LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098917.D
Acq On : 28 Sep 2017 20:07
Operator : SJ/JU
Sample : I5447-03 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-ENV-115-5(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	2.204	18	20	33	rVB2	59636	116560	7.39%	0.597%
2	2.310	36	38	44	rVB	28069	35138	2.23%	0.180%
3	4.022	324	329	333	rVB	20472	23938	1.52%	0.123%
4	4.528	411	415	423	rBV	41178	46823	2.97%	0.240%
5	5.134	514	518	529	rBV	404195	426792	27.04%	2.187%
6	5.534	582	586	589	rBV	1723926	1508685	95.59%	7.732%
7	6.534	752	756	765	rBV	1576206	1531517	97.04%	7.849%
8	6.681	777	781	785	rBV	1779291	1578273	100.00%	8.089%
9	6.916	817	821	824	rBV	1010946	801226	50.77%	4.106%
10	7.069	843	847	851	rBV	1414044	1212371	76.82%	6.214%
11	7.475	911	916	919	rBV	1091514	941300	59.64%	4.824%
12	8.198	1035	1039	1042	rBV	1197921	974929	61.77%	4.997%
13	9.269	1215	1221	1224	rBV	1975899	1573211	99.68%	8.063%
14	9.663	1284	1288	1296	rVB	239788	223565	14.17%	1.146%
15	9.875	1319	1324	1328	rVB2	27582	29395	1.86%	0.151%
16	9.951	1333	1337	1341	rBV	1017055	903050	57.22%	4.628%
17	10.374	1406	1409	1411	rVB	36849	29793	1.89%	0.153%
18	10.739	1467	1471	1481	rVB	749007	664188	42.08%	3.404%
19	10.845	1486	1489	1495	rBV2	38316	38707	2.45%	0.198%
20	11.292	1562	1565	1568	rBV3	23085	20617	1.31%	0.106%
21	11.386	1577	1581	1584	rBV2	21997	25237	1.60%	0.129%
22	11.439	1586	1590	1593	rBV	942654	775099	49.11%	3.973%
23	11.463	1593	1594	1597	rVB	69094	38887	2.46%	0.199%
24	11.951	1672	1677	1683	rBV4	63217	96683	6.13%	0.496%
25	12.051	1691	1694	1696	rBV2	20588	20969	1.33%	0.107%
26	12.492	1764	1769	1772	rBV4	24996	39840	2.52%	0.204%
27	12.651	1793	1796	1800	rBV	227296	188944	11.97%	0.968%
28	12.739	1808	1811	1816	rBV5	22087	24887	1.58%	0.128%
29	12.880	1829	1835	1839	rBV	209233	224784	14.24%	1.152%
30	12.933	1841	1844	1848	rVB2	58151	55539	3.52%	0.285%
31	13.021	1855	1859	1862	rBV	1410656	1175546	74.48%	6.025%
32	13.092	1869	1871	1875	rBV4	14197	20140	1.28%	0.103%
33	13.210	1888	1891	1894	rVB2	29945	31404	1.99%	0.161%
34	13.310	1905	1908	1911	rBV2	21465	21913	1.39%	0.112%

LSC Area Percent Report

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Data File : BF098917.D
Acq On : 28 Sep 2017 20:07
Operator : SJ/JU
Sample : I5447-03 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-ENV-115-5(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	13.363	1915	1917	1921	rBV5	20445	23025	1.46%	0.118%
36	13.592	1953	1956	1961	rBV	75778	77577	4.92%	0.398%
37	13.698	1970	1974	1981	rBV2	186962	221335	14.02%	1.134%
38	13.904	2007	2009	2013	rBV4	45495	64251	4.07%	0.329%
39	13.939	2013	2015	2019	rVB	45275	38261	2.42%	0.196%
40	14.051	2031	2034	2035	rBV	50642	50380	3.19%	0.258%
41	14.080	2035	2039	2042	rVV	929152	922035	58.42%	4.726%
42	14.104	2042	2043	2045	rVV	127187	86786	5.50%	0.445%
43	14.133	2045	2048	2055	rVB	919041	842245	53.36%	4.317%
44	14.468	2102	2105	2109	rBV	597250	524164	33.21%	2.686%
45	15.127	2214	2217	2221	rBV	112735	172870	10.95%	0.886%
46	15.445	2267	2271	2275	rBV	70720	87716	5.56%	0.450%
47	15.504	2278	2281	2288	rVV	98363	140494	8.90%	0.720%
48	15.574	2288	2293	2301	rVB	606458	840173	53.23%	4.306%

