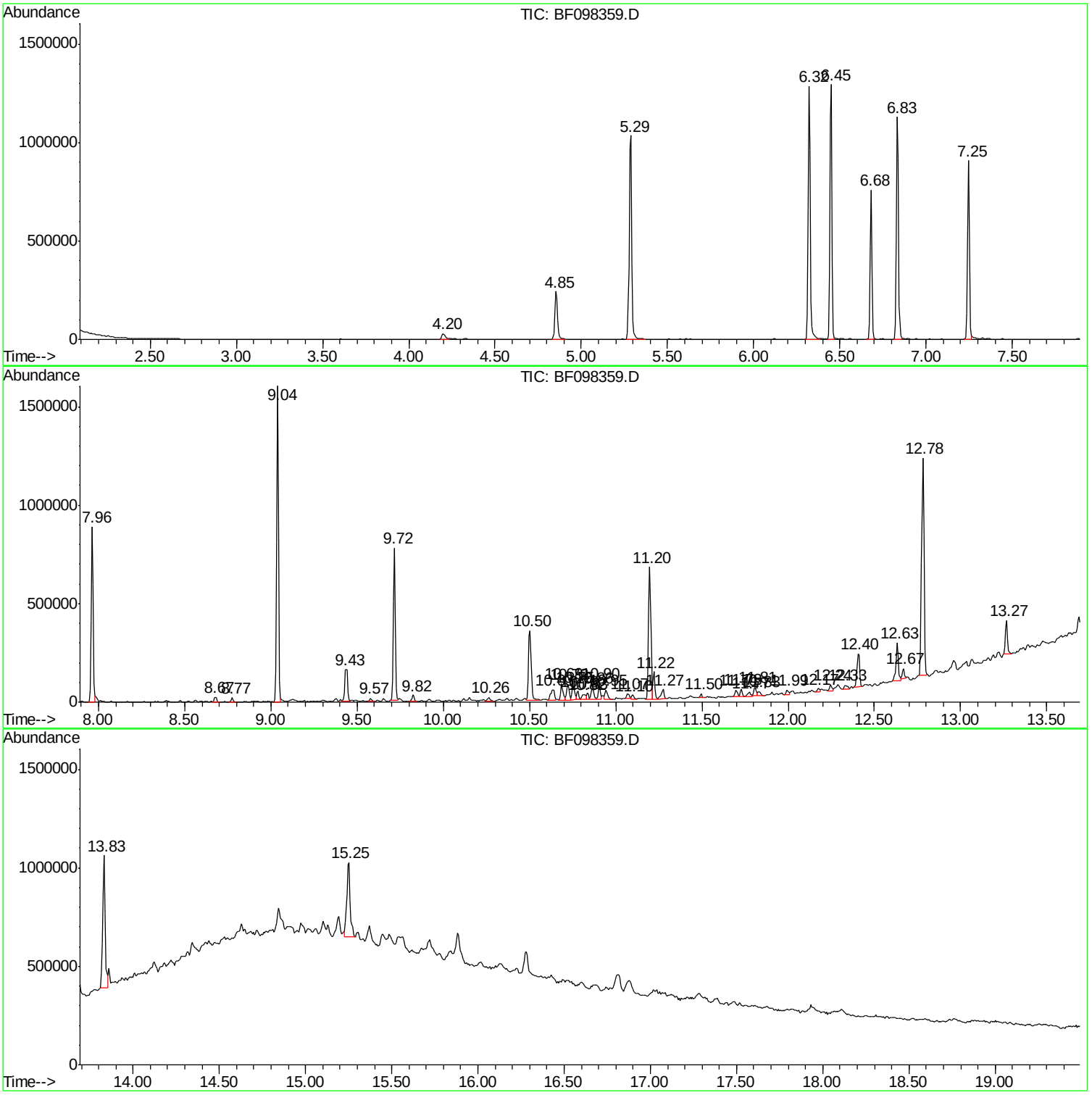
Instrument : BNA_F
ClientSampleId : G58A-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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\BF090817\
Data File : BF098359.D
Acq On : 8 Sep 2017 19:15
Operator : SJ/JU
Sample : I5071-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

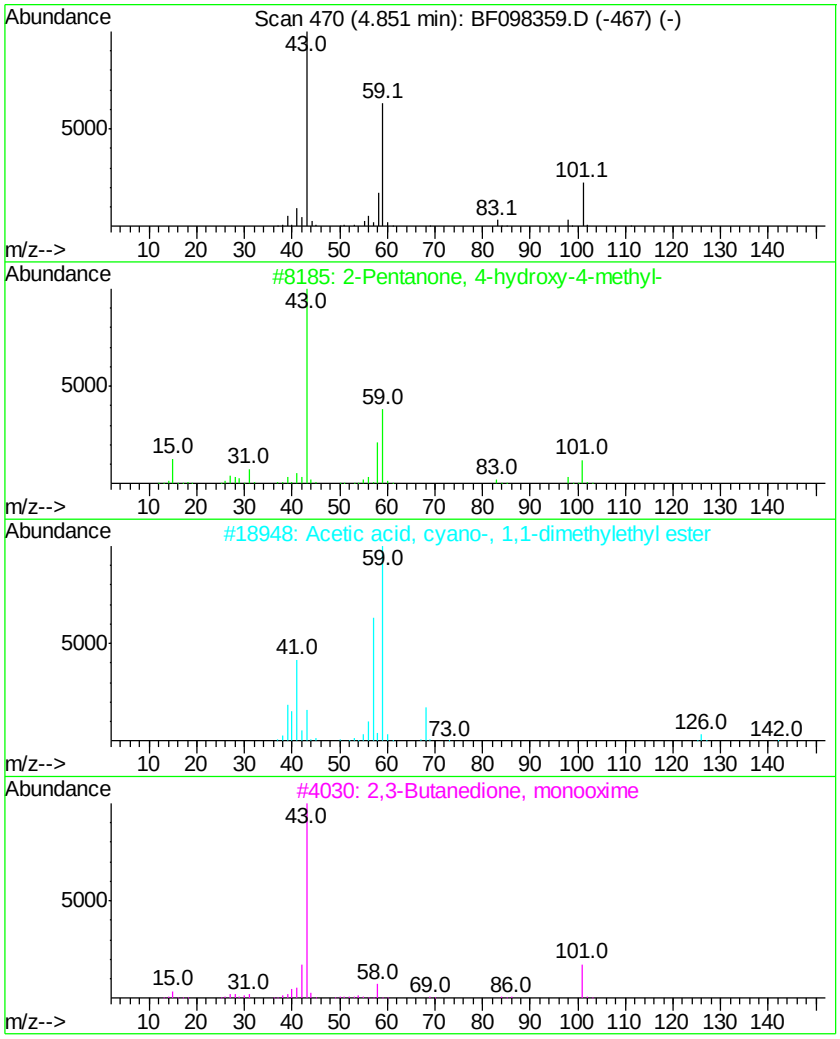
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

