LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102160.D
Acq On : 17 Jan 2018 19:53
Operator : SJ/JU
Sample : J1167-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-12000

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	4.928	478	483	492	rVB	195442	286500	8.01%	0.941%
2	5.334	547	552	555	rBV	3298186	3401085	95.09%	11.170%
3	6.363	721	727	731	rBV	3095009	3473007	97.10%	11.406%
4	6.493	744	749	752	rBV	3679165	3447614	96.39%	11.323%
5	6.722	784	788	791	rVB	1075482	911292	25.48%	2.993%
6	6.875	810	814	818	rBV	2876992	2687390	75.13%	8.826%
7	7.287	878	884	887	rBV	2165436	2134973	59.69%	7.012%
8	8.004	1001	1006	1009	rBV	1346921	1205242	33.70%	3.958%
9	8.557	1097	1100	1104	rBV	213274	179096	5.01%	0.588%
10	9.081	1183	1189	1192	rBV	4027674	3576773	100.00%	11.747%
11	9.475	1252	1256	1259	rBV	465814	375441	10.50%	1.233%
12	9.757	1299	1304	1307	rBV	1282490	1164497	32.56%	3.824%
13	10.469	1421	1425	1428	rBV	706958	562197	15.72%	1.846%
14	10.545	1433	1438	1441	rBV	1921958	1807002	50.52%	5.935%
15	11.233	1551	1555	1558	rBV	1079159	936615	26.19%	3.076%
16	12.822	1820	1825	1828	rBV	2491899	2240692	62.65%	7.359%
17	13.710	1973	1976	1982	rBV	174470	187535	5.24%	0.616%
18	13.869	1998	2003	2006	rBV	779067	765928	21.41%	2.515%
19	14.498	2107	2110	2115	rBV3	46049	78258	2.19%	0.257%
20	15.286	2239	2244	2248	rBV	614617	791188	22.12%	2.598%
21	15.715	2315	2317	2322	rVB2	61626	88610	2.48%	0.291%
22	16.751	2488	2493	2496	rBV3	71735	147638	4.13%	0.485%

Sum of corrected areas: 30448573

LSC Report - Integrated Chromatogram

Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102160.D
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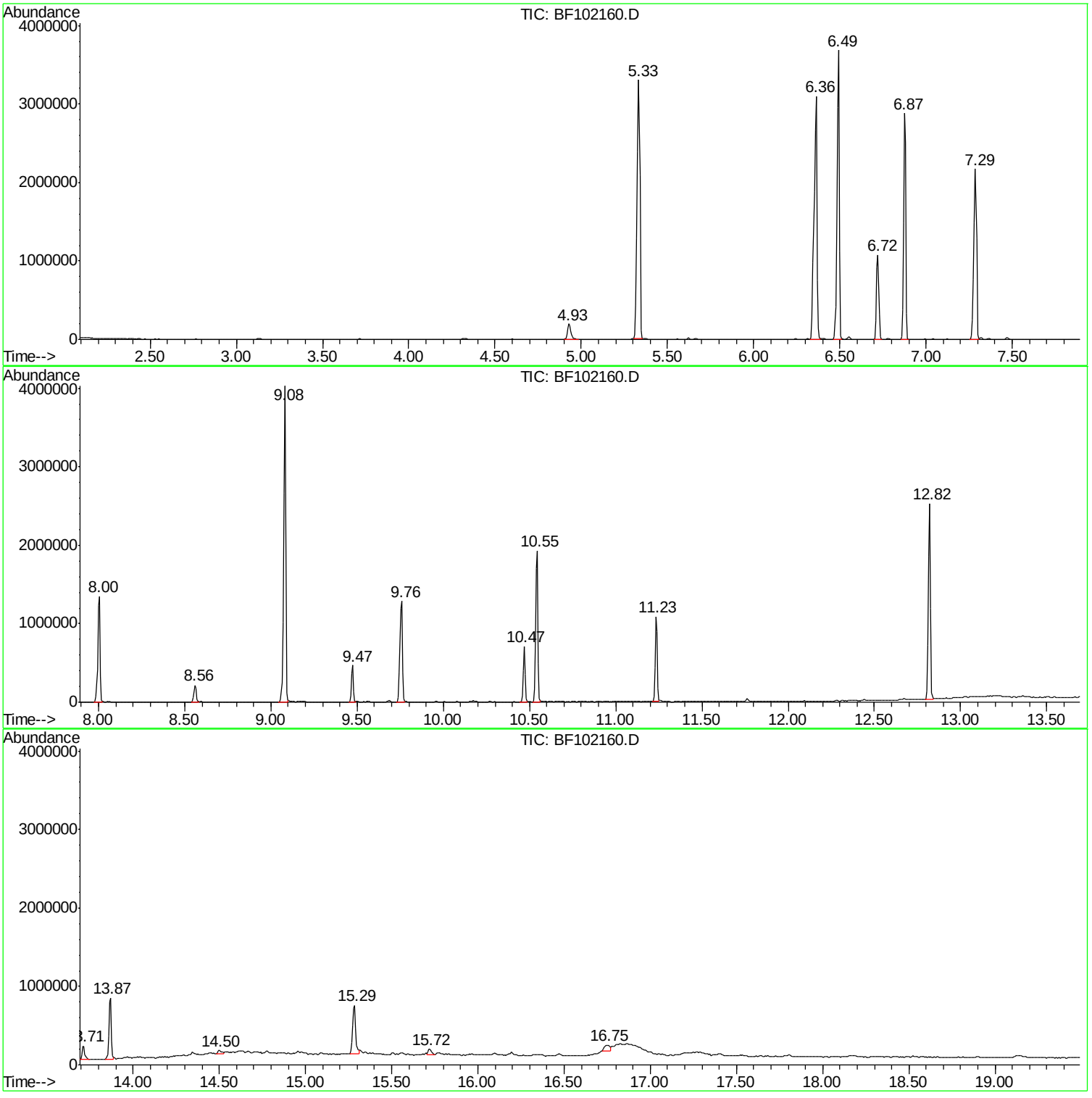
Operator : SJ/JU
Sample : J1167-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-12000

