LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090617\
Data File : BF098297.D
Acq On : 7 Sep 2017 2:44
Operator : SJ/JU
Sample : I5053-01 10X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-46A-0-3-COMP

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	4.863	469	472	481	rBV	36341	41053	5.11%	0.670%
2	5.098	508	512	515	rVB	19271	18052	2.25%	0.294%
3	5.298	542	546	556	rVB	133225	144578	18.00%	2.358%
4	6.334	719	722	731	rBV	185235	174439	21.71%	2.845%
5	6.463	741	744	752	rBV	200291	163825	20.39%	2.672%
6	6.698	780	784	787	rBV	716716	658617	81.98%	10.742%
7	6.851	806	810	816	rBV	150656	127844	15.91%	2.085%
8	7.257	876	879	884	rBV	96548	83265	10.36%	1.358%
9	7.981	998	1002	1005	rBV	1011488	803344	100.00%	13.103%
10	9.057	1181	1185	1194	rBV	171064	170310	21.20%	2.778%
11	9.139	1194	1199	1205	rVB3	7646	13462	1.68%	0.220%
12	9.457	1248	1253	1256	rBV2	17917	21236	2.64%	0.346%
13	9.733	1296	1300	1308	rBV	800858	733199	91.27%	11.959%
14	10.386	1407	1411	1414	rBV2	14204	14300	1.78%	0.233%
15	10.445	1417	1421	1424	rBV	27426	25229	3.14%	0.411%
16	10.522	1430	1434	1437	rVB3	31804	27106	3.37%	0.442%
17	10.651	1451	1456	1462	rBV2	66892	68690	8.55%	1.120%
18	10.704	1462	1465	1467	rBV	67060	54956	6.84%	0.896%
19	10.739	1467	1471	1474	rVV3	72116	92604	11.53%	1.510%
20	10.769	1474	1476	1479	rVV2	71226	72357	9.01%	1.180%
21	10.792	1479	1480	1483	rVV	39431	32588	4.06%	0.532%
22	10.833	1483	1487	1489	rVV2	24774	39817	4.96%	0.649%
23	10.851	1489	1490	1492	rVV	29699	19227	2.39%	0.314%
24	10.880	1492	1495	1499	rVV2	56291	67500	8.40%	1.101%
25	10.922	1499	1502	1507	rVV	70098	84538	10.52%	1.379%
26	10.963	1507	1509	1513	rVB	41675	36562	4.55%	0.596%
27	11.086	1527	1530	1532	rBV3	14525	14822	1.85%	0.242%
28	11.116	1532	1535	1539	rVB3	27980	28307	3.52%	0.462%
29	11.216	1548	1552	1555	rBV	798993	676647	84.23%	11.036%
30	11.463	1590	1594	1597	rBV3	9684	11982	1.49%	0.195%
31	11.510	1600	1602	1606	rVB2	13808	12062	1.50%	0.197%
32	11.780	1644	1648	1650	rBV	15551	13293	1.65%	0.217%
33	11.916	1669	1671	1674	rBV	15467	12928	1.61%	0.211%
34	12.304	1734	1737	1743	rVB3	22330	20688	2.58%	0.337%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090617\
Data File : BF098297.D
Acq On : 7 Sep 2017 2:44
Operator : SJ/JU
Sample : I5053-01 10X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-46A-0-3-COMP

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	12.422	1754	1757	1761	rBV	34562	31108	3.87%	0.507%
36	12.651	1793	1796	1798	rBV	38812	28819	3.59%	0.470%
37	12.680	1798	1801	1804	rVV2	27345	25137	3.13%	0.410%
38	12.792	1817	1820	1828	rBV	161705	160534	19.98%	2.618%
39	13.033	1858	1861	1866	rVB2	28158	28244	3.52%	0.461%
40	13.374	1916	1919	1922	rBV2	33965	32714	4.07%	0.534%
41	13.704	1972	1975	1978	rBV2	29879	30430	3.79%	0.496%
42	13.845	1995	1999	2003	rBV	695474	720252	89.66%	11.748%
43	15.257	2235	2239	2247	rBV	368062	494437	61.55%	8.064%

