LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092618\
Data File : BF109342.D
Acq On : 26 Sep 2018 17:45
Operator : JU/SJ
Sample : J5070-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RT-4005

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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	4.893	474	477	488	rVB	56298	73513	3.51%	0.362%
2	5.316	544	549	552	rBV	1928749	1760972	83.96%	8.667%
3	6.346	719	724	733	rVB	1982842	1913166	91.22%	9.416%
4	6.475	742	746	749	rBV	2229488	1879195	89.60%	9.249%
5	6.540	755	757	766	rVB	27547	25953	1.24%	0.128%
6	6.704	782	785	789	rBV	753975	583366	27.81%	2.871%
7	6.863	808	812	815	rBV	1793484	1453927	69.32%	7.156%
8	7.263	876	880	883	rBV	1241180	1176854	56.11%	5.792%
9	7.987	999	1003	1006	rBV	963498	748488	35.69%	3.684%
10	9.063	1182	1186	1189	rBV	2644045	2097326	100.00%	10.322%
11	9.457	1249	1253	1256	rBV	766158	581083	27.71%	2.860%
12	9.734	1297	1300	1304	rBV	952831	850366	40.55%	4.185%
13	10.522	1430	1434	1437	rBV	1544897	1318564	62.87%	6.489%
14	10.710	1463	1466	1468	rBV	36520	27527	1.31%	0.135%
15	10.745	1468	1472	1475	rVV2	31297	39270	1.87%	0.193%
16	10.798	1479	1481	1485	rVB2	37194	35516	1.69%	0.175%
17	10.886	1493	1496	1500	rBV2	27004	27258	1.30%	0.134%
18	10.922	1500	1502	1507	rBV	30482	29678	1.42%	0.146%
19	11.210	1548	1551	1554	rBV	907458	838699	39.99%	4.128%
20	11.233	1554	1555	1558	rVB	52181	32816	1.56%	0.162%
21	11.751	1639	1643	1647	rBV2	159949	149320	7.12%	0.735%
22	12.416	1753	1756	1761	rBV	138659	130341	6.21%	0.641%
23	12.533	1773	1776	1780	rBV	31986	31542	1.50%	0.155%
24	12.645	1789	1795	1798	rBV	122296	124073	5.92%	0.611%
25	12.680	1798	1801	1809	rVB5	15377	26866	1.28%	0.132%
26	12.792	1816	1820	1824	rVB	1861878	1659094	79.11%	8.165%
27	13.039	1855	1862	1864	rBV5	23304	29544	1.41%	0.145%
28	13.704	1969	1975	1984	rBV3	127995	250677	11.95%	1.234%
29	13.780	1984	1988	1991	rVV	69358	78787	3.76%	0.388%
30	13.839	1993	1998	2001	rVV	814972	779121	37.15%	3.835%
31	13.863	2001	2002	2004	rVB	67946	33686	1.61%	0.166%
32	14.469	2101	2105	2109	rBV	56868	66894	3.19%	0.329%
33	14.686	2136	2142	2147	rBV3	112746	154427	7.36%	0.760%
34	14.845	2165	2169	2172	rBV	111163	157018	7.49%	0.773%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092618\
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Acq On : 26 Sep 2018 17:45
Operator : JU/SJ
Sample : J5070-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RT-4005

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.939	2181	2185	2188	rVB2	34084	42976	2.05%	0.212%
36	15.121	2212	2216	2221	rVB	92894	118342	5.64%	0.582%
37	15.180	2222	2226	2232	rBV	78829	129069	6.15%	0.635%
38	15.239	2232	2236	2240	rBV2	597969	703986	33.57%	3.465%
39	15.445	2268	2271	2278	rVB7	21733	35602	1.70%	0.175%
40	15.686	2309	2312	2315	rBV2	26961	33383	1.59%	0.164%
41	16.580	2460	2464	2469	rBV2	29380	51470	2.45%	0.253%
42	16.980	2529	2532	2539	rVB2	24124	38873	1.85%	0.191%