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



Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102160.D
Acq On : 17 Jan 2018 19:53
Operator : SJ/JU
Sample : J1167-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-12000

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

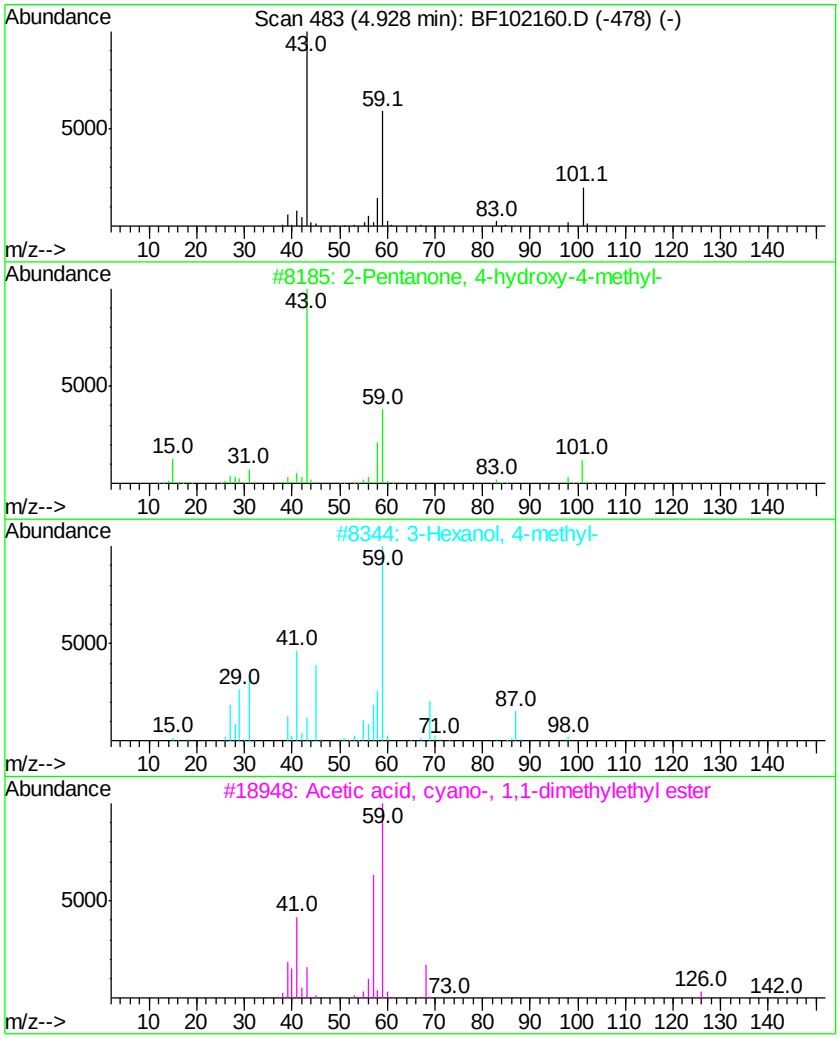
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

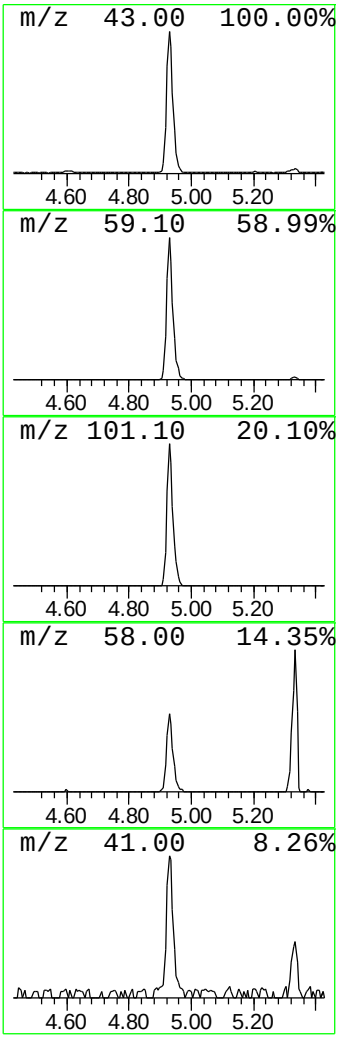
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	6.29 ng	286500	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	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102160.D
Acq On : 17 Jan 2018 19:53
Operator : SJ/JU
Sample : J1167-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-12000

