LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102243.D
Acq On : 20 Jan 2018 3:19
Operator : SJ/JU
Sample : J1114-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-27-2.0-2.5

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	4.933	480	484	494	rVB	215858	347544	7.95%	0.950%
2	5.339	547	553	556	rBV	3852842	4276753	97.84%	11.692%
3	6.369	721	728	731	rBV	3336479	4371222	100.00%	11.951%
4	6.492	744	749	752	rBV	4219142	4333418	99.14%	11.847%
5	6.716	784	787	791	rBV	973500	839084	19.20%	2.294%
6	6.875	810	814	817	rBV	3489631	3277245	74.97%	8.960%
7	7.286	878	884	887	rBV	2529754	2862500	65.49%	7.826%
8	7.998	1001	1005	1009	rBV	1273634	1108830	25.37%	3.031%
9	9.080	1183	1189	1192	rBV	4322288	4147430	94.88%	11.339%
10	9.468	1251	1255	1258	rBV	313206	281913	6.45%	0.771%
11	9.686	1288	1292	1295	rBV	95182	75317	1.72%	0.206%
12	9.751	1299	1303	1307	rVB	1250906	1137633	26.03%	3.110%
13	10.186	1373	1377	1380	rVB	129112	111919	2.56%	0.306%
14	10.404	1408	1414	1416	rBV	34739	44727	1.02%	0.122%
15	10.545	1431	1438	1441	rBV	2492683	2417400	55.30%	6.609%
16	10.657	1454	1457	1465	rVB	123280	117117	2.68%	0.320%
17	11.233	1552	1555	1559	rBV	1075110	970462	22.20%	2.653%
18	12.645	1791	1795	1798	rBV	392654	295690	6.76%	0.808%
19	12.721	1805	1808	1812	rVB	82805	66635	1.52%	0.182%
20	12.821	1821	1825	1829	rBV	2728583	2739790	62.68%	7.490%
21	13.304	1898	1907	1911	rBV	44647	54848	1.25%	0.150%
22	13.351	1911	1915	1918	rBV	216129	181530	4.15%	0.496%
23	13.715	1973	1977	1989	rBV	401738	415086	9.50%	1.135%
24	13.868	1997	2003	2007	rBV	797970	744771	17.04%	2.036%
25	14.039	2028	2032	2038	rBV	55775	53603	1.23%	0.147%
26	14.345	2080	2084	2091	rBV2	69432	95579	2.19%	0.261%
27	14.956	2185	2188	2197	rBV	38433	55685	1.27%	0.152%
28	15.292	2240	2245	2249	rBV	683434	779275	17.83%	2.130%
29	15.727	2315	2319	2323	rBV2	38360	53549	1.23%	0.146%
30	15.774	2323	2327	2335	rVB3	50124	82386	1.88%	0.225%
31	16.197	2394	2399	2404	rBV3	33637	67694	1.55%	0.185%
32	16.750	2489	2493	2500	rVB3	22674	45913	1.05%	0.126%
33	17.209	2565	2571	2583	rVB3	54403	125168	2.86%	0.342%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102243.D
Acq On : 20 Jan 2018 3:19
Operator : SJ/JU
Sample : J1114-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-27-2.0-2.5

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

Sum of corrected areas: 36577716

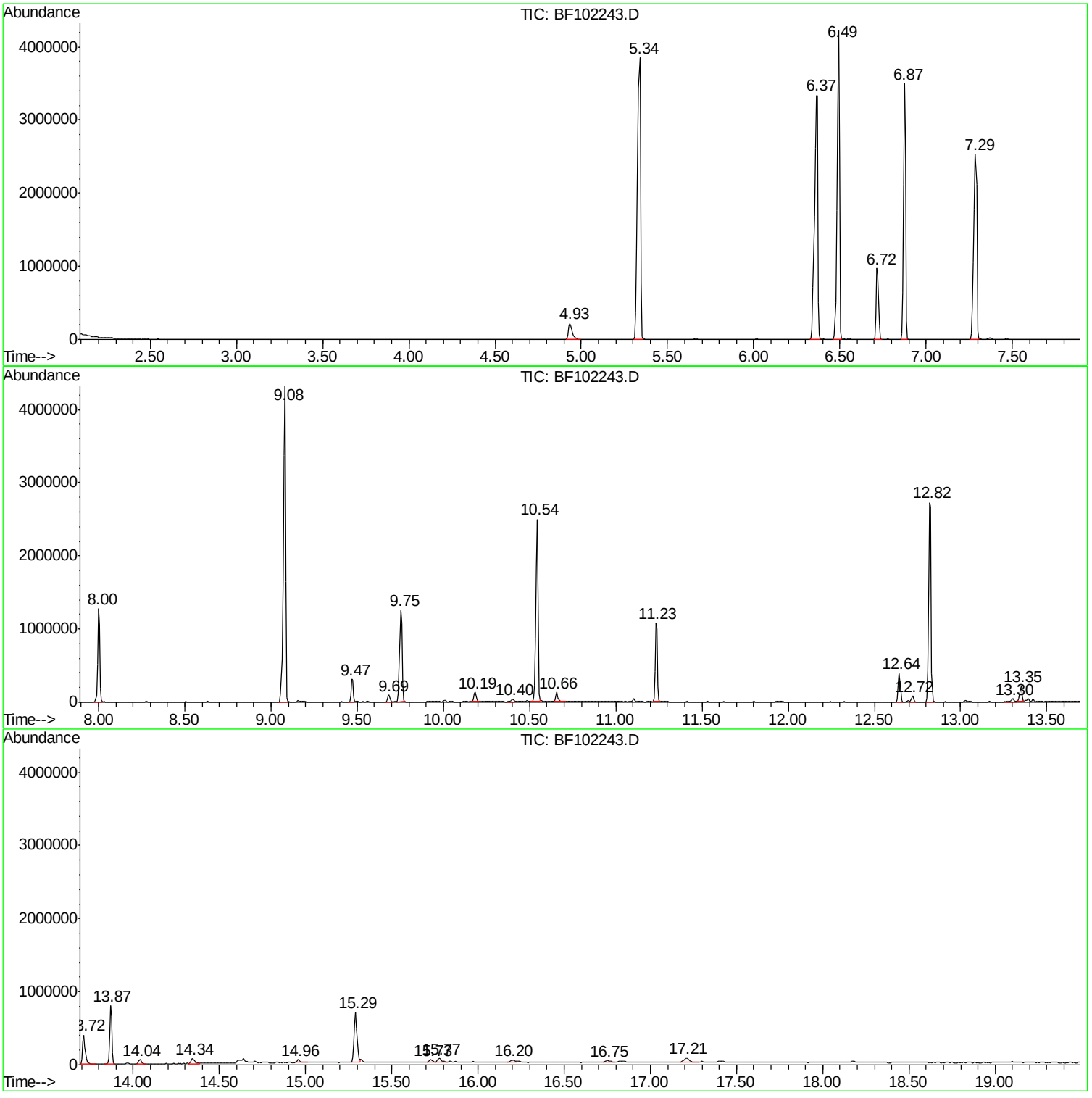
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102243.D
Acq On : 20 Jan 2018 3:19
Operator : SJ/JU
Sample : J1114-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-27-2.0-2.5

