LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102264.D
Acq On : 20 Jan 2018 14:31
Operator : SJ/JU
Sample : J1115-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-36-2.5-3.0

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	490	rBV	173332	255259	7.29%	0.859%
2	5.334	547	552	555	rBV	3350034	3410612	97.43%	11.483%
3	6.363	721	727	731	rBV	3066231	3500550	100.00%	11.786%
4	6.493	744	749	752	rBV	3577553	3423224	97.79%	11.526%
5	6.716	784	787	791	rBV	984182	855372	24.44%	2.880%
6	6.875	810	814	817	rBV	3013632	2618596	74.81%	8.817%
7	7.287	879	884	887	rBV	2198796	2173110	62.08%	7.317%
8	7.381	895	900	911	rVB	55578	69481	1.98%	0.234%
9	7.998	1001	1005	1009	rBV	1231417	1111622	31.76%	3.743%
10	9.081	1183	1189	1192	rBV	3695907	3354233	95.82%	11.293%
11	9.157	1198	1202	1204	rBV	49487	37599	1.07%	0.127%
12	9.469	1252	1255	1258	rBV	543538	476727	13.62%	1.605%
13	9.686	1288	1292	1295	rBV	134273	109612	3.13%	0.369%
14	9.751	1299	1303	1307	rVB	1195620	1070641	30.58%	3.605%
15	10.157	1369	1372	1374	rBV	43373	37483	1.07%	0.126%
16	10.186	1374	1377	1380	rVB	139023	118866	3.40%	0.400%
17	10.404	1409	1414	1416	rBV	36083	44769	1.28%	0.151%
18	10.545	1431	1438	1441	rBV	1744706	1685083	48.14%	5.674%
19	10.657	1454	1457	1464	rBV	118221	120764	3.45%	0.407%
20	11.104	1530	1533	1536	rBV	75715	65841	1.88%	0.222%
21	11.233	1552	1555	1559	rBV	956078	877055	25.05%	2.953%
22	11.528	1602	1605	1608	rBV	40170	35543	1.02%	0.120%
23	12.822	1821	1825	1829	rVB	2413872	2233859	63.81%	7.521%
24	13.716	1973	1977	1981	rBV	352695	358266	10.23%	1.206%
25	13.869	1999	2003	2007	rBV	834720	795251	22.72%	2.678%
26	14.351	2080	2085	2092	rBV5	36198	52228	1.49%	0.176%
27	15.292	2240	2245	2249	rBV	623036	732880	20.94%	2.468%
28	15.774	2324	2327	2333	rVB4	47095	76157	2.18%	0.256%

Sum of corrected areas: 29700683

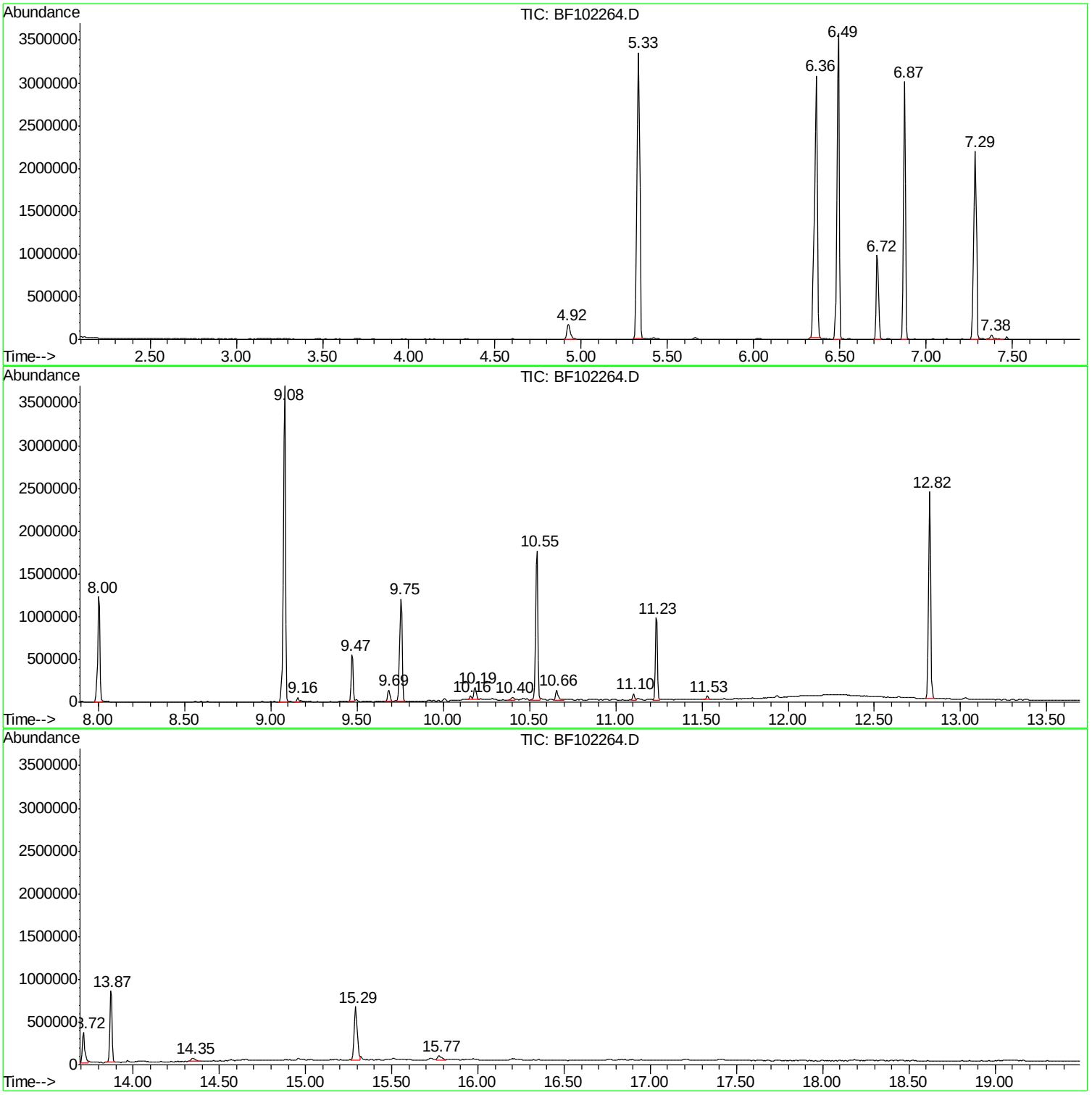
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102264.D
Acq On : 20 Jan 2018 14:31
Operator : SJ/JU
Sample : J1115-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-36-2.5-3.0