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

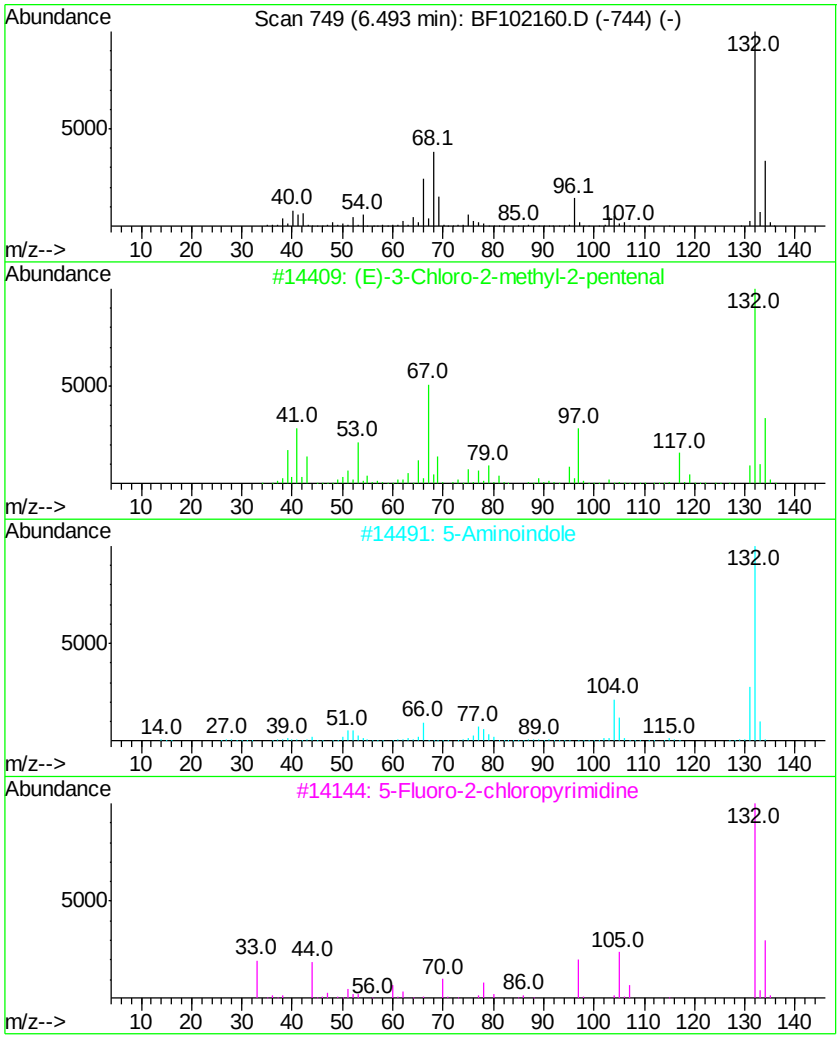
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

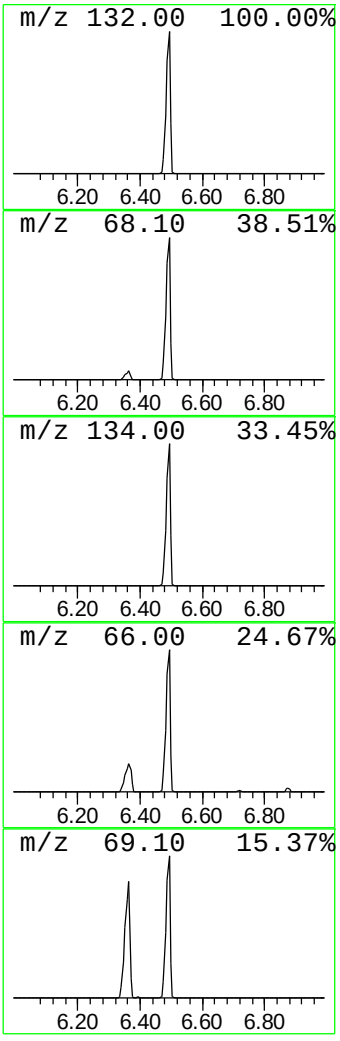
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	75.66 ng	3447610	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	17
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102160.D
Acq On : 17 Jan 2018 19:53
Operator : SJ/JU
Sample : J1167-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-12000