Sum of corrected areas: 19511262

LSC Report - Integrated Chromatogram

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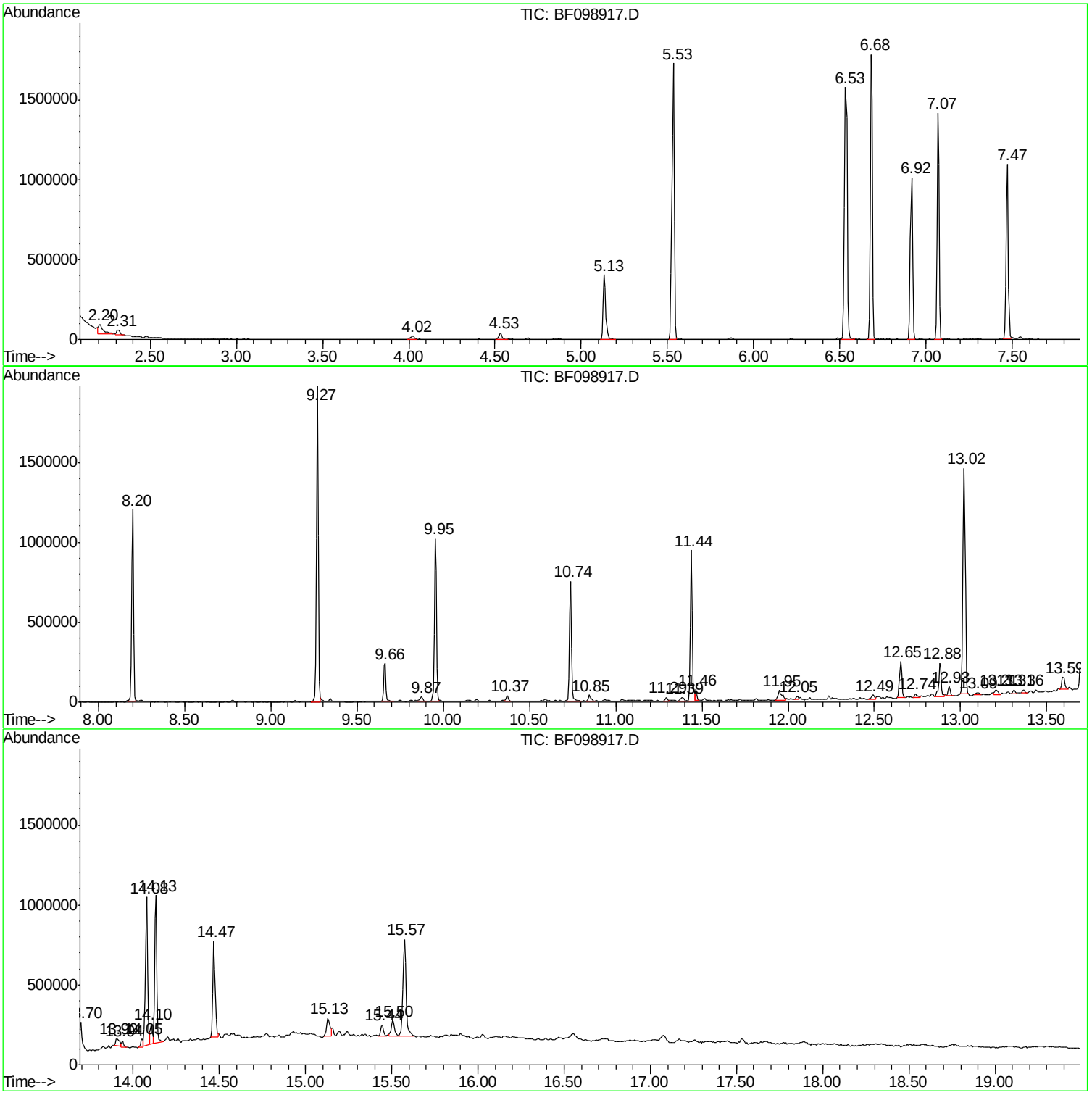
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-ENV-115-5(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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098917.D
Acq On : 28 Sep 2017 20:07
Operator : SJ/JU
Sample : I5447-03 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-ENV-115-5(0-5)

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

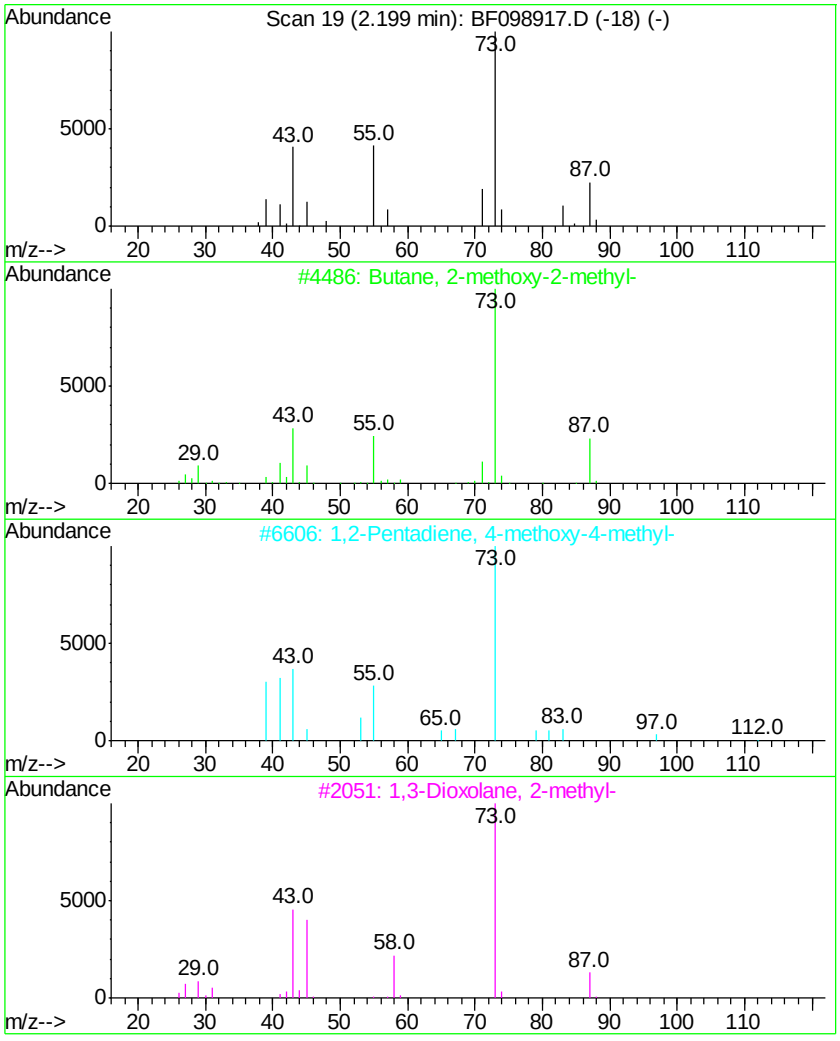
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