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102243.D
Acq On : 20 Jan 2018 3:19
Operator : SJ/JU
Sample : J1114-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-27-2.0-2.5

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

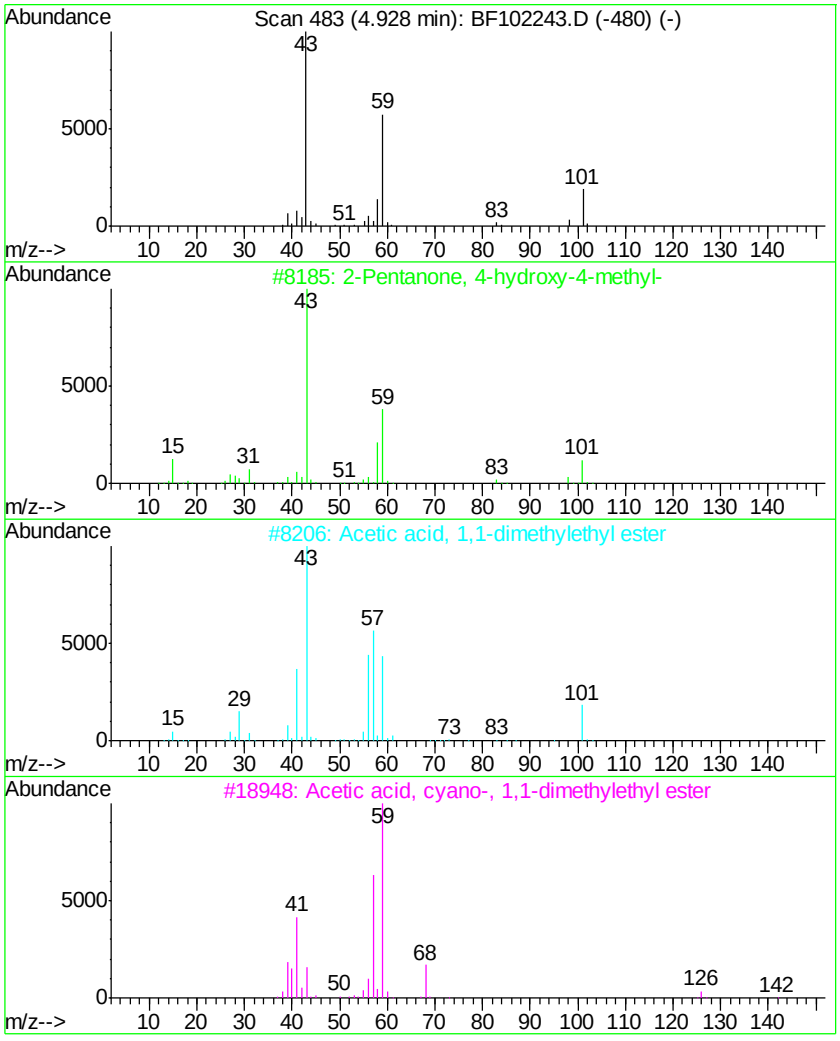
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

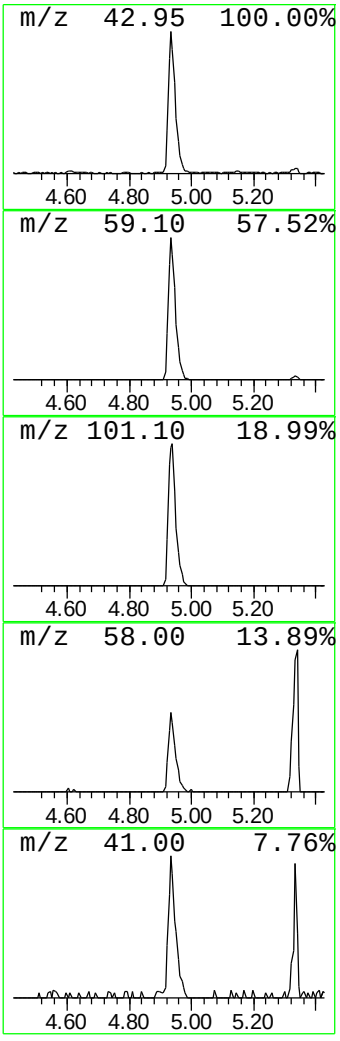
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	8.28 ng	347544	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	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102243.D
Acq On : 20 Jan 2018 3:19
Operator : SJ/JU
Sample : J1114-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-27-2.0-2.5

