LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
Data File : BF094692.D
Acq On : 28 Apr 2017 19:11
Operator : SJ/MA
Sample : I2895-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02-3.0-4.0

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-BF041717.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	3.948	337	342	354	rBV	460497	607123	17.47%	2.251%
2	4.337	403	408	425	rBV	3098892	3301031	95.00%	12.240%
3	4.713	469	472	481	rVB	38421	41760	1.20%	0.155%
4	5.407	585	590	593	rBV	2731534	3250103	93.54%	12.051%
5	5.531	606	611	614	rBV	3376862	3394286	97.69%	12.586%
6	5.772	648	652	659	rVB	505264	454274	13.07%	1.684%
7	5.948	677	682	686	rBV	2784970	2631689	75.74%	9.758%
8	6.425	757	763	766	rBV	2004449	2054529	59.13%	7.618%
9	7.260	901	905	911	rBV	661370	577858	16.63%	2.143%
10	8.583	1125	1130	1134	rBV	3225304	3474643	100.00%	12.883%
11	9.083	1212	1215	1219	rBV	235583	222123	6.39%	0.824%
12	9.395	1258	1268	1281	rBV2	626320	639042	18.39%	2.369%
13	9.989	1366	1369	1374	rVB	49810	51472	1.48%	0.191%
14	10.377	1430	1435	1438	rBV	1667491	1760962	50.68%	6.529%
15	10.577	1465	1469	1477	rBV	64499	87025	2.50%	0.323%
16	11.130	1559	1563	1565	rBV	46756	41315	1.19%	0.153%
17	11.219	1574	1578	1586	rBV	529148	513840	14.79%	1.905%
18	11.954	1699	1703	1710	rBV2	147043	175371	5.05%	0.650%
19	12.918	1863	1867	1874	rBV2	26889	44121	1.27%	0.164%
20	13.201	1909	1915	1918	rBV	2355807	2571553	74.01%	9.535%
21	14.359	2108	2112	2124	rBV	113002	210122	6.05%	0.779%
22	14.471	2127	2131	2135	rVV	419443	453628	13.06%	1.682%
23	15.859	2365	2367	2373	rBV3	28720	34836	1.00%	0.129%
24	16.101	2404	2408	2417	rVB	311770	377050	10.85%	1.398%