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102264.D
Acq On : 20 Jan 2018 14:31
Operator : SJ/JU
Sample : J1115-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-36-2.5-3.0

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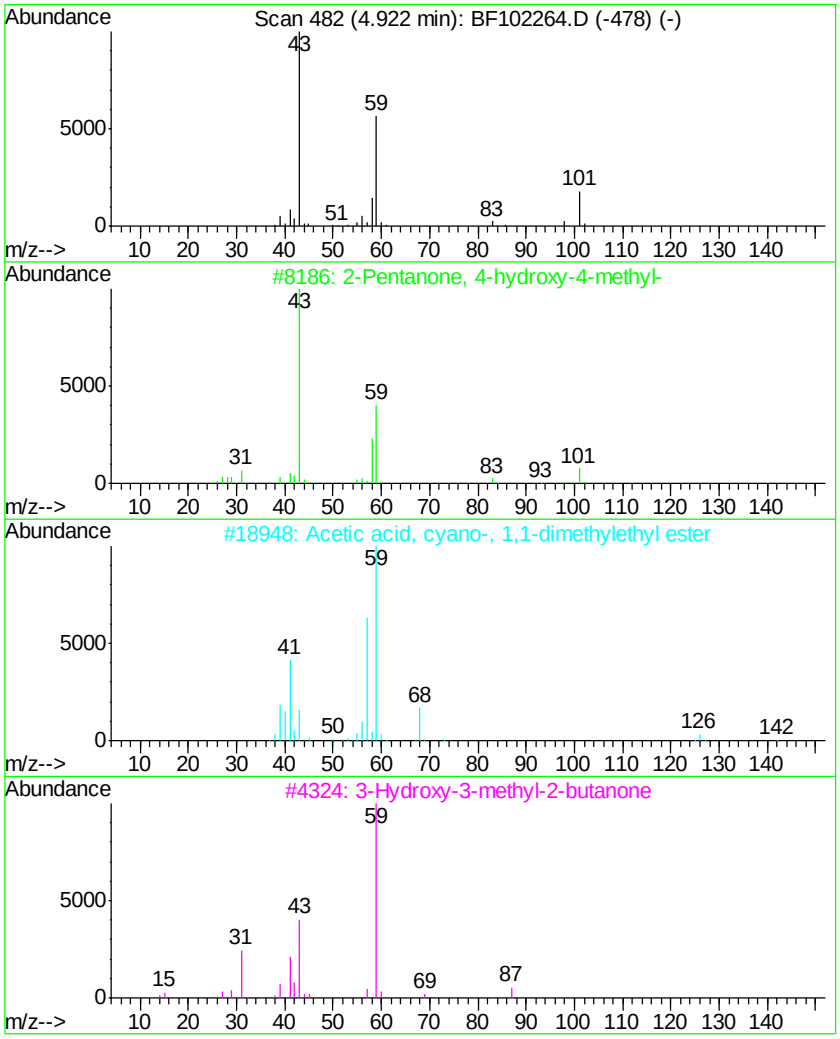
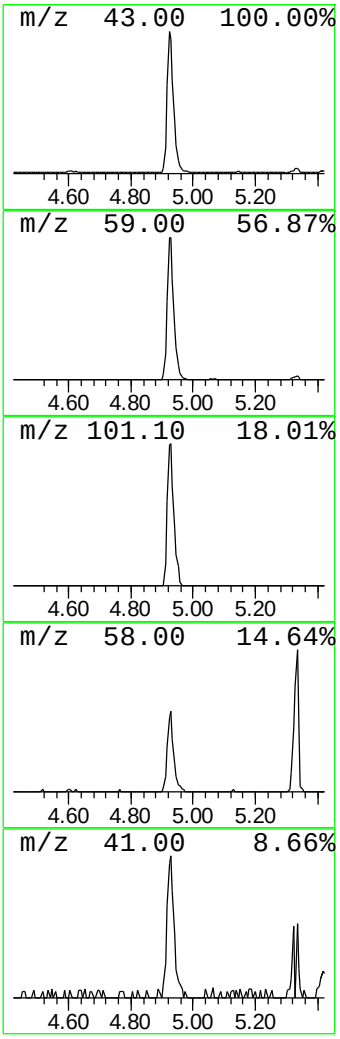
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	5.97 ng	255259	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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
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Sample : J1115-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-36-2.5-3.0

