LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102258.D
Acq On : 20 Jan 2018 11:49
Operator : SJ/JU
Sample : J1114-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-23-2.5-3.0

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-BF010918.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	4.922	478	482	489	rBV	161478	225582	7.21%	0.842%
2	5.334	547	552	555	rBV	3086657	3108538	99.40%	11.608%
3	6.363	722	727	731	rBV	2879291	3124967	99.93%	11.669%
4	6.493	744	749	752	rBV	3370781	3127272	100.00%	11.677%
5	6.722	784	788	791	rBV	968776	870694	27.84%	3.251%
6	6.875	810	814	817	rBV	2834301	2435873	77.89%	9.096%
7	7.287	879	884	887	rBV	2084554	1942253	62.11%	7.253%
8	8.004	1001	1006	1009	rBV	1190715	1103214	35.28%	4.119%
9	9.081	1184	1189	1192	rBV	3422804	3030808	96.92%	11.317%
10	9.475	1251	1256	1259	rBV	248126	225670	7.22%	0.843%
11	9.686	1289	1292	1295	rVB	138442	100991	3.23%	0.377%
12	9.751	1300	1303	1308	rVB	1109470	1053020	33.67%	3.932%
13	10.186	1373	1377	1380	rVB	145374	125638	4.02%	0.469%
14	10.404	1410	1414	1416	rBV	37201	37109	1.19%	0.139%
15	10.545	1433	1438	1441	rBV	1529848	1447707	46.29%	5.406%
16	10.657	1454	1457	1467	rVB	132374	143995	4.60%	0.538%
17	11.104	1530	1533	1536	rBV2	39130	40493	1.29%	0.151%
18	11.239	1552	1556	1559	rBV	970668	835044	26.70%	3.118%
19	12.645	1792	1795	1799	rBV	137910	116012	3.71%	0.433%
20	12.822	1821	1825	1829	rBV	2099352	1922156	61.46%	7.177%
21	13.304	1905	1907	1911	rVB	46091	45281	1.45%	0.169%
22	13.351	1912	1915	1918	rVV	78509	68862	2.20%	0.257%
23	13.716	1974	1977	1981	rBV	164497	164842	5.27%	0.616%
24	13.874	2000	2004	2007	rBV	808554	731633	23.40%	2.732%
25	15.298	2241	2246	2255	rBV	547045	698538	22.34%	2.608%
26	15.727	2317	2319	2324	rVB5	42366	54198	1.73%	0.202%