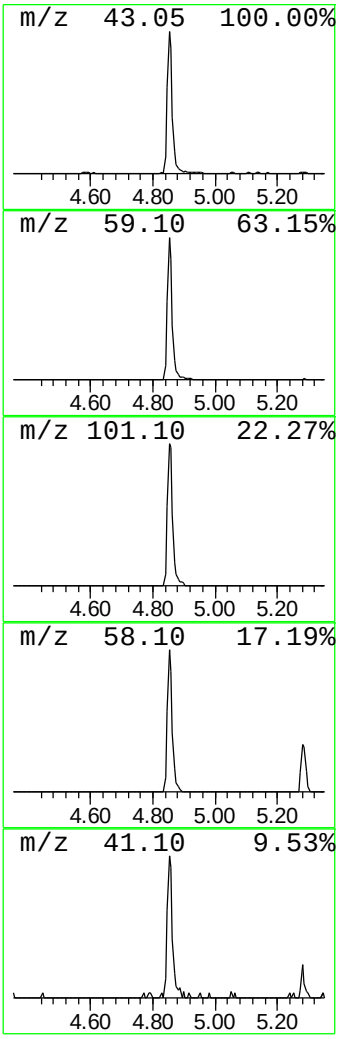
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	9.26 ng	276475	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
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	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090817\
Data File : BF098359.D
Acq On : 8 Sep 2017 19:15
Operator : SJ/JU
Sample : I5071-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

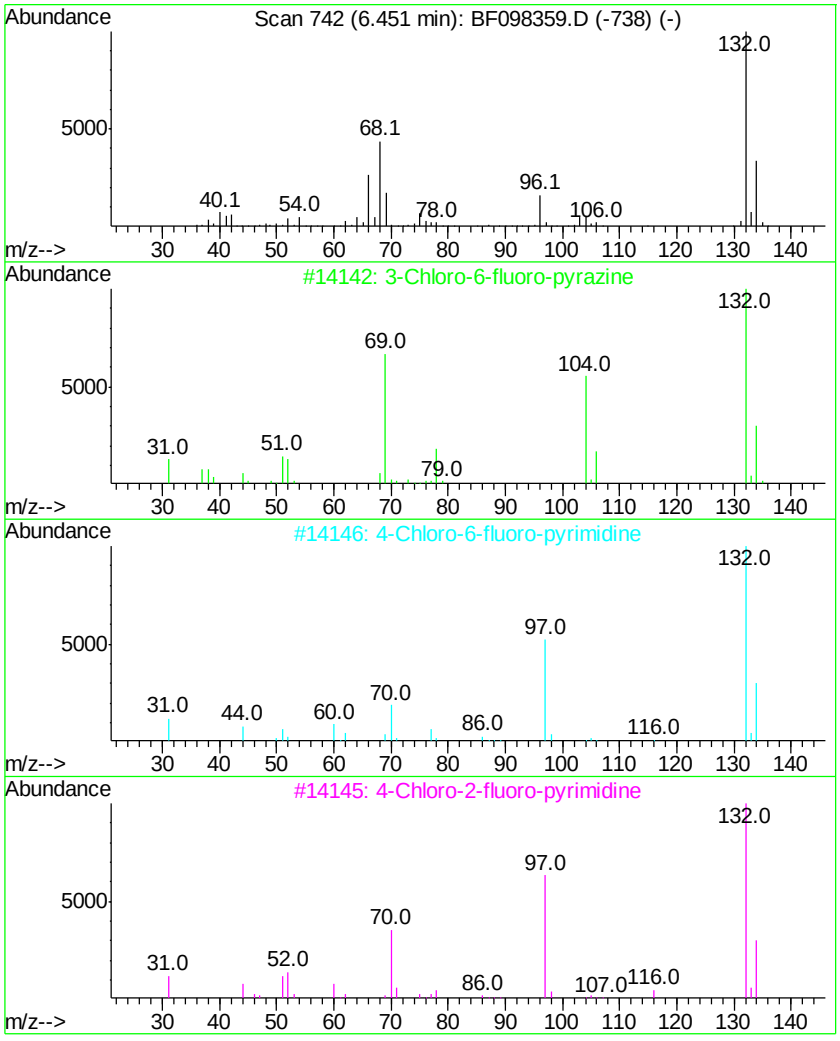
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

