LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111117\
Data File : BF100432.D
Acq On : 11 Nov 2017 11:27
Operator : SJ/JU
Sample : I6399-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-A-13-B

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-BF110817.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	5.122	512	516	526	rVB	383196	432095	20.19%	2.103%
2	5.516	579	583	587	rBV	2059979	2095058	97.89%	10.196%
3	6.522	749	754	761	rBV	2107447	2140280	100.00%	10.416%
4	6.669	775	779	783	rBV	2349809	2103847	98.30%	10.239%
5	6.904	815	819	822	rBV	1096166	896275	41.88%	4.362%
6	7.057	841	845	849	rBV	1881041	1654210	77.29%	8.051%
7	7.463	909	914	917	rBV	1505199	1269219	59.30%	6.177%
8	8.186	1033	1037	1040	rVB	1222366	1016819	47.51%	4.949%
9	8.469	1079	1085	1092	rBV6	12544	27298	1.28%	0.133%
10	8.598	1104	1107	1109	rBV	33108	27801	1.30%	0.135%
11	8.769	1133	1136	1140	rVB	44434	35644	1.67%	0.173%
12	9.257	1215	1219	1229	rBV	2298804	1990740	93.01%	9.689%
13	9.333	1229	1232	1235	rVB	51375	39113	1.83%	0.190%
14	9.645	1283	1285	1289	rBV	118626	115921	5.42%	0.564%
15	9.780	1305	1308	1309	rBV	36494	28549	1.33%	0.139%
16	9.798	1309	1311	1314	rVV	50347	39170	1.83%	0.191%
17	9.863	1314	1322	1326	rVB	47185	47432	2.22%	0.231%
18	9.939	1331	1335	1339	rBV	1074981	911345	42.58%	4.435%
19	10.251	1384	1388	1391	rBV4	18864	27509	1.29%	0.134%
20	10.310	1395	1398	1401	rVV	48894	42286	1.98%	0.206%
21	10.363	1404	1407	1409	rVB	44322	34268	1.60%	0.167%
22	10.580	1440	1444	1450	rVB2	23448	28544	1.33%	0.139%
23	10.722	1464	1468	1472	rBV	994495	887207	41.45%	4.318%
24	10.839	1484	1488	1493	rBV2	62912	96020	4.49%	0.467%
25	11.280	1560	1563	1566	rBV	27209	27307	1.28%	0.133%
26	11.316	1566	1569	1572	rVB2	25686	29025	1.36%	0.141%
27	11.427	1584	1588	1590	rBV	847268	767978	35.88%	3.738%
28	11.445	1590	1591	1595	rVB	44209	37286	1.74%	0.181%
29	11.710	1634	1636	1640	rVB	29542	23215	1.08%	0.113%
30	11.939	1670	1675	1684	rBV2	167015	225898	10.55%	1.099%
31	12.116	1703	1705	1708	rBV	30912	27574	1.29%	0.134%
32	12.504	1769	1771	1774	rBV2	34173	31341	1.46%	0.153%
33	12.639	1791	1794	1798	rBV	93370	81900	3.83%	0.399%
34	12.727	1806	1809	1813	rBV3	61752	71805	3.35%	0.349%

LSC Area Percent Report

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Acq On : 11 Nov 2017 11:27
Operator : SJ/JU
Sample : I6399-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-A-13-B

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-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.868	1830	1833	1837	rVB	77790	78445	3.67%	0.382%
36	13.010	1853	1857	1860	rBV	1501773	1347856	62.98%	6.560%
37	13.898	2005	2008	2013	rBV	184971	195135	9.12%	0.950%
38	14.063	2033	2036	2039	rBV	856200	851153	39.77%	4.142%
39	15.551	2285	2289	2297	rVB	559511	764468	35.72%	3.721%