Sum of corrected areas: 20318628

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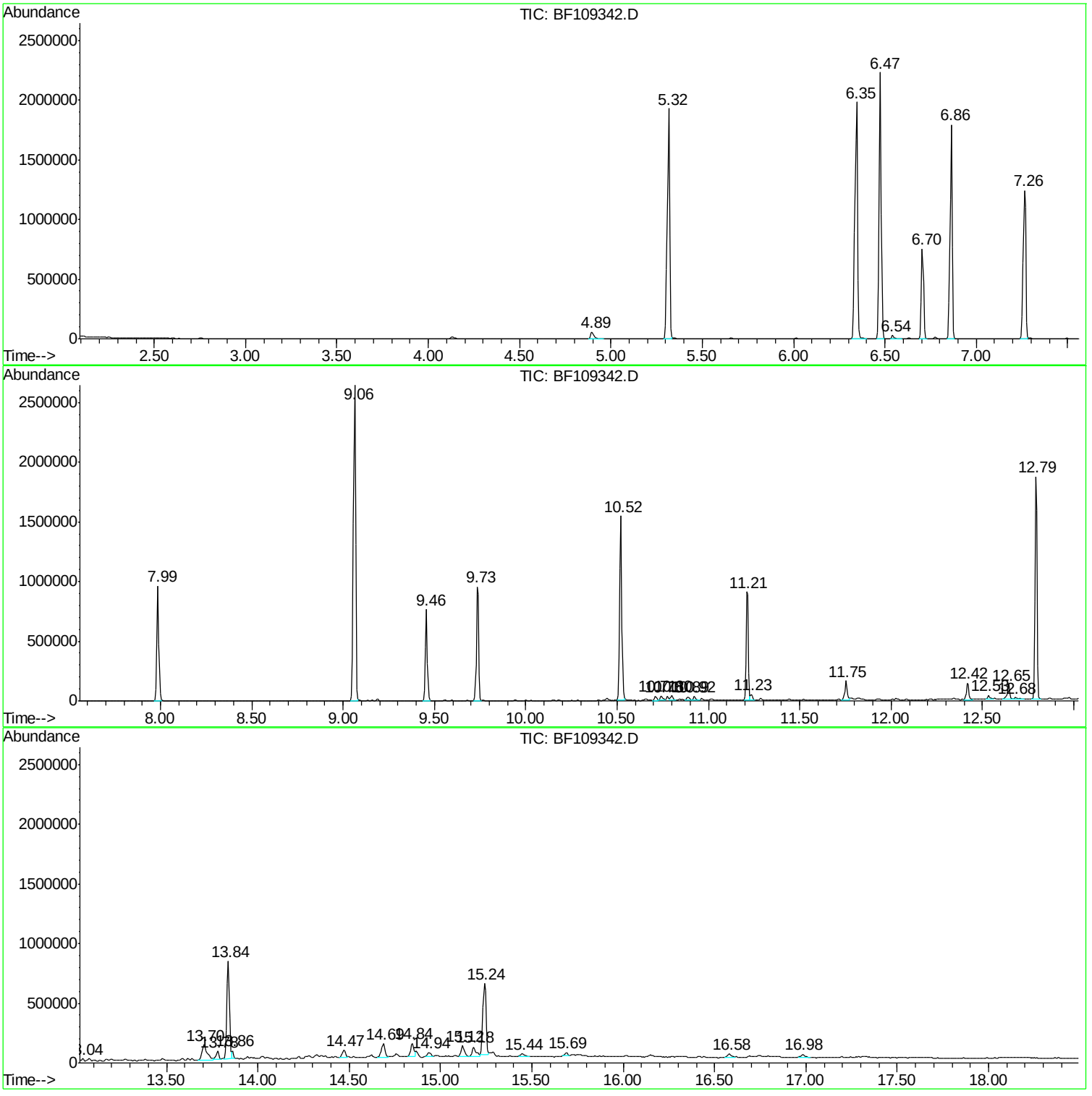
ClientSampleId : CS-RT-4005

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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 : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092618\
Data File : BF109342.D
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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : CS-RT-4005

