LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020718\
Data File : BF102842.D
Acq On : 8 Feb 2018 3:58
Operator : SJ/JU
Sample : J1458-03
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03

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-BF020318.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	2.181	9	16	24	rVB	432666	578535	12.79%	1.548%
2	5.122	513	516	525	rVB	113436	145042	3.21%	0.388%
3	5.504	576	581	584	rBV	4421600	4521978	100.00%	12.102%
4	6.510	747	752	755	rBV	3898766	4429053	97.95%	11.854%
5	6.657	772	777	780	rVB	4152483	4329183	95.74%	11.586%
6	6.887	812	816	819	rVB	1172649	1079467	23.87%	2.889%
7	7.039	838	842	846	rBV	3613577	3374474	74.62%	9.031%
8	7.445	906	911	914	rBV	2870902	2782239	61.53%	7.446%
9	8.163	1029	1033	1037	rBV	1428918	1341516	29.67%	3.590%
10	9.239	1211	1216	1226	rBV	4225069	4167905	92.17%	11.155%
11	9.316	1226	1229	1231	rVB	65647	52678	1.16%	0.141%
12	9.628	1279	1282	1286	rBV	406501	379319	8.39%	1.015%
13	9.845	1312	1319	1322	rBV	184624	152583	3.37%	0.408%
14	9.922	1328	1332	1341	rBV	1485582	1275751	28.21%	3.414%
15	10.345	1397	1404	1407	rBV	191193	169139	3.74%	0.453%
16	10.563	1436	1441	1444	rBV	45685	59834	1.32%	0.160%
17	10.710	1462	1466	1477	rVB	2113221	2059682	45.55%	5.512%
18	10.816	1480	1484	1493	rVB2	178083	218928	4.84%	0.586%
19	11.269	1558	1561	1563	rBV	51557	47609	1.05%	0.127%
20	11.410	1581	1585	1589	rBV	1231494	1046525	23.14%	2.801%
21	11.927	1669	1673	1677	rBV	121692	113313	2.51%	0.303%
22	12.992	1850	1854	1858	rBV	2832664	2823097	62.43%	7.555%
23	13.880	2001	2005	2015	rBV	471692	545391	12.06%	1.460%
24	14.051	2030	2034	2039	rBV	955671	917849	20.30%	2.456%
25	15.533	2280	2286	2297	rBV	524859	753805	16.67%	2.017%

Sum of corrected areas: 37364895

LSC Report - Integrated Chromatogram

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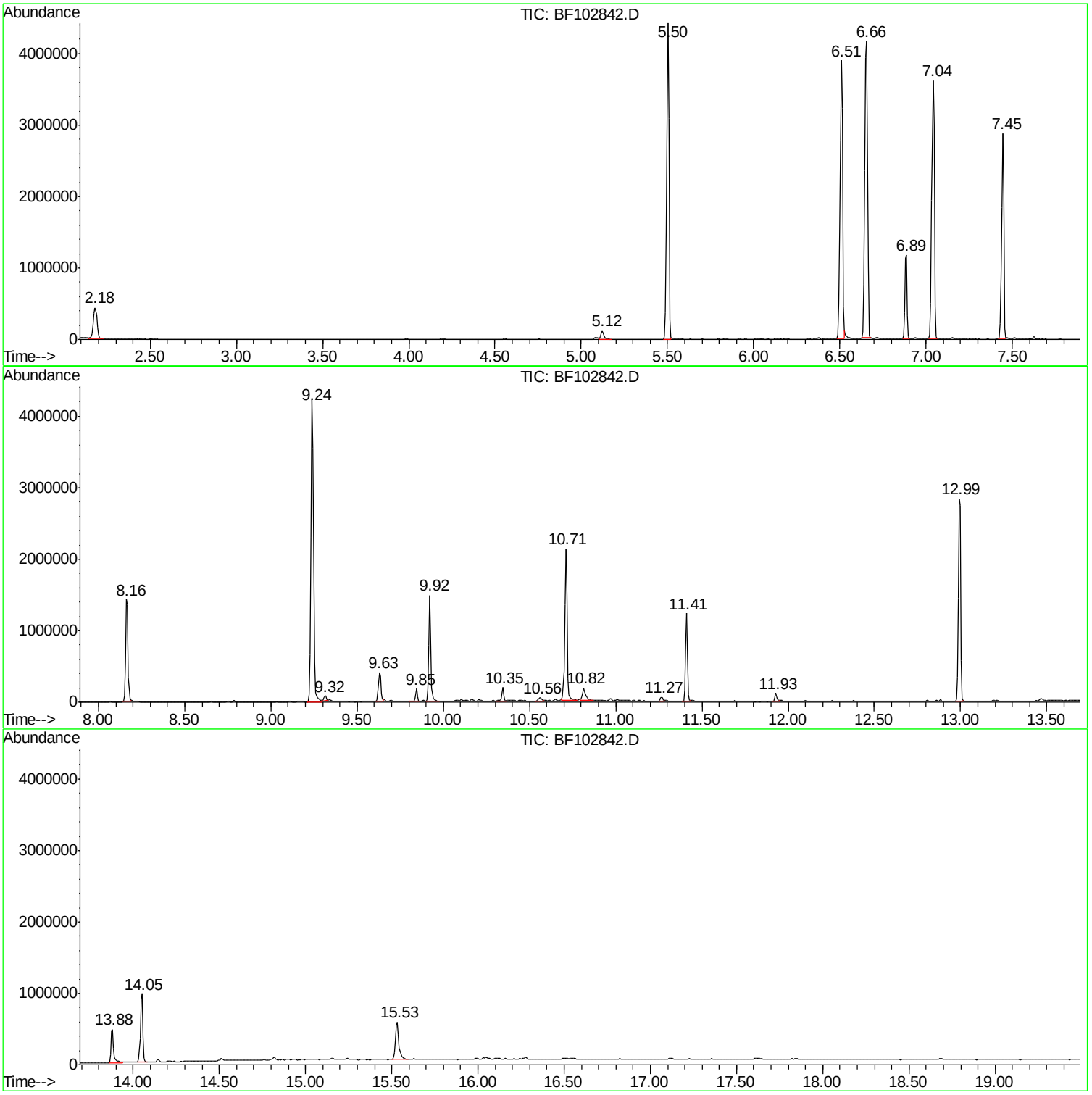
Operator : SJ/JU
Sample : J1458-03
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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Data File : BF102842.D
Acq On : 8 Feb 2018 3:58
Operator : SJ/JU
Sample : J1458-03
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