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

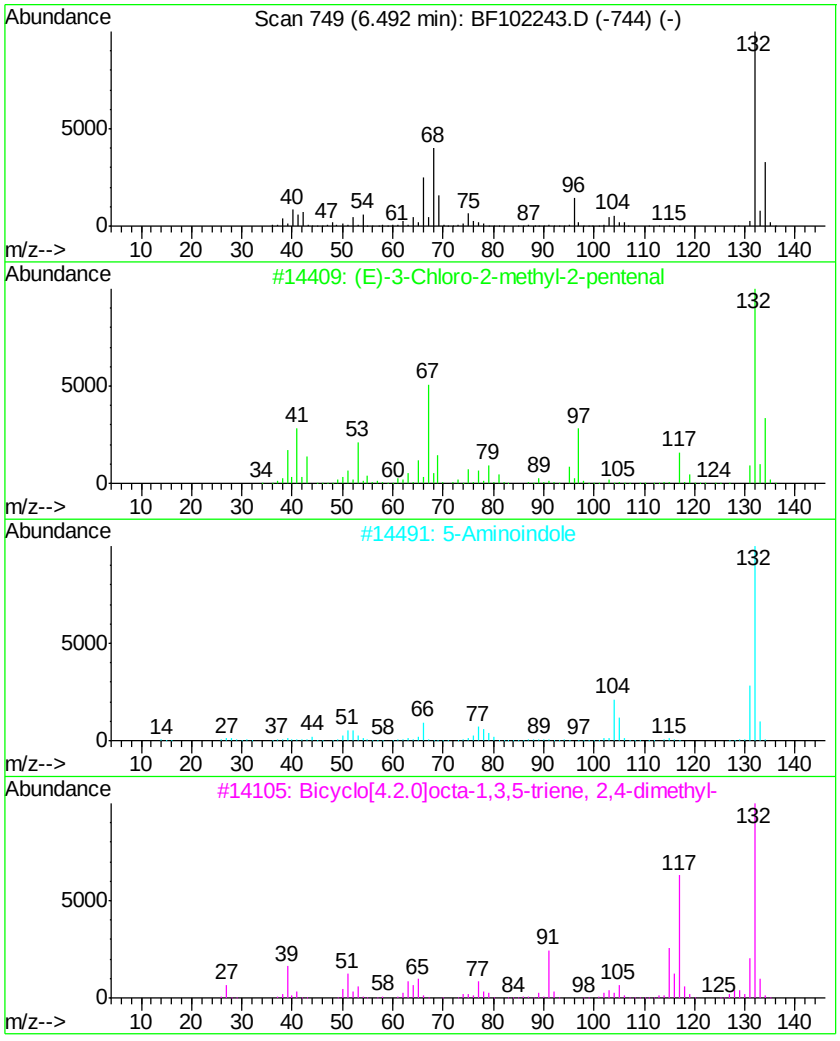
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

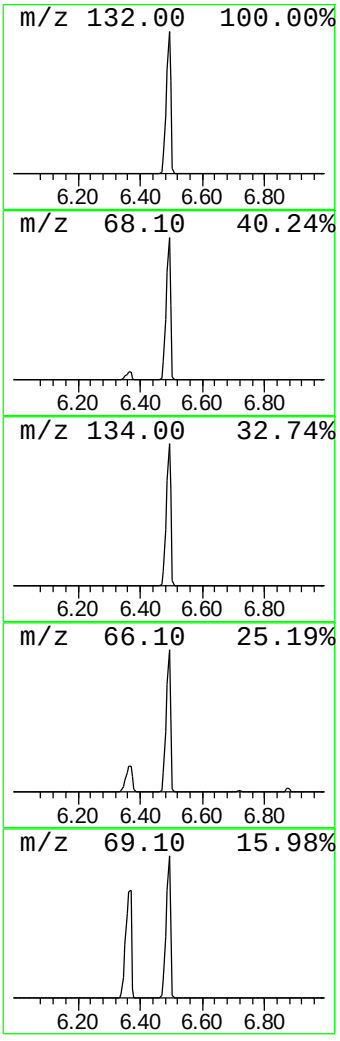
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	103.29 ng	4333420	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102243.D
Acq On : 20 Jan 2018 3:19
Operator : SJ/JU
Sample : J1114-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-27-2.0-2.5

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

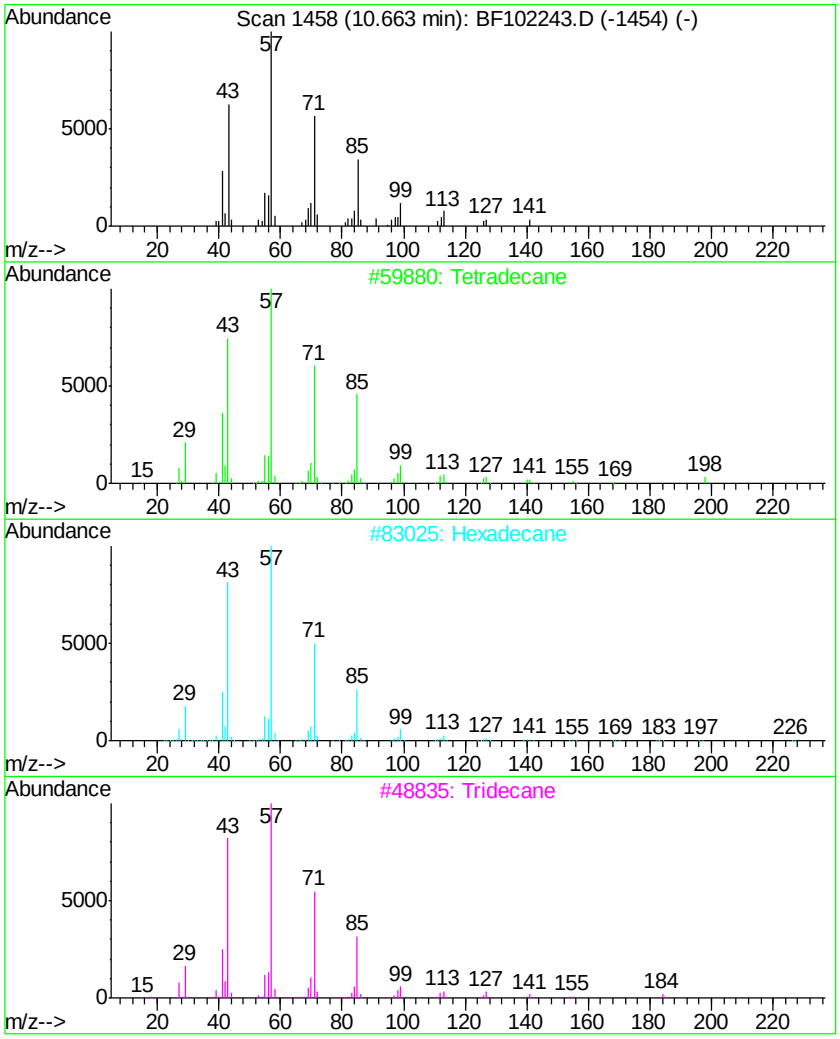
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