Sum of corrected areas: 20547036

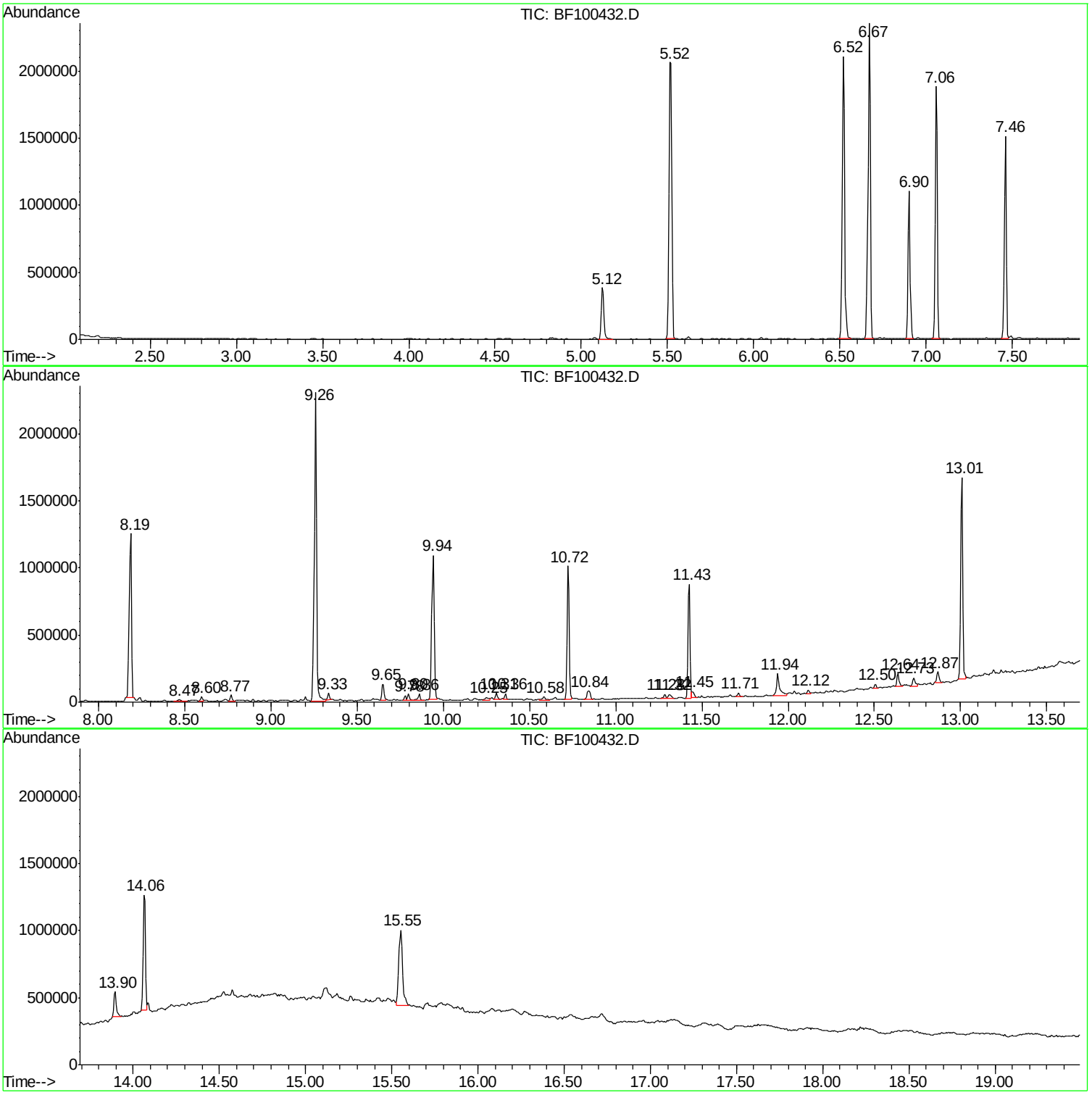
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111117\
Data File : BF100432.D
Acq On : 11 Nov 2017 11:27
Operator : SJ/JU
Sample : I6399-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-13-A-13-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111117\
Data File : BF100432.D
Acq On : 11 Nov 2017 11:27