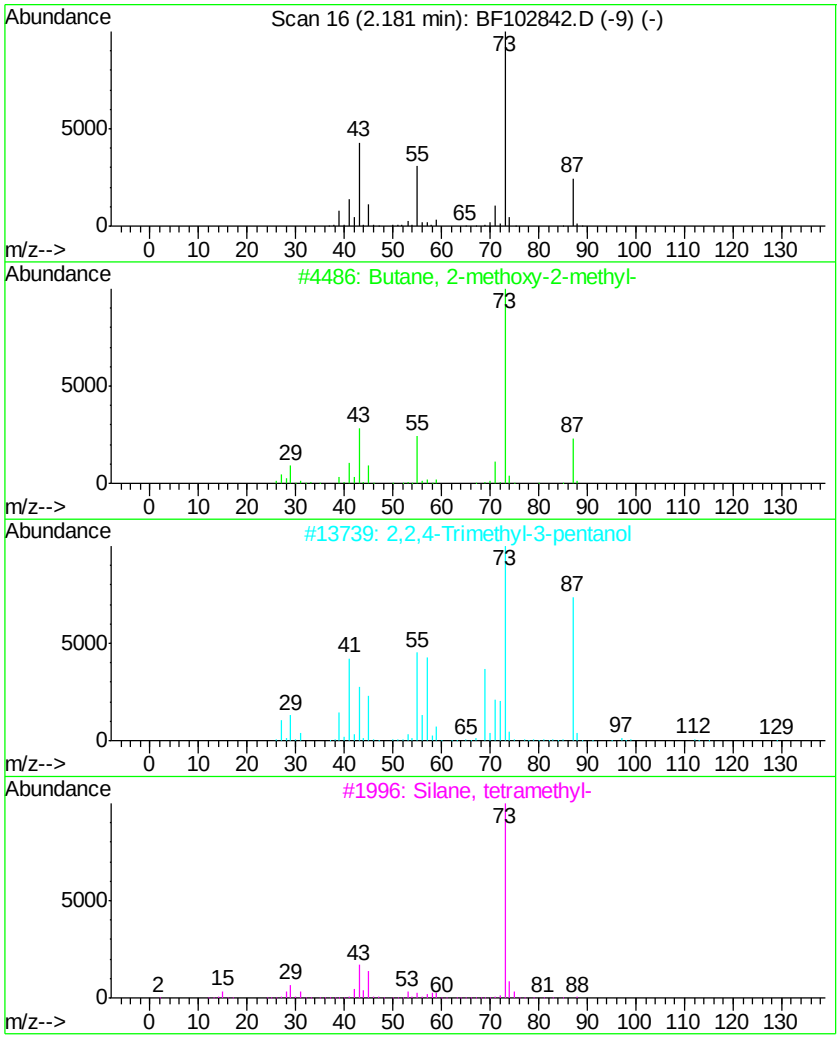
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