Sum of corrected areas: 26969756

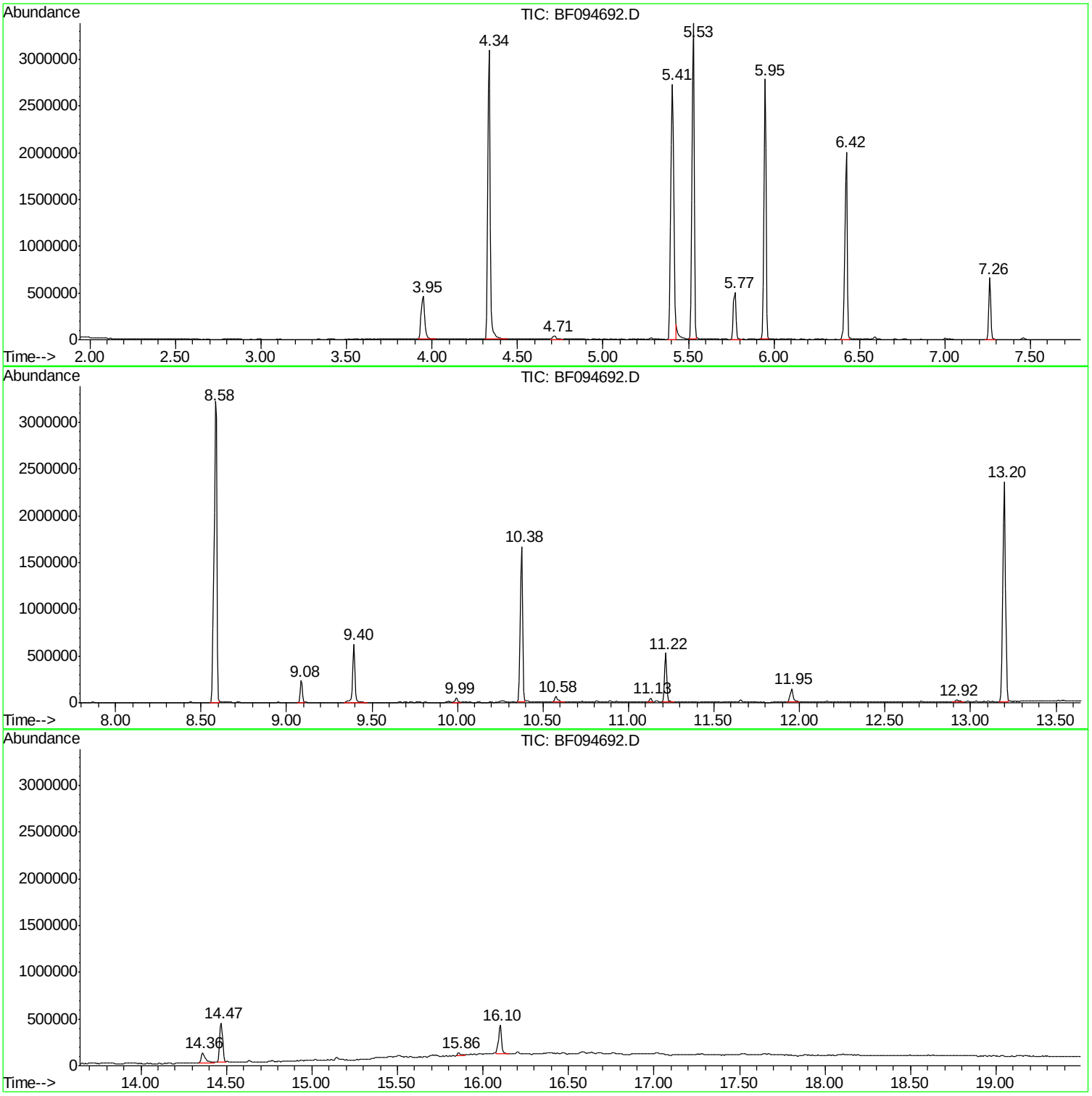
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
Data File : BF094692.D
Acq On : 28 Apr 2017 19:11
Operator : SJ/MA
Sample : I2895-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02-3.0-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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\BF042817\
Data File : BF094692.D
Acq On : 28 Apr 2017 19:11
Operator : SJ/MA
Sample : I2895-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02-3.0-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

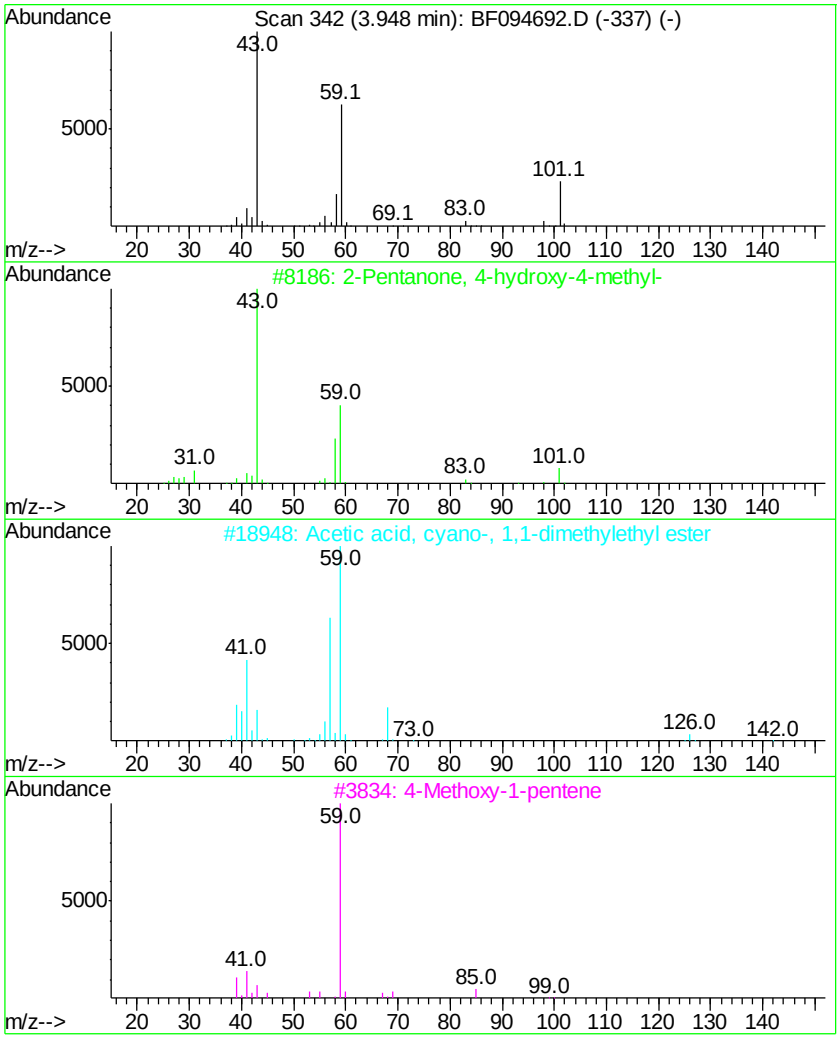
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