Sum of corrected areas: 26780390

LSC Report - Integrated Chromatogram

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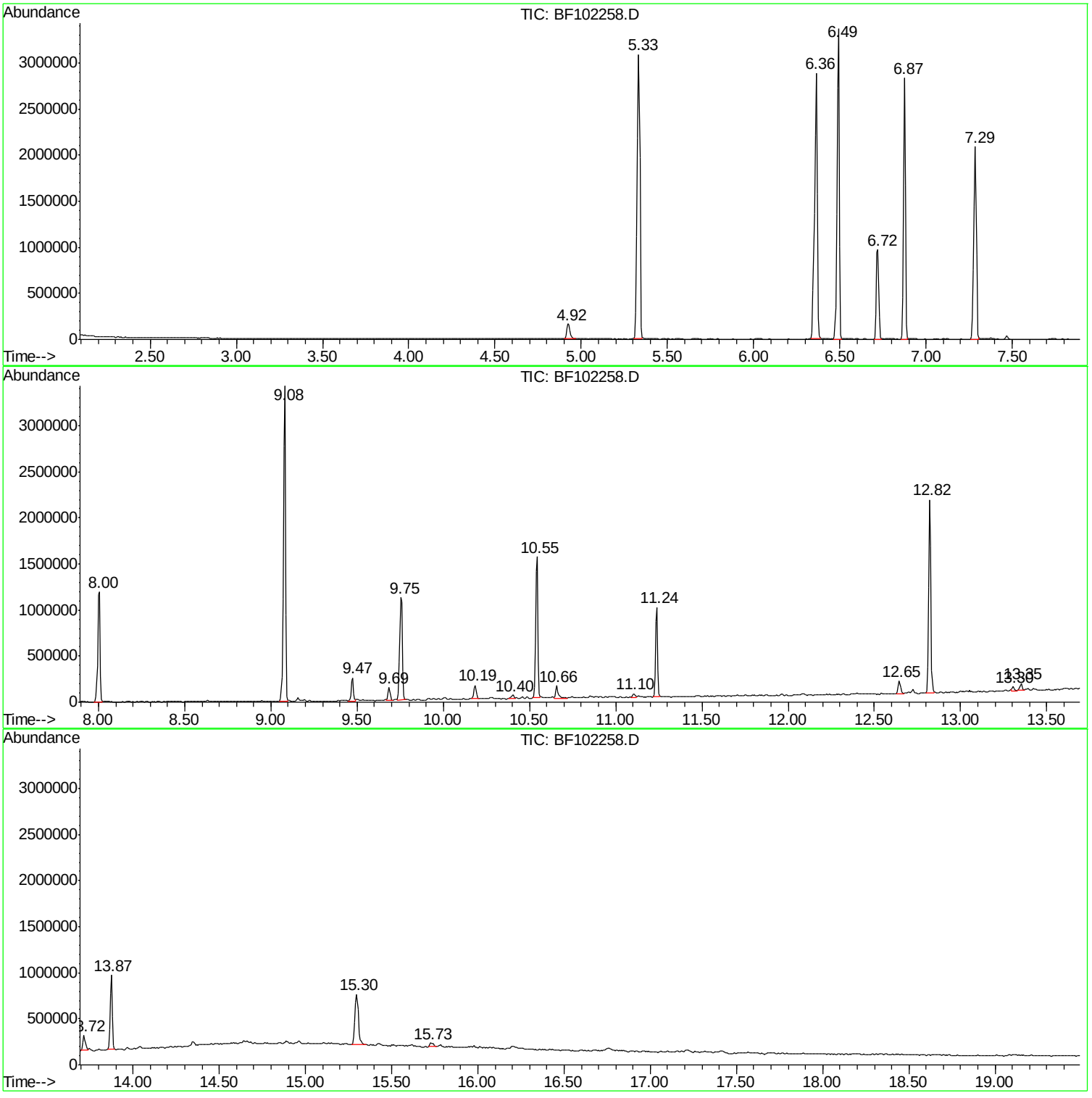
Instrument : BNA_F