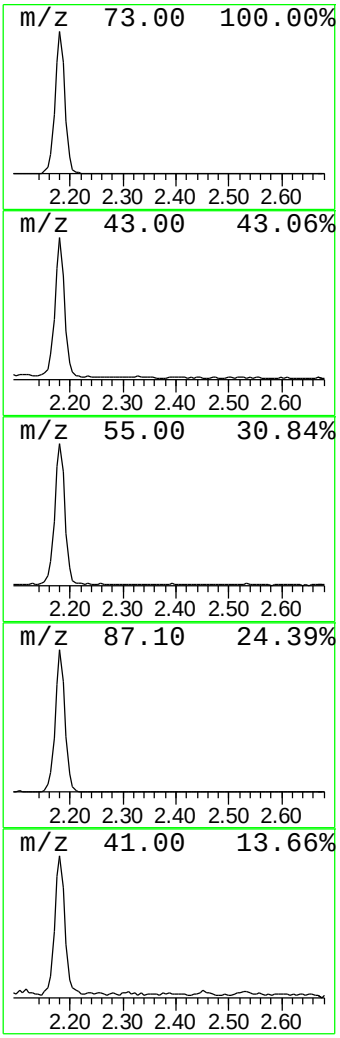
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	10.72 ng	578535	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Acq On : 8 Feb 2018 3:58
Operator : SJ/JU
Sample : J1458-03
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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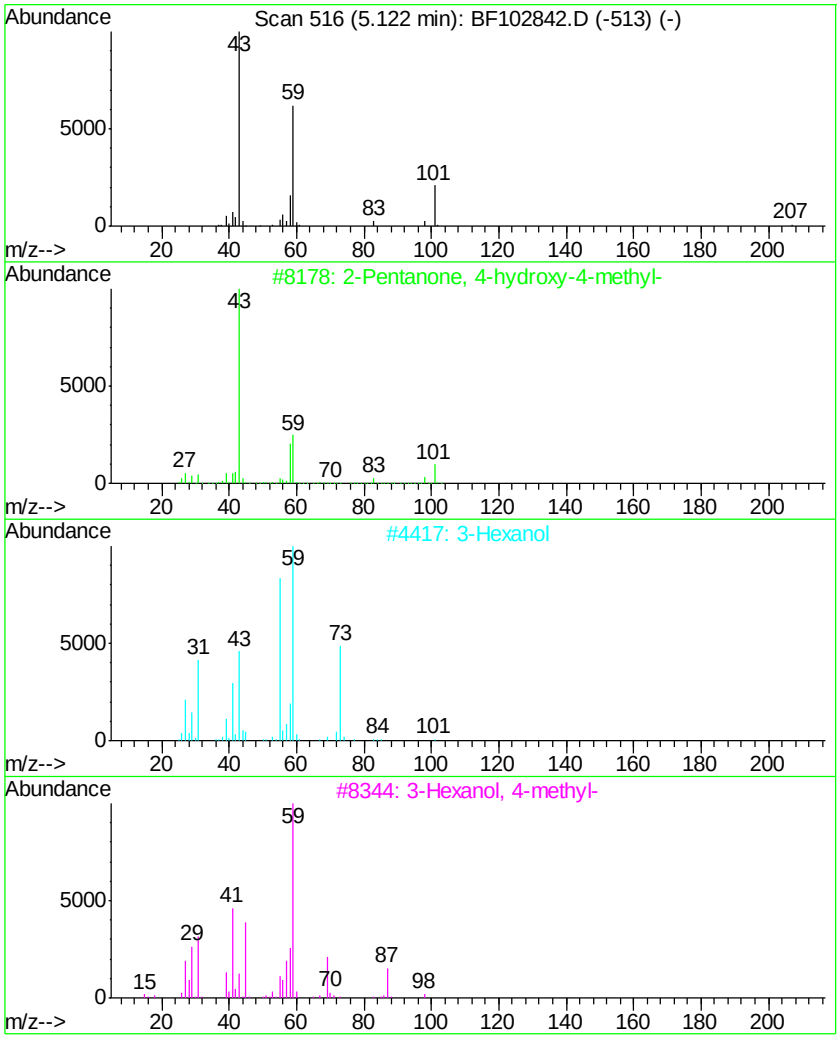
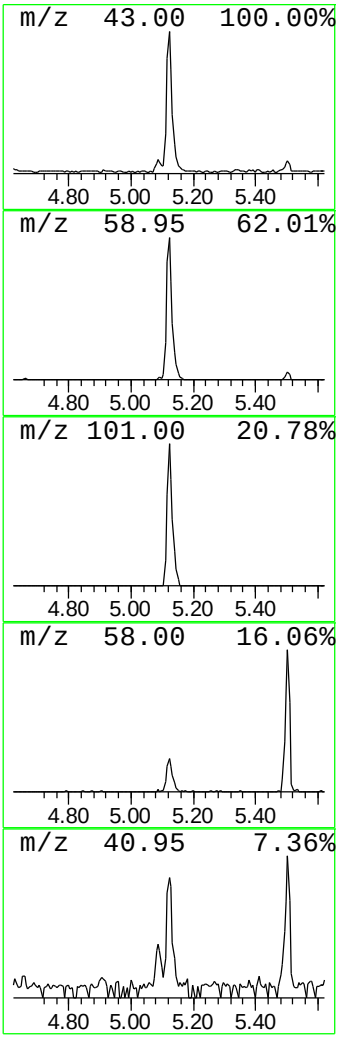
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.69 ng	145042	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol	102	C6H14O	000623-37-0	28
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Butane	58	C4H10	000106-97-8	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020718\
Data File : BF102842.D
Acq On : 8 Feb 2018 3:58
Operator : SJ/JU
Sample : J1458-03
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