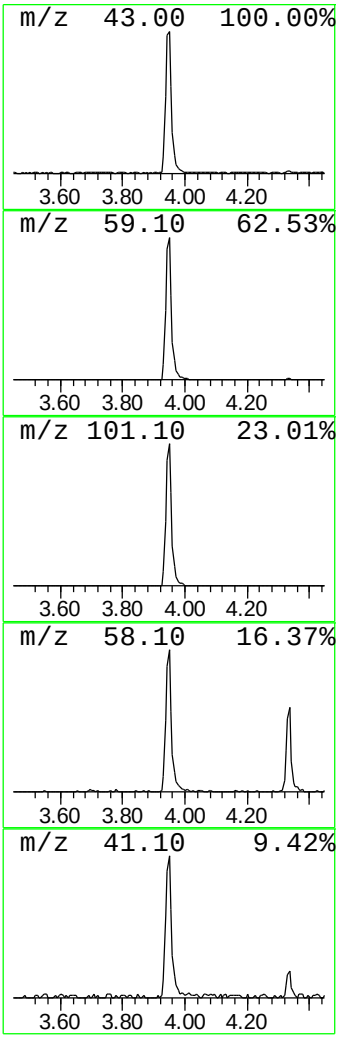
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.95	26.73 ng	607123	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
Data File : BF094692.D
Acq On : 28 Apr 2017 19:11
Operator : SJ/MA
Sample : I2895-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02-3.0-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

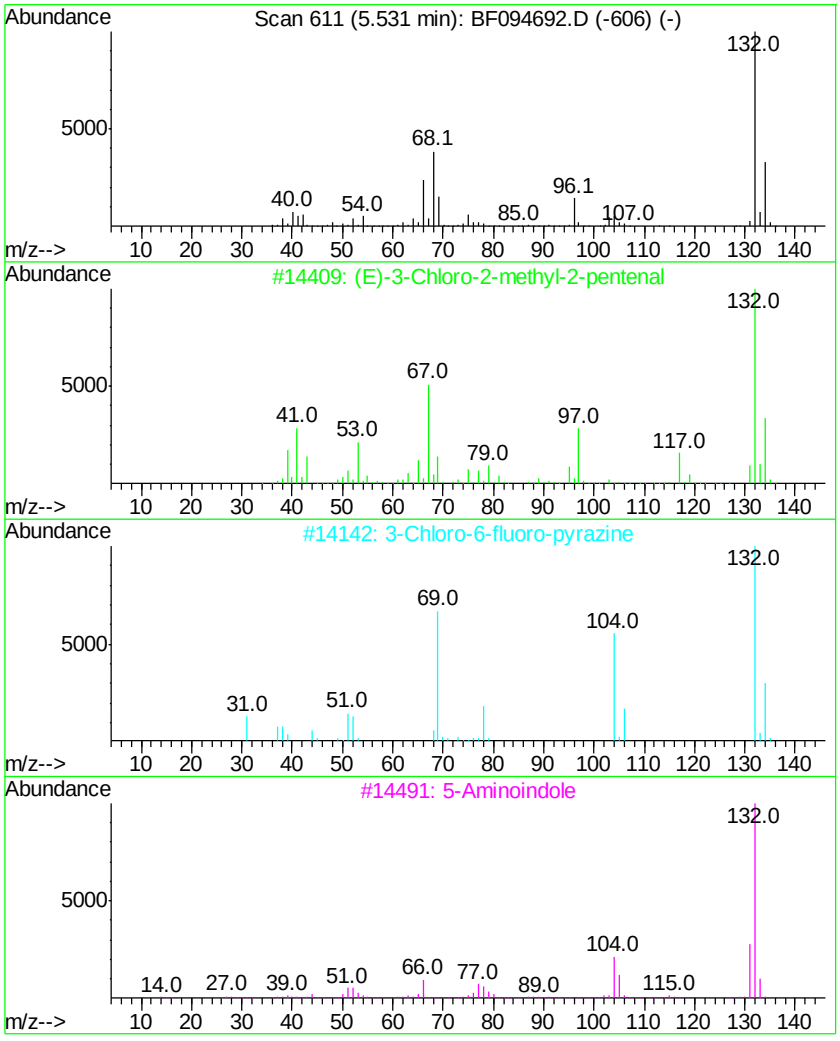
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