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

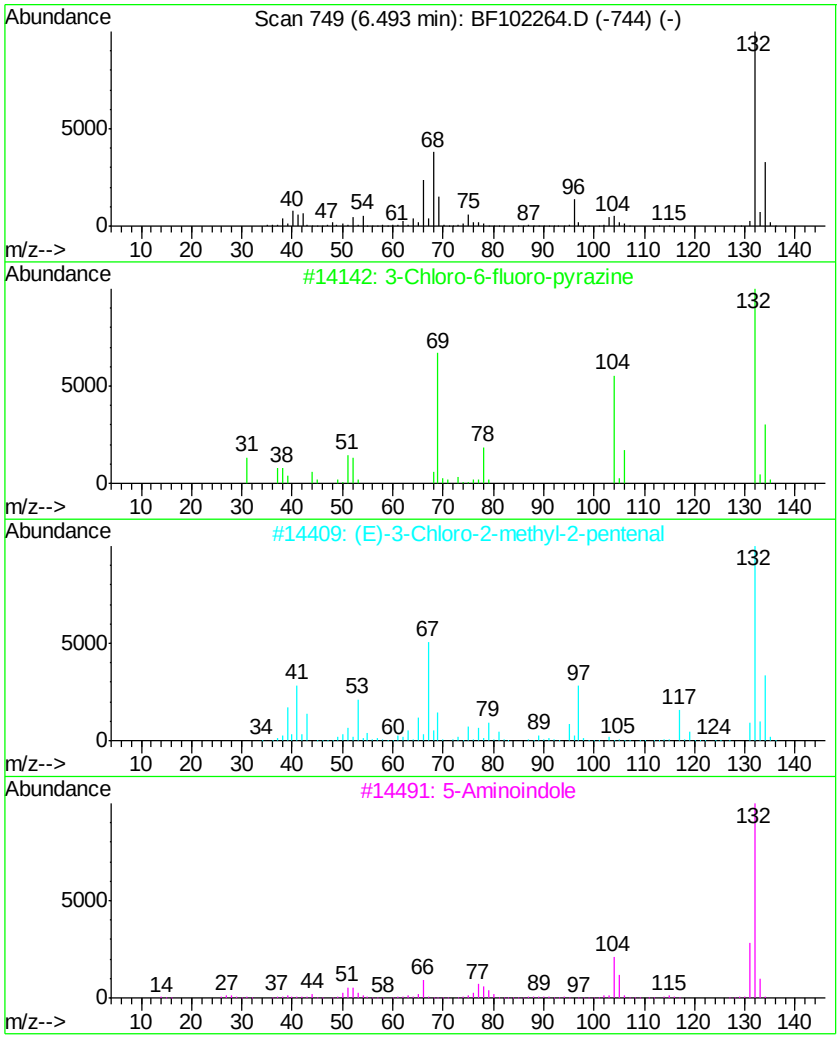
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