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

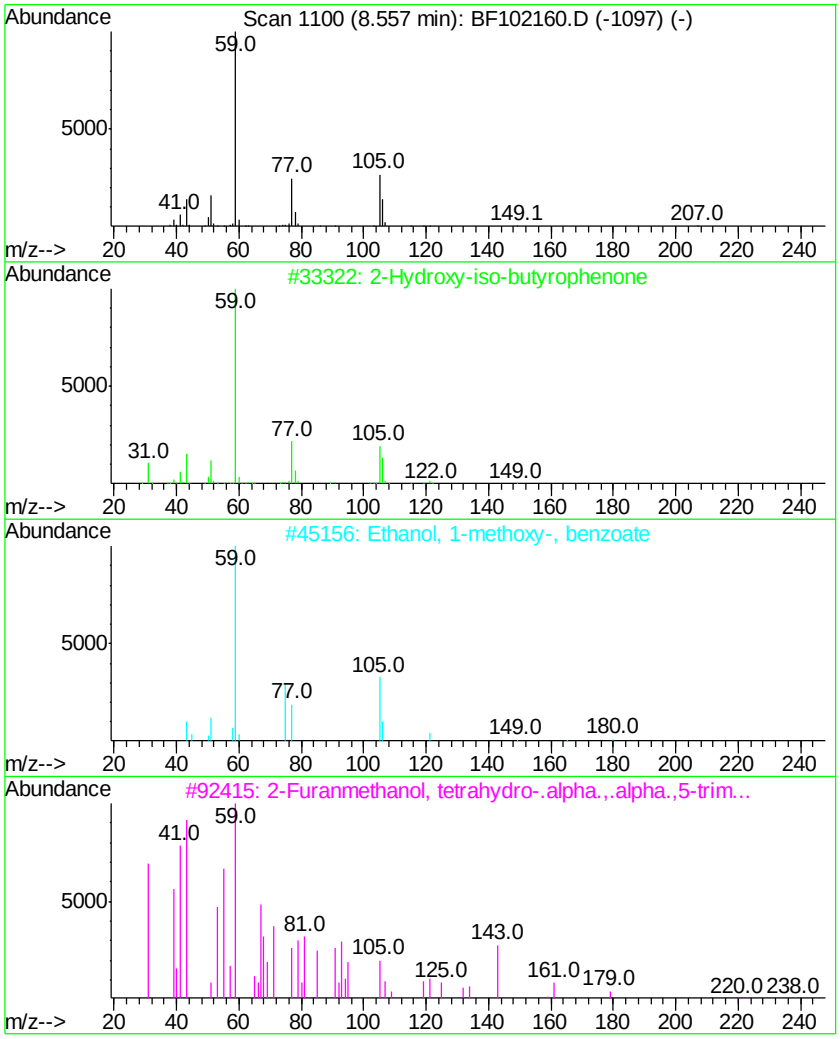
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

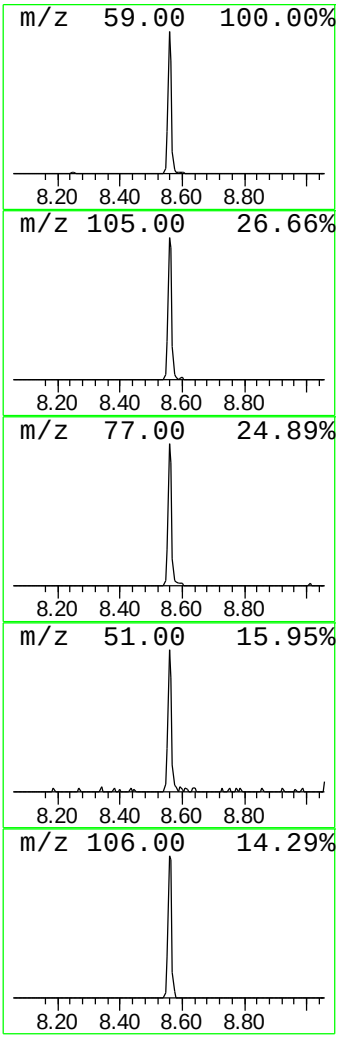
****

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.56	2.97 ng	179096	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3	2-Furanmethanol, tetrahydro-.alp...	238	C15H26O2	026184-88-3	28
4	Guanidine	59	CH5N3	000113-00-8	9
5	Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102160.D
Acq On : 17 Jan 2018 19:53
Operator : SJ/JU
Sample : J1167-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-12000

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

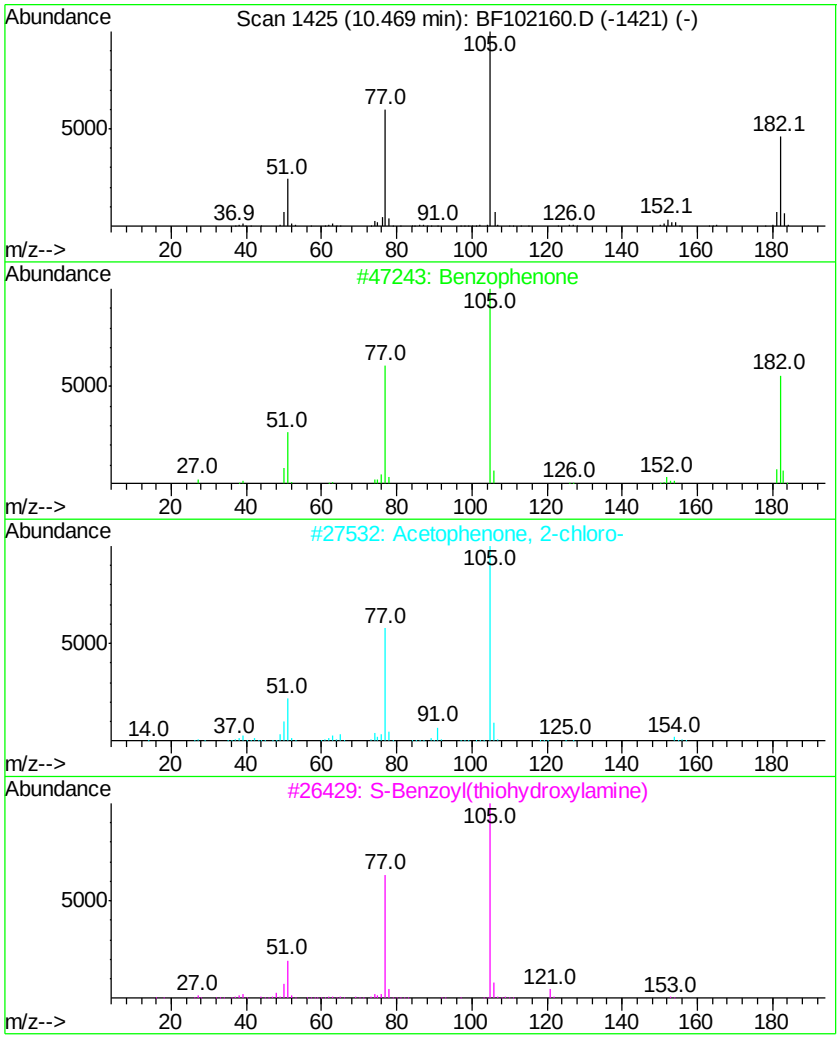
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