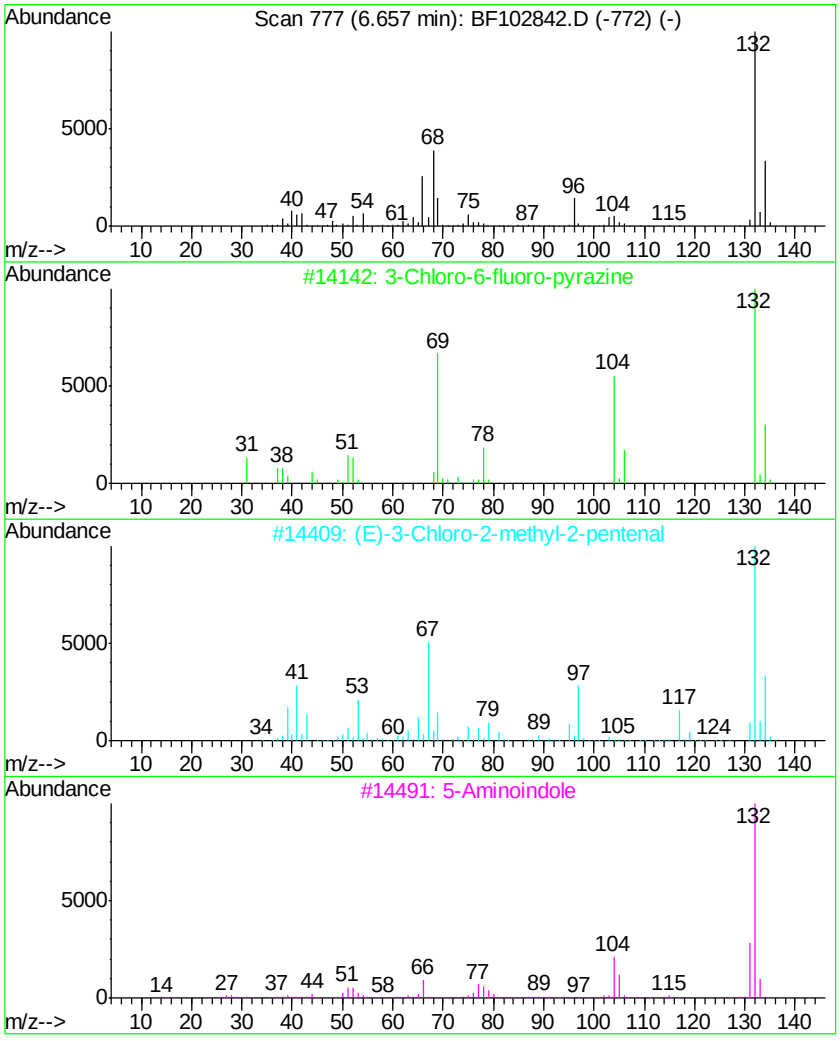
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

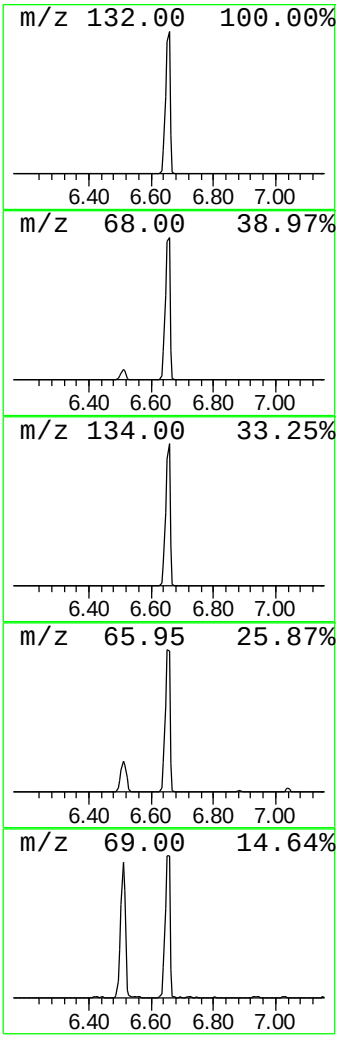
****

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	80.21 ng	4329180	1,4-Dichlorobenzene-d4	6.89

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Acq On : 8 Feb 2018 3:58
Operator : SJ/JU
Sample : J1458-03
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

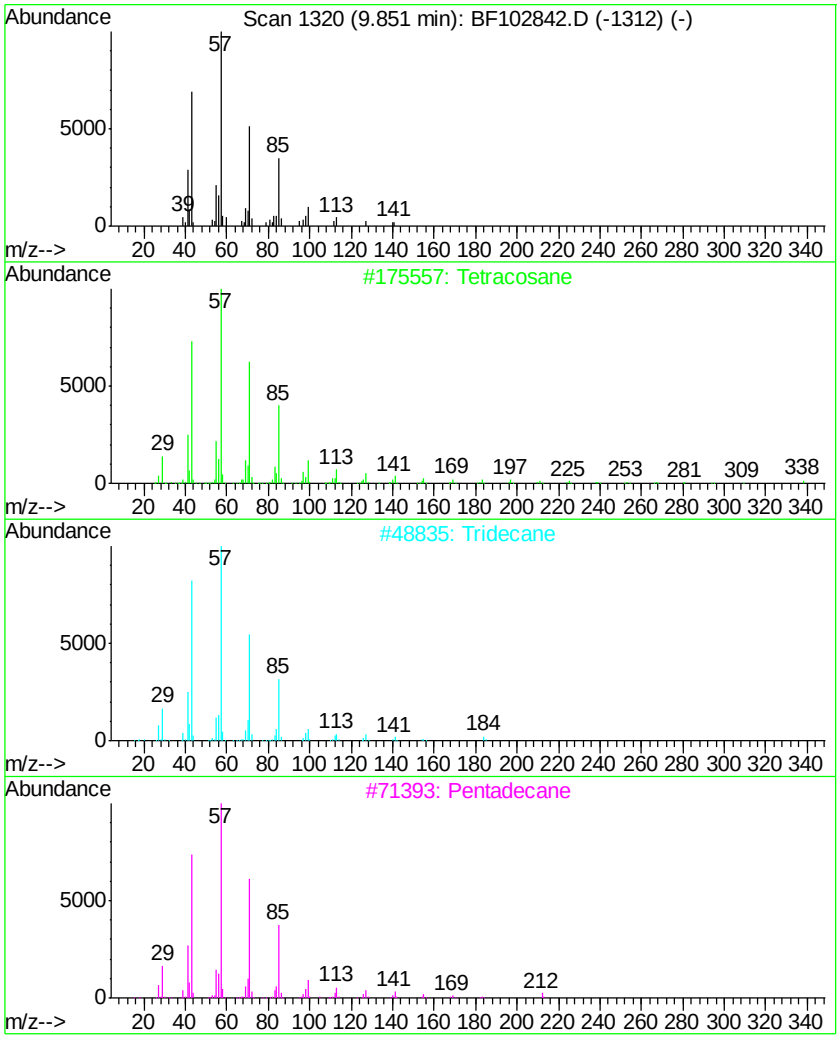
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