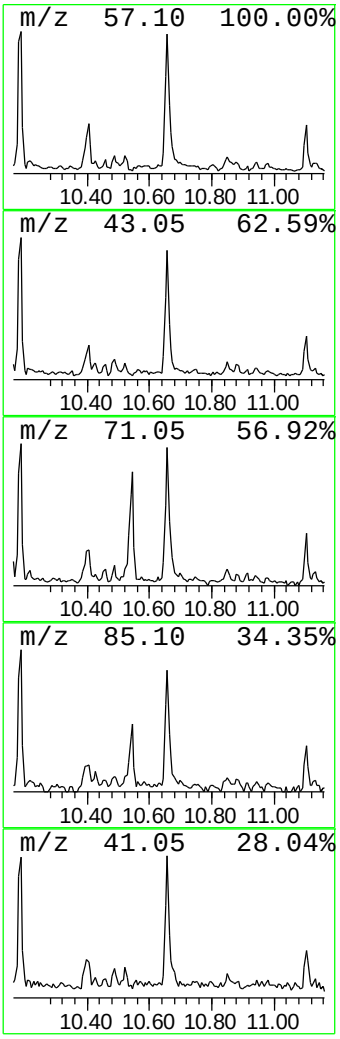
****

Peak Number 4 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	2.41 ng	117117	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tridecane	184	C13H28	000629-50-5	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Nonadecane	268	C19H40	000629-92-5	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102243.D
Acq On : 20 Jan 2018 3:19
Operator : SJ/JU
Sample : J1114-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-27-2.0-2.5

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

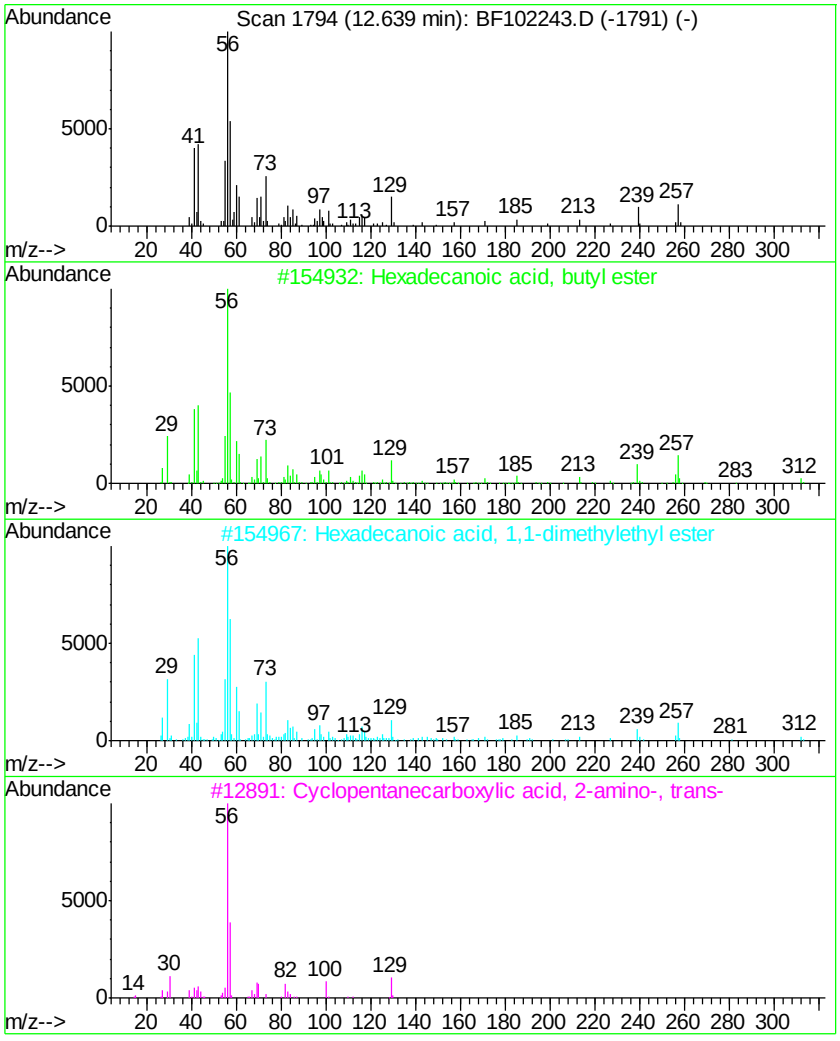
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

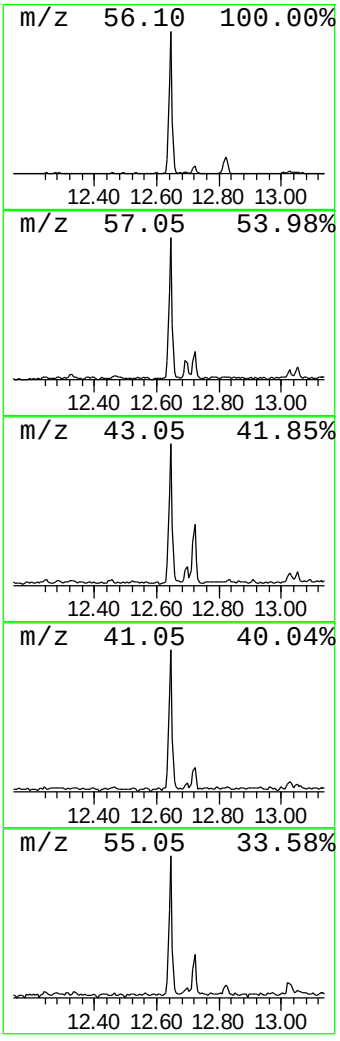
****

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	7.94 ng	295690	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	46
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38
4	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	35
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102243.D
Acq On : 20 Jan 2018 3:19
Operator : SJ/JU
Sample : J1114-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-27-2.0-2.5