Operator : SJ/JU
Sample : I6399-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-A-13-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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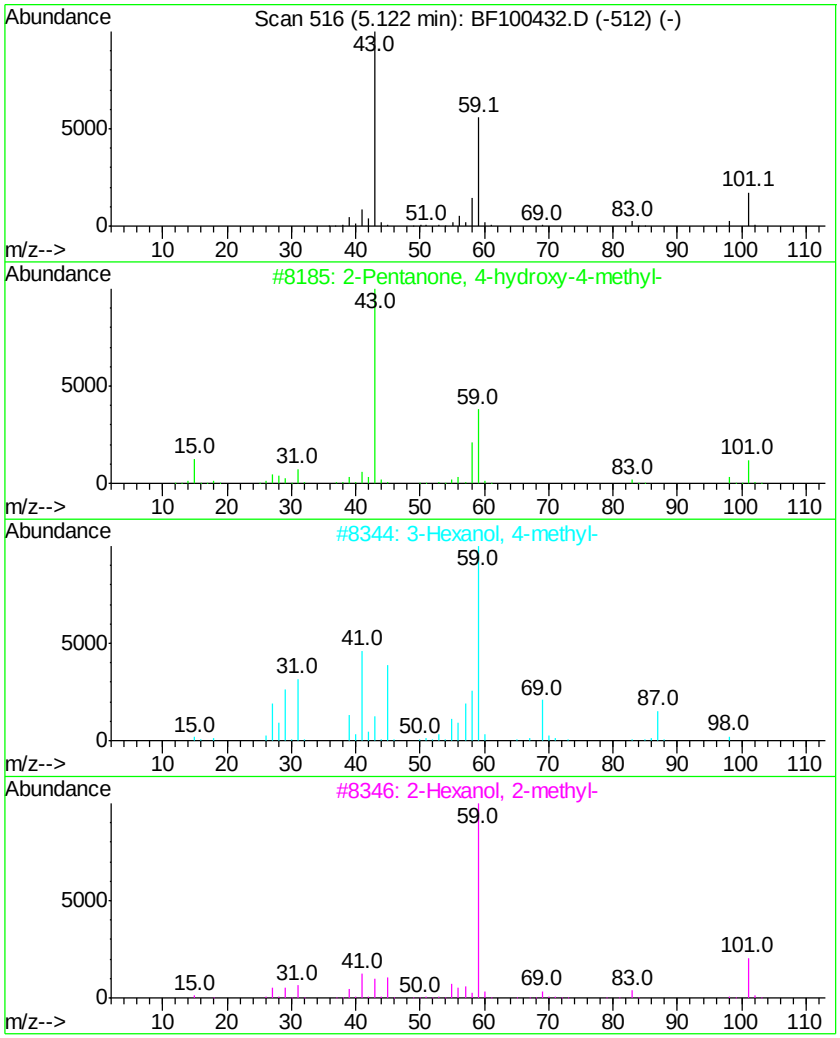
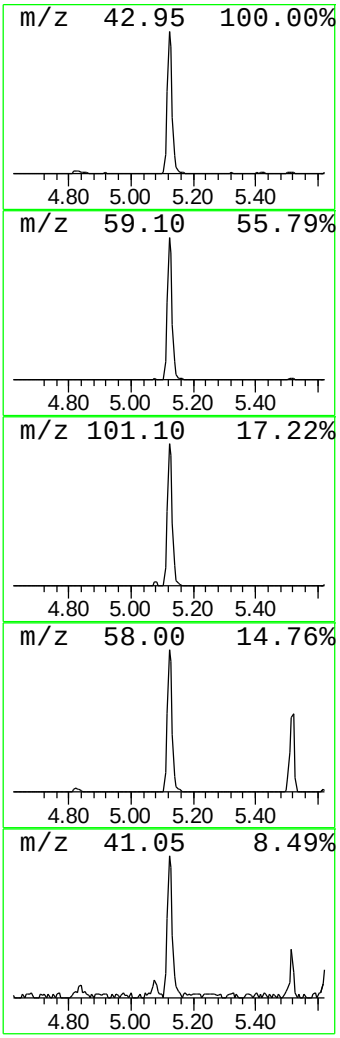
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	9.64 ng	432095	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