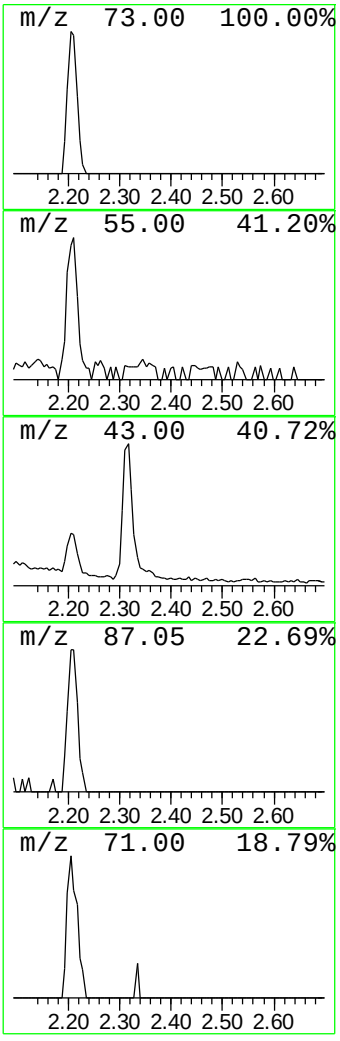
****

Peak Number 1 unknown2.20 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	2.91 ng	116560	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	45
2	1,2-Pentadiene, 4-methoxy-4-methyl-	112	C7H12O	049833-91-2	9
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	4
5	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	4





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098917.D
Acq On : 28 Sep 2017 20:07
Operator : SJ/JU
Sample : I5447-03 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-ENV-115-5(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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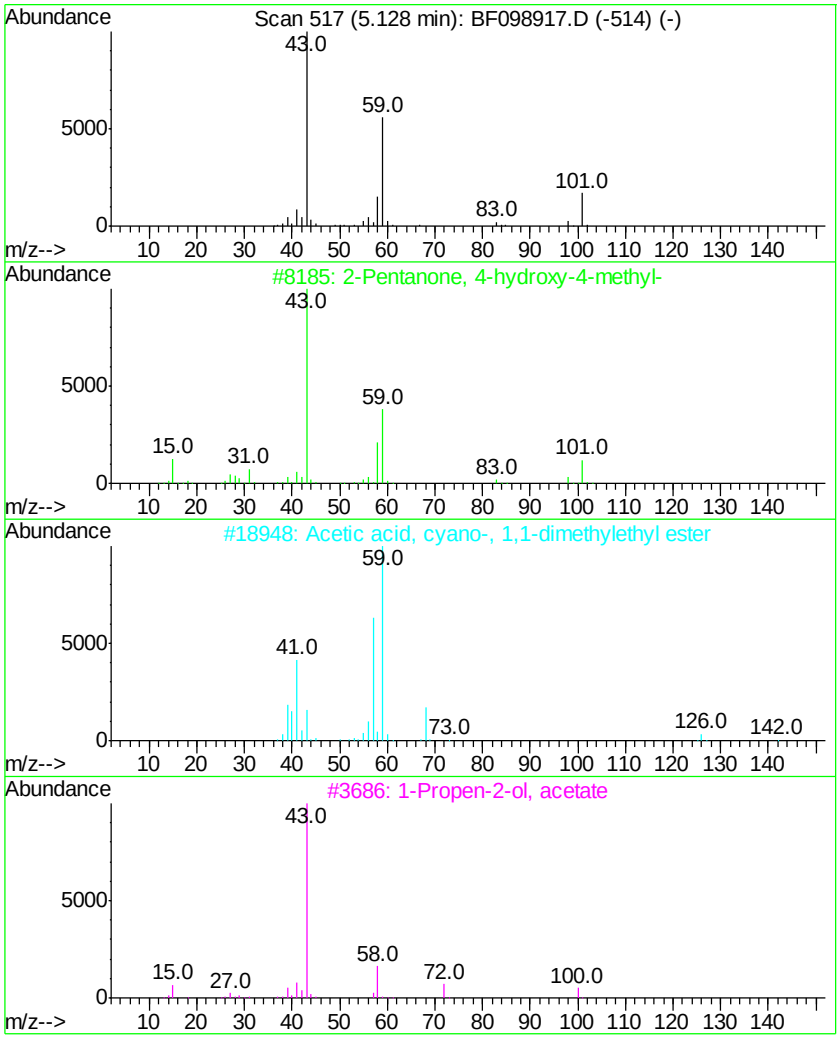
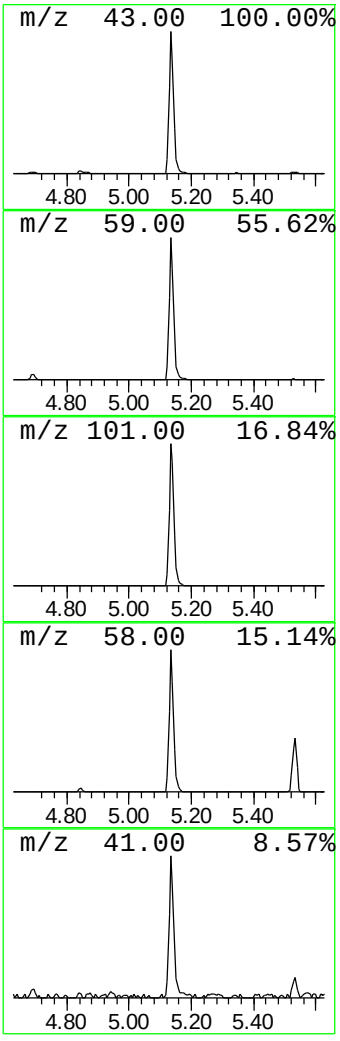
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	10.65 ng	426792	1,4-Dichlorobenzene-d4	6.92