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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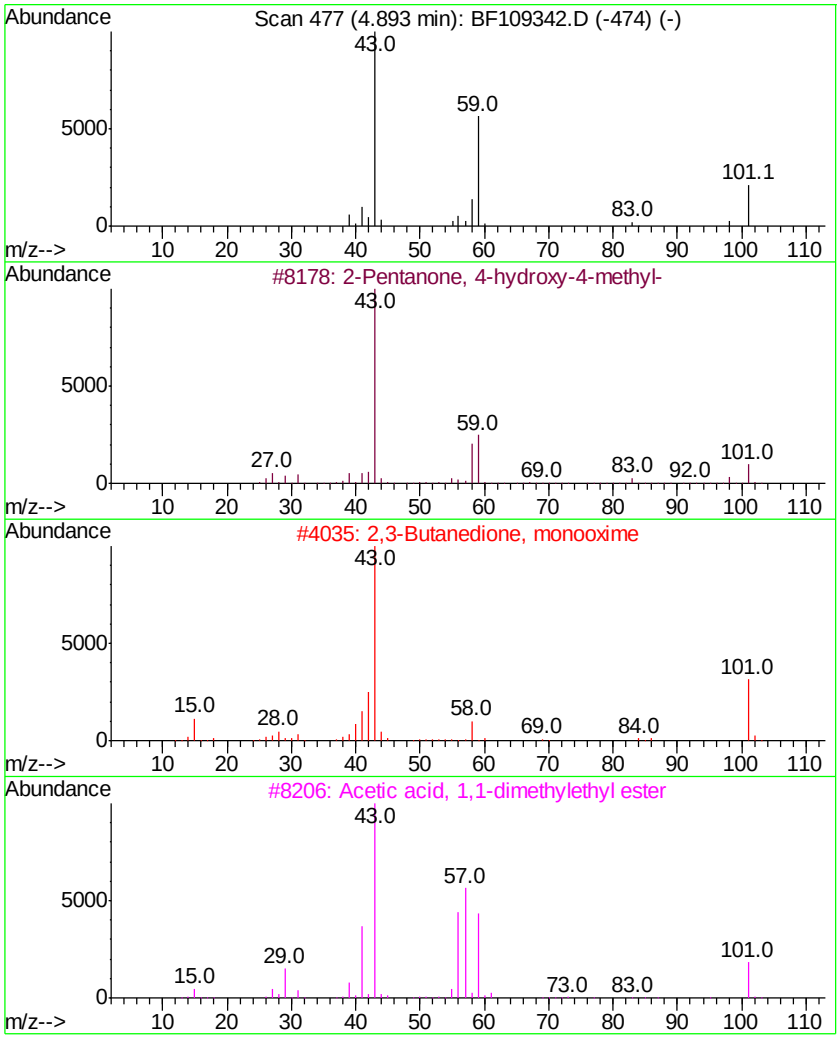
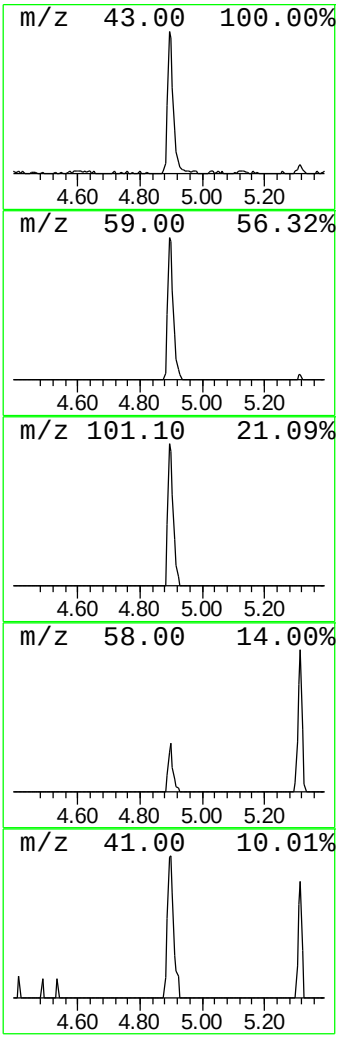
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	2.52 ng	73513	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4	Silane, trimethyl-	74	C3H10Si	000993-07-7	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092618\
Data File : BF109342.D
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Operator : JU/SJ
Sample : J5070-07
Misc :
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Instrument : BNA_F
ClientSampleId : CS-RT-4005

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

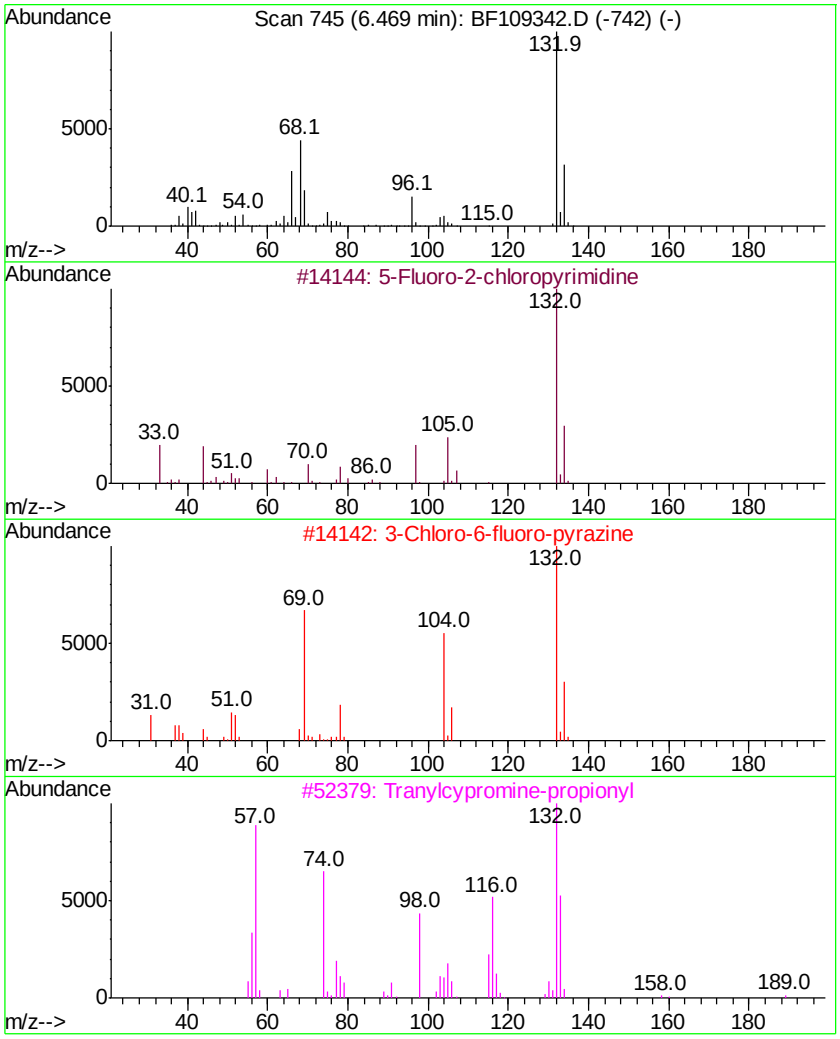
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