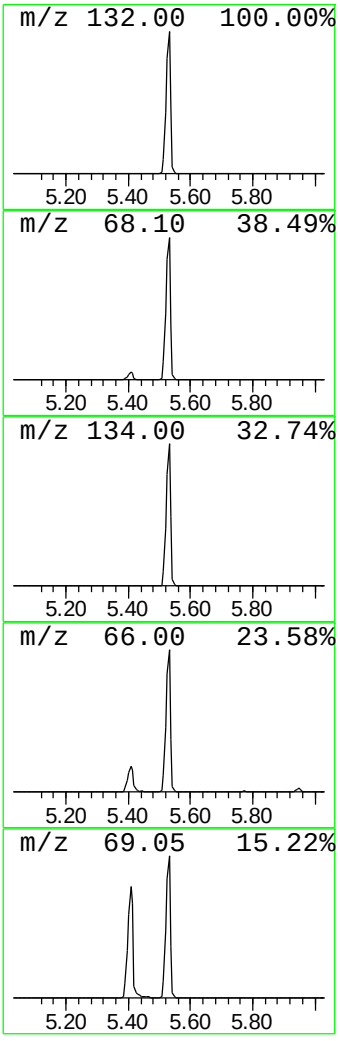
****

Peak Number 2 unknown5.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.53	149.44 ng	3394290	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
Data File : BF094692.D
Acq On : 28 Apr 2017 19:11
Operator : SJ/MA
Sample : I2895-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02-3.0-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