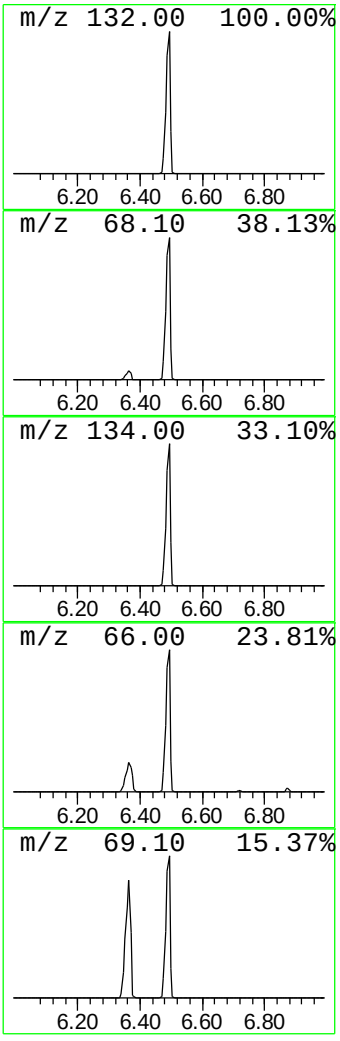
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	80.04 ng	3423220	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	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
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\BF012018\
Data File : BF102264.D
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Operator : SJ/JU
Sample : J1115-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-36-2.5-3.0

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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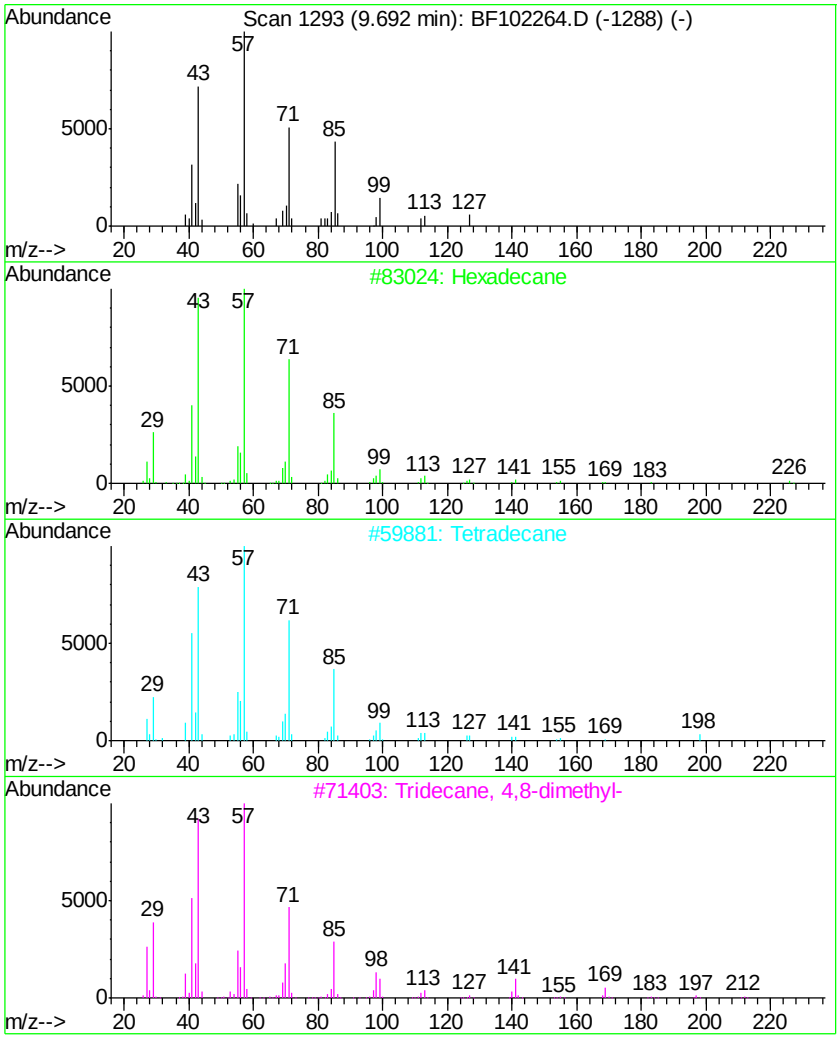
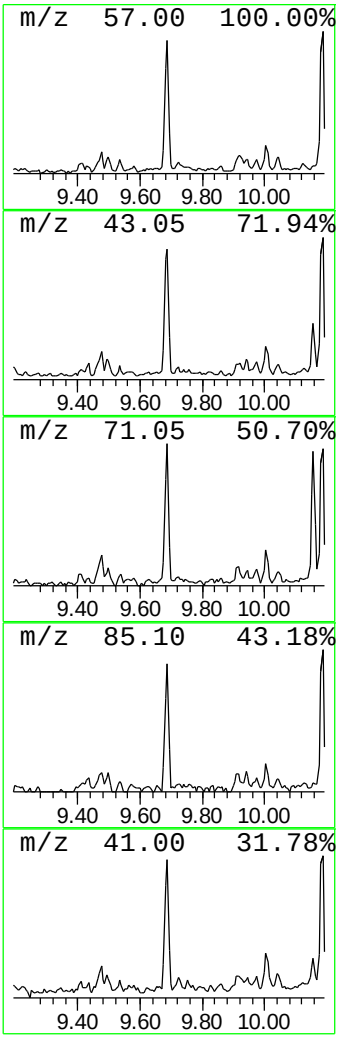
Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.69	2.05 ng	109612	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tetradecane	198	C14H30	000629-59-4	86
3	Tridecane, 4,8-dimethyl-	212	C15H32	055030-62-1	80
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102264.D
Acq On : 20 Jan 2018 14:31
Operator : SJ/JU
Sample : J1115-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-36-2.5-3.0