ClientSampleId : SB-23-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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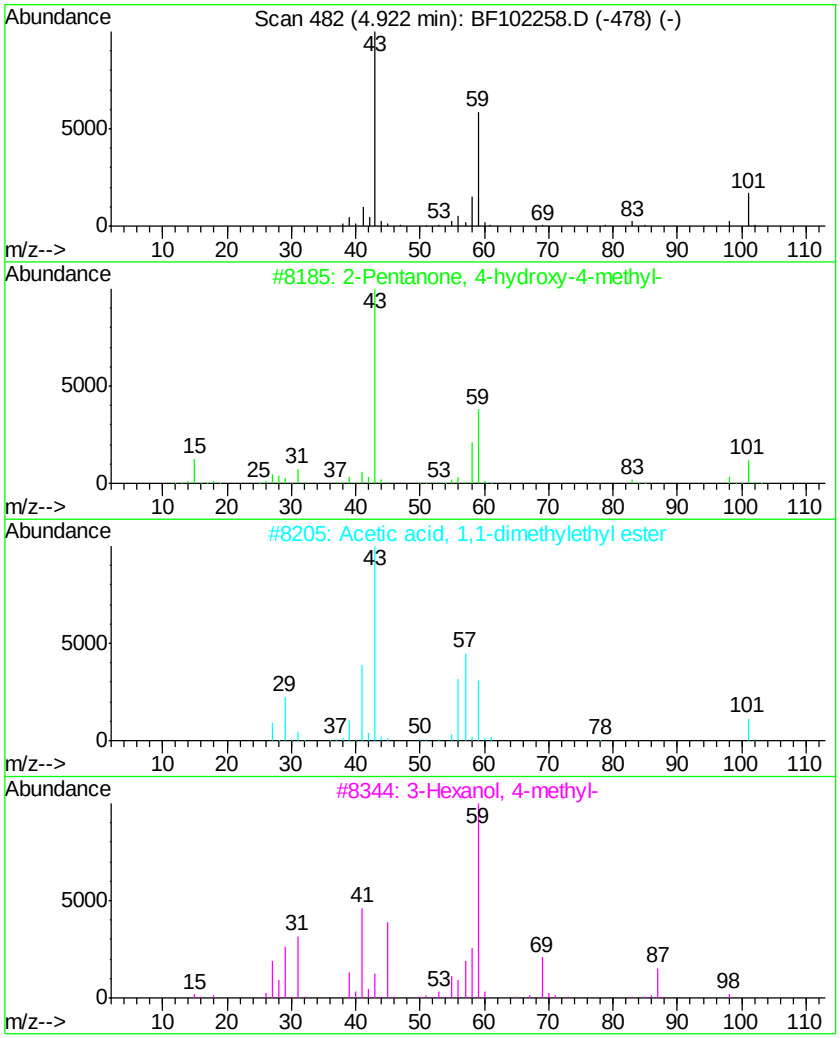
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