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

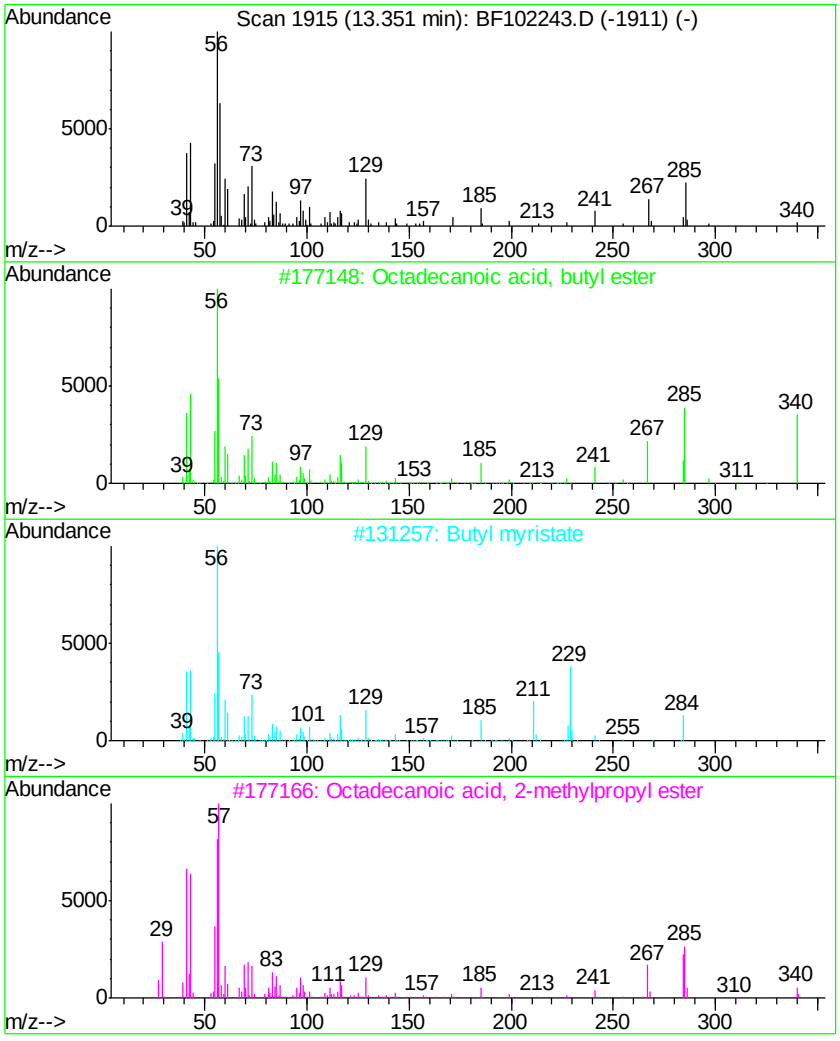
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

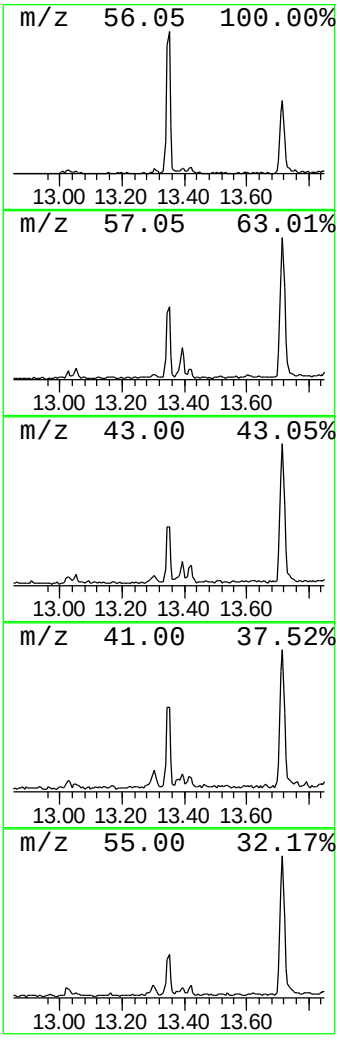
****

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	4.87 ng	181530	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	94
2	Butyl myristate	284	C18H36O2	000110-36-1	64
3	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	43
4	Piperidin-4-carboxylic acid	129	C6H11NO2	000498-94-2	38
5	Propan-2-one O-(2-chloro-1-methy...	149	C6H12ClNO	1000186-05-6	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102243.D
Acq On : 20 Jan 2018 3:19
Operator : SJ/JU
Sample : J1114-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-27-2.0-2.5