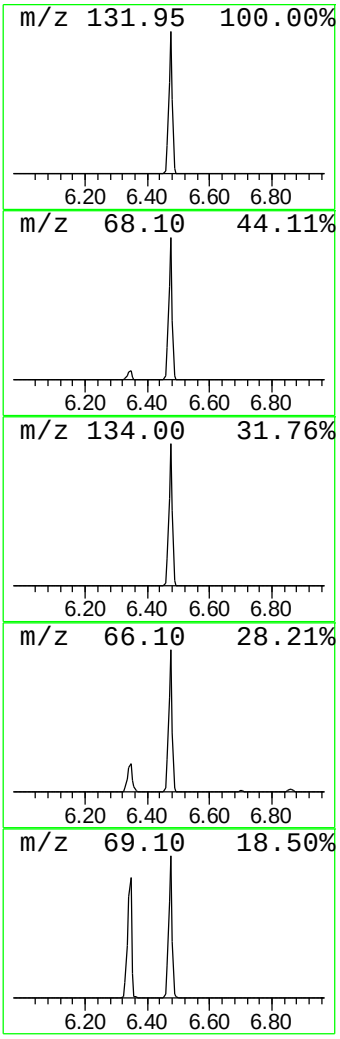
****

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	64.43 ng	1879200	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092618\
Data File : BF109342.D
Acq On : 26 Sep 2018 17:45
Operator : JU/SJ
Sample : J5070-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RT-4005

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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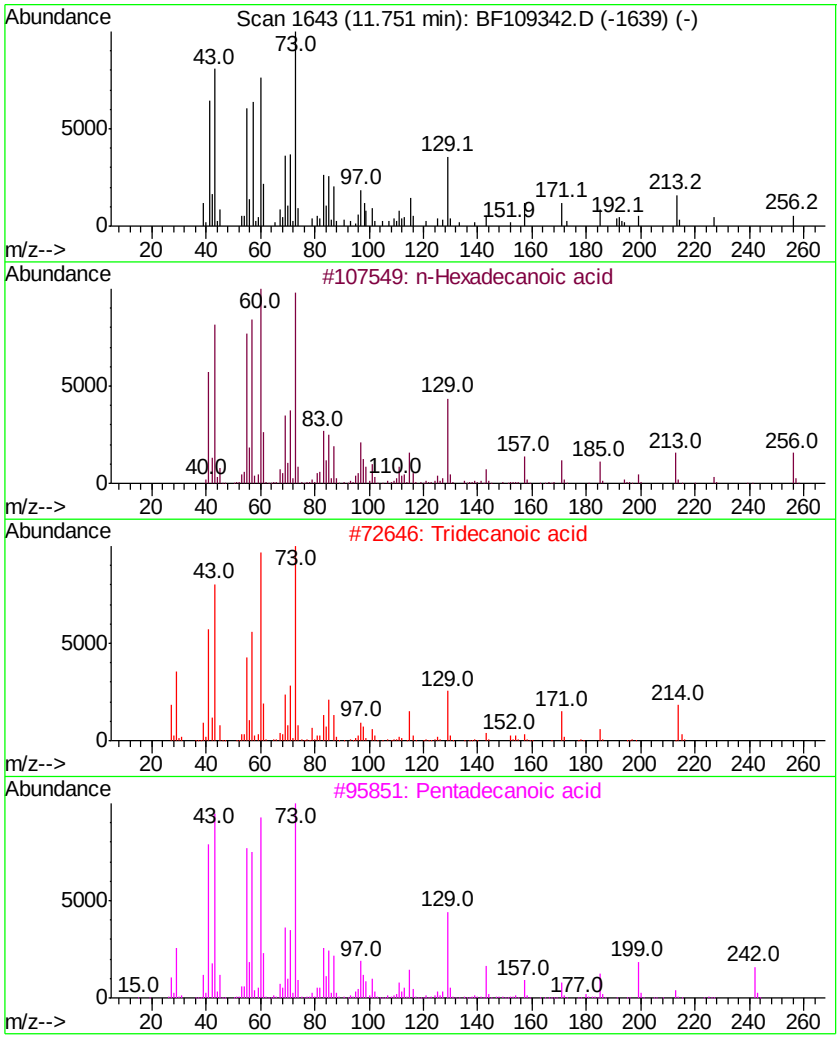
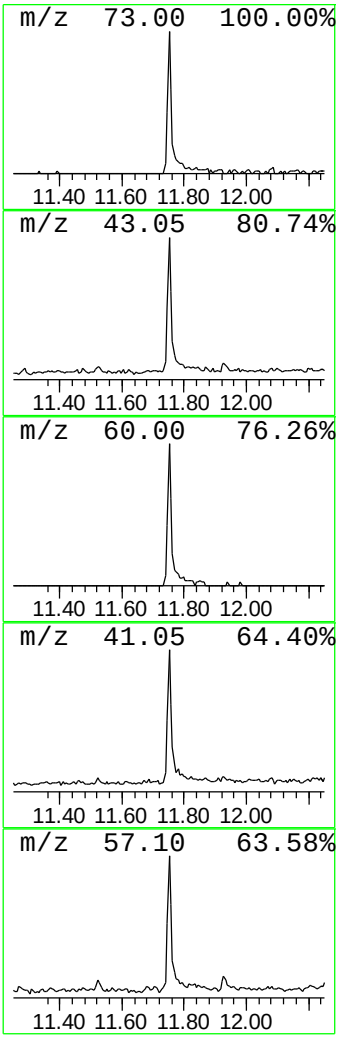
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	3.56 ng	149320	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Trehalose	342	C12H22O11	000099-20-7	50