Sum of corrected areas: 6131102

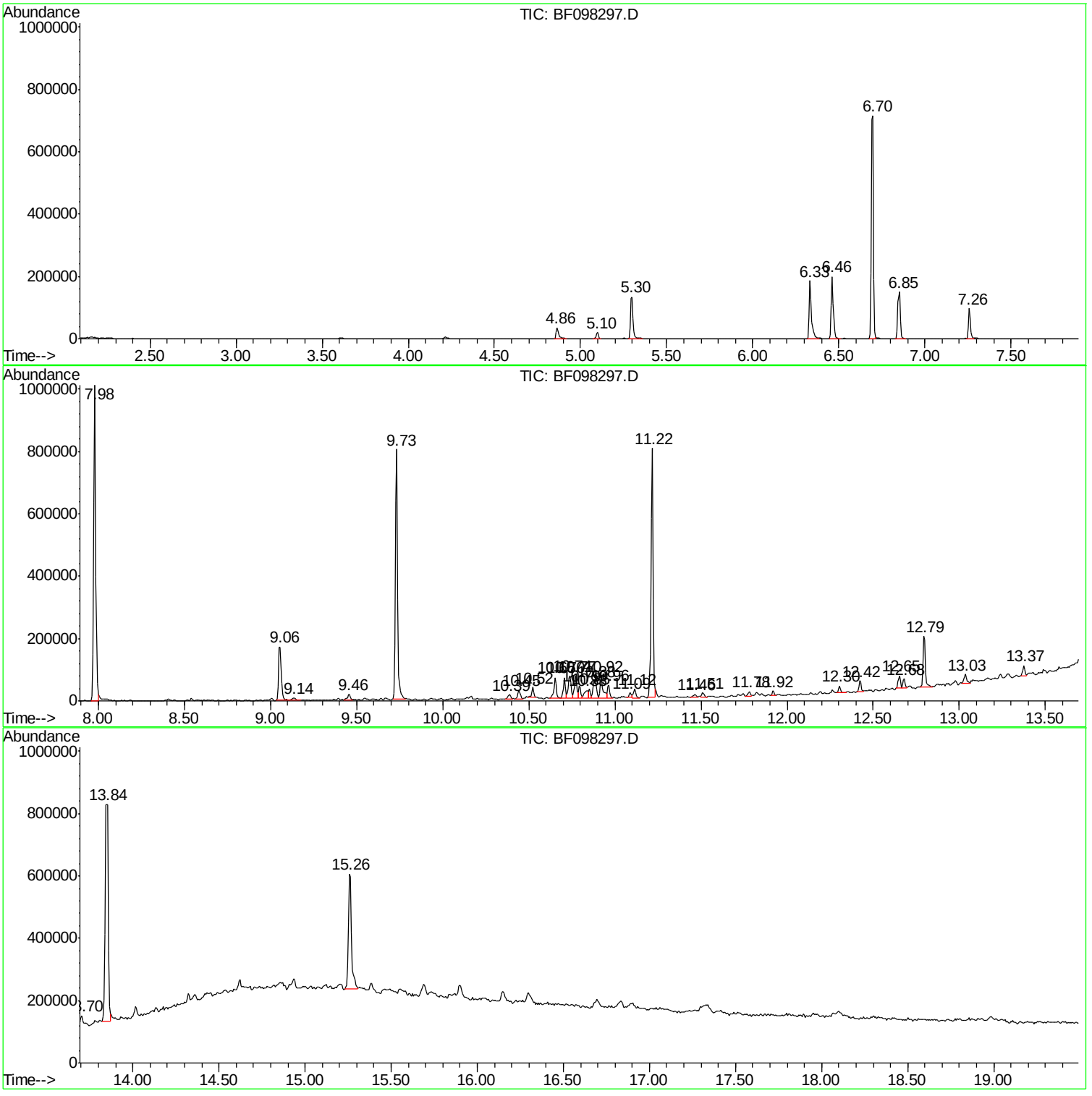
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090617\
Data File : BF098297.D
Acq On : 7 Sep 2017 2:44
Operator : SJ/JU
Sample : I5053-01 10X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-46A-0-3-COMP