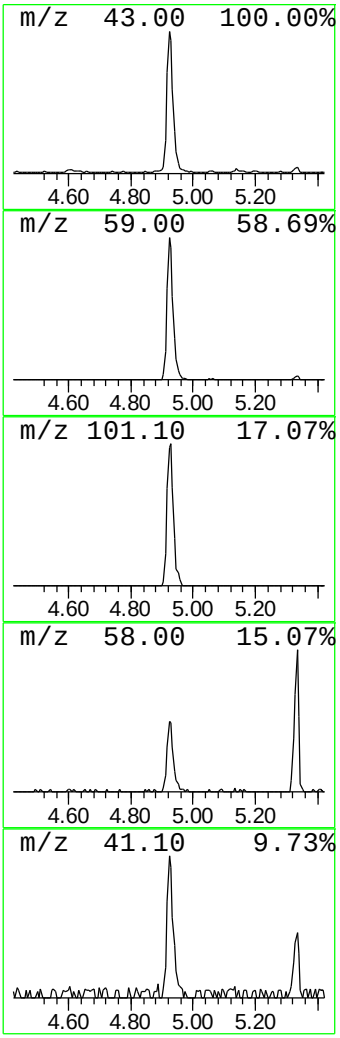
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	5.18 ng	225582	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27





Library Search Compound Report

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Data File : BF102258.D
Acq On : 20 Jan 2018 11:49
Operator : SJ/JU
Sample : J1114-05
Misc :
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Instrument : BNA_F
ClientSampleId : SB-23-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

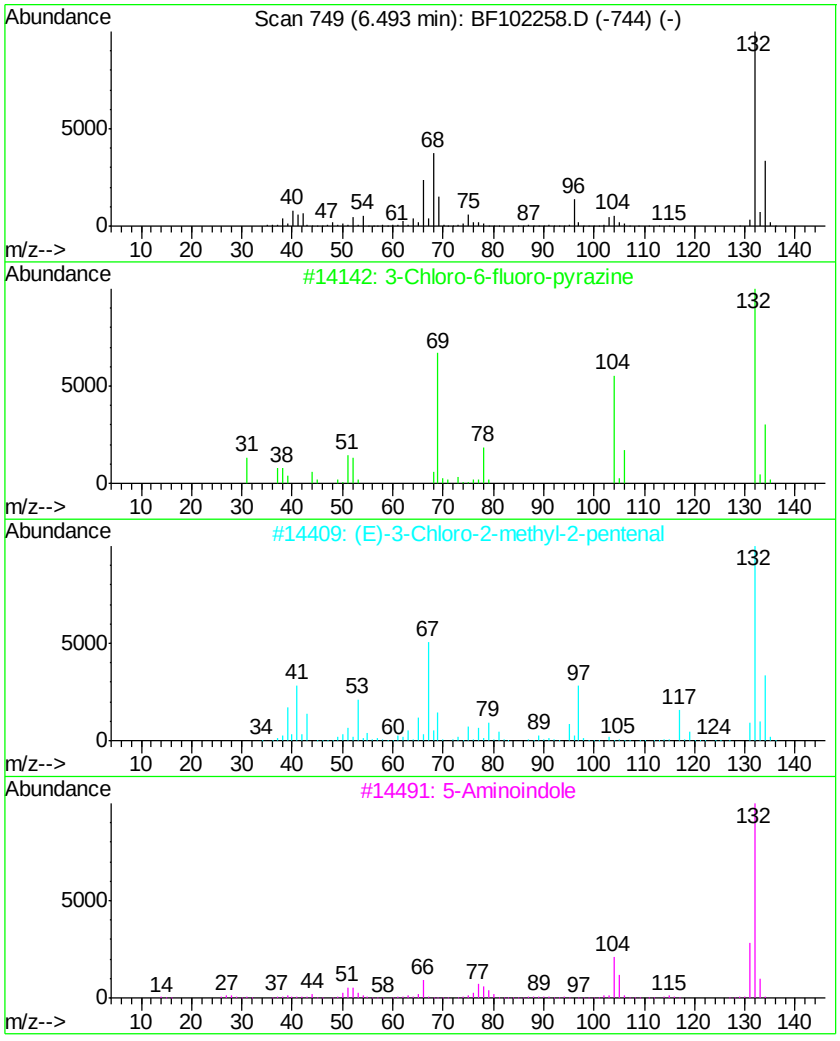
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