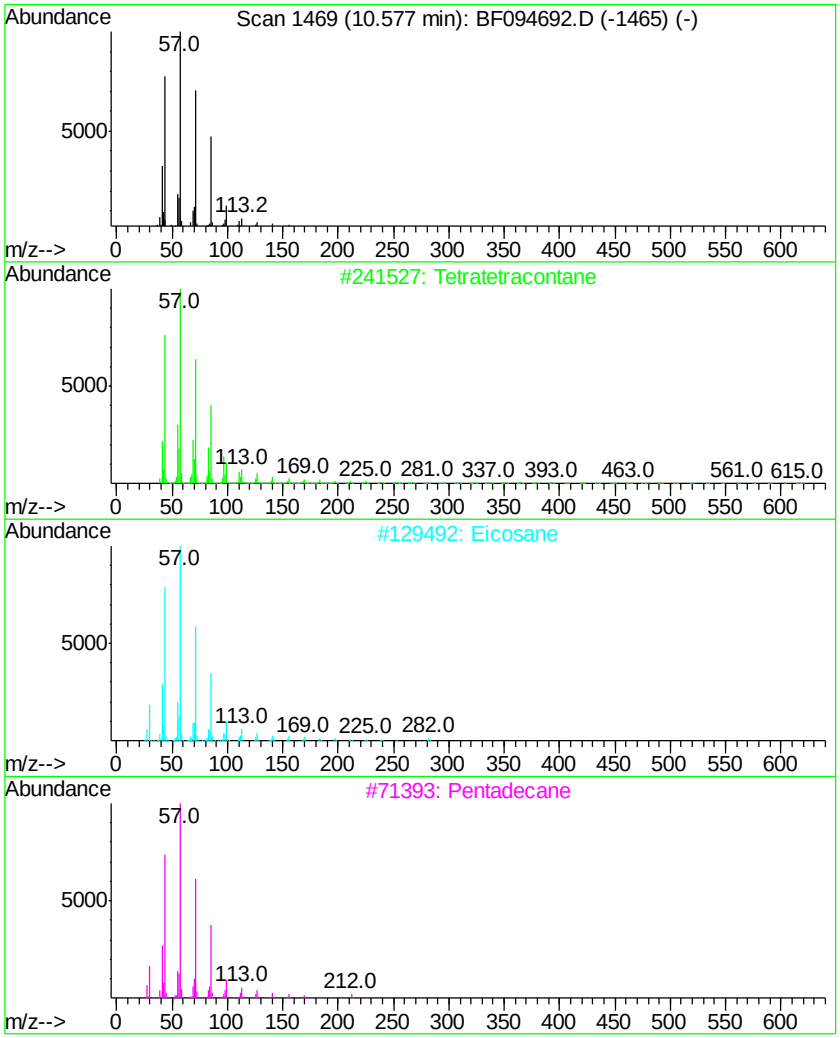
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

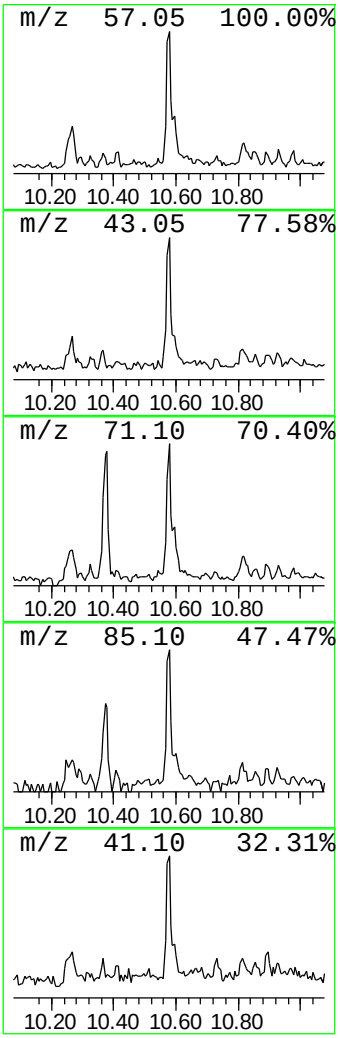
****

Peak Number 4 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.58	3.39 ng	87025	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	90
2	Eicosane	282	C20H42	000112-95-8	86
3	Pentadecane	212	C15H32	000629-62-9	86
4	Hexadecane	226	C16H34	000544-76-3	86
5	Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
Data File : BF094692.D
Acq On : 28 Apr 2017 19:11
Operator : SJ/MA
Sample : I2895-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02-3.0-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