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\BF090617\
Data File : BF098297.D
Acq On : 7 Sep 2017 2:44
Operator : SJ/JU
Sample : I5053-01 10X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-46A-0-3-COMP

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

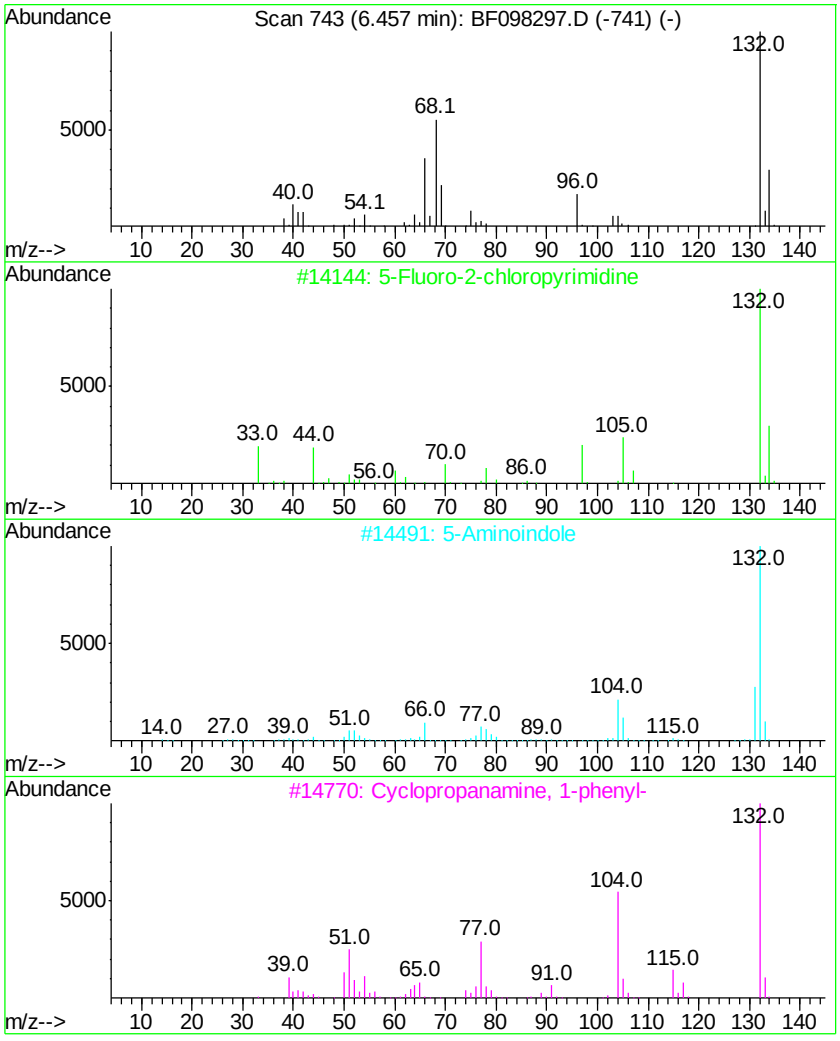
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