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	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
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Acq On : 28 Sep 2017 20:07
Operator : SJ/JU
Sample : I5447-03 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-ENV-115-5(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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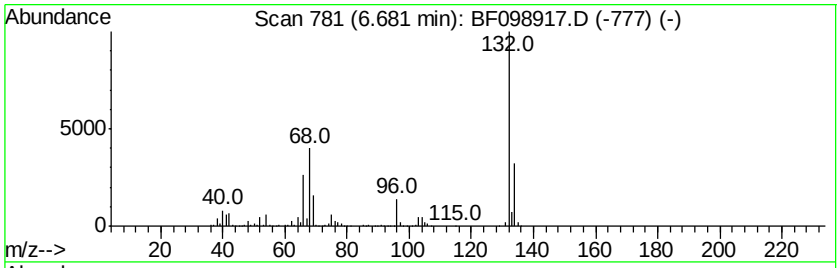
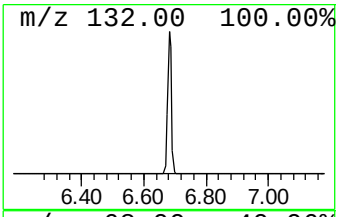
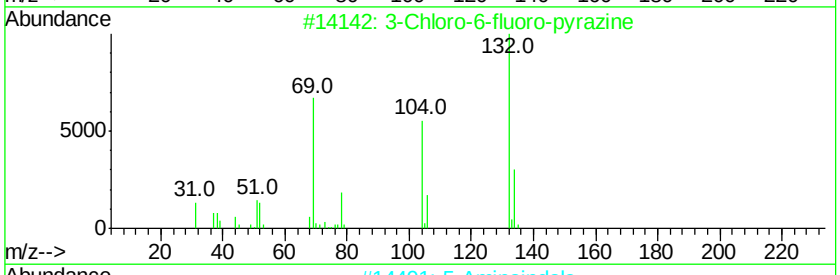
Peak Number 3 unknown6.68 Concentration Rank 1

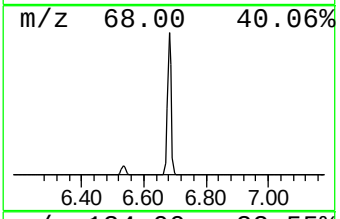
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	39.40 ng	1578270	1,4-Dichlorobenzene-d4	6.92

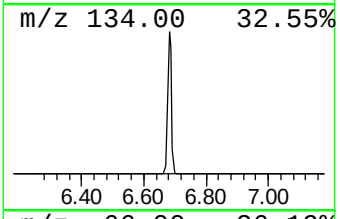
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Benzeneethanamine, .alpha.-methy...	223	C16H17N	002980-02-1	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9