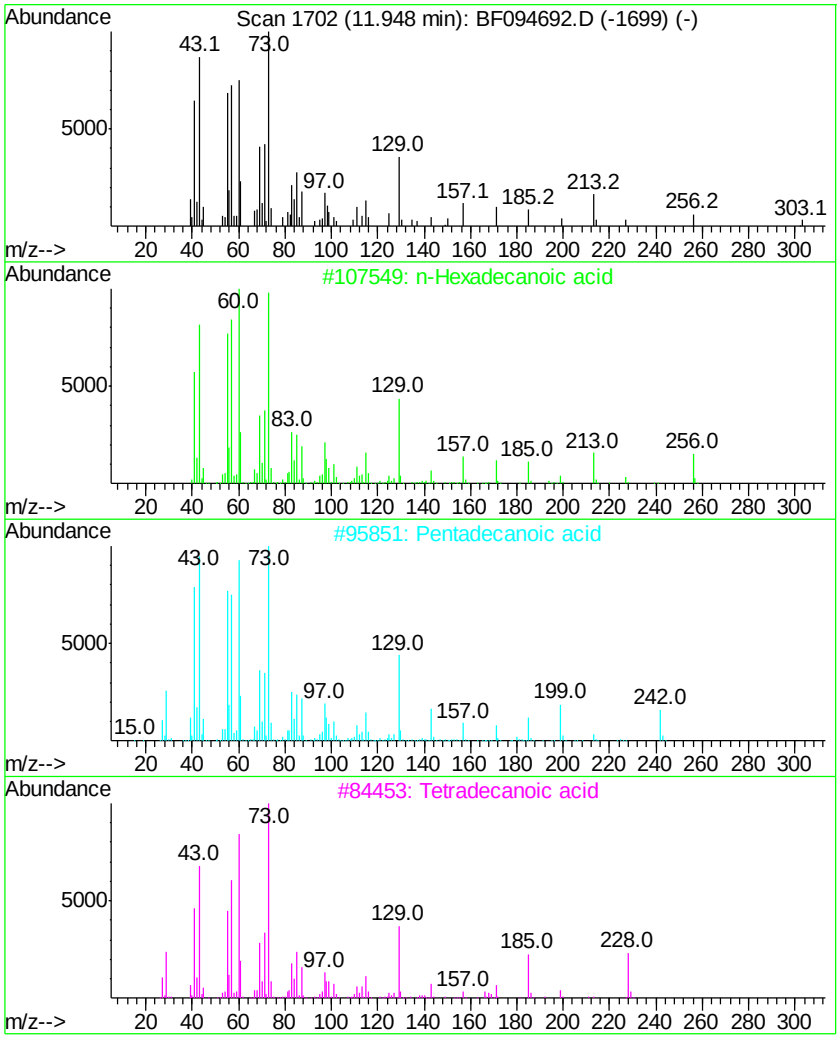
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

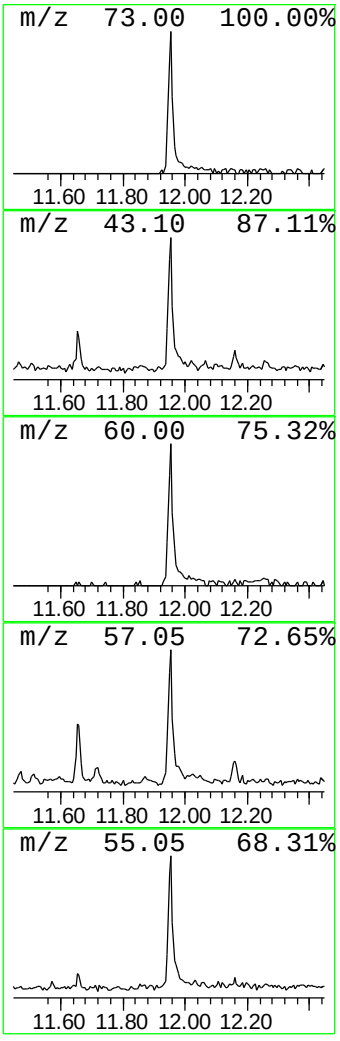
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	6.83 ng	175371	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
Data File : BF094692.D
Acq On : 28 Apr 2017 19:11
Operator : SJ/MA
Sample : I2895-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02-3.0-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

