LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099946.D
Acq On : 29 Oct 2017 6:32
Operator : SJ/JU
Sample : I6100-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-D-B

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-BF102317.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	5.004	493	496	509	rBV	87282	122461	4.17%	0.714%
2	5.410	562	565	592	rBV	679313	853870	29.06%	4.976%
3	6.428	736	738	754	rBV	442429	583587	19.86%	3.401%
4	6.557	757	760	766	rVV	1670989	1512534	51.47%	8.814%
5	6.786	796	799	808	rBV	662273	607219	20.66%	3.538%
6	6.939	821	825	842	rBV	2157510	2116782	72.03%	12.335%
7	7.357	892	896	899	rBV	1493357	1511612	51.44%	8.808%
8	8.069	1013	1017	1020	rBV	904908	814811	27.73%	4.748%
9	8.627	1109	1112	1123	rBB	94515	82695	2.81%	0.482%
10	9.145	1195	1200	1203	rBV	3048626	2938709	100.00%	17.124%
11	9.539	1264	1267	1276	rVB	70181	56408	1.92%	0.329%
12	9.821	1306	1315	1319	rBV	933635	800539	27.24%	4.665%
13	9.857	1319	1321	1327	rVB	44190	39644	1.35%	0.231%
14	10.374	1406	1409	1416	rBB	34561	30252	1.03%	0.176%
15	10.492	1425	1429	1433	rBV	116610	89353	3.04%	0.521%
16	10.533	1433	1436	1444	rVB	339486	274842	9.35%	1.602%
17	10.615	1447	1450	1464	rBV	843793	747366	25.43%	4.355%
18	11.315	1565	1569	1571	rBV	652183	594323	20.22%	3.463%
19	11.339	1571	1573	1578	rVB	80042	70150	2.39%	0.409%
20	12.704	1801	1805	1808	rBV	221981	194088	6.60%	1.131%
21	12.774	1814	1817	1822	rVB2	53745	52009	1.77%	0.303%
22	12.898	1833	1838	1841	rBV	2058667	1858879	63.25%	10.832%
23	13.404	1921	1924	1928	rBV	168883	136429	4.64%	0.795%
24	13.774	1984	1987	1997	rVB	39143	43290	1.47%	0.252%
25	13.962	2015	2019	2026	rBV	594512	527630	17.95%	3.075%
26	15.421	2263	2267	2280	rVB	377444	501784	17.07%	2.924%

Sum of corrected areas: 17161266

LSC Report - Integrated Chromatogram

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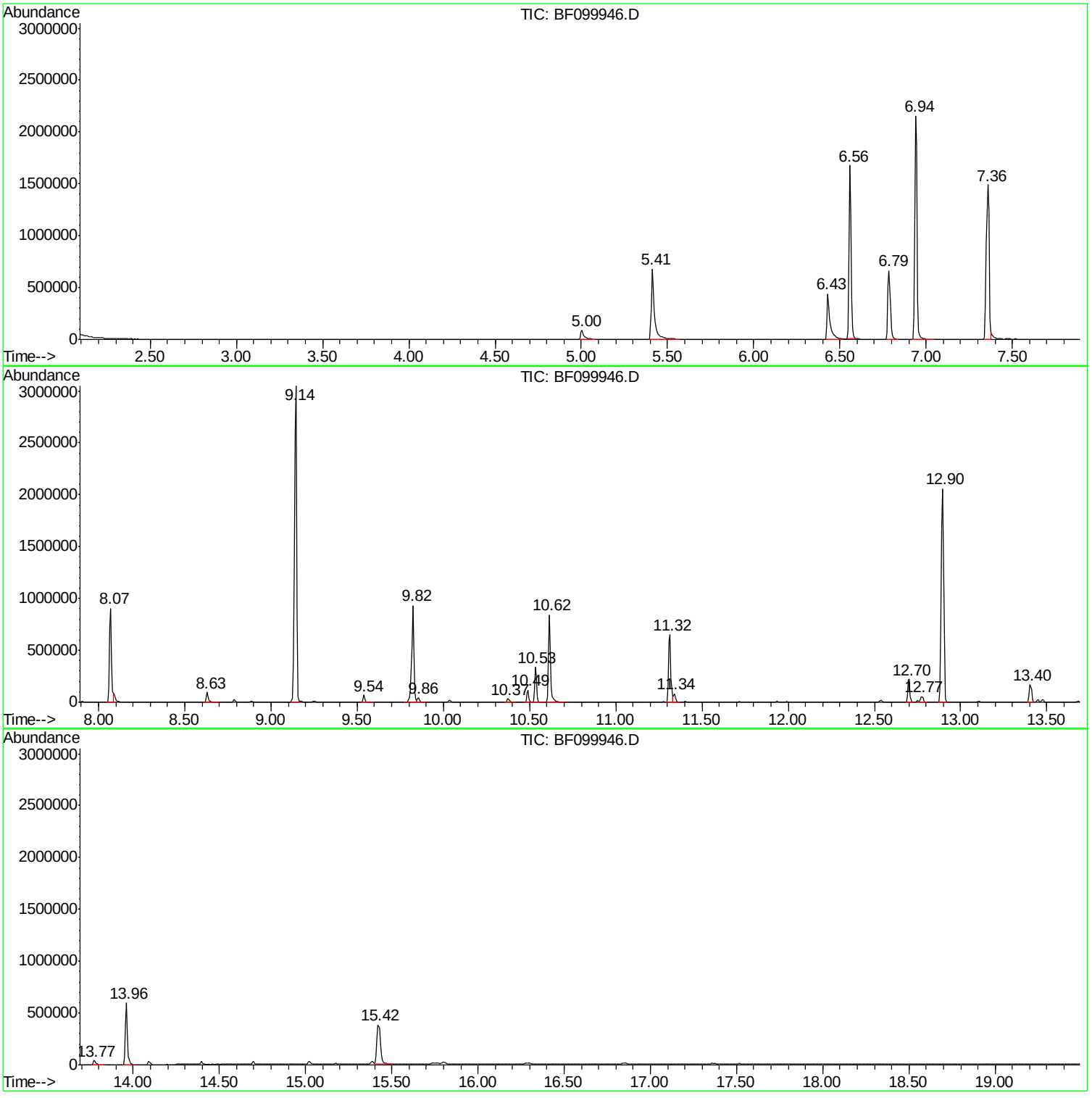