Library Search Compound Report

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Sample : J5070-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RT-4005

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
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TIC Library : C:\DATABASE\NIST11.L
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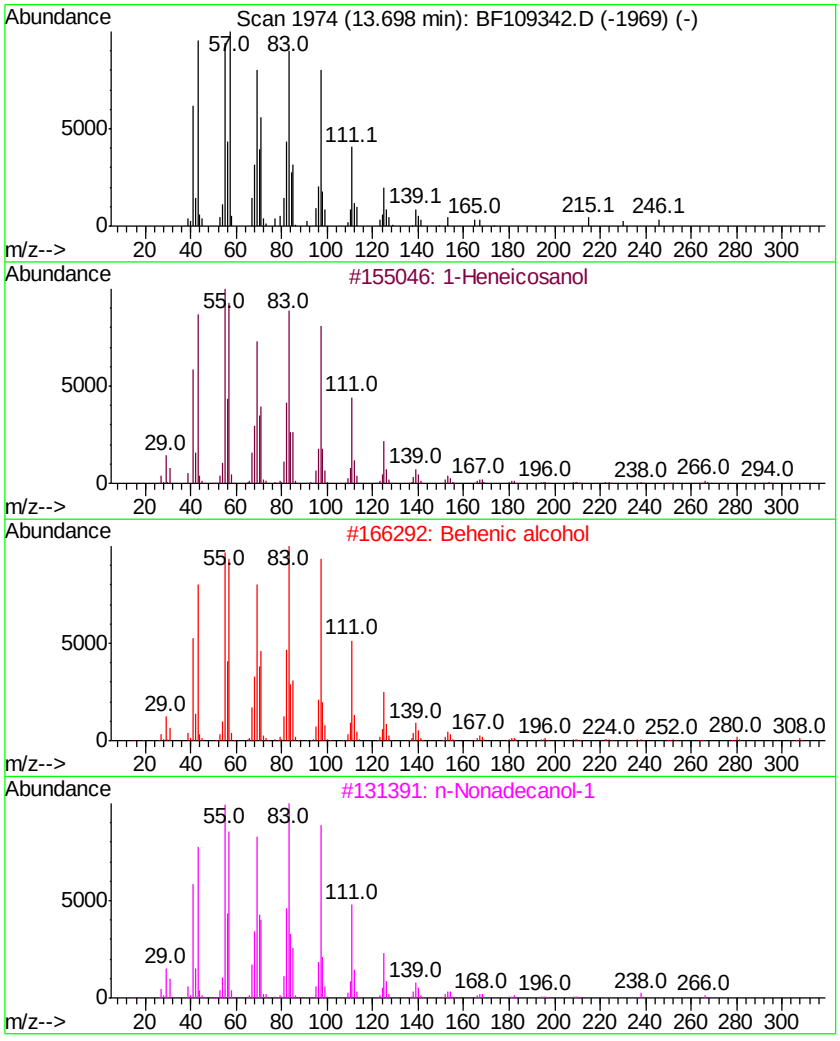
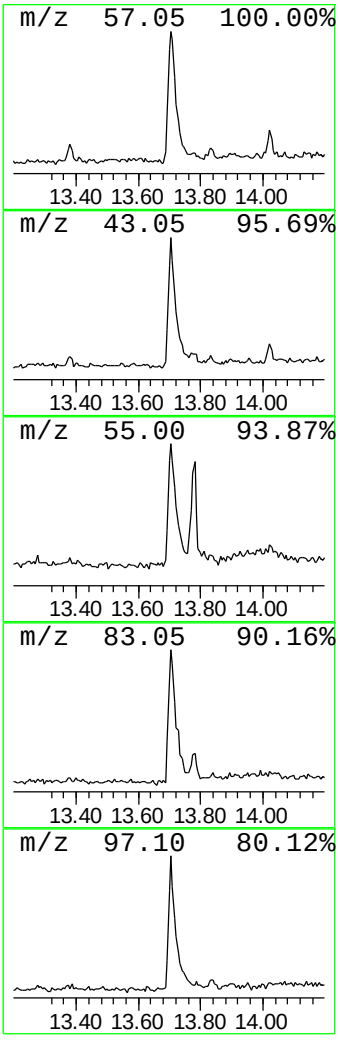
Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	6.43 ng	250677	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4	1-Heptacosanol	396	C27H56O	002004-39-9	93
5	Octacosanol	410	C28H58O	000557-61-9	92