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Data File : BF100432.D
Acq On : 11 Nov 2017 11:27
Operator : SJ/JU
Sample : I6399-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-A-13-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

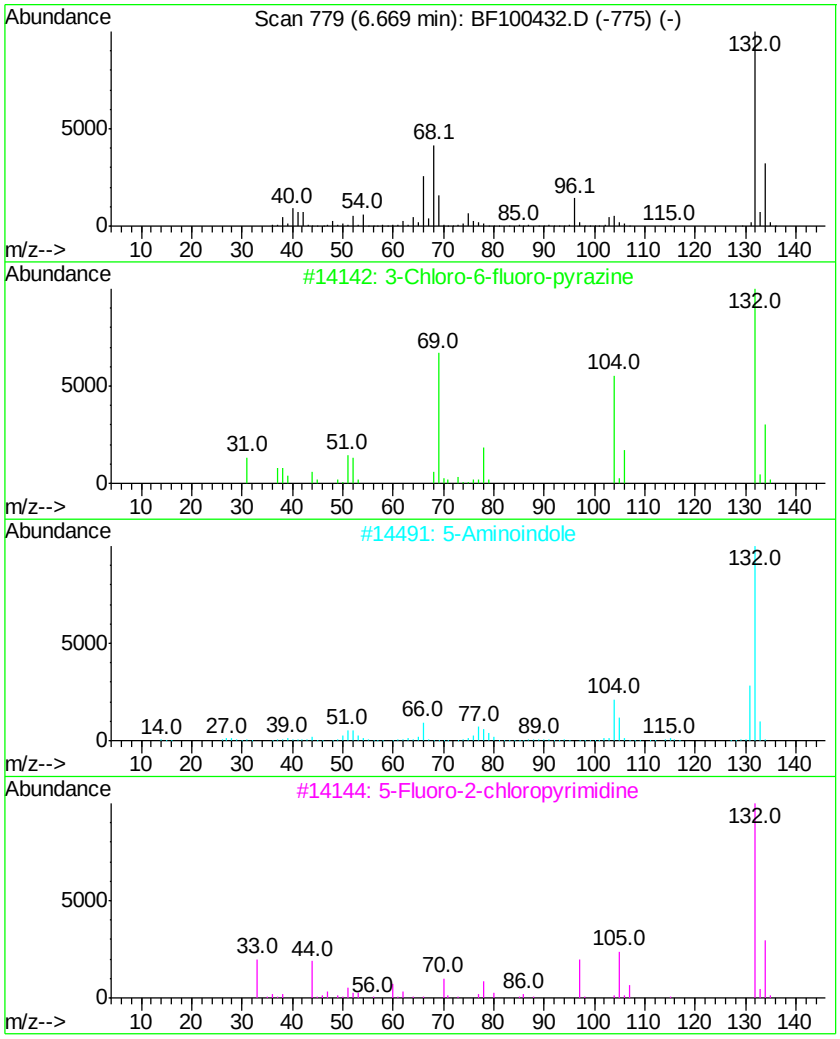
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

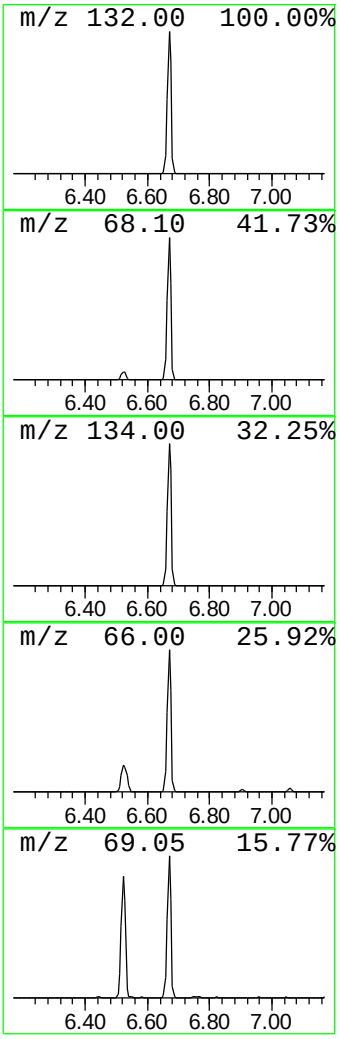
****

Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	46.95 ng	2103850	1,4-Dichlorobenzene-d4	6.90

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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Library Search Compound Report