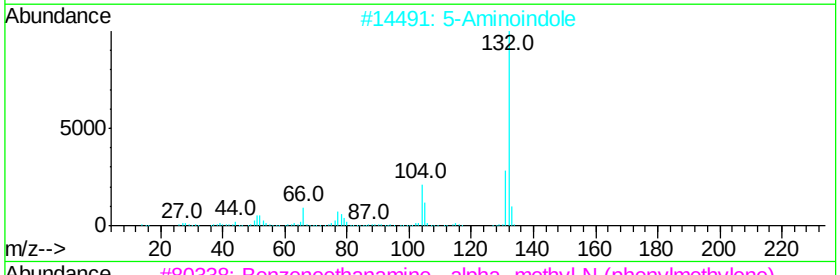


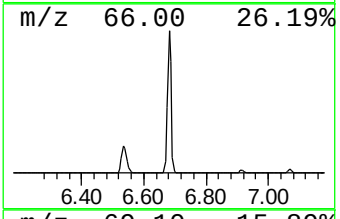


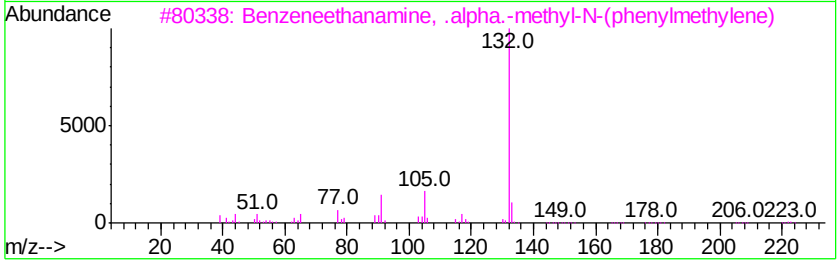


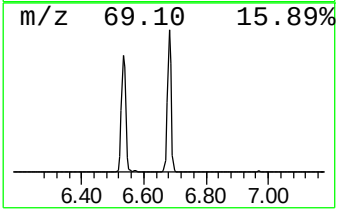












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Operator : SJ/JU
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-ENV-115-5(0-5)

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

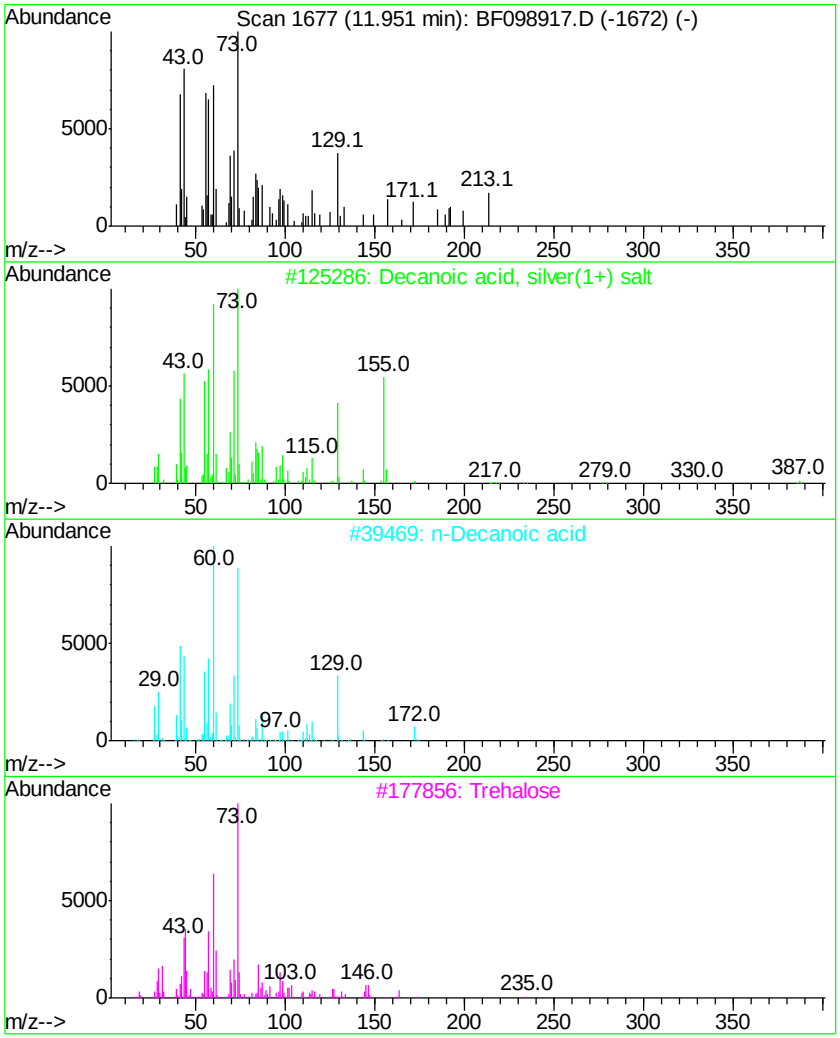
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

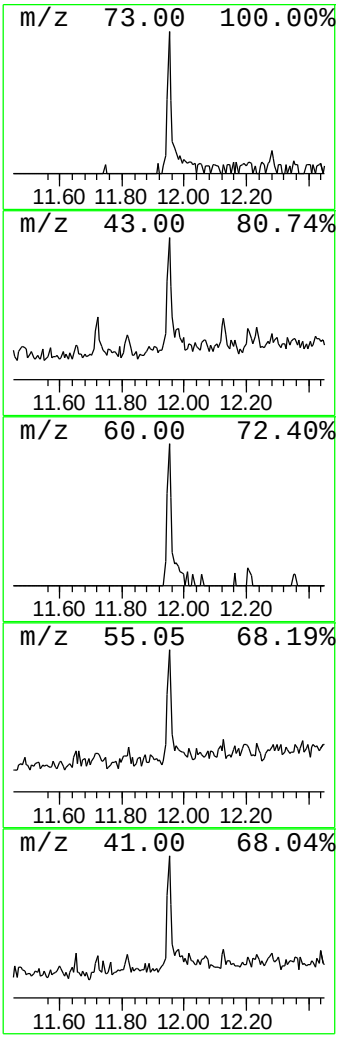
****

Peak Number 5 Decanoic acid, silver(1+) salt Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	2.49 ng	96683	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59
2	n-Decanoic acid	172	C10H20O2	000334-48-5	50
3	Trehalose	342	C12H22O11	000099-20-7	38
4	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	22
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	22