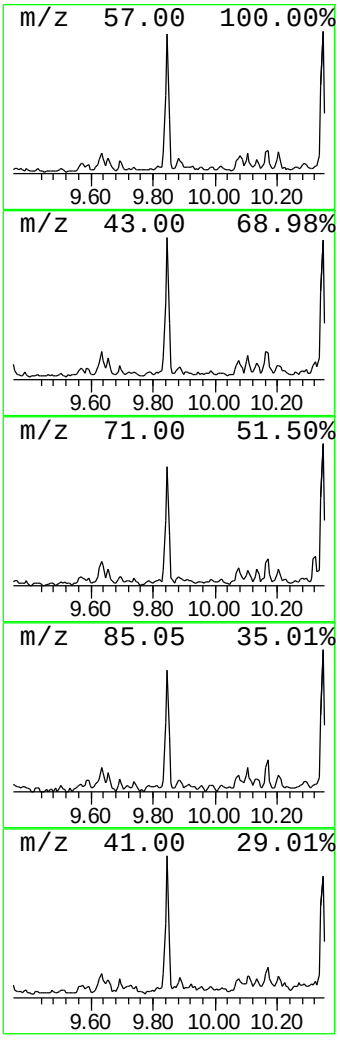
****

Peak Number 5 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	2.39 ng	152583	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Tridecane	184	C13H28	000629-50-5	86
3	Pentadecane	212	C15H32	000629-62-9	86
4	Hexadecane	226	C16H34	000544-76-3	86
5	Tetradecane	198	C14H30	000629-59-4	80





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Data File : BF102842.D
Acq On : 8 Feb 2018 3:58
Operator : SJ/JU
Sample : J1458-03
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

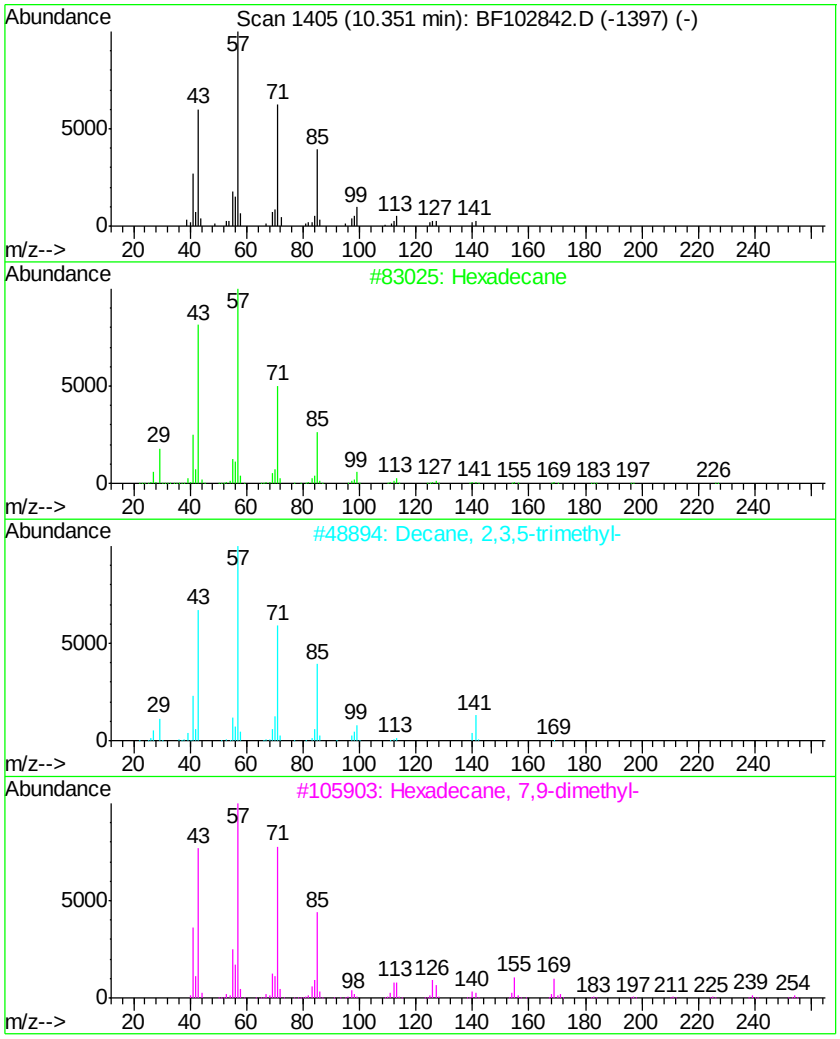
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