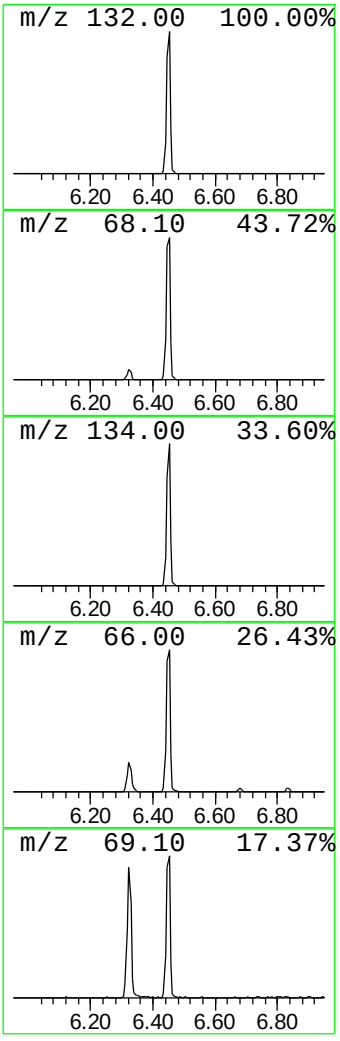
****

Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	37.57 ng	1121380	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	Xenon	132	Xe	007440-63-3	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090817\
Data File : BF098359.D
Acq On : 8 Sep 2017 19:15
Operator : SJ/JU
Sample : I5071-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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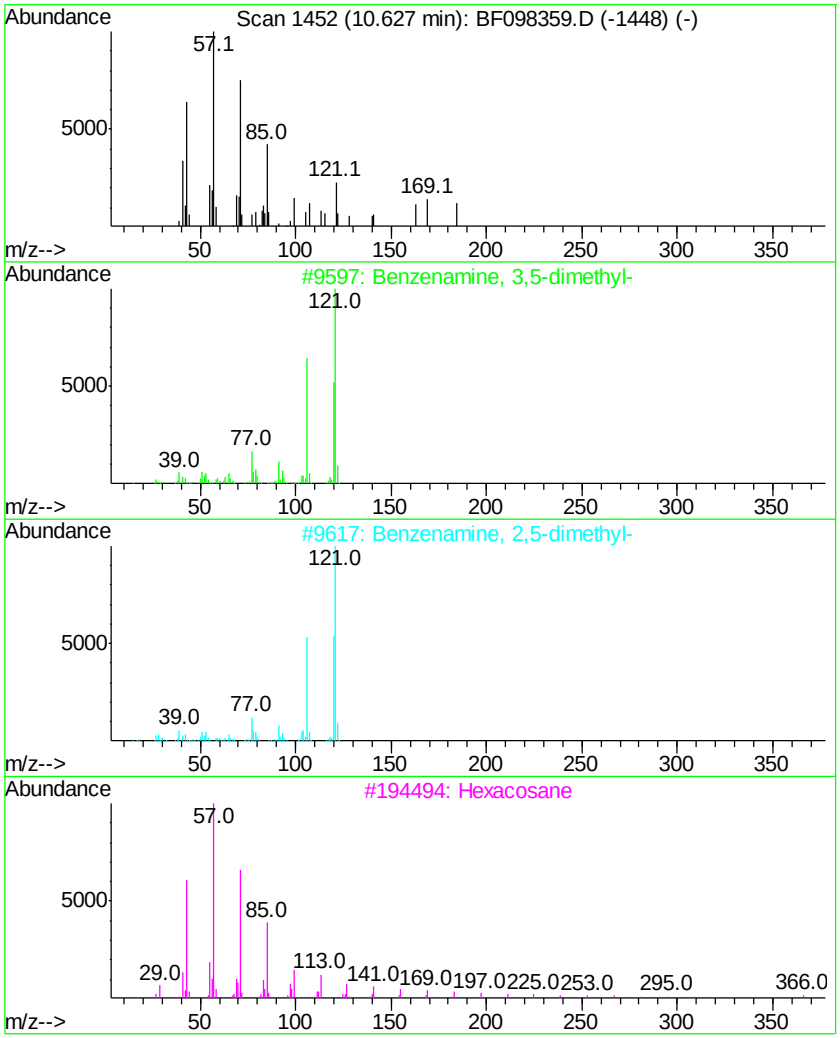
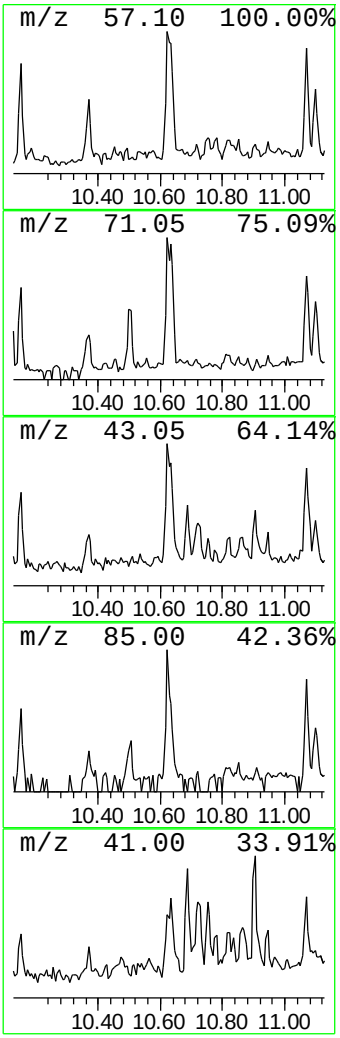
Peak Number 4 unknown10.63 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	2.52 ng	70947	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 3,5-dimethyl-	121	C8H11N	000108-69-0	22
2	Benzenamine, 2,5-dimethyl-	121	C8H11N	000095-78-3	22
3	Hexacosane	366	C26H54	000630-01-3	18
4	Hentriacontane	437	C31H64	000630-04-6	18
5	Tridecane	184	C13H28	000629-50-5	15