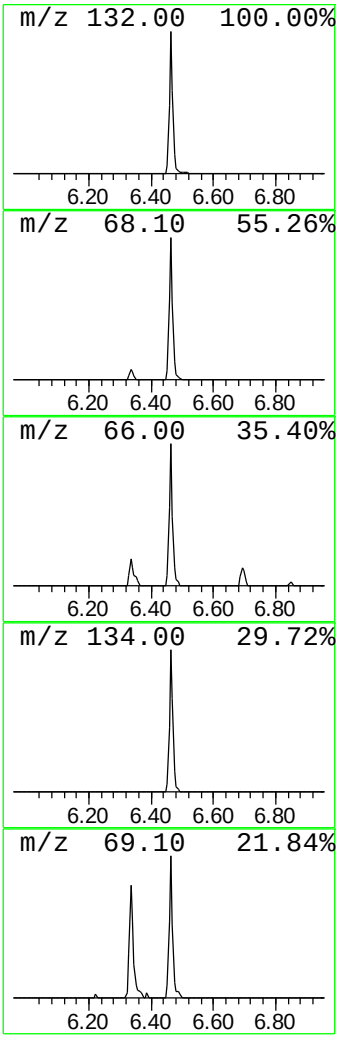
****

Peak Number 1 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	4.97 ng	163825	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	12
2	5-Aminoindole	132	C8H8N2	005192-03-0	10
3	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	Xenon	132	Xe	007440-63-3	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090617\
Data File : BF098297.D
Acq On : 7 Sep 2017 2:44
Operator : SJ/JU
Sample : I5053-01 10X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-46A-0-3-COMP

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

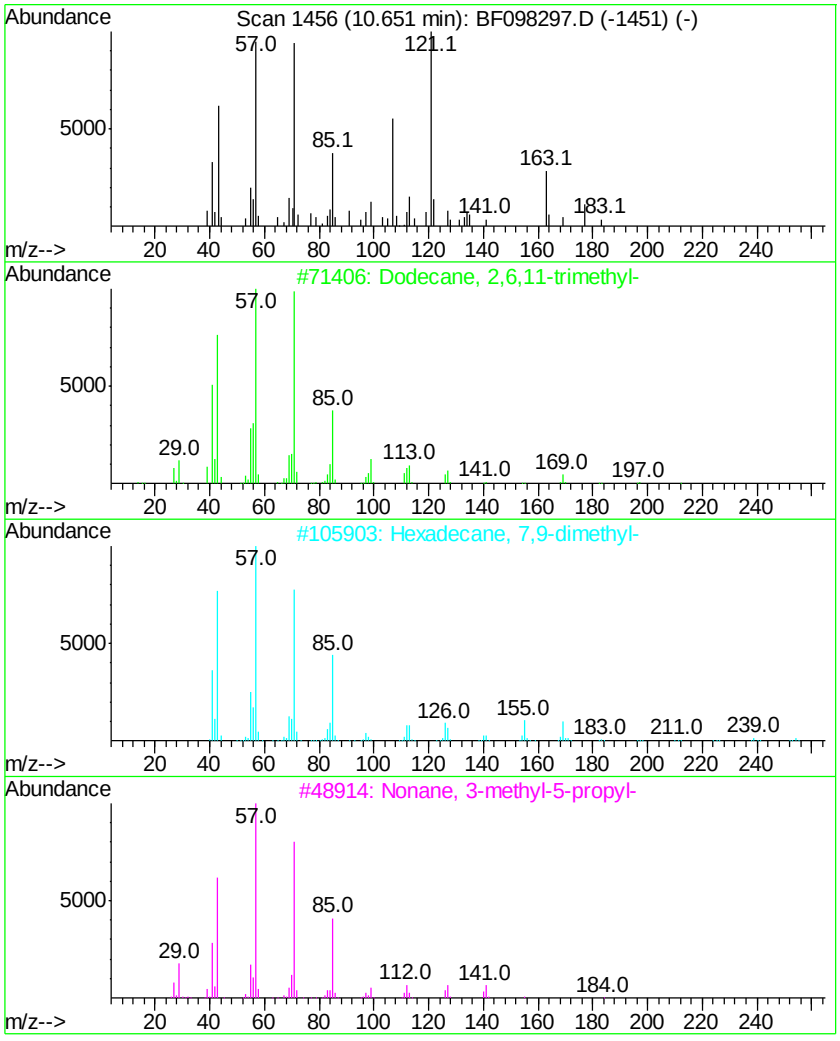
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