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

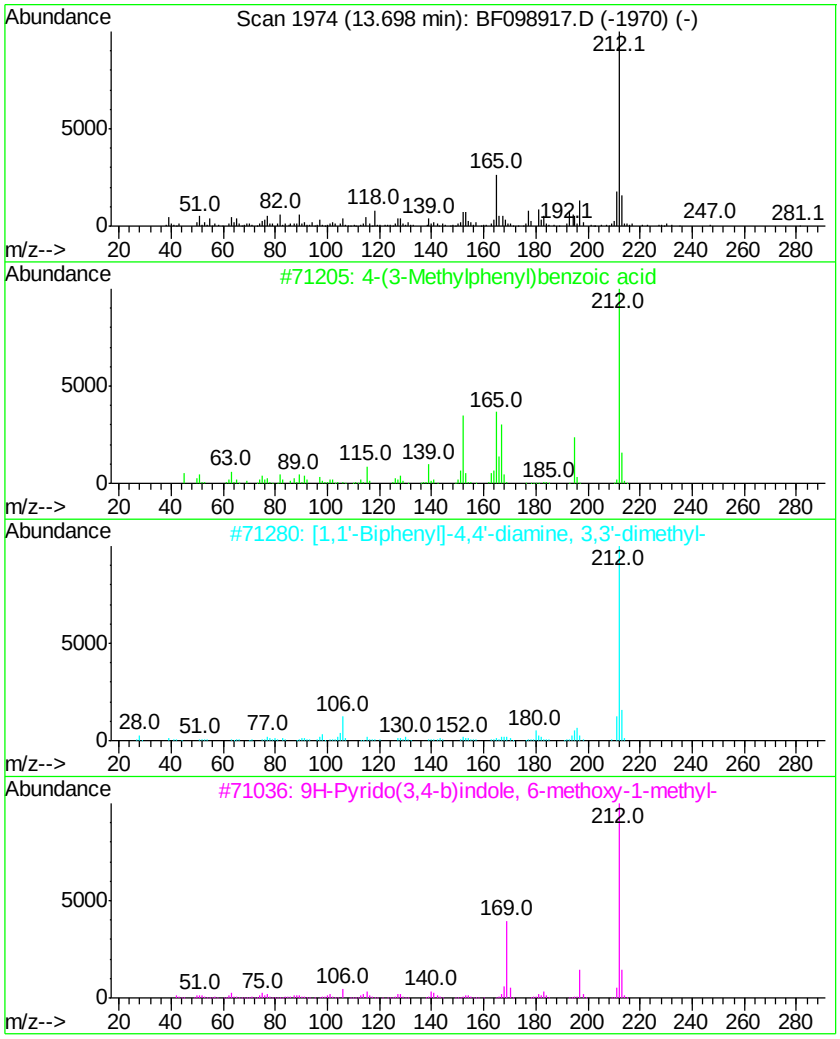
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

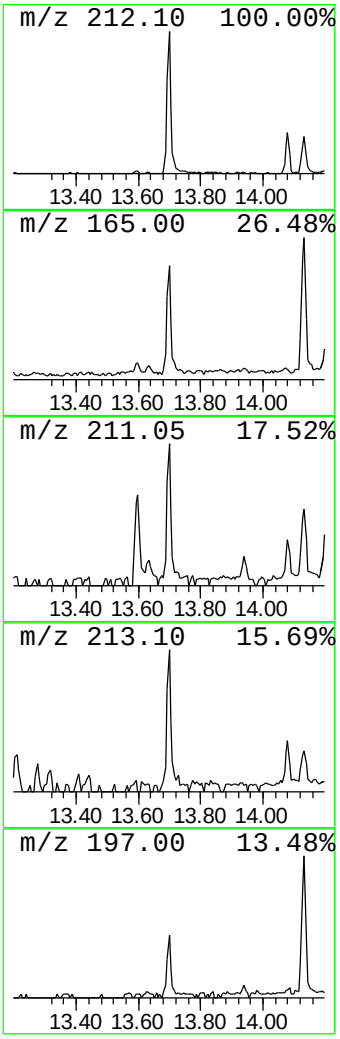
****

Peak Number 6 4-(3-Methylphenyl)benzoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	4.80 ng	221335	Chrysene-d12	14.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(3-Methylphenyl)benzoic acid	212	C14H12O2	1000305-27-3	72
2	[1,1'-Biphenyl]-4,4'-diamine, 3,...	212	C14H16N2	000119-93-7	68
3	9H-Pyrido(3,4-b)indole, 6-methox...	212	C13H12N2O	003589-72-8	64
4	Benzaldehyde, 2-butoxy-5-(4-meth...	268	C18H20O2	1000276-88-3	64
5	2,4'-Dihydroxy-stilbene	212	C14H12O2	1000147-73-5	64