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090817\
Data File : BF098359.D
Acq On : 8 Sep 2017 19:15
Operator : SJ/JU
Sample : I5071-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

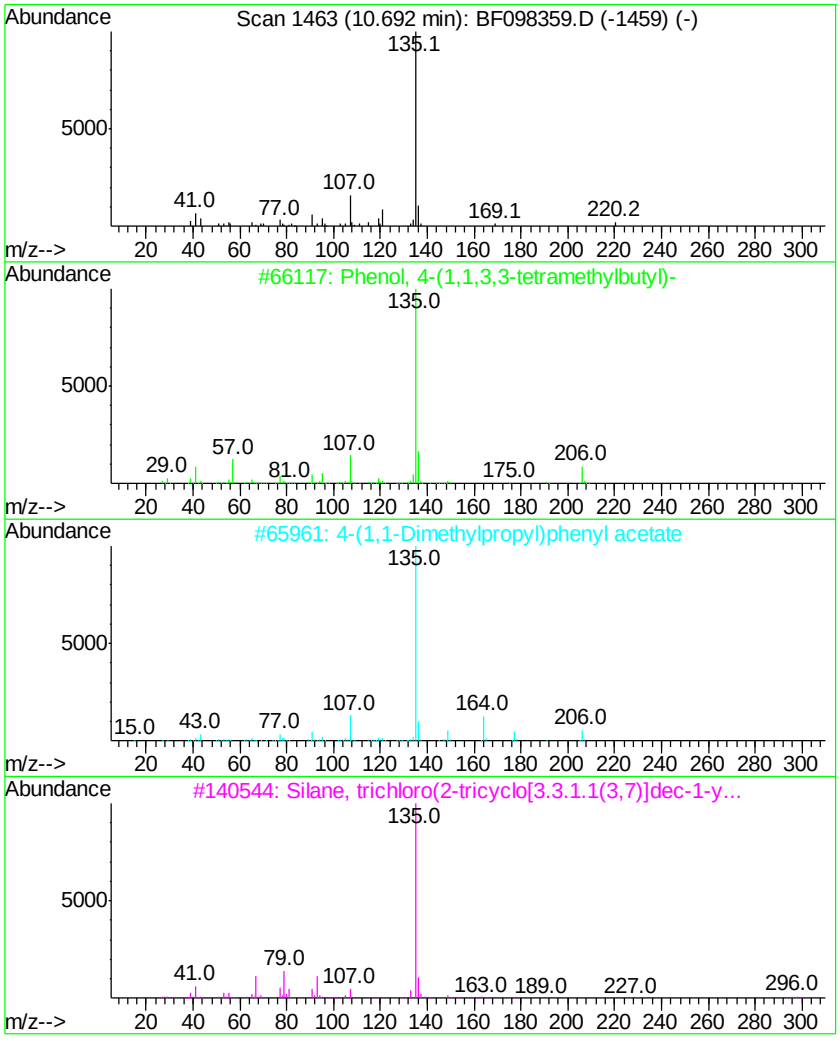
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

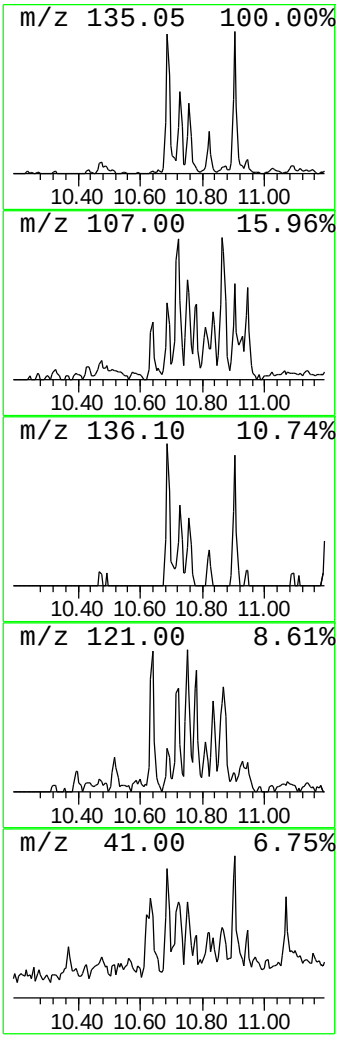
****

Peak Number 5 Phenol, 4-(1,1,3,3-tetramet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.69	2.58 ng	72761	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	83
2	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	64
3	Silane, trichloro(2-tricyclo[3.3...	296	C12H19Cl3Si	037843-11-1	59
4	1-Adamantanecarboxylic acid chlo...	198	C11H15ClO	002094-72-6	59
5	4-Methoxybenzoic acid, 2,6-dimet...	422	C19H16F6O4	1000304-50-0	59





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090817\
Data File : BF098359.D
Acq On : 8 Sep 2017 19:15
Operator : SJ/JU
Sample : I5071-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