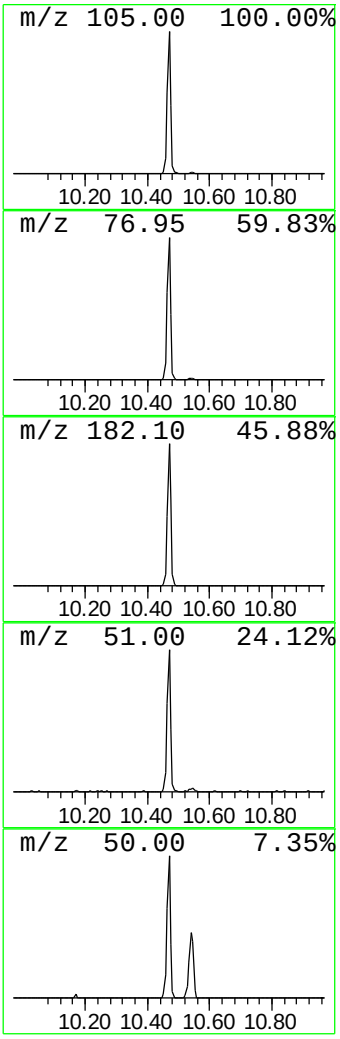
****

Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.47	9.66 ng	562197	Acenaphthene-d10	9.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	47
4	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5	5-[N-Benzoylaminomethyl]tetrazole	203	C9H9N5O	1000227-36-3	47





Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102160.D
Acq On : 17 Jan 2018 19:53
Operator : SJ/JU
Sample : J1167-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-12000

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

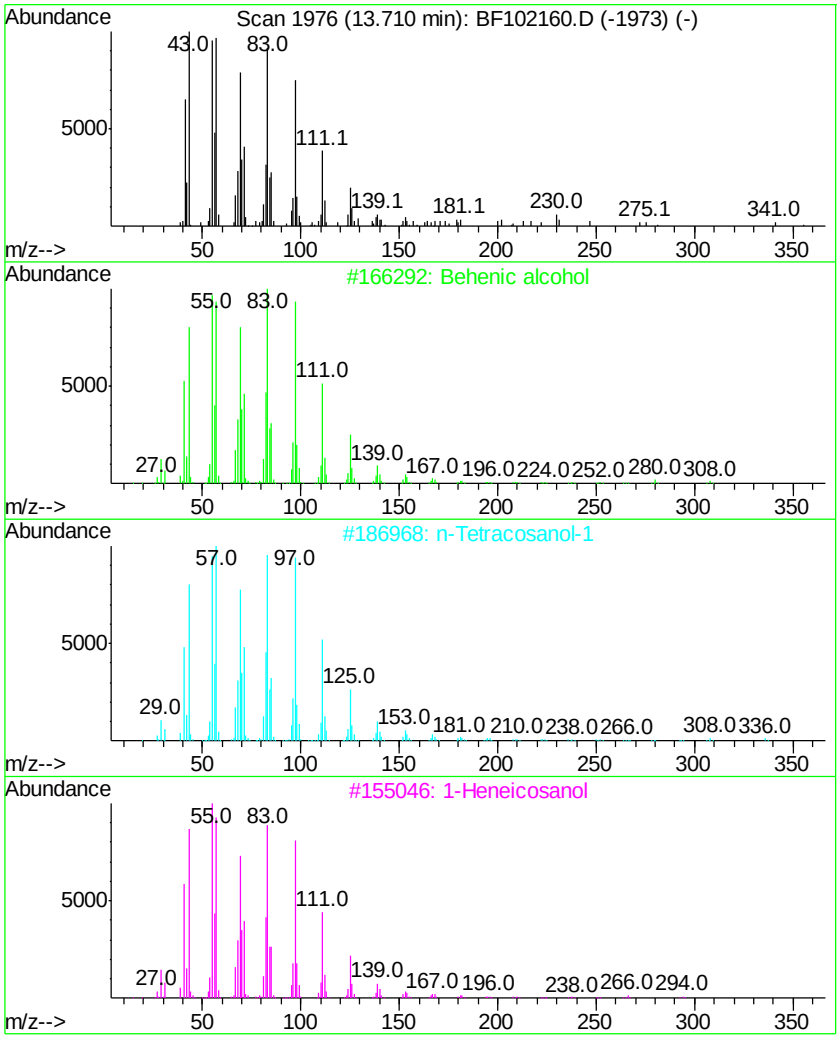
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