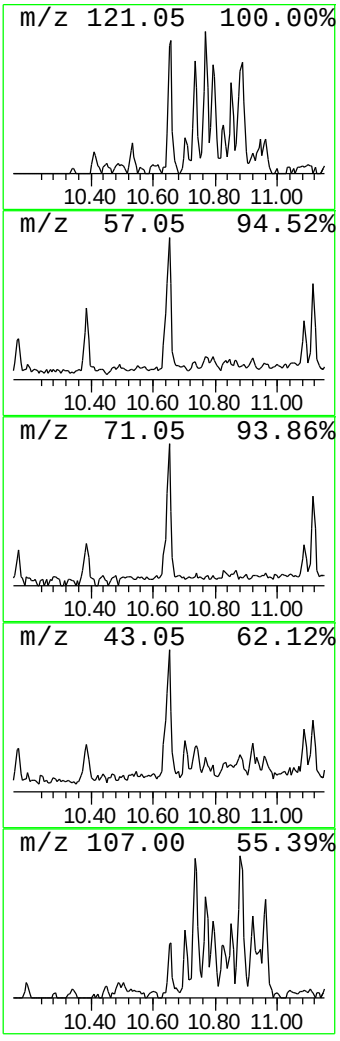
****

Peak Number 3 unknown10.65 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	2.03 ng	68690	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	35
2	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	27
3	Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	22
4	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	22
5	3-Heptanone, 4-methyl-	128	C8H16O	006137-11-7	18





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090617\
Data File : BF098297.D
Acq On : 7 Sep 2017 2:44
Operator : SJ/JU
Sample : I5053-01 10X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-46A-0-3-COMP

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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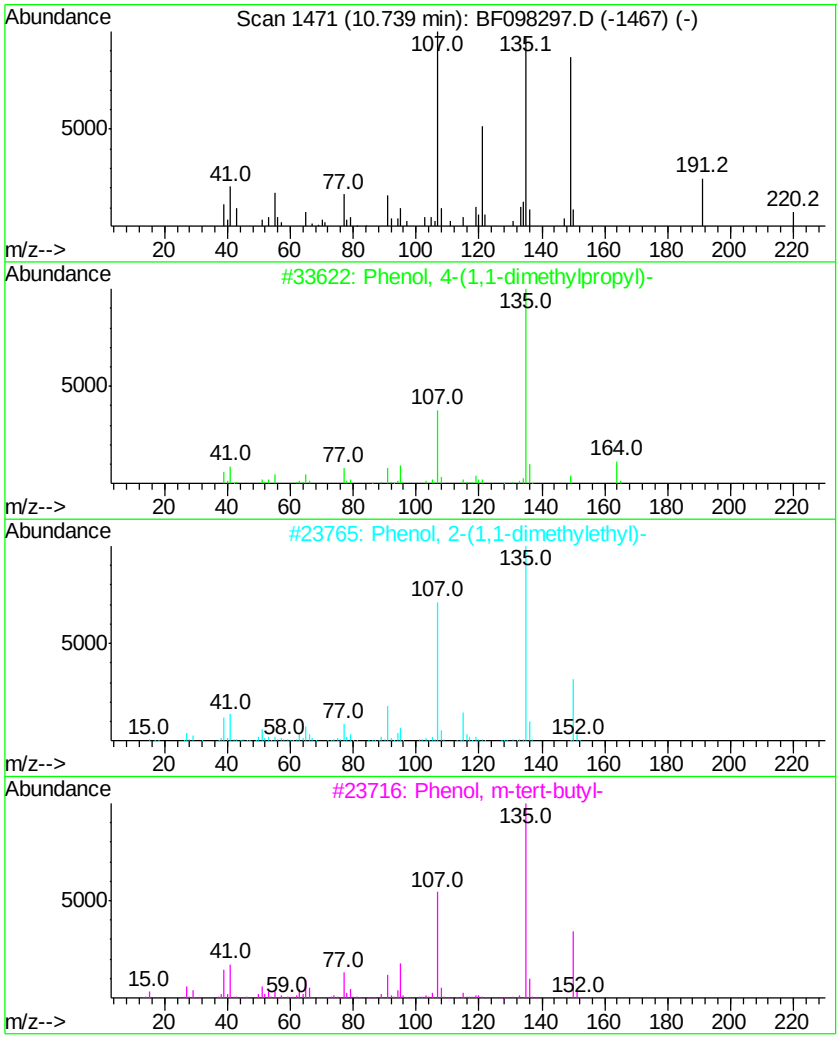
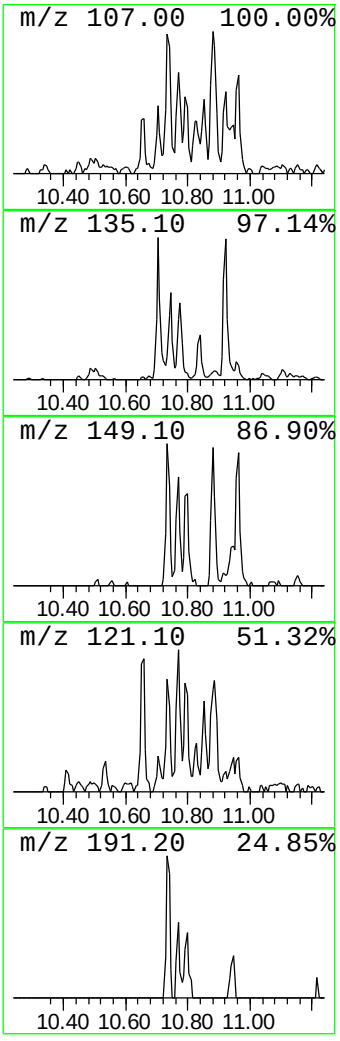
Peak Number 4 unknown10.74 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	2.74 ng	92604	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	47
2	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	46
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	46
4	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	43
5	Hexestrol, O-heptafluorobutyryl-	466	C22H21F7O3	1000365-31-9	43