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Sample : J5070-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RT-4005

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

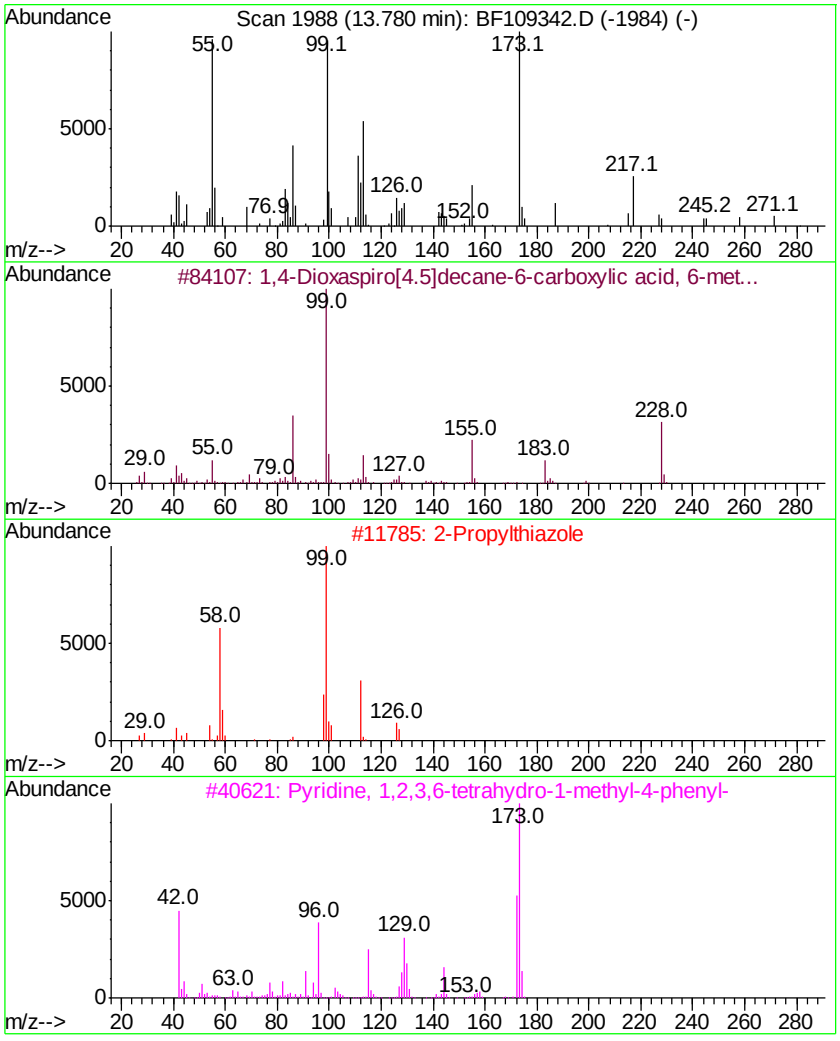
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

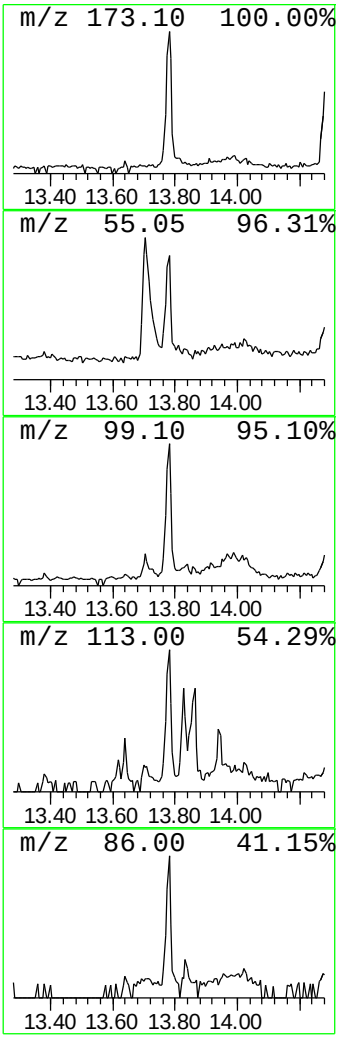
****

Peak Number 6 unknown13.78 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	2.02 ng	78787	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dioxaspiro[4.5]decane-6-carb...	228	C12H20O4	013839-77-5	35
2	2-Propylthiazole	127	C6H9NS	017626-75-4	14
3	Pyridine, 1,2,3,6-tetrahydro-1-m...	173	C12H15N	028289-54-5	11
4	2(1H)-Quinolinone, 3,4-dimethyl-	173	C11H11NO	017336-90-2	10
5	Spiro[1,3-dioxolane-2,2'-[6,7]di...	182	C9H14N2O2	1000142-34-9	10