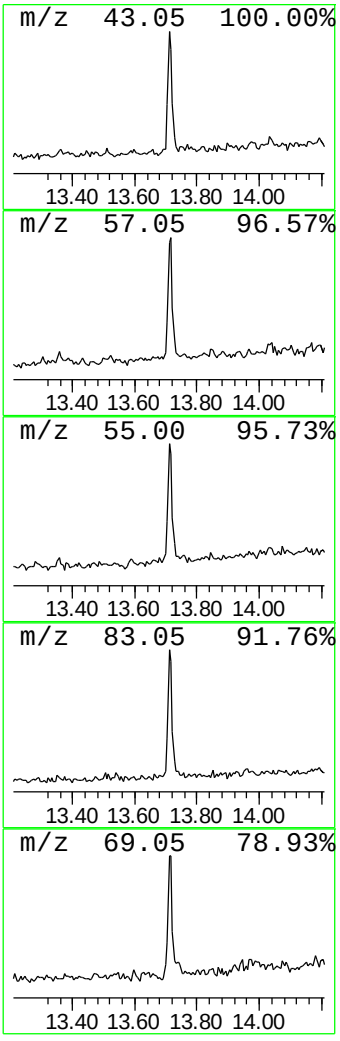
****

Peak Number 6 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	4.90 ng	187535	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
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	91





Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102160.D
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Operator : SJ/JU
Sample : J1167-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-12000

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

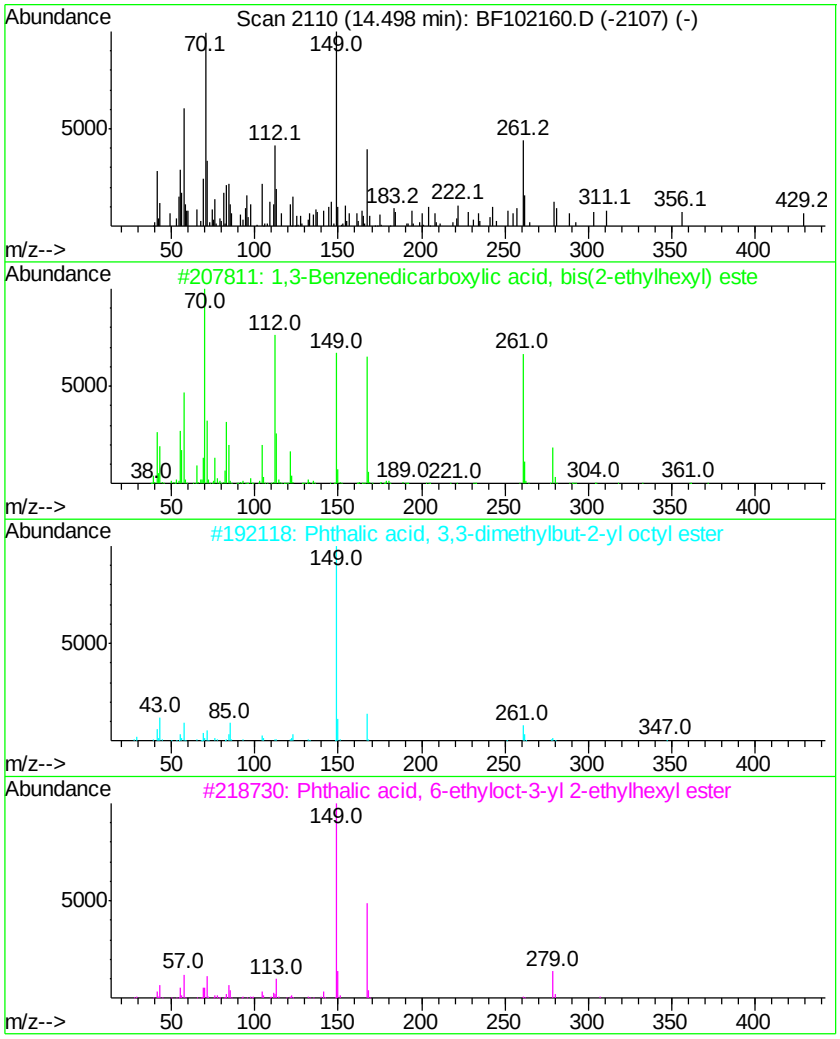
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

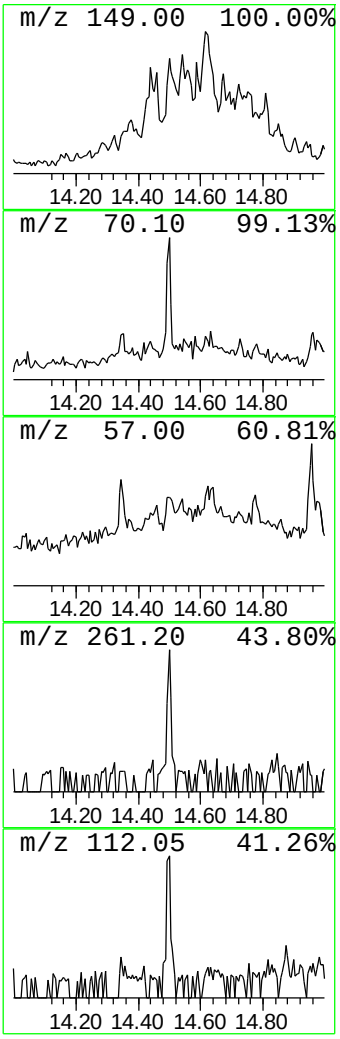
****

Peak Number 7 unknown14.50 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	2.04 ng	78258	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	38
2	Phthalic acid, 3,3-dimethylbut-2...	362	C22H34O4	1000357-00-7	25
3	Phthalic acid, 6-ethyloct-3-yl 2...	418	C26H42O4	1000315-53-8	22
4	(3-Aminopropyl)dipropylborane	155	C9H22BN	060993-56-8	22
5	Cyclopentane, 1,2,4-trimethyl-, ...	112	C8H16	016883-48-0	22





Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
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Sample : J1167-03
Misc :
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Instrument : BNA_F
ClientSampleId : RO-72-12000

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

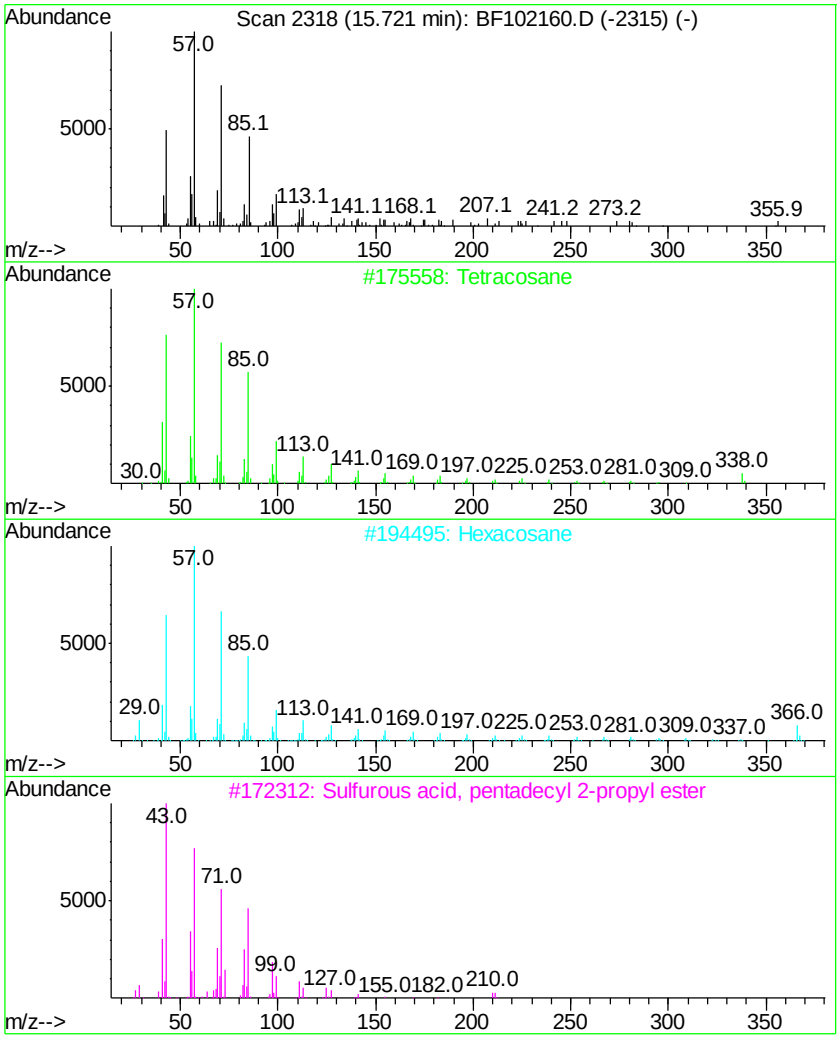
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

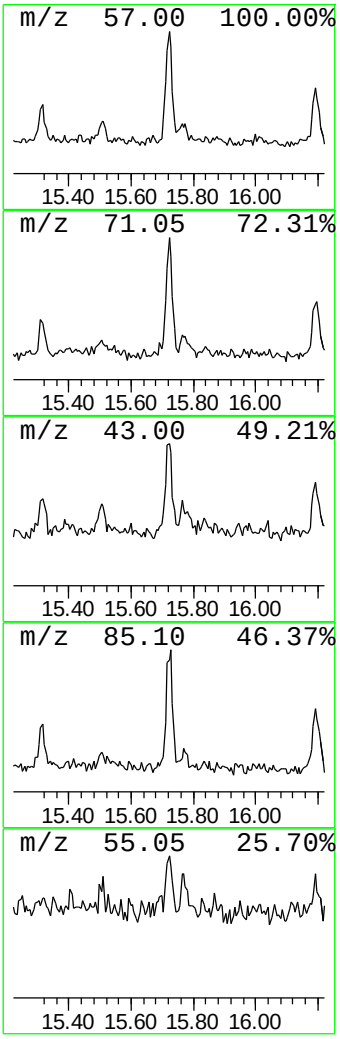
****

Peak Number 8 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	2.24 ng	88610	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	59
2	Hexacosane	366	C26H54	000630-01-3	53
3	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	53
4	Heptacosane	380	C27H56	000593-49-7	50
5	Heneicosane	296	C21H44	000629-94-7	50





Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102160.D
Acq On : 17 Jan 2018 19:53
Operator : SJ/JU
Sample : J1167-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-12000