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

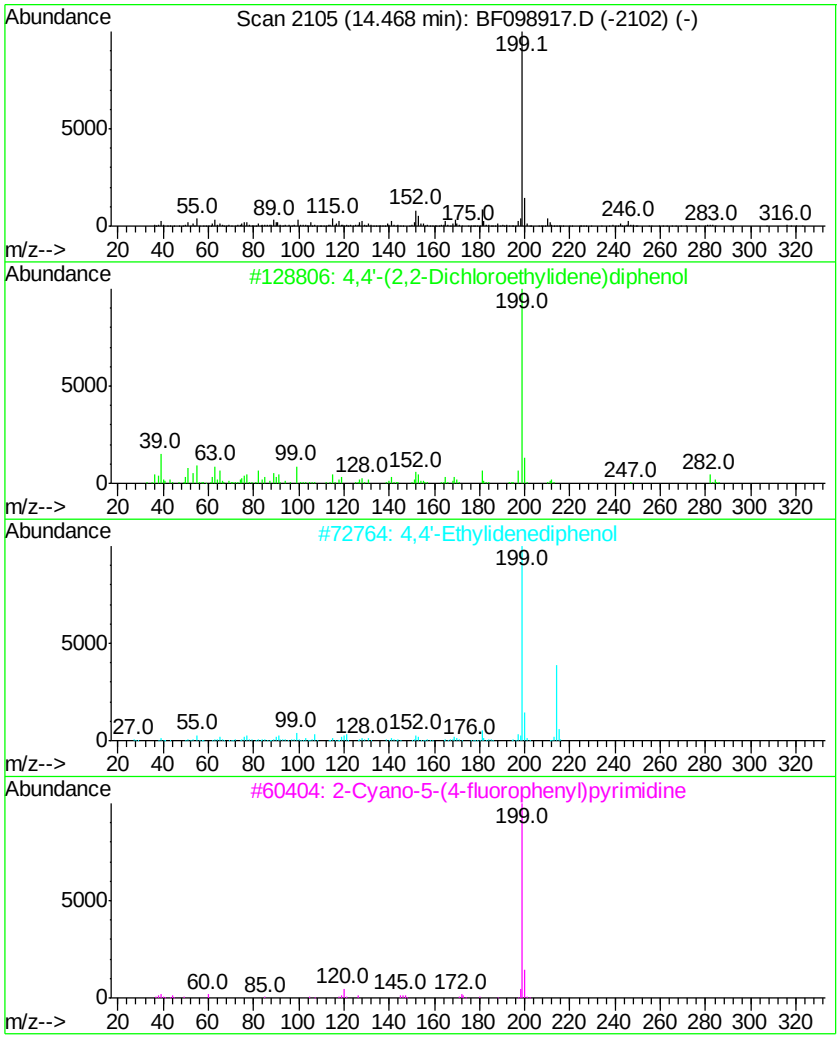
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

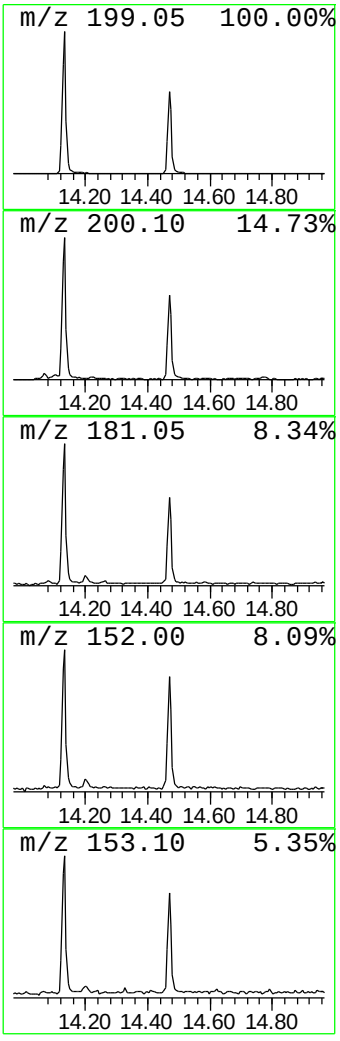
****

Peak Number 7 4,4'-(2,2-Dichloroethyliden... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	11.37 ng	524164	Chrysene-d12	14.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-(2,2-Dichloroethylidene)dip...	282	C14H12Cl2O2	013005-40-8	72
2	4,4'-Ethylidenediphenol	214	C14H14O2	002081-08-5	72
3	2-Cyano-5-(4-fluorophenyl)pyrimi...	199	C11H6FN3	1000078-56-5	64
4	2-Amino-5-methyl[1,2,4]triazolo[...	199	C10H9N5	018732-09-7	64
5	1-(3,4-Dihydro-2-naphthyl)-pyrro...	199	C14H17N	021403-95-2	62