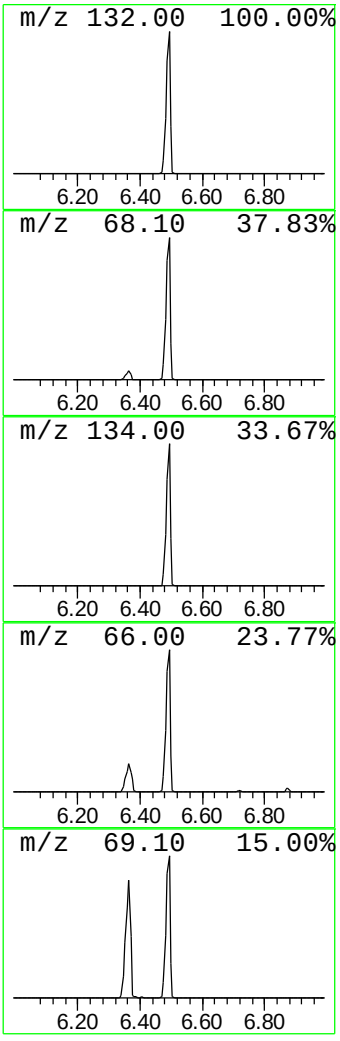
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	71.83 ng	3127270	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Operator : SJ/JU
Sample : J1114-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-23-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
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TIC Library : C:\DATABASE\NIST11.L
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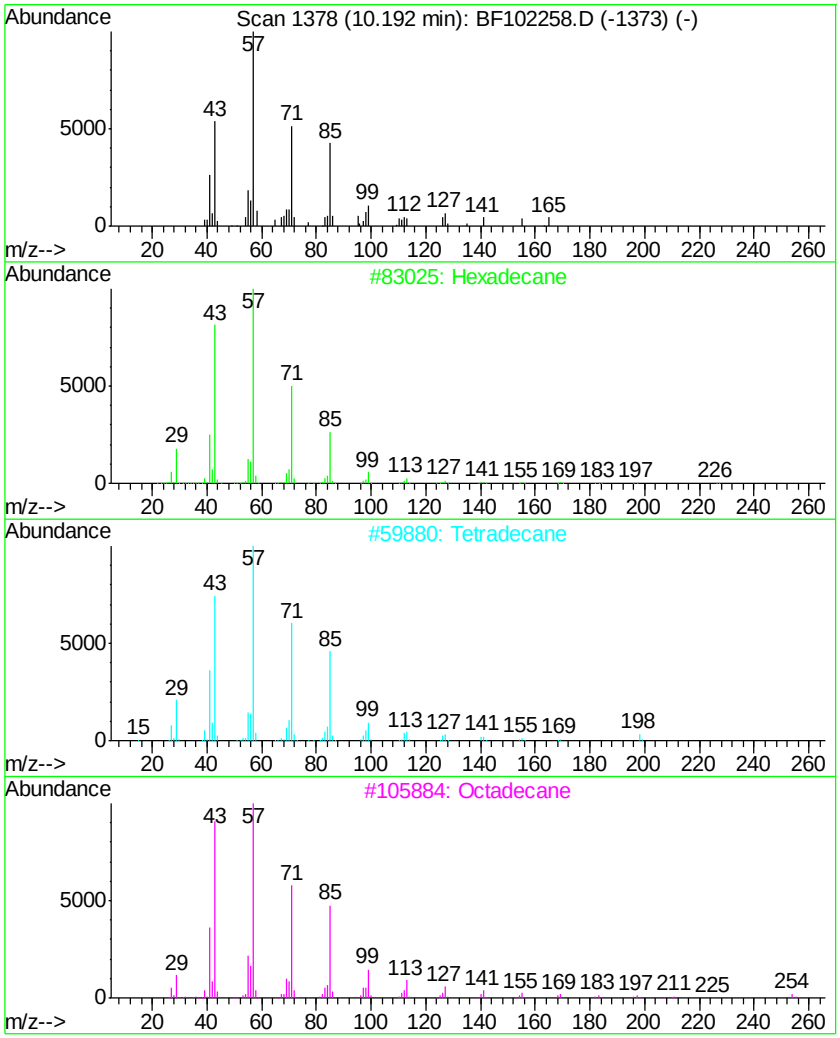
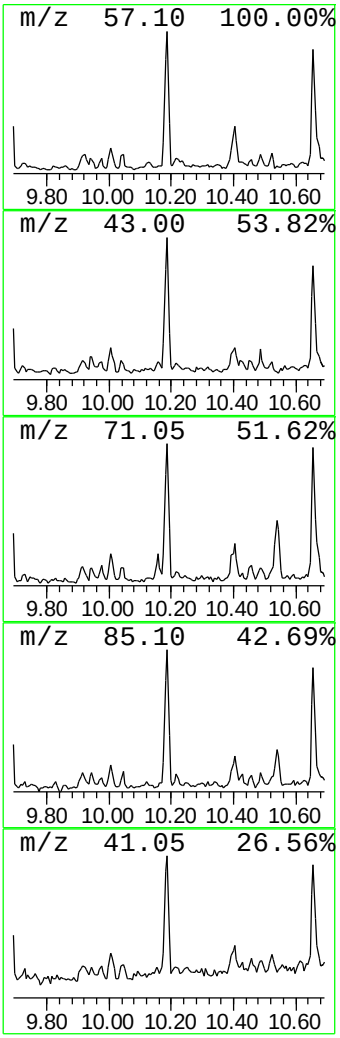
Peak Number 4 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.19	2.39 ng	125638	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	97
2	Tetradecane	198	C14H30	000629-59-4	91
3	Octadecane	254	C18H38	000593-45-3	90
4	Tridecane	184	C13H28	000629-50-5	90
5	Pentadecane	212	C15H32	000629-62-9	90