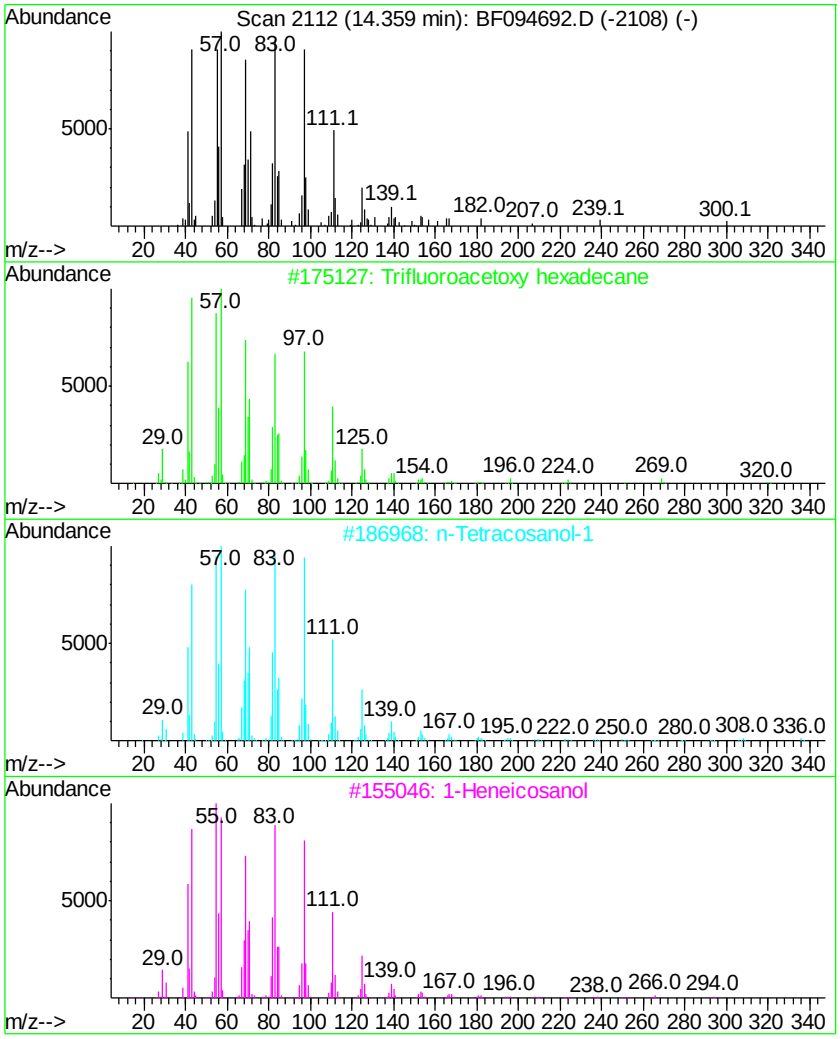
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

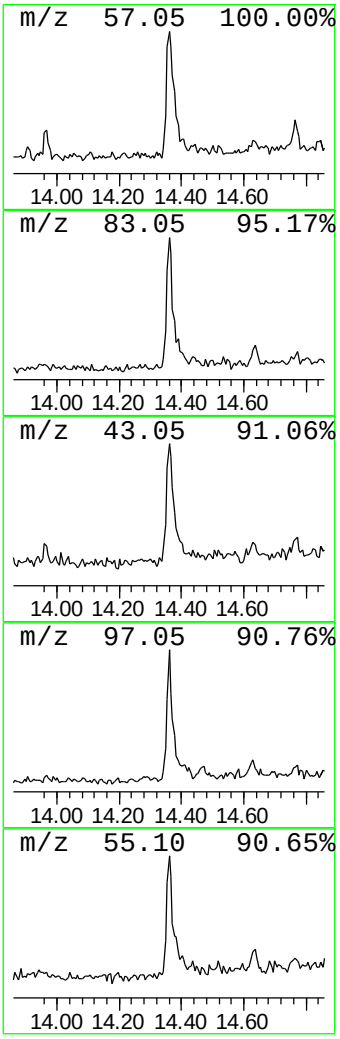
****

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	9.26 ng	210122	Chrysene-d12	14.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042817\
Data File : BF094692.D
Acq On : 28 Apr 2017 19:11
Operator : SJ/MA
Sample : I2895-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02-3.0-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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...	3.95	26.7	ng	607123	1	5.77	454274	20.0
unknown5.53	5.53	149.4	ng	3394290	1	5.77	454274	20.0
Tetratetracontane	10.58	3.4	ng	87025	4	11.22	513840	20.0
n-Hexadecanoic acid	11.95	6.8	ng	175371	4	11.22	513840	20.0
Trifluoroacetoxy ...	14.36	9.3	ng	210122	5	14.47	453628	20.0