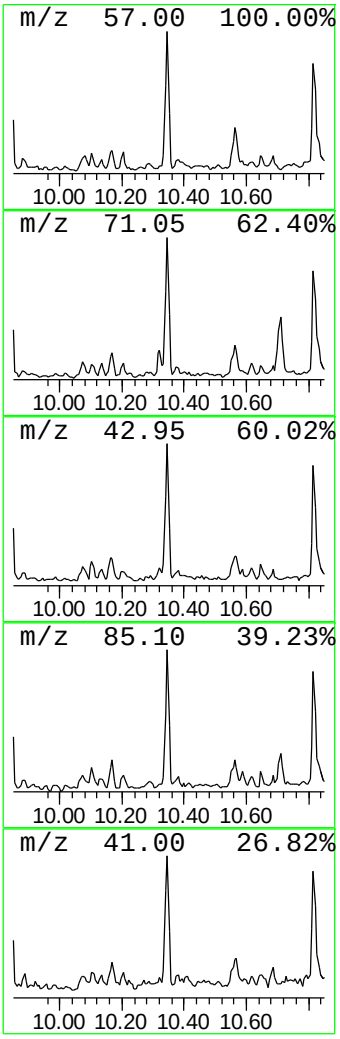
****

Peak Number 6 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	2.65 ng	169139	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
3	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	72
4	Nonane, 5-(1-methylpropyl)-	184	C13H28	062185-54-0	64
5	Nonane, 5-butyl-	184	C13H28	017312-63-9	64





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Misc :
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Instrument : BNA_F
ClientSampleId : SB-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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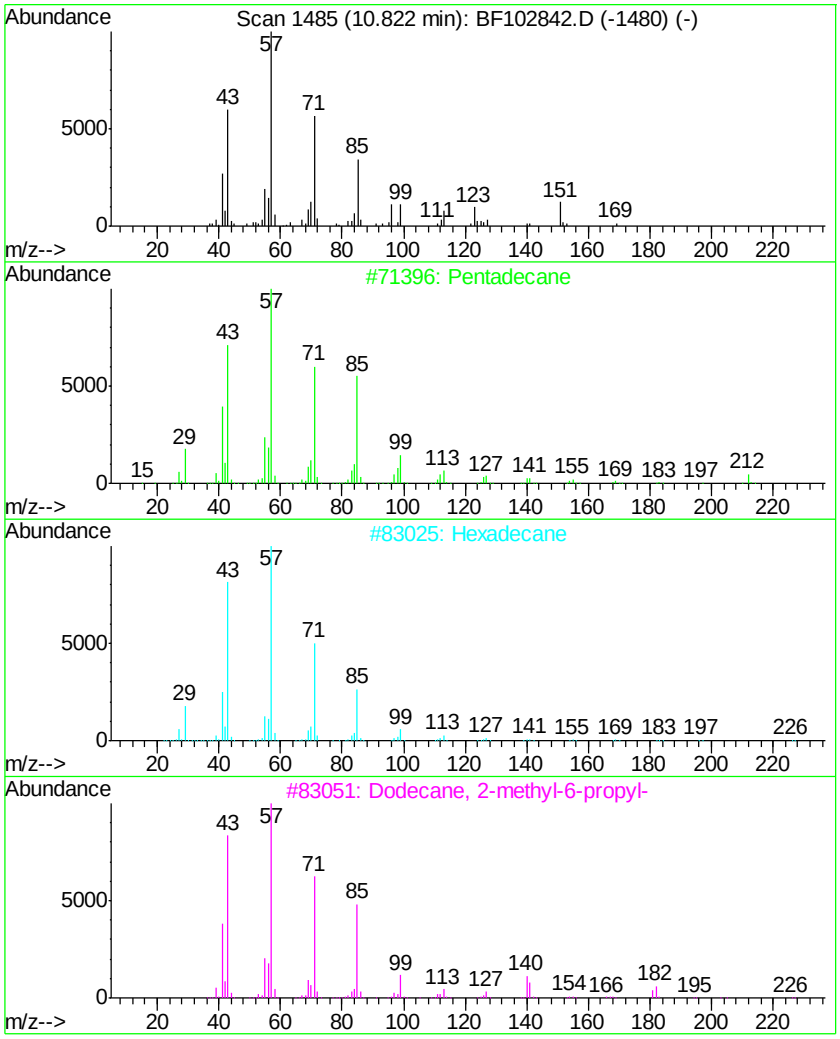
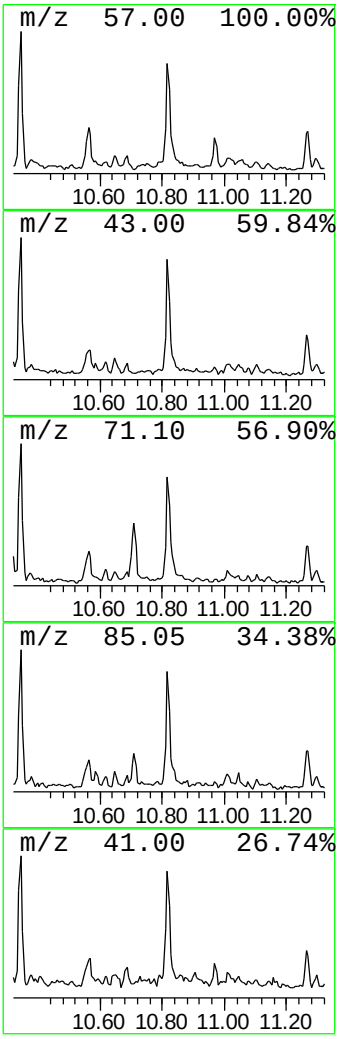
Peak Number 7 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	4.18 ng	218928	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	72
2	Hexadecane	226	C16H34	000544-76-3	64
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	64
4	Tetracosane	338	C24H50	000646-31-1	64
5	Tetratetracontane	619	C44H90	007098-22-8	64