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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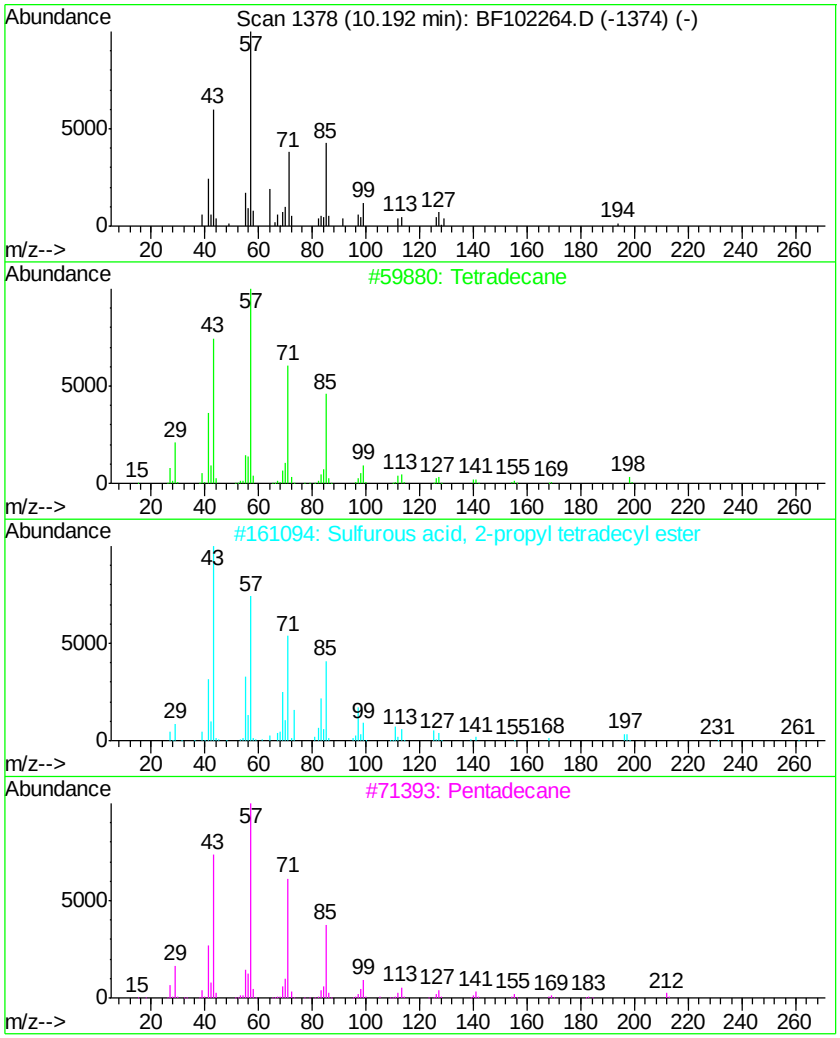
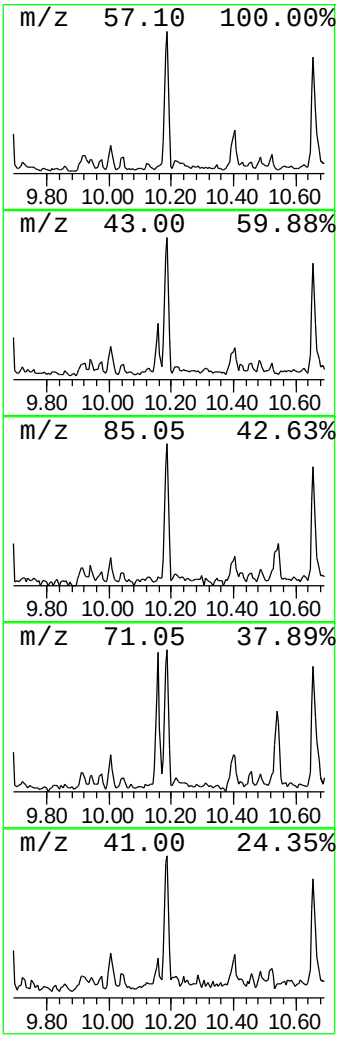
Peak Number 5 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.19	2.22 ng	118866	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	86
3	Pentadecane	212	C15H32	000629-62-9	83
4	Tridecane	184	C13H28	000629-50-5	80
5	Hexadecane	226	C16H34	000544-76-3	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102264.D
Acq On : 20 Jan 2018 14:31
Operator : SJ/JU
Sample : J1115-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-36-2.5-3.0