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

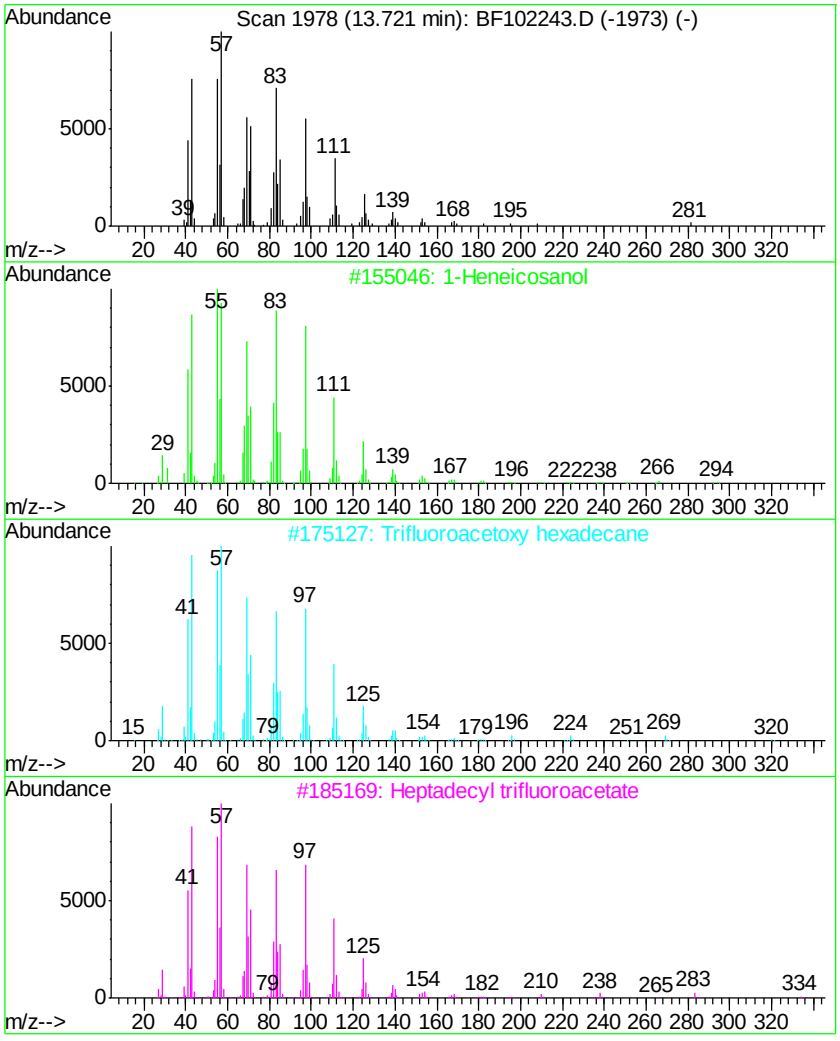
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

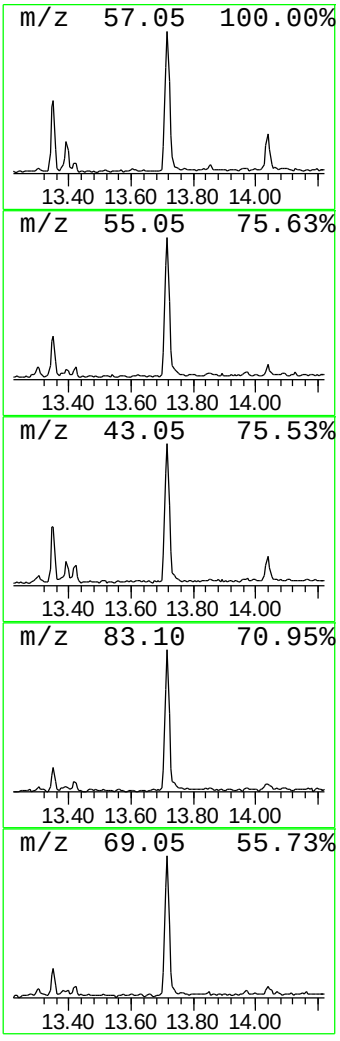
****

Peak Number 7 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	11.15 ng	415086	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102243.D
Acq On : 20 Jan 2018 3:19
Operator : SJ/JU
Sample : J1114-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-27-2.0-2.5

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

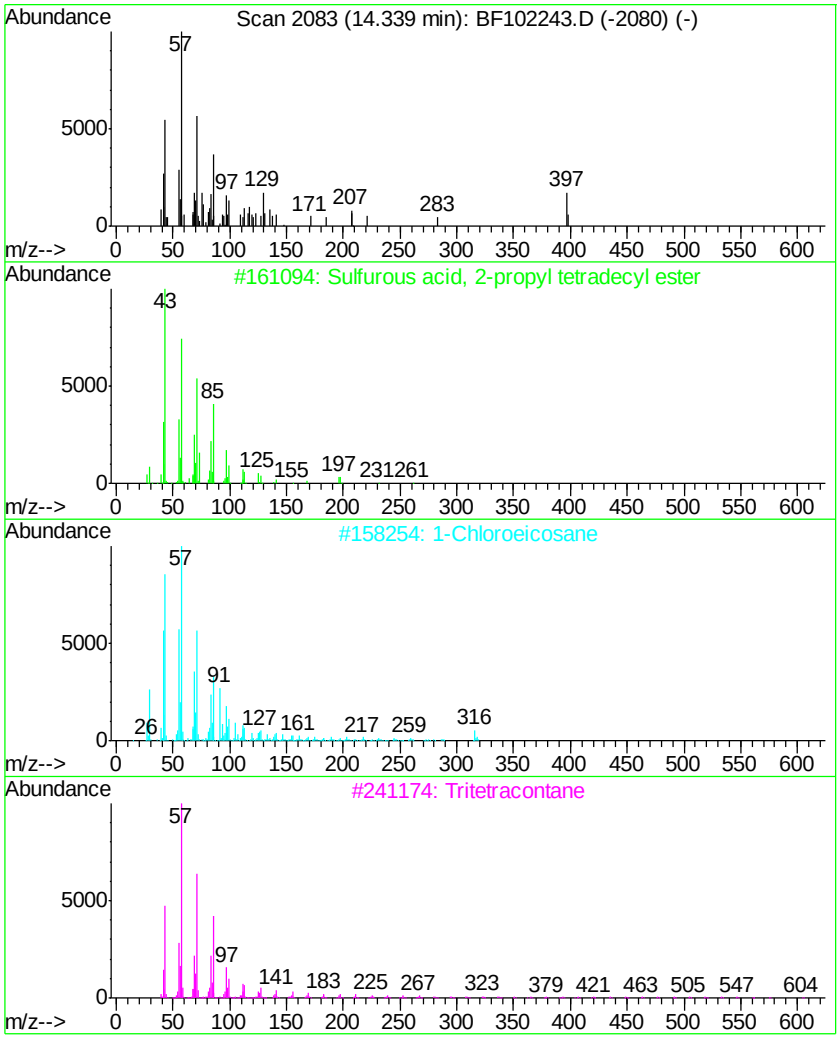
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