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TIC Library : C:\DATABASE\NIST11.L
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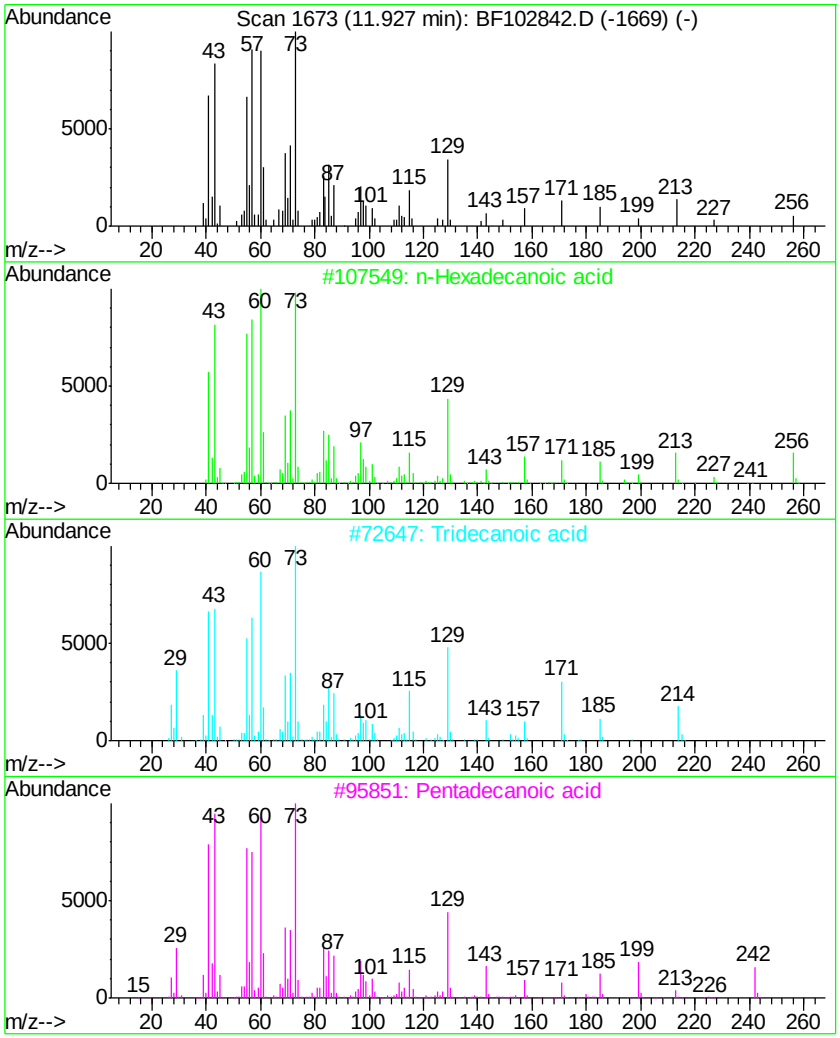
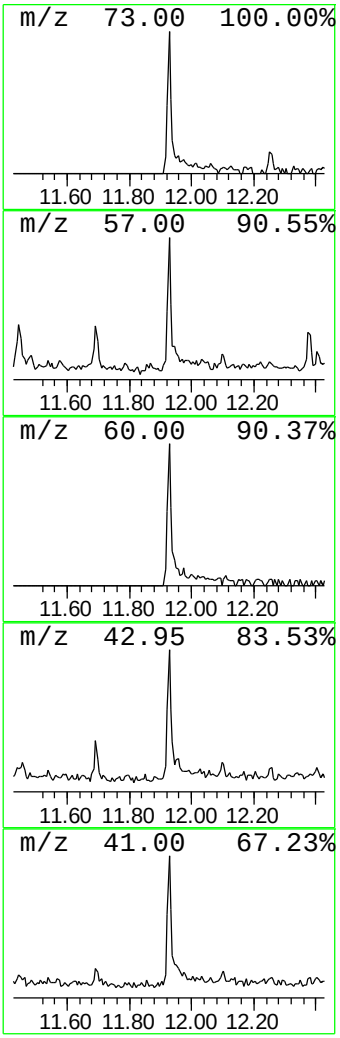
Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	2.17 ng	113313	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	80
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	25
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20