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098917.D
Acq On : 28 Sep 2017 20:07
Operator : SJ/JU
Sample : I5447-03 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-ENV-115-5(0-5)

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

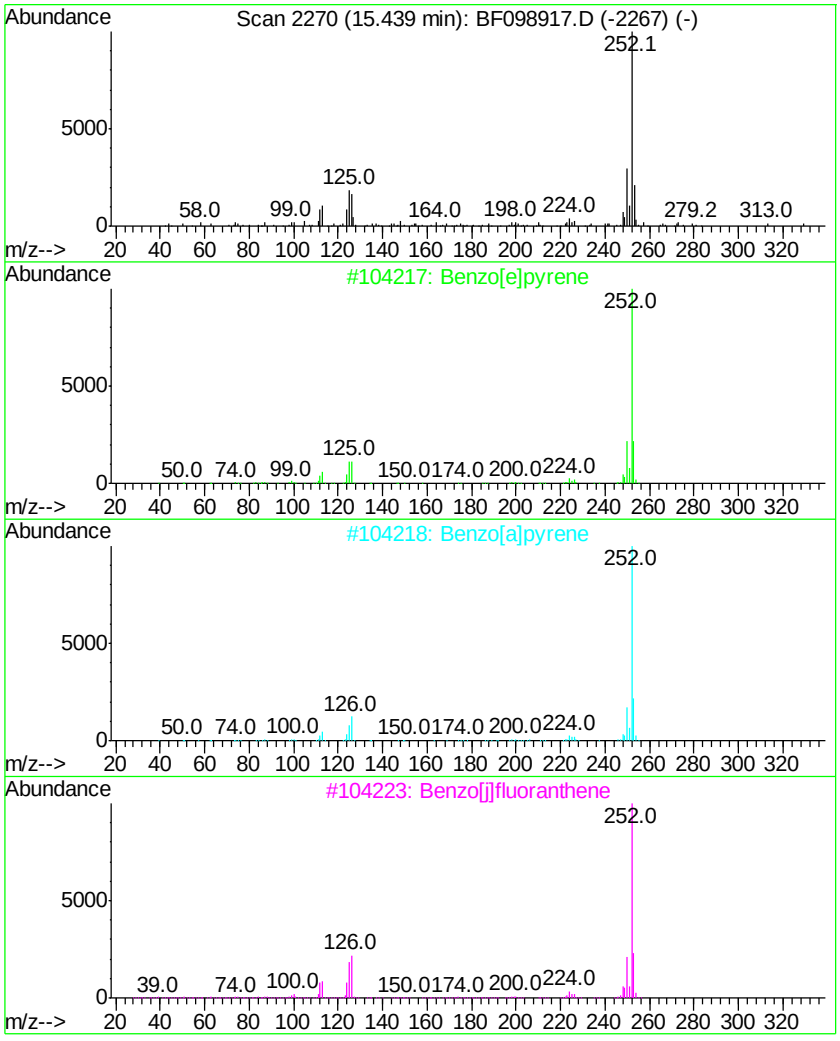
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

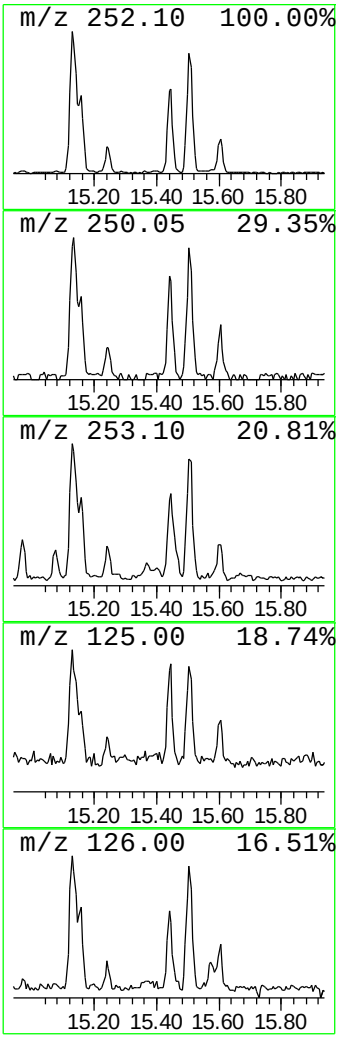
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.44	2.09 ng	87716	Perylene-d12	15.57

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	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098917.D
Acq On : 28 Sep 2017 20:07
Operator : SJ/JU
Sample : I5447-03 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-ENV-115-5(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
unknown2.20	2.20	2.9	ng	116560	1	6.92	801226	20.0
2-Pentanone, 4-hy...	5.13	10.7	ng	426792	1	6.92	801226	20.0
unknown6.68	6.68	39.4	ng	1578270	1	6.92	801226	20.0
Decanoic acid, si...	11.95	2.5	ng	96683	4	11.44	775099	20.0
4-(3-Methylphenyl...	13.70	4.8	ng	221335	5	14.08	922035	20.0
4,4'-(2,2-Dichlor...	14.47	11.4	ng	524164	5	14.08	922035	20.0
Benzo[e]pyrene	15.44	2.1	ng	87716	6	15.57	840173	20.0