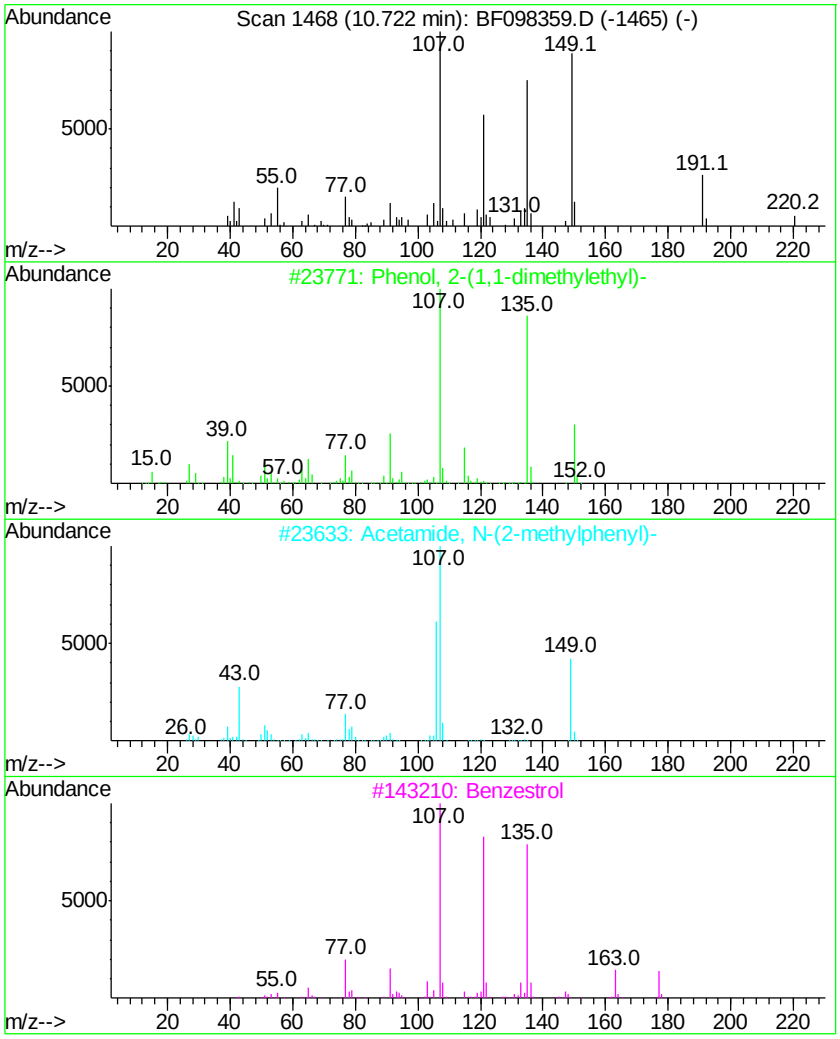
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

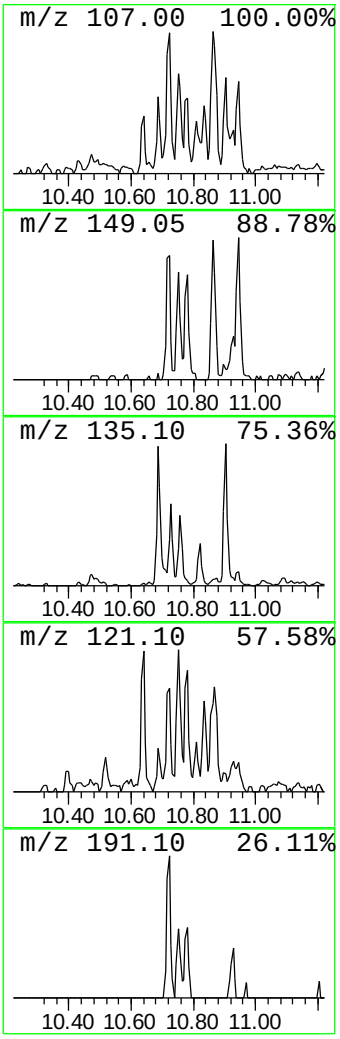
****

Peak Number 6 unknown10.72 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	3.26 ng	91926	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	46
2	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	46
3	Benzestrol	298	C20H26O2	000085-95-0	46
4	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	43
5	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	43





Library Search Compound Report

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Data File : BF098359.D
Acq On : 8 Sep 2017 19:15
Operator : SJ/JU
Sample : I5071-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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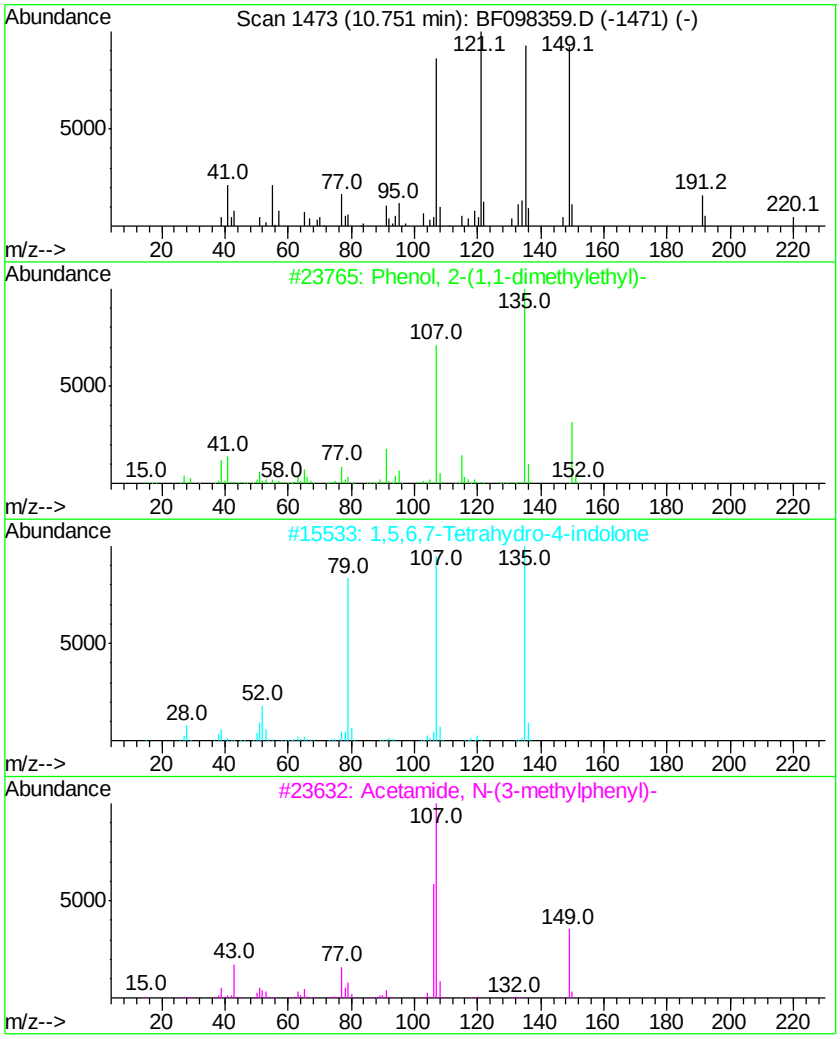
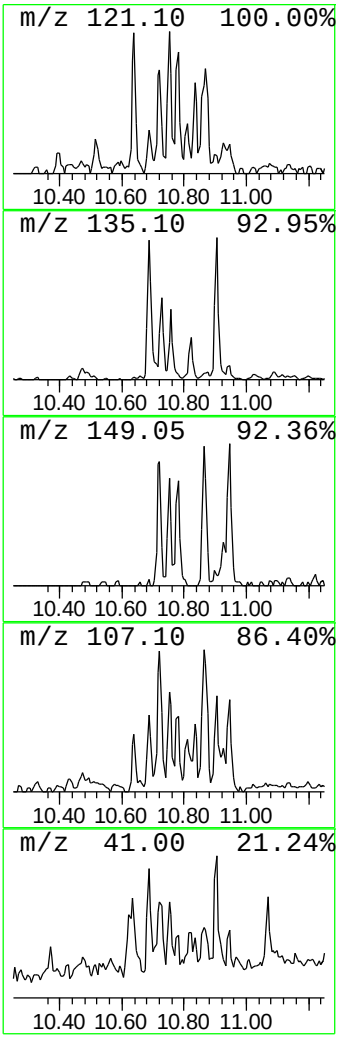
Peak Number 7 unknown10.75 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.50 ng	70493	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	38
2	1,5,6,7-Tetrahydro-4-indolone	135	C8H9NO	013754-86-4	38
3	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	38
4	Hexestrol	270	C18H22O2	005635-50-7	22
5	1-(4-Hydroxymethylphenyl)ethanone	150	C9H10O2	075633-63-5	18