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : CS-RT-4005

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

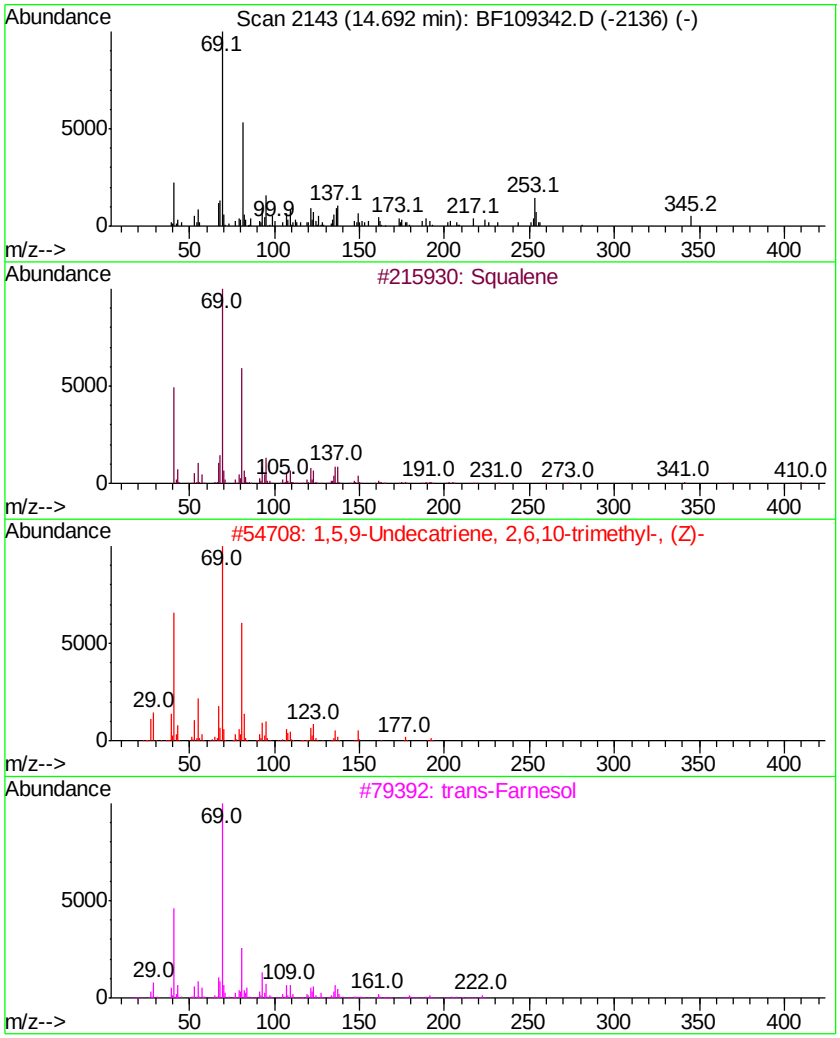
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

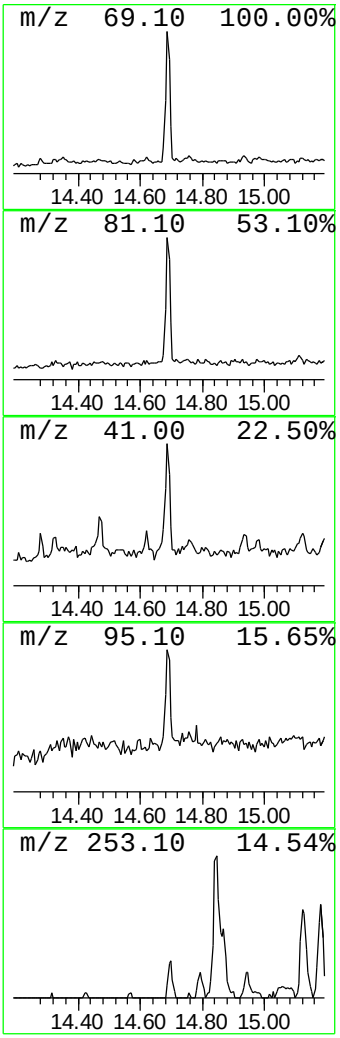
****

Peak Number 7 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	4.39 ng	154427	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	64
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	52
3	trans-Farnesol	222	C15H26O	000106-28-5	50
4	Methacrylic acid, ethyl ester	114	C6H10O2	000097-63-2	50
5	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	50





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Misc :
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Instrument : BNA_F
ClientSampleId : CS-RT-4005