Library Search Compound Report

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Operator : SJ/JU
Sample : J1114-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-23-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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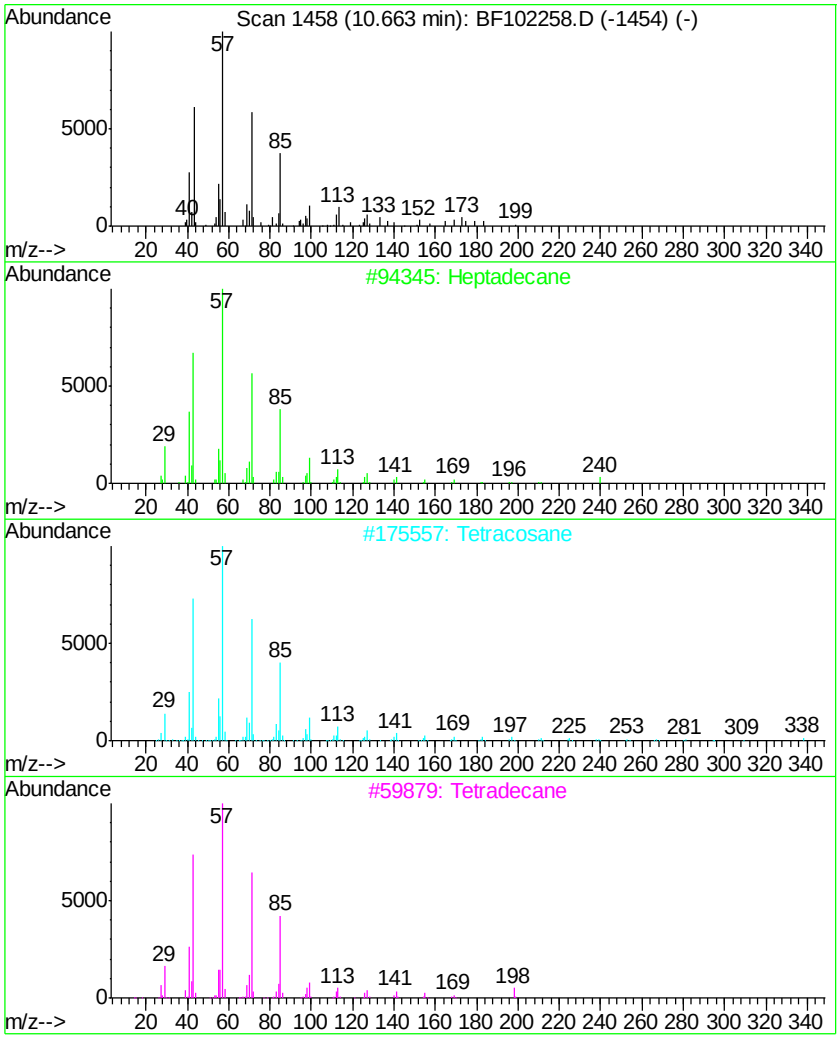
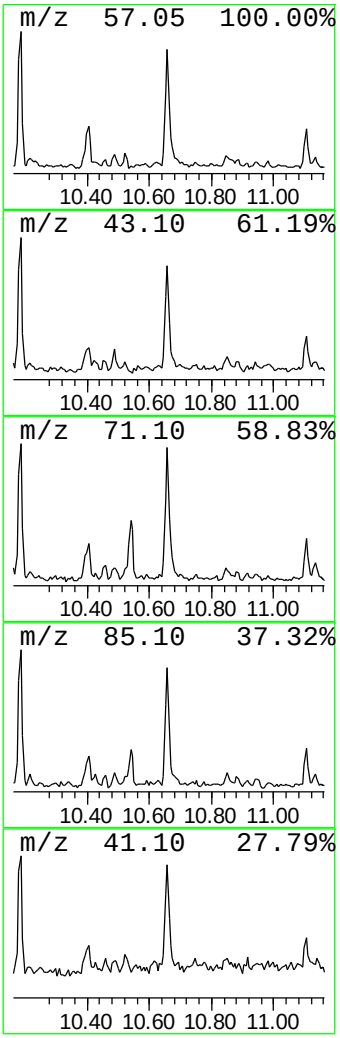
Peak Number 5 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	3.45 ng	143995	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Tetradecane	198	C14H30	000629-59-4	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Nonadecane	268	C19H40	000629-92-5	87





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Operator : SJ/JU
Sample : J1114-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-23-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

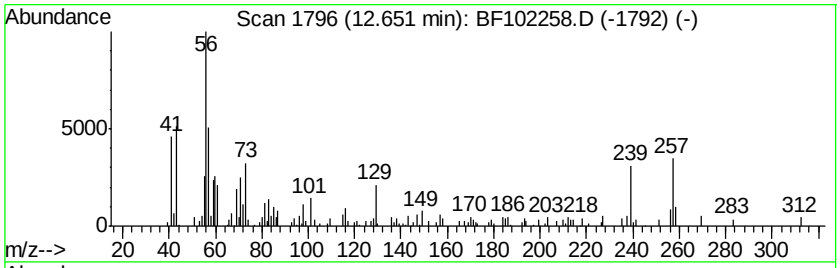
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

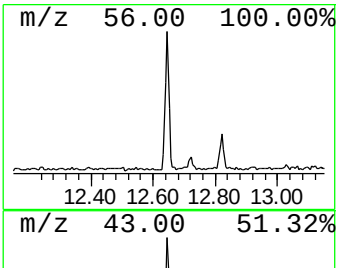
****

Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	3.17 ng	116012	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	41
3	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
4	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	38
5	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	35