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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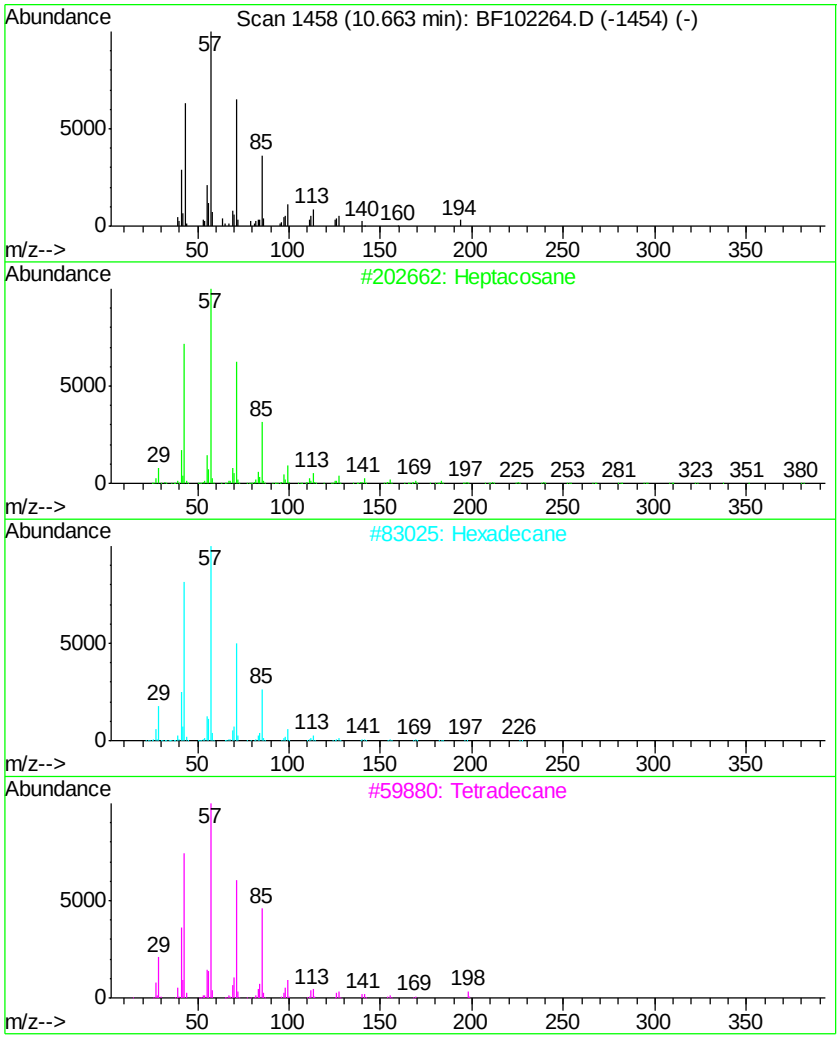
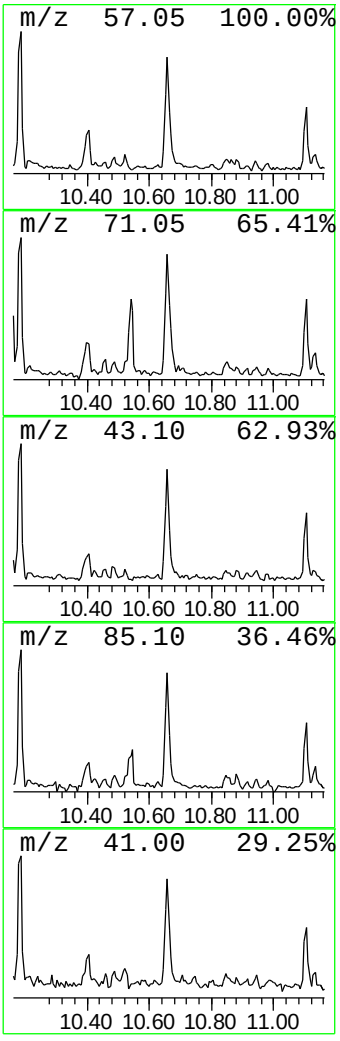
Peak Number 6 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	2.75 ng	120764	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tetradecane	198	C14H30	000629-59-4	87
4	Eicosane	282	C20H42	000112-95-8	87
5	Pentadecane	212	C15H32	000629-62-9	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
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Operator : SJ/JU
Sample : J1115-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-36-2.5-3.0