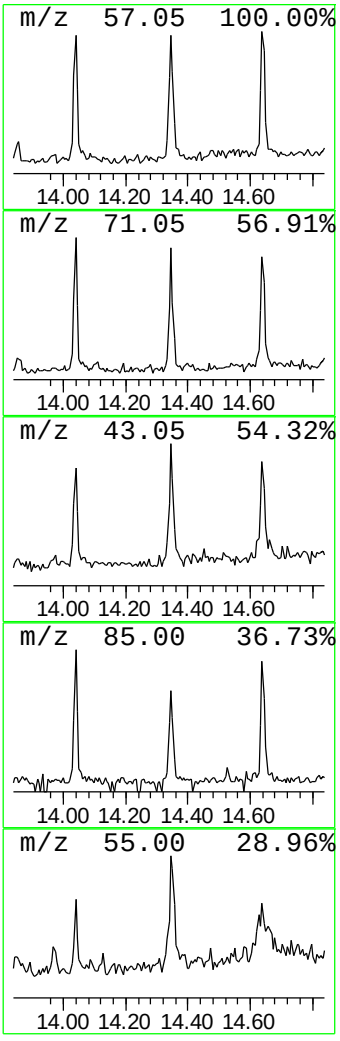
****

Peak Number 8 Sulfurous acid, 2-propyl te... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.57 ng	95579	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	80
2	1-Chloroeicosane	316	C20H41Cl	042217-02-7	74
3	Tritetracontane	605	C43H88	007098-21-7	74
4	Tetracosane, 1-bromo-	416	C24H49Br	006946-24-3	72
5	Tetratetracontane	619	C44H90	007098-22-8	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102243.D
Acq On : 20 Jan 2018 3:19
Operator : SJ/JU
Sample : J1114-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-27-2.0-2.5

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

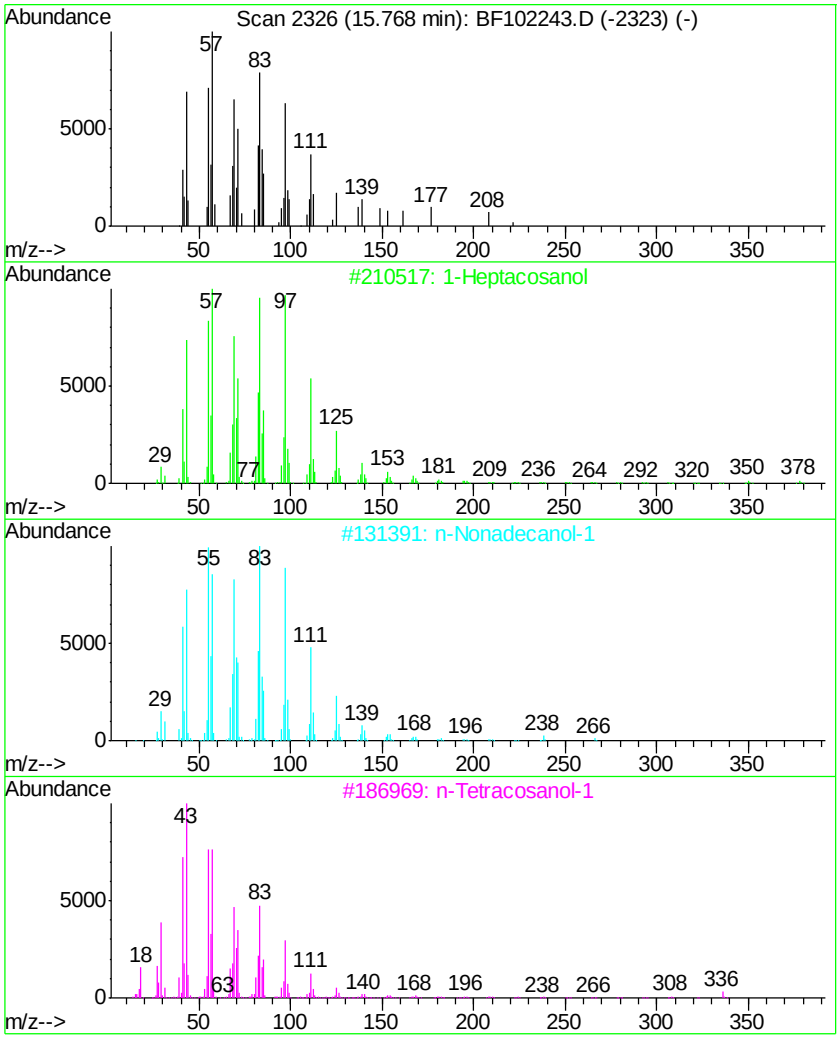
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

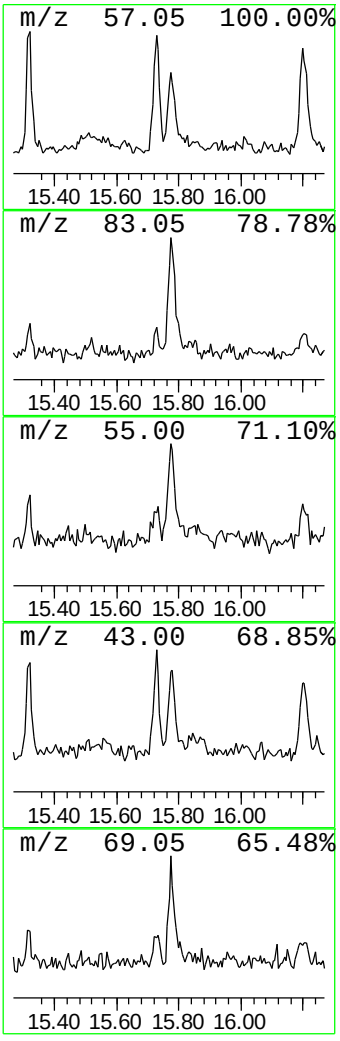
****

Peak Number 9 1-Heptacosanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	2.11 ng	82386	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	91
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	87
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	86
4	1-Hexadecanol	242	C16H34O	036653-82-4	83
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	81