Sample : I6100-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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\BF102817\
Data File : BF099946.D
Acq On : 29 Oct 2017 6:32
Operator : SJ/JU
Sample : I6100-01
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Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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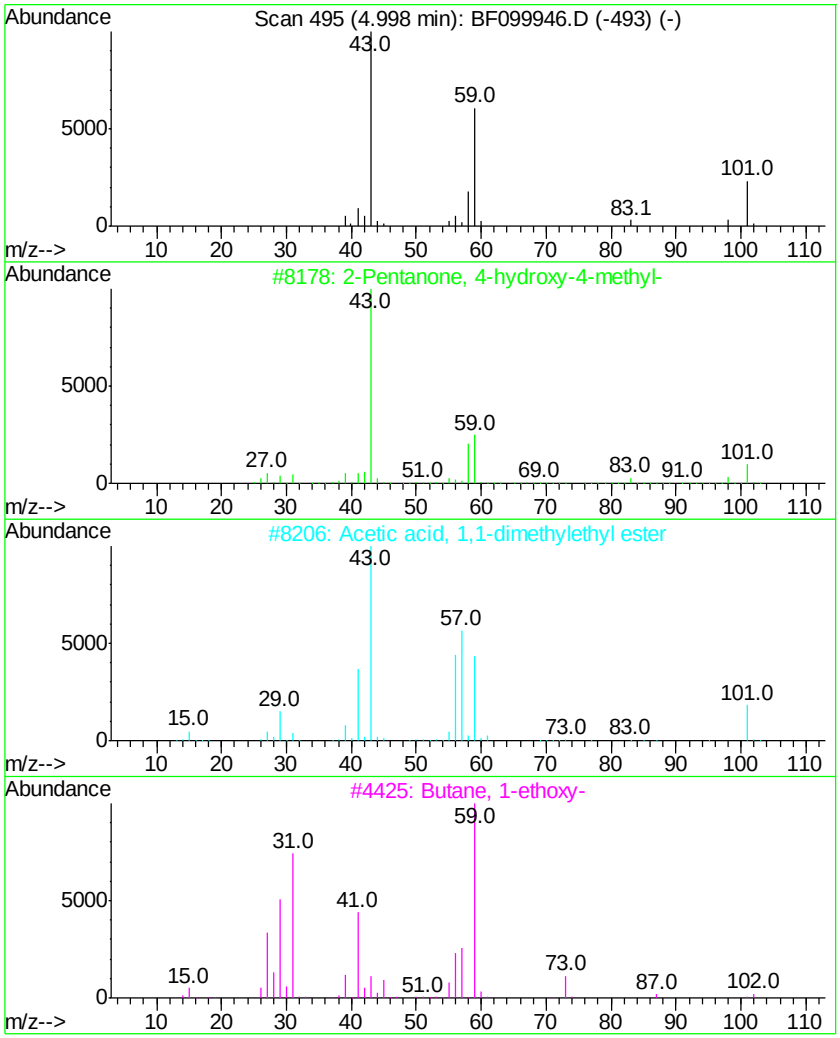
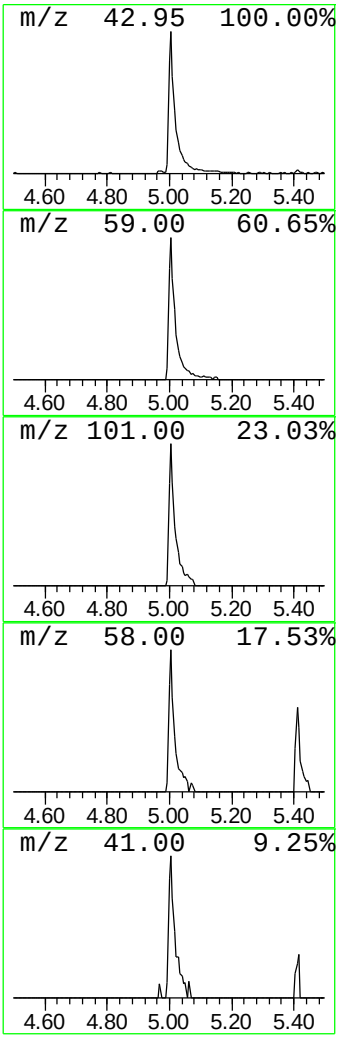
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	4.03 ng	122461	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Acetone	58	C3H6O	000067-64-1	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BF099946.D
Acq On : 29 Oct 2017 6:32
Operator : SJ/JU
Sample : I6100-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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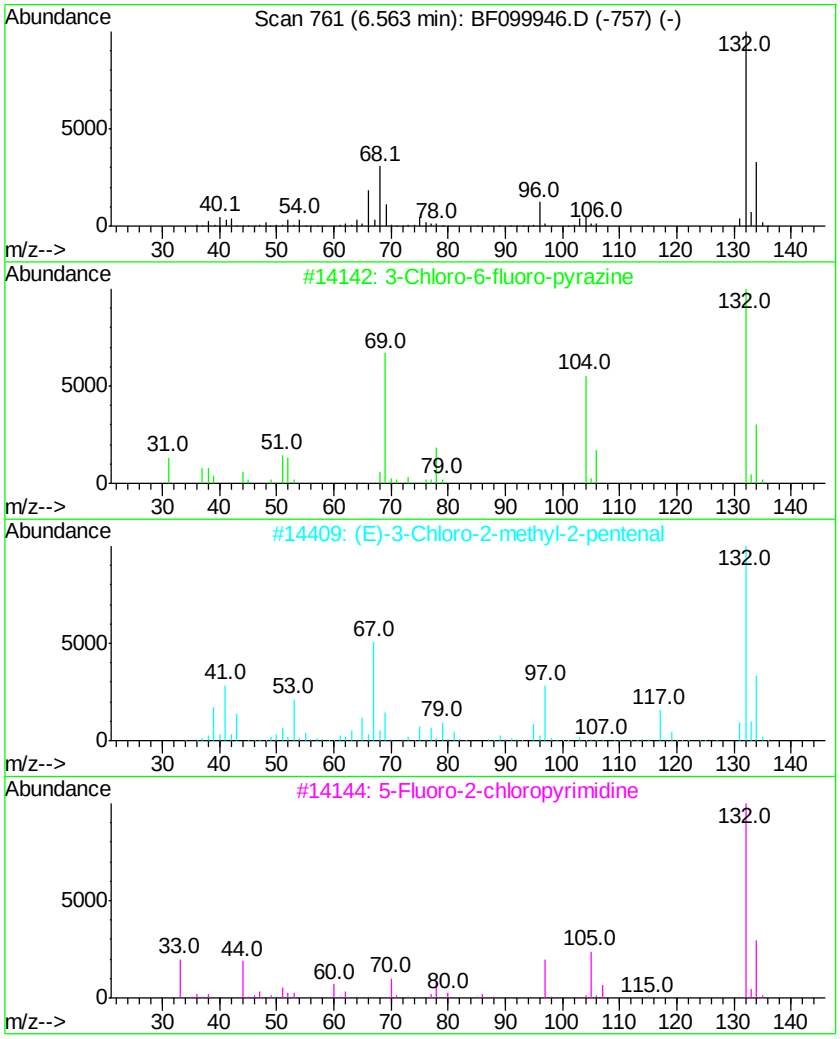
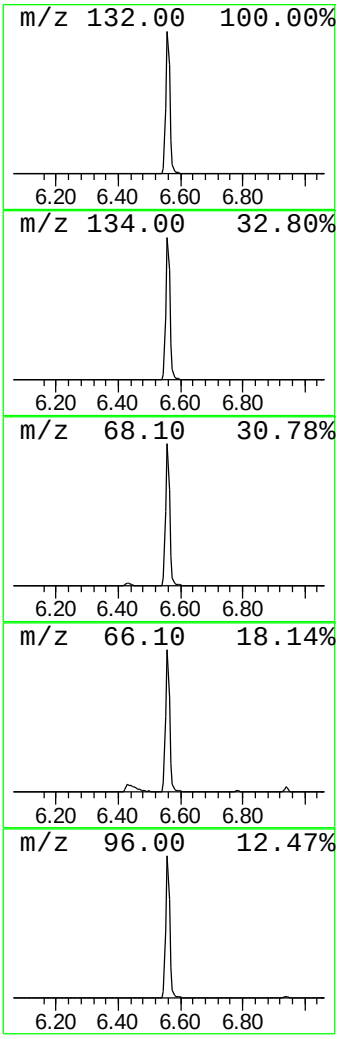
Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	49.82 ng	