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090617\
Data File : BF098297.D
Acq On : 7 Sep 2017 2:44
Operator : SJ/JU
Sample : I5053-01 10X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-46A-0-3-COMP

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

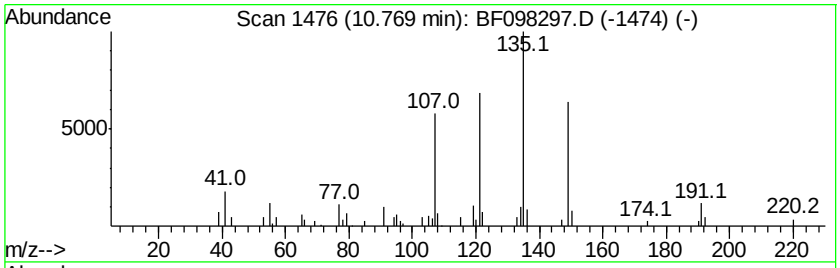
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

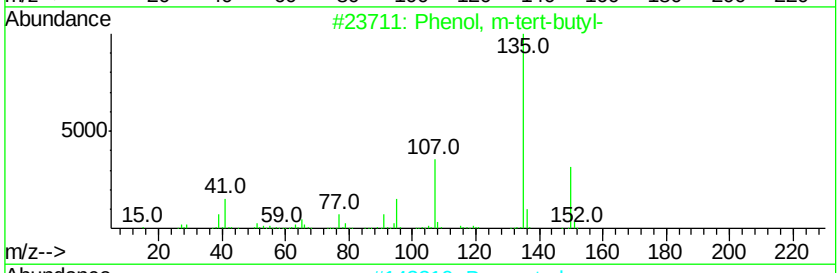
****

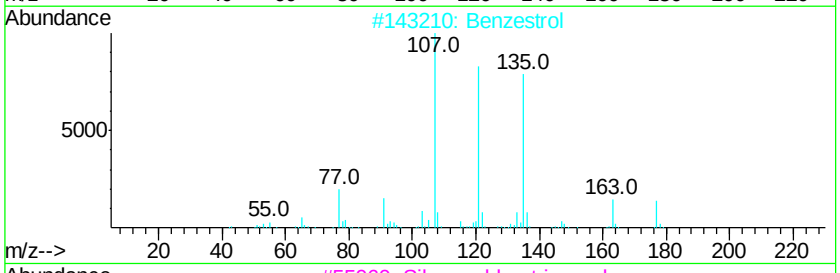
Peak Number 5 unknown10.77 Concentration Rank 5