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

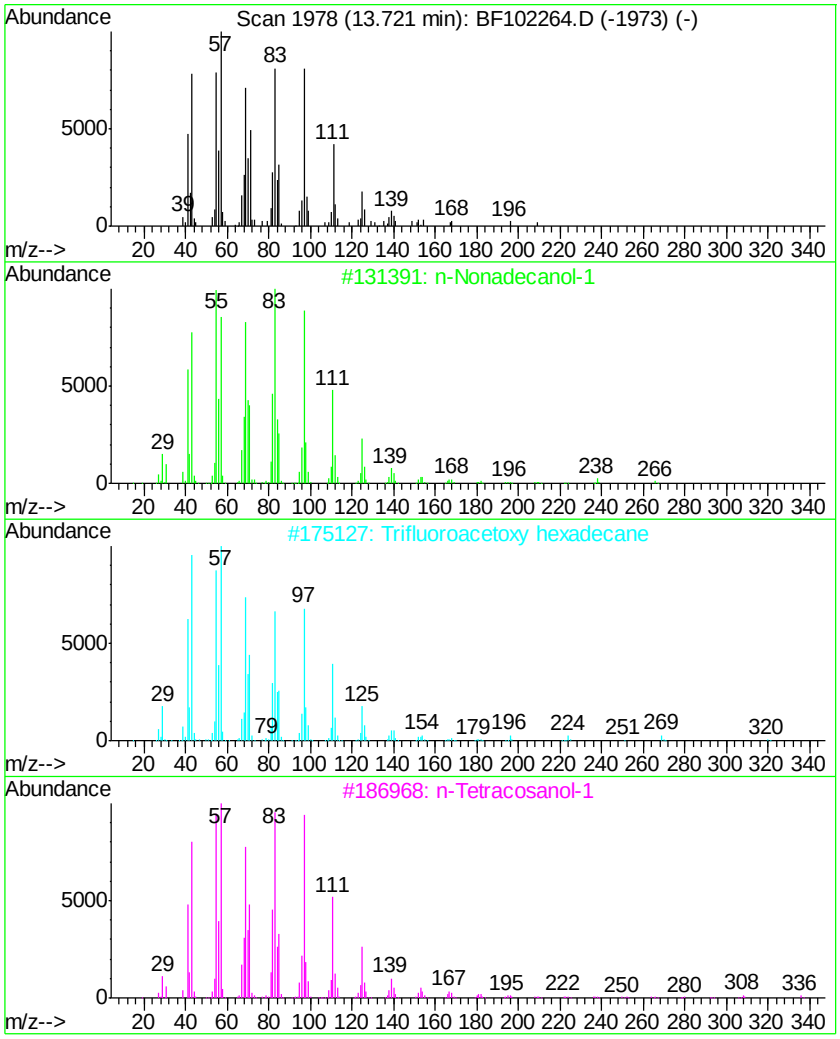
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

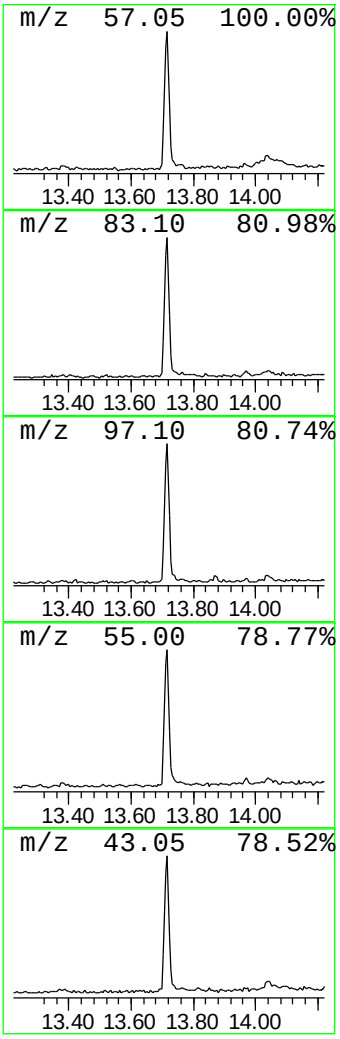
****

Peak Number 7 n-Nonadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	9.01 ng	358266	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
5	1-Heneicosanol	312	C21H44O	015594-90-8	91





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Sample : J1115-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-36-2.5-3.0