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Sample : I6399-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-A-13-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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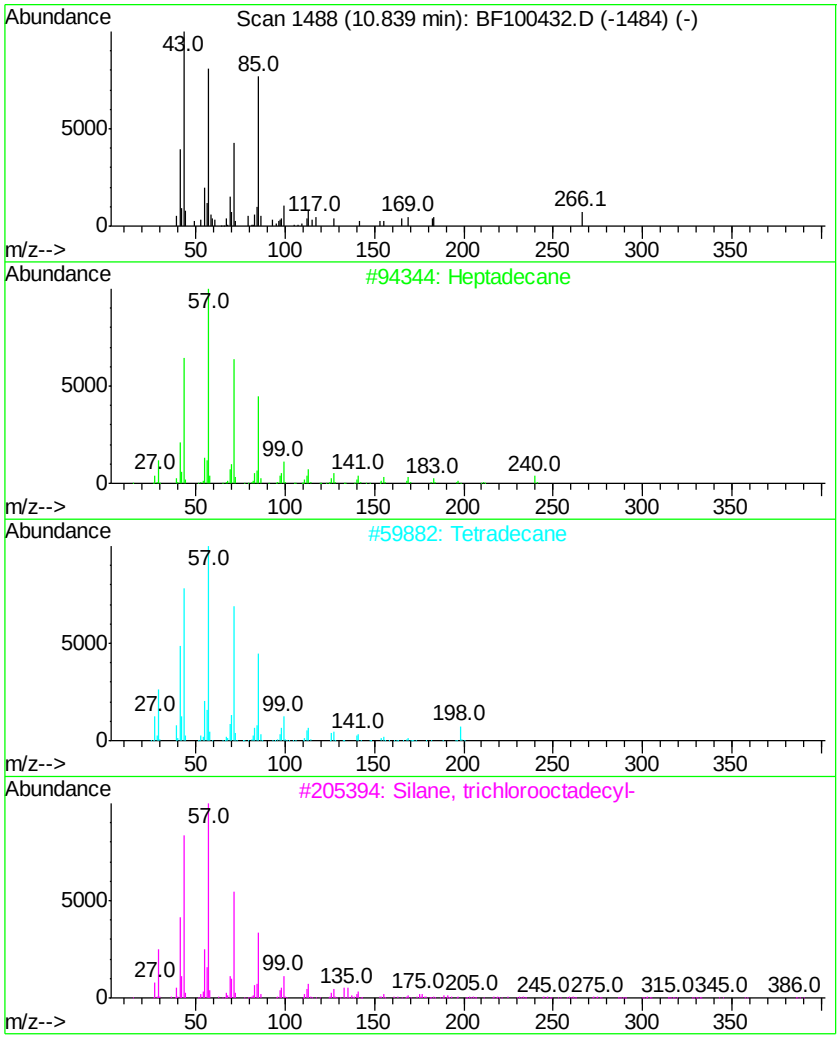
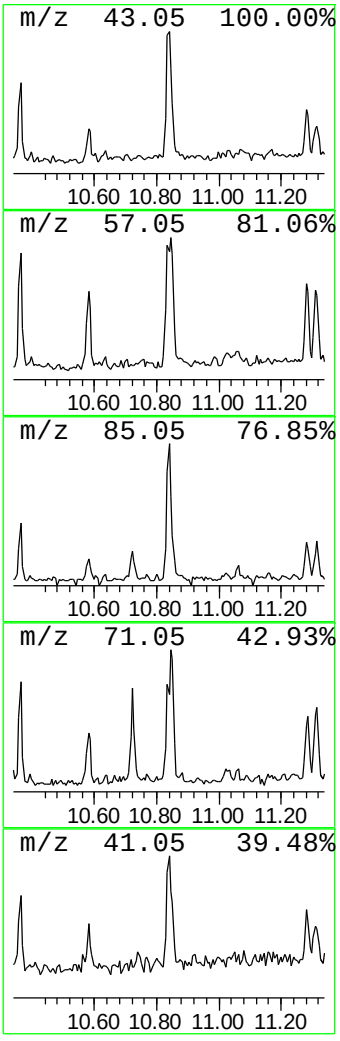
Peak Number 4 unknown10.84 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	2.50 ng	96020	Phenanthrene-d10	11.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	46
2	Tetradecane	198	C14H30	000629-59-4	46
3	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	46
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	43
5	Octacosane	394	C28H58	000630-02-4	43