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102243.D
Acq On : 20 Jan 2018 3:19
Operator : SJ/JU
Sample : J1114-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-27-2.0-2.5

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

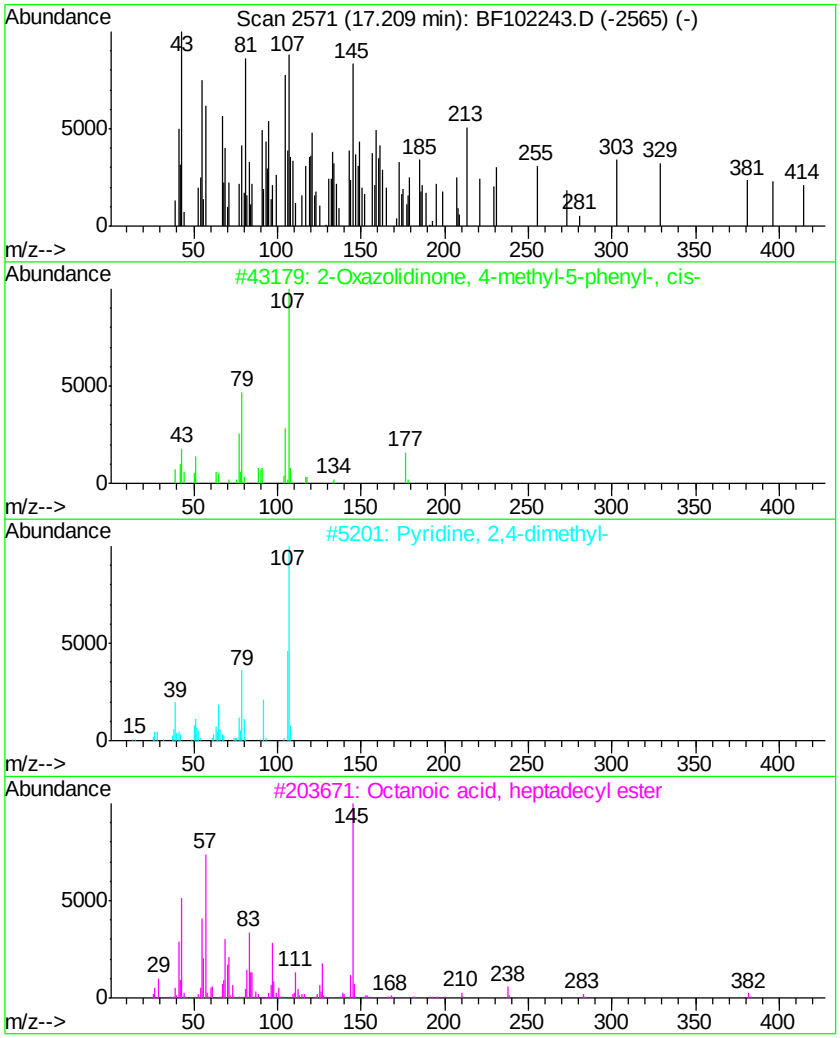
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

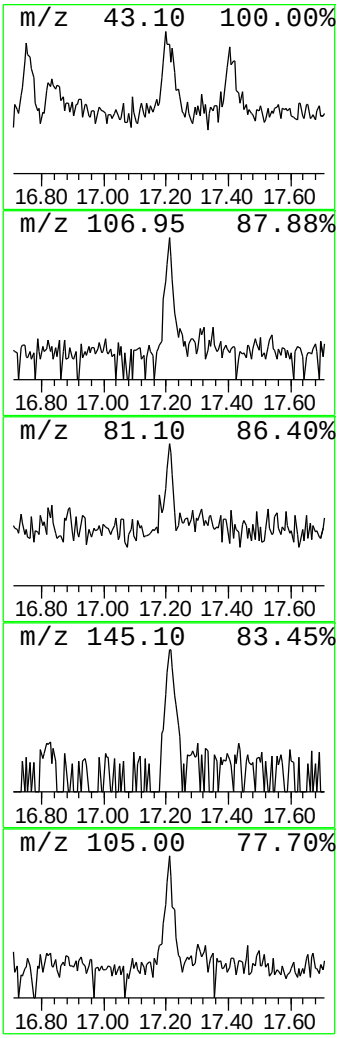
****

Peak Number 10 unknown17.21 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.21	3.21 ng	125168	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Oxazolidinone, 4-methyl-5-phen...	177	C10H11NO2	028044-22-6	11
2	Pyridine, 2,4-dimethyl-	107	C7H9N	000108-47-4	11
3	Octanoic acid, heptadecyl ester	382	C25H50O2	042231-43-6	10
4	Phosphine oxide, dicyclopentyl-	186	C10H19OP	187344-97-4	10
5	Benzene, (2,2-dimethyl-1-methyle...	160	C12H16	005676-29-9	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
Data File : BF102243.D
Acq On : 20 Jan 2018 3:19
Operator : SJ/JU
Sample : J1114-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-27-2.0-2.5

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	8.3	ng	347544	1	6.72	839084	20.0
unknown6.49	6.49	103.3	ng	4333420	1	6.72	839084	20.0
Tetradecane	10.66	2.4	ng	117117	4	11.23	970462	20.0
Hexadecanoic acid...	12.64	7.9	ng	295690	5	13.87	744771	20.0
Octadecanoic acid...	13.35	4.9	ng	181530	5	13.87	744771	20.0
1-Heneicosanol	13.72	11.2	ng	415086	5	13.87	744771	20.0
Sulfurous acid, 2...	14.34	2.6	ng	95579	5	13.87	744771	20.0
1-Heptacosanol	15.77	2.1	ng	82386	6	15.29	779275	20.0
unknown17.21	17.21	3.2	ng	125168	6	15.29	779275	20.0