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

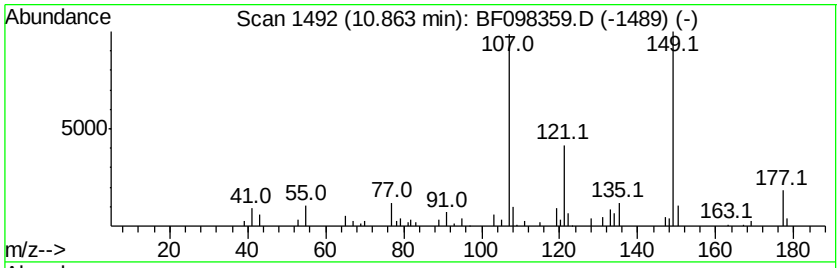
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

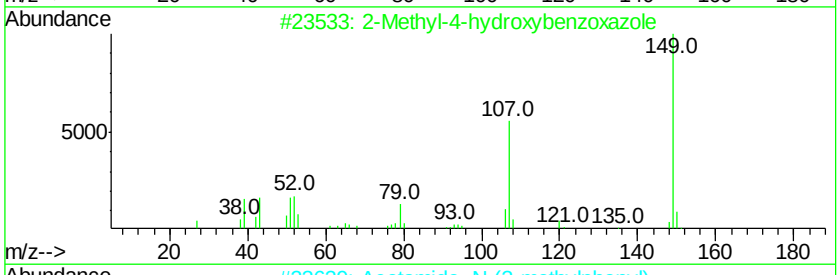
****

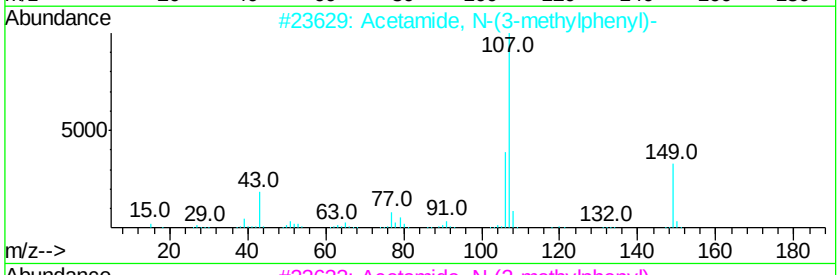
Peak Number 8 2-Methyl-4-hydroxybenzoxazole Concentration Rank 7

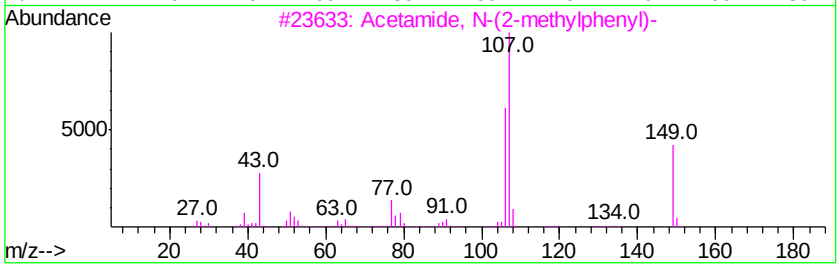
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.86	2.54 ng	71642	Phenanthrene-d10	11.20

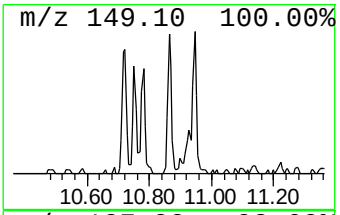
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	64
2	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	64
3	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	59
4	1-(6-Methyl-2-pyridyl)propan-2-one	149	C9H11NO	065702-08-1	59
5	Benzeneamine, 3-hexyl-	177	C12H19N	036042-29-2	46