Library Search Compound Report

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Sample : I6399-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-A-13-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
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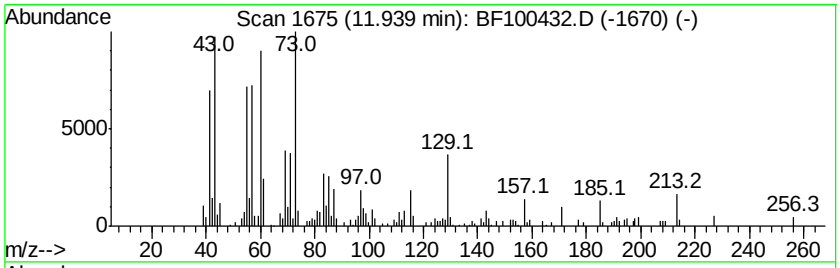
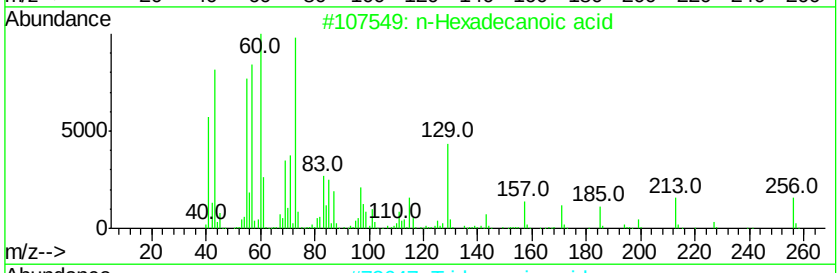
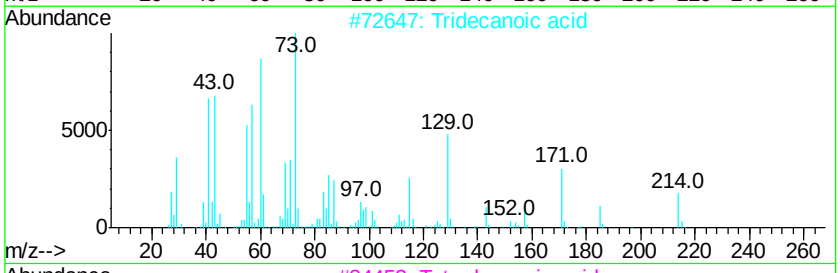
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

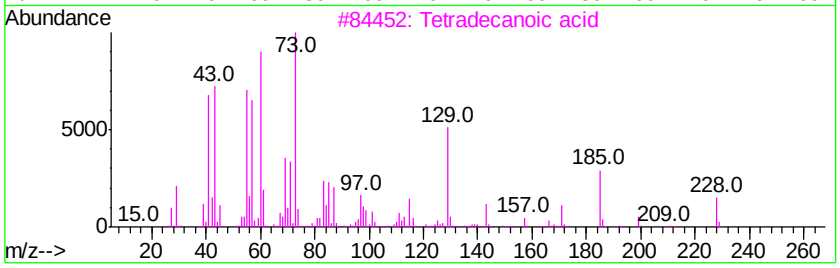
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	5.88 ng	225898	Phenanthrene-d10	11.43

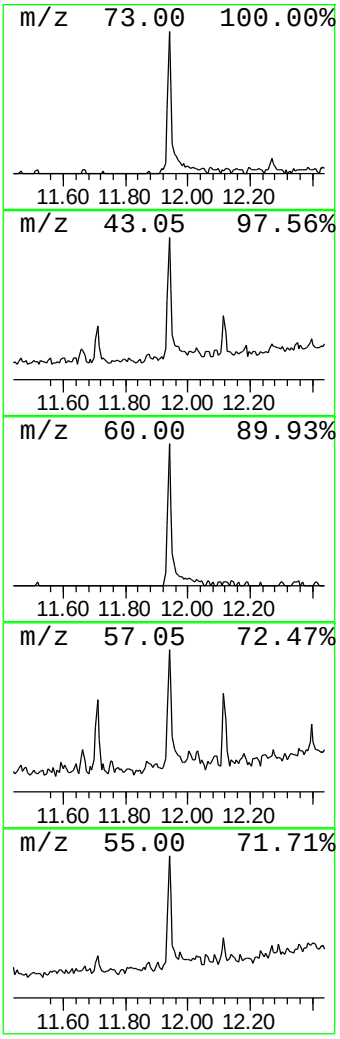
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Undecanoic acid	186	C11H22O2	000112-37-8	72











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Instrument : BNA_F
ClientSampleId : TP-13-A-13-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