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

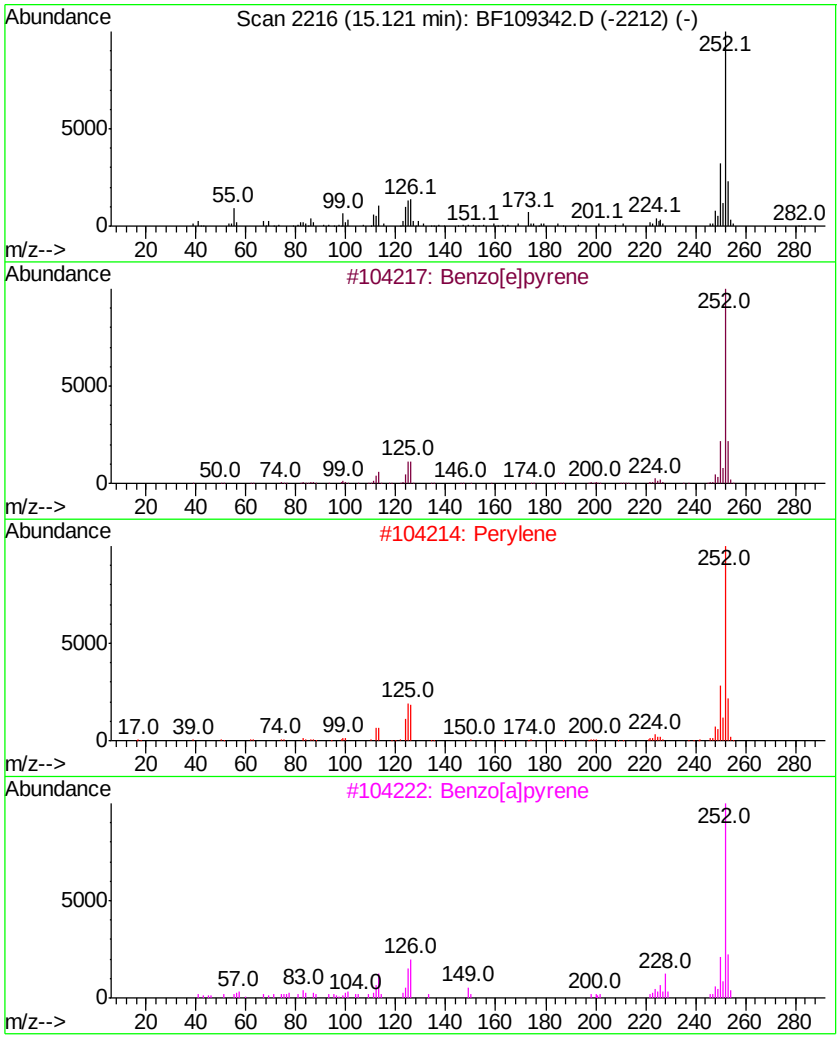
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

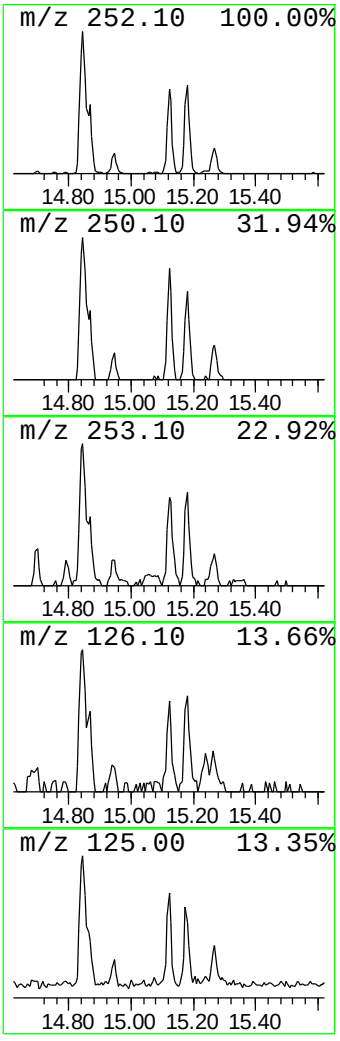
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	3.36 ng	118342	Perylene-d12	15.24

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





Tentatively Identified Compound (LSC) summary

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Operator : JU/SJ
Sample : J5070-07
Misc :
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Instrument : BNA_F
ClientSampleId : CS-RT-4005

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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...	4.89	2.5	ng	73513	1	6.70	583366	20.0
unknown6.47	6.47	64.4	ng	1879200	1	6.70	583366	20.0
n-Hexadecanoic acid	11.75	3.6	ng	149320	4	11.21	838699	20.0
1-Heneicosanol	13.70	6.4	ng	250677	5	13.84	779121	20.0
unknown13.78	13.78	2.0	ng	78787	5	13.84	779121	20.0
Squalene	14.69	4.4	ng	154427	6	15.24	703986	20.0
Benzo[e]pyrene	15.12	3.4	ng	118342	6	15.24	703986	20.0