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

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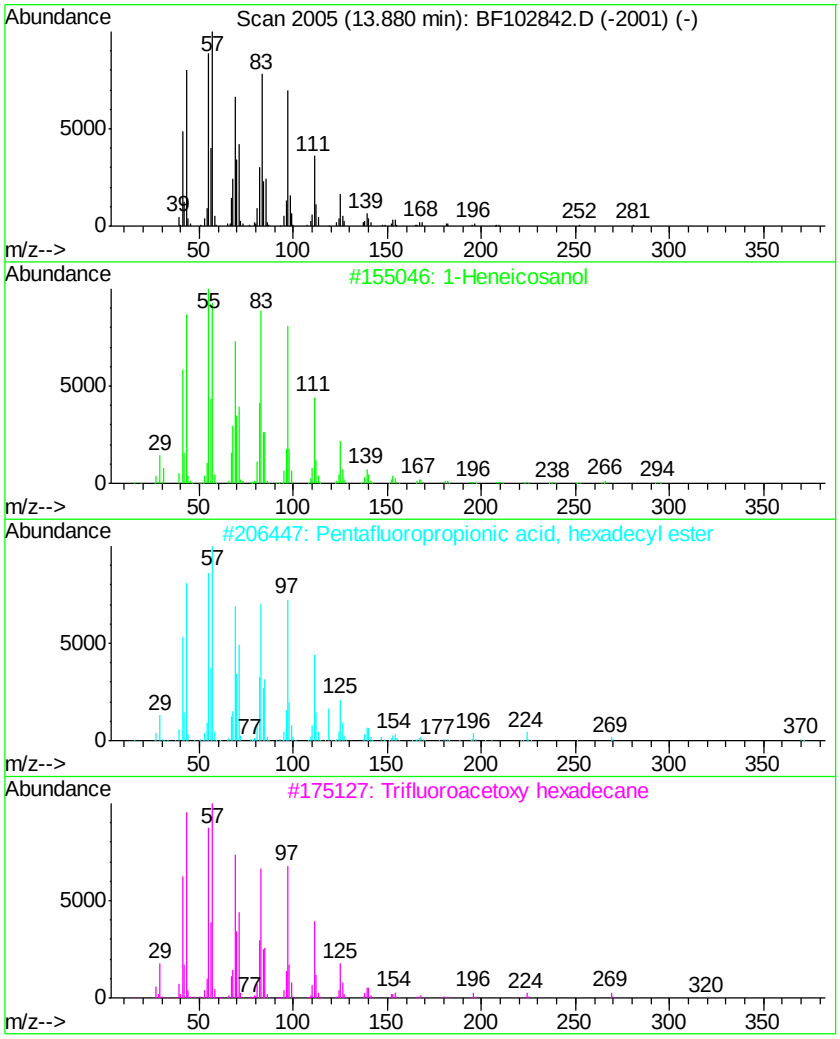
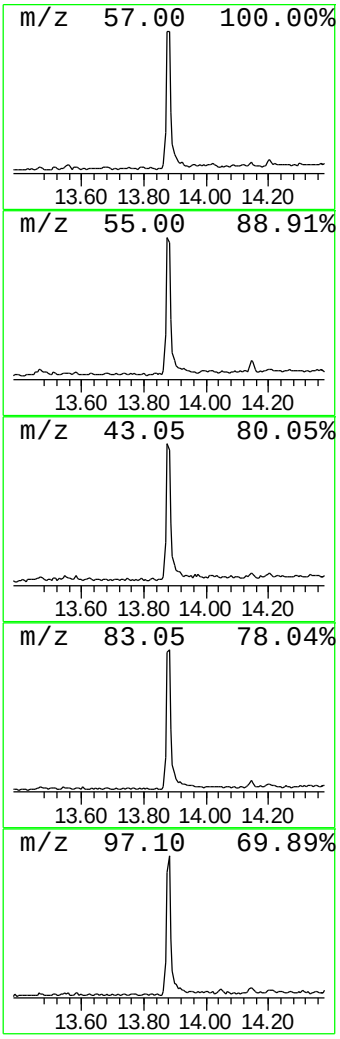
Peak Number 9 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	11.88 ng	545391	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93





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
Butane, 2-methoxy...	2.18	10.7	ng	578535	1	6.89	1079470	20.0
2-Pentanone, 4-hy...	5.12	2.7	ng	145042	1	6.89	1079470	20.0
unknown6.66	6.66	80.2	ng	4329180	1	6.89	1079470	20.0
Tetracosane	9.85	2.4	ng	152583	3	9.92	1275750	20.0
Hexadecane	10.35	2.6	ng	169139	3	9.92	1275750	20.0
Pentadecane	10.82	4.2	ng	218928	4	11.41	1046530	20.0
n-Hexadecanoic acid	11.93	2.2	ng	113313	4	11.41	1046530	20.0
1-Heneicosanol	13.88	11.9	ng	545391	5	14.05	917849	20.0