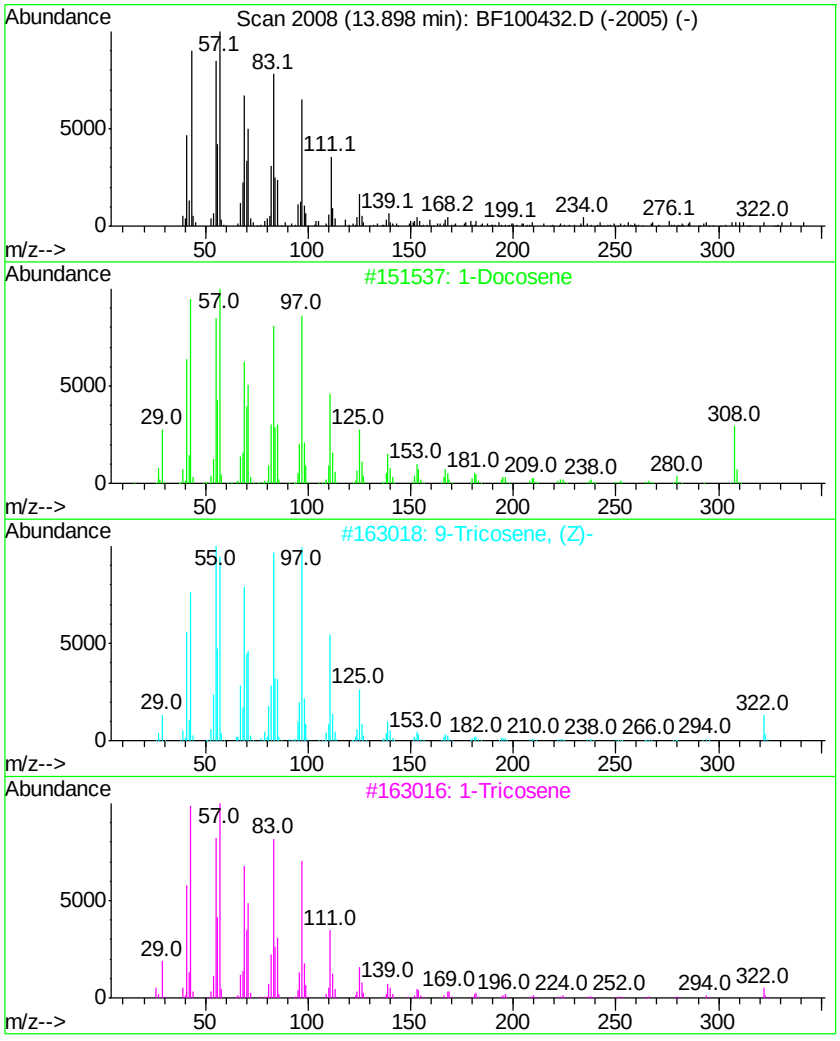
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

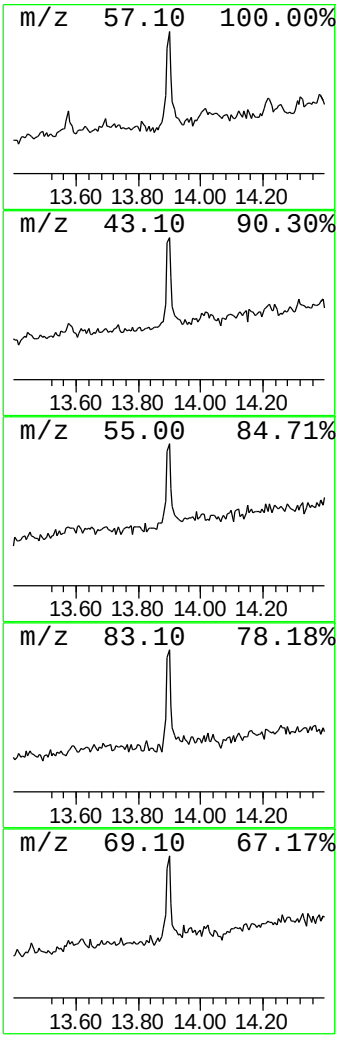
****

Peak Number 6 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	4.59 ng	195135	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	96
2	9-Tricosene, (Z)-	322	C23H46	027519-02-4	95
3	1-Tricosene	322	C23H46	018835-32-0	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5	2-Methyl-2-docosene	322	C23H46	1000131-16-9	91





Tentatively Identified Compound (LSC) summary

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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...	5.12	9.6	ng	432095	1	6.90	896275	20.0
unknown6.67	6.67	47.0	ng	2103850	1	6.90	896275	20.0
unknown10.84	10.84	2.5	ng	96020	4	11.43	767978	20.0
n-Hexadecanoic acid	11.94	5.9	ng	225898	4	11.43	767978	20.0
1-Docosene	13.90	4.6	ng	195135	5	14.07	851153	20.0