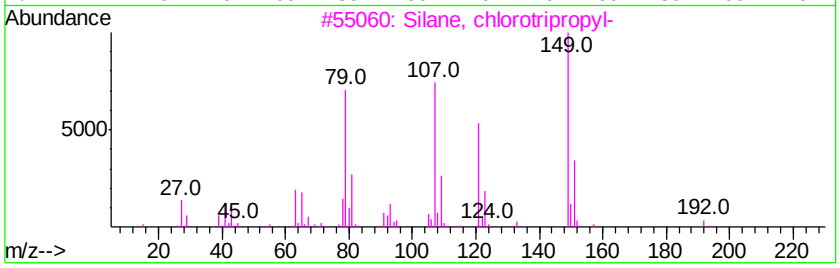
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	2.14 ng	72357	Phenanthrene-d10	11.22

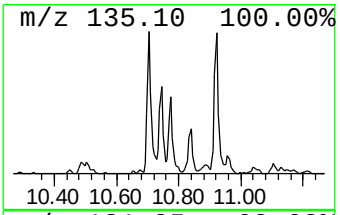
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	47
2	Benzestrol	298	C20H26O2	000085-95-0	38
3	Silane, chlorotripropyl-	192	C9H21ClSi	000995-25-5	38
4	4-n-Butoxyphenyl isocyanate	207	C11H13NOS	1000342-44-4	35
5	.alpha. Isomethyl ionone	206	C14H22O	000127-51-5	35

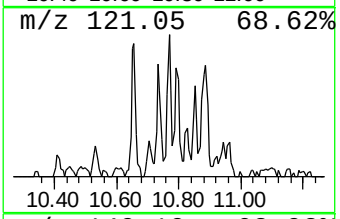


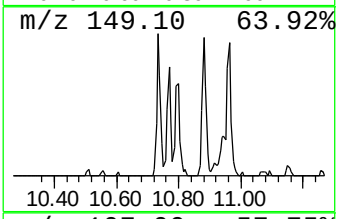


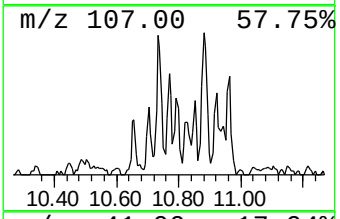


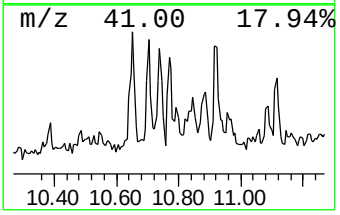












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ClientSampleId : G-46A-0-3-COMP