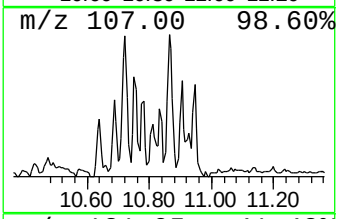


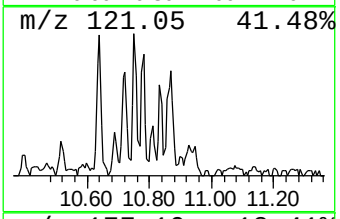


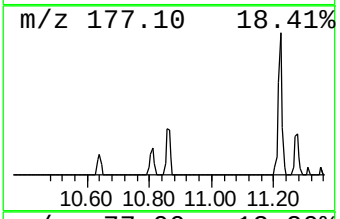


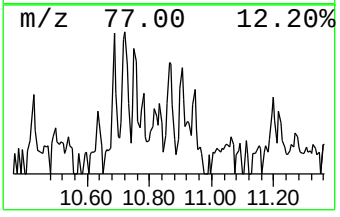












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Acq On : 8 Sep 2017 19:15
Operator : SJ/JU
Sample : I5071-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

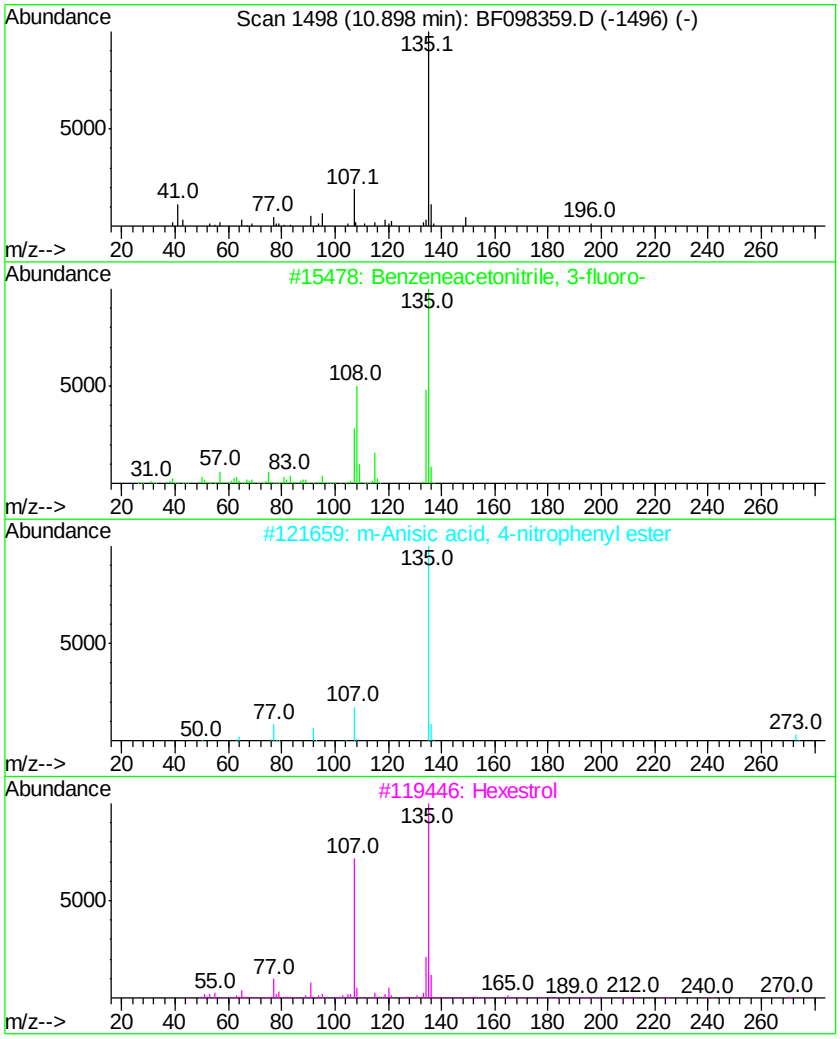
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

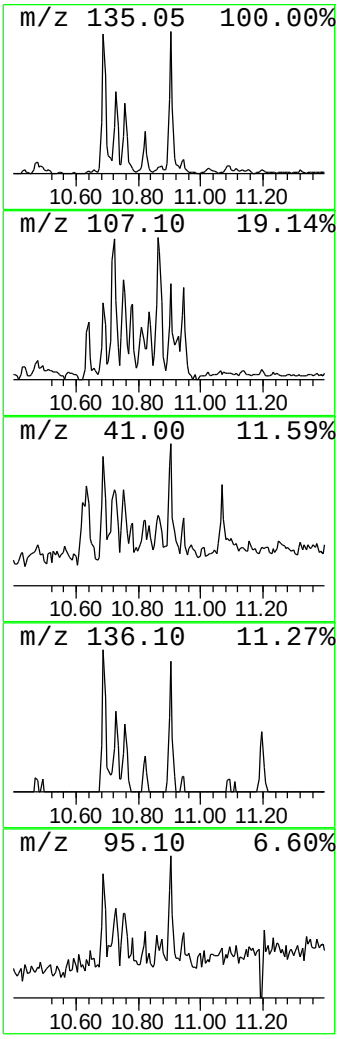
****

Peak Number 9 Benzeneacetonitrile, 3-fluoro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	2.45 ng	69034	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetonitrile, 3-fluoro-	135	C8H6FN	000501-00-8	72
2	m-Anisic acid, 4-nitrophenyl ester	273	C14H11NO5	1000307-80-4	56
3	Hexestrol	270	C18H22O2	000084-16-2	56
4	Benzeneacetonitrile, 2-fluoro-	135	C8H6FN	000326-62-5	56
5	Carbamic acid, N-[1,1-bis(triflu...	413	C19H25F6NO2	296242-69-8	45