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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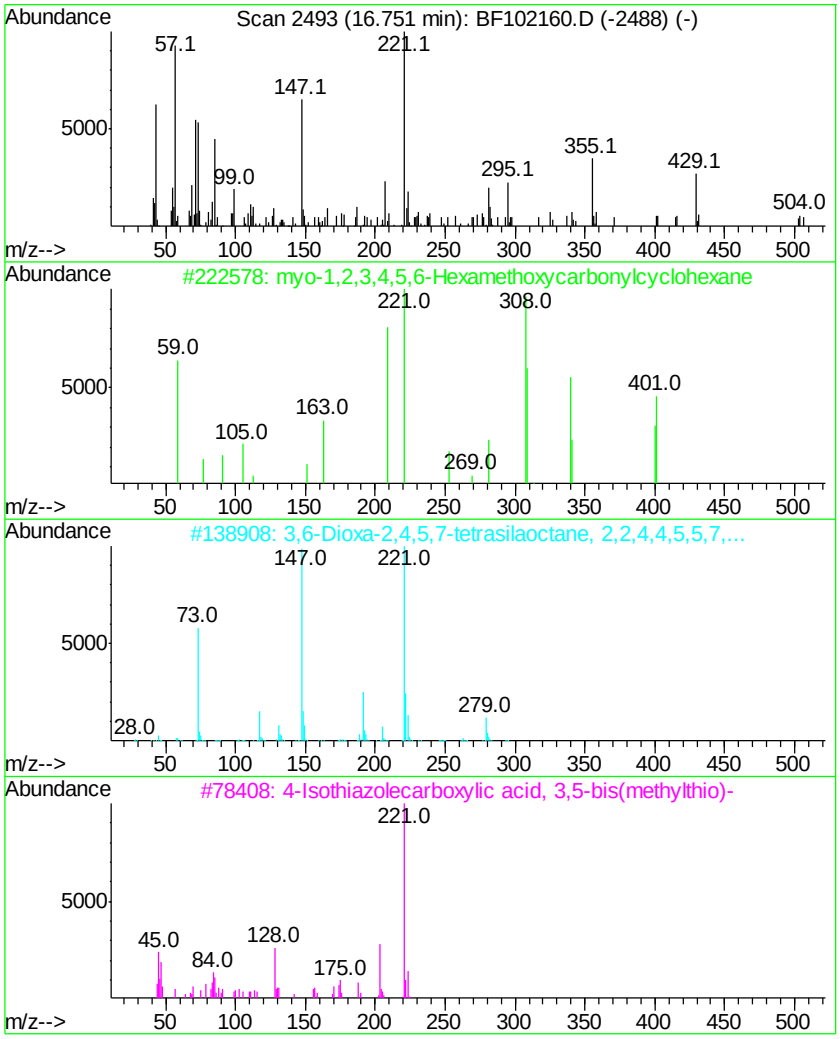
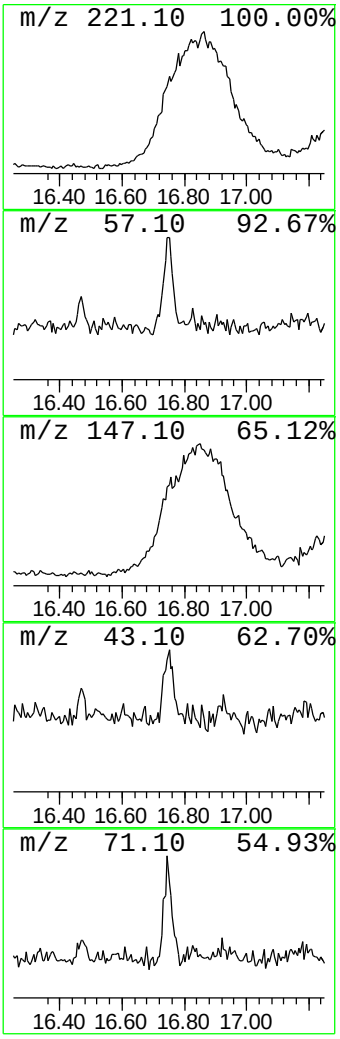
Peak Number 9 unknown16.75 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.75	3.73 ng	147638	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	myo-1,2,3,4,5,6-Hexamethoxycarbo...	432	C18H24O12	1000147-86-4	27
2	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	25
3	4-Isothiazolecarboxylic acid, 3,...	221	C6H7NO2S3	004886-15-1	22
4	4-Hydroxy-beta-phenylcinnamonitrile	221	C15H11NO	016281-90-6	14
5	Pyrido[1,2-a]benzimidazole-4-car...	221	C14H11N3	016314-95-7	14





Tentatively Identified Compound (LSC) summary

Data Path : U:\HPCHEM1\BNA_F\DATA\BF011718\
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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...	4.93	6.3	ng	286500	1	6.72	911292	20.0
unknown6.49	6.49	75.7	ng	3447610	1	6.72	911292	20.0
2-Hydroxy-iso-but...	8.56	3.0	ng	179096	2	8.00	1205240	20.0
Benzophenone	10.47	9.7	ng	562197	3	9.76	1164500	20.0
Behenic alcohol	13.71	4.9	ng	187535	5	13.87	765928	20.0
unknown14.50	14.50	2.0	ng	78258	5	13.87	765928	20.0
Tetracosane	15.72	2.2	ng	88610	6	15.29	791188	20.0
unknown16.75	16.75	3.7	ng	147638	6	15.29	791188	20.0