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

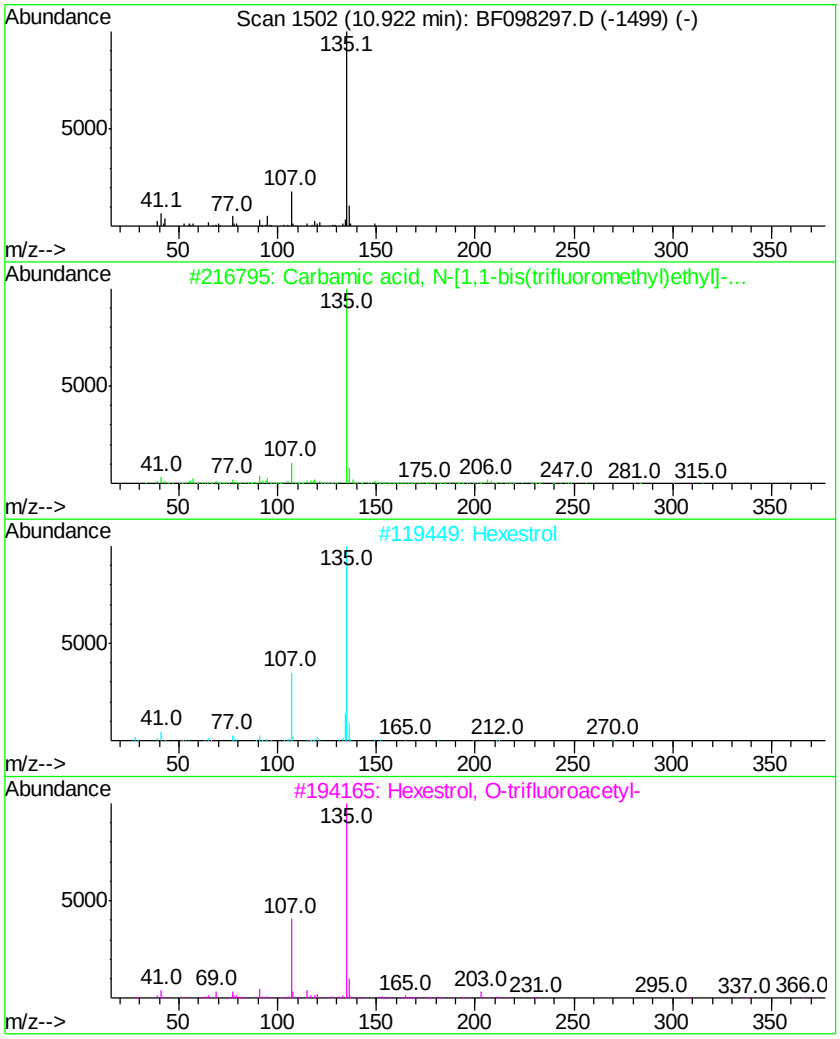
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

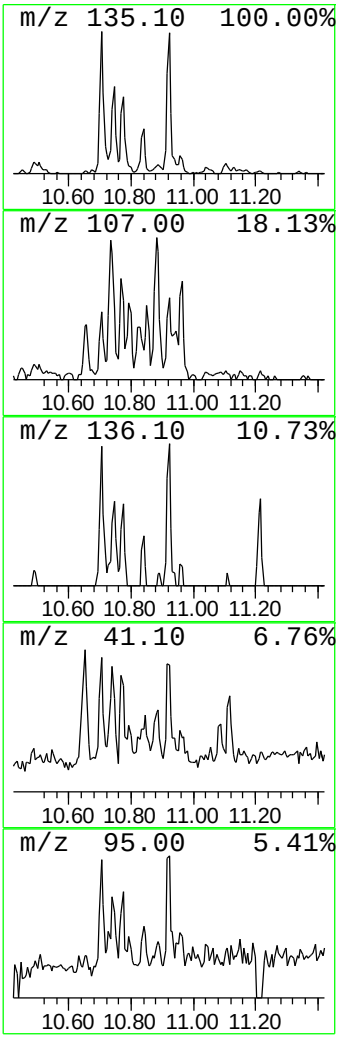
****

Peak Number 6 Carbamic acid, N-[1,1-bis(t... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.92	2.50 ng	84538	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbamic acid, N-[1,1-bis(triflu...	413	C19H25F6NO2	296242-69-8	78
2	Hexestrol	270	C18H22O2	000084-16-2	72
3	Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	45
4	Hexestrol	270	C18H22O2	005635-50-7	45
5	Benzene, 1-(1,3-dimethyl-3-buten...	190	C13H18O	074672-05-2	42





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF090617\
Data File : BF098297.D
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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-46A-0-3-COMP

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
unknown6.46	6.46	5.0	ng	163825	1	6.70	658617	20.0
unknown10.65	10.65	2.0	ng	68690	4	11.22	676647	20.0
unknown10.74	10.74	2.7	ng	92604	4	11.22	676647	20.0
unknown10.77	10.77	2.1	ng	72357	4	11.22	676647	20.0
Carbamic acid, N-...	10.92	2.5	ng	84538	4	11.22	676647	20.0