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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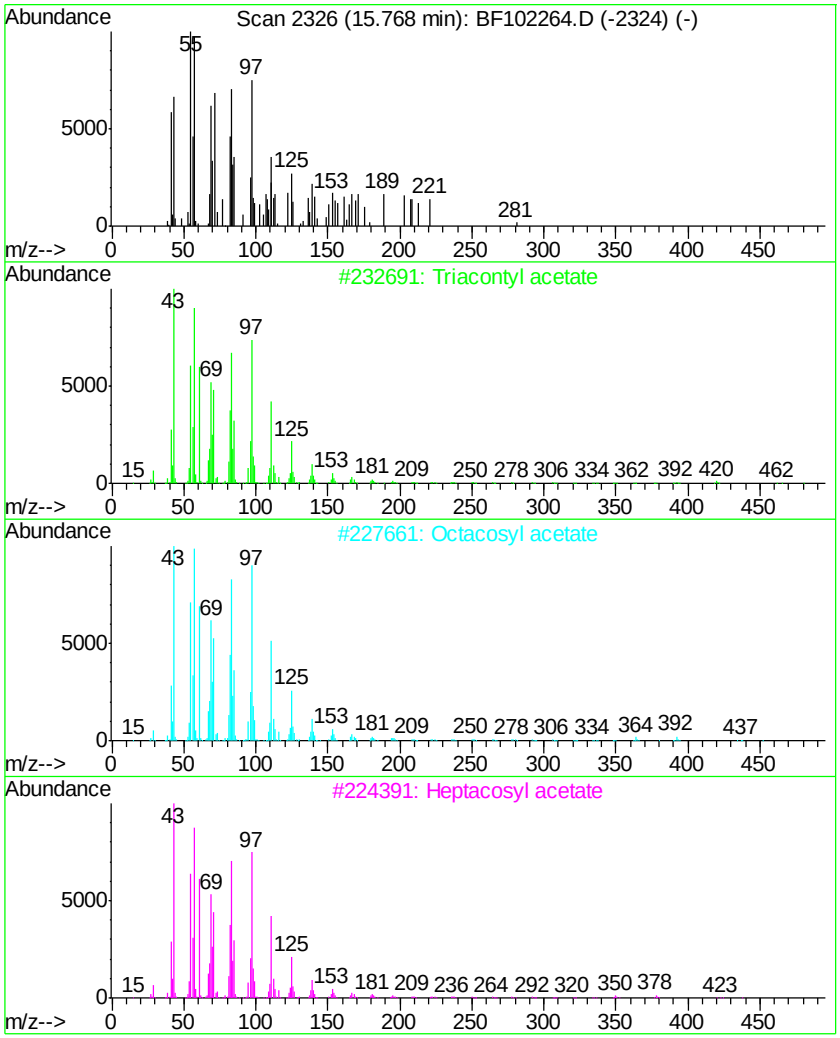
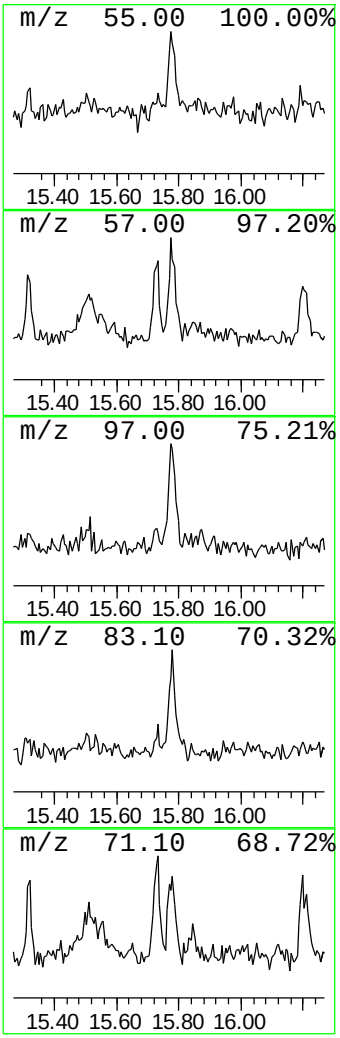
Peak Number 8 Triacontyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	2.08 ng	76157	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontyl acetate	480	C32H64O2	041755-58-2	81
2	Octacosyl acetate	452	C30H60O2	018206-97-8	81
3	Heptacosyl acetate	438	C29H58O2	1000351-78-2	81
4	17-Pentatriacontene	491	C35H70	006971-40-0	80
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
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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...	4.92	6.0	ng	255259	1	6.72	855372	20.0
unknown6.49	6.49	80.0	ng	3423220	1	6.72	855372	20.0
Hexadecane	9.69	2.0	ng	109612	3	9.75	1070640	20.0
Tetradecane	10.19	2.2	ng	118866	3	9.75	1070640	20.0
Heptacosane	10.66	2.8	ng	120764	4	11.23	877055	20.0
n-Nonadecanol-1	13.72	9.0	ng	358266	5	13.87	795251	20.0
Triacontyl acetate	15.77	2.1	ng	76157	6	15.29	732880	20.0