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090817\
Data File : BF098359.D
Acq On : 8 Sep 2017 19:15
Operator : SJ/JU
Sample : I5071-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

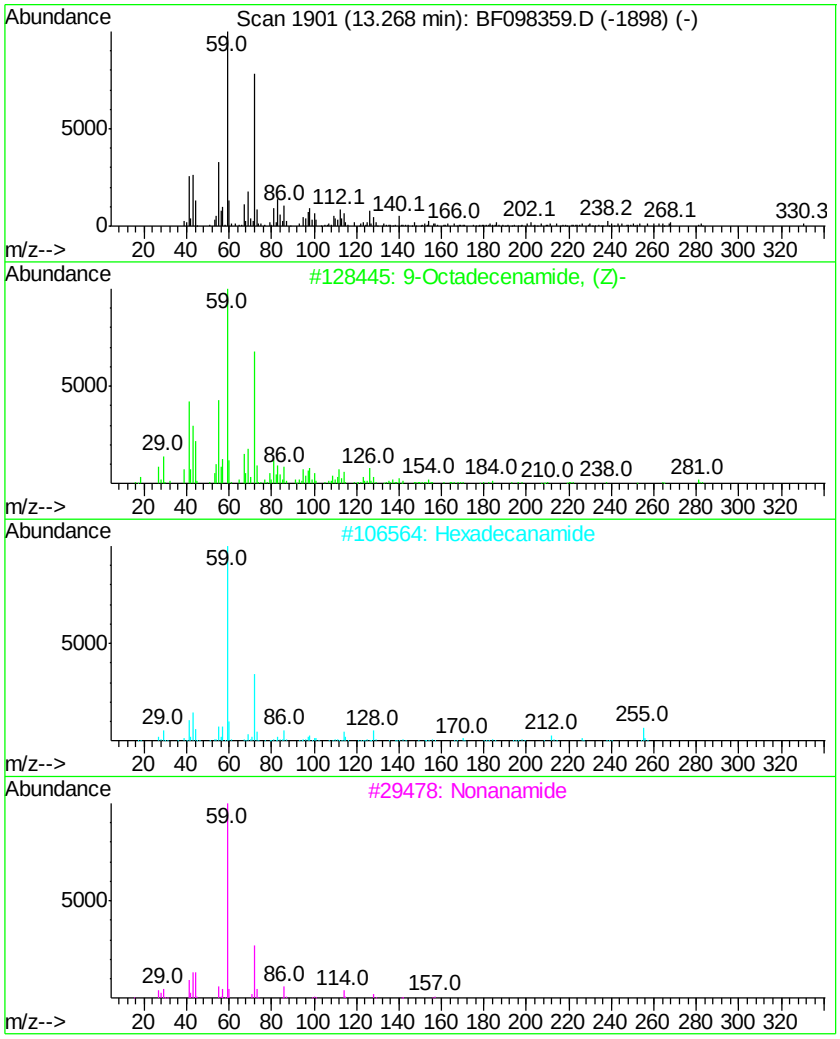
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

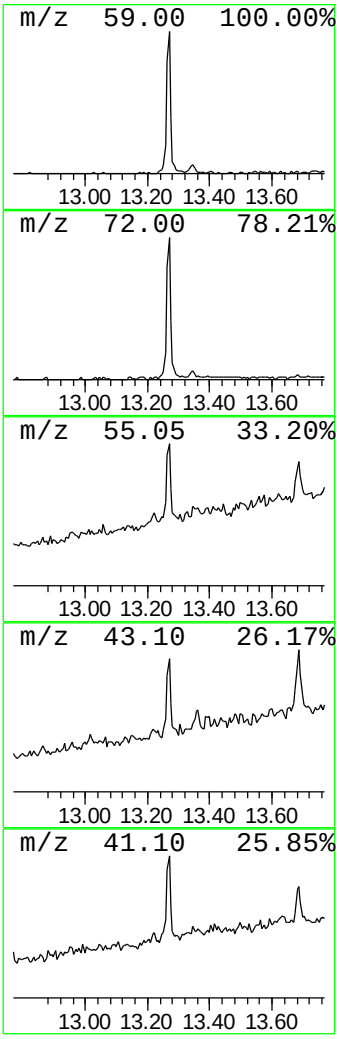
****

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.27	4.34 ng	151449	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Hexadecanamide	255	C16H33NO	000629-54-9	47
3	Nonanamide	157	C9H19NO	001120-07-6	46
4	1,1,3-Trimethyl-1-silacyclobutane	114	C6H14Si	002295-13-8	38
5	2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	35





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF090817\
Data File : BF098359.D
Acq On : 8 Sep 2017 19:15
Operator : SJ/JU
Sample : I5071-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G58A-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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...	4.85	9.3	ng	276475	1	6.68	596951	20.0
unknown6.45	6.45	37.6	ng	1121380	1	6.68	596951	20.0
unknown10.63	10.63	2.5	ng	70947	4	11.20	563489	20.0
Phenol, 4-(1,1,3,...	10.69	2.6	ng	72761	4	11.20	563489	20.0
unknown10.72	10.72	3.3	ng	91926	4	11.20	563489	20.0
unknown10.75	10.75	2.5	ng	70493	4	11.20	563489	20.0
2-Methyl-4-hydrox...	10.86	2.5	ng	71642	4	11.20	563489	20.0
Benzeneacetonitri...	10.90	2.5	ng	69034	4	11.20	563489	20.0
9-Octadecenamide,...	13.27	4.3	ng	151449	5	13.83	698695	20.0