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ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-23-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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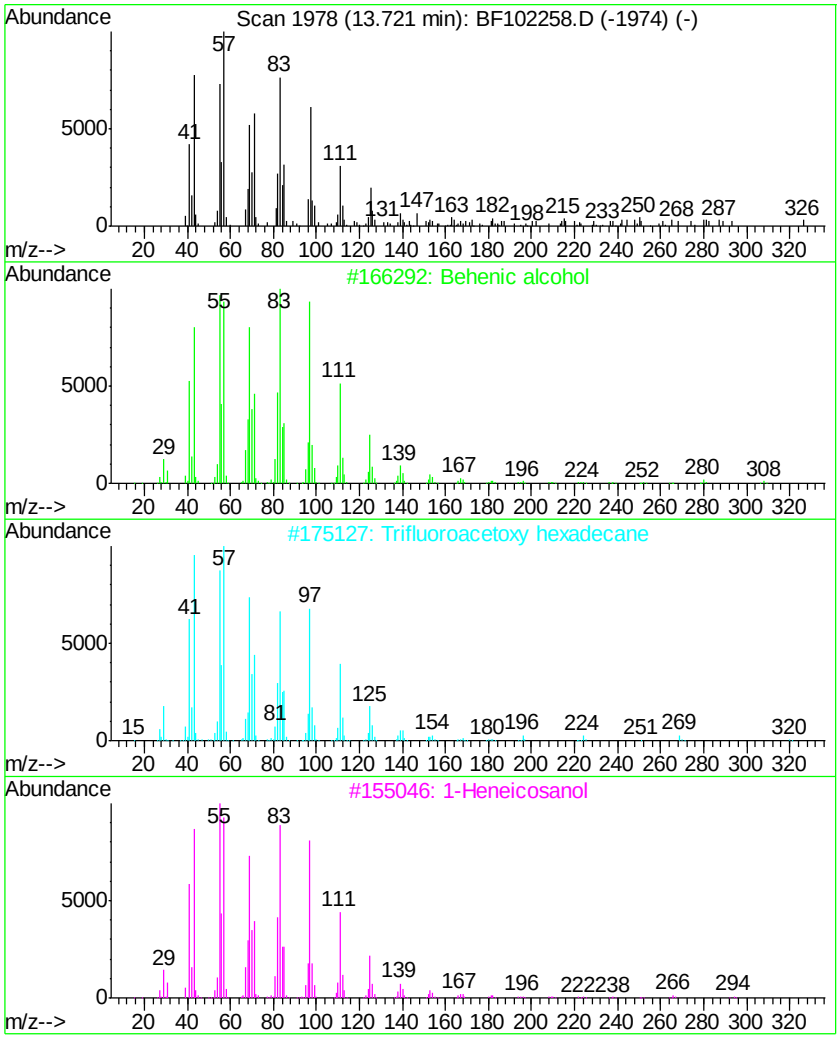
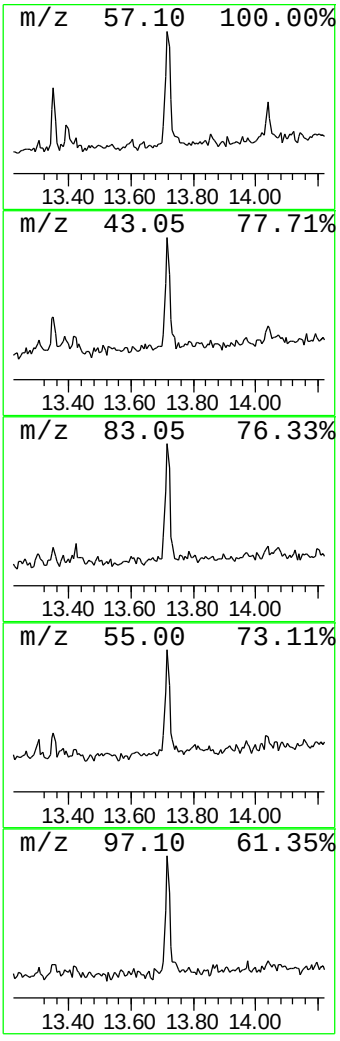
Peak Number 7 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.51 ng	164842	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94





Tentatively Identified Compound (LSC) summary

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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...	4.92	5.2	ng	225582	1	6.72	870694	20.0
unknown6.49	6.49	71.8	ng	3127270	1	6.72	870694	20.0
Hexadecane	10.19	2.4	ng	125638	3	9.75	1053020	20.0
Heptadecane	10.66	3.5	ng	143995	4	11.24	835044	20.0
Hexadecanoic acid...	12.65	3.2	ng	116012	5	13.87	731633	20.0
Behenic alcohol	13.72	4.5	ng	164842	5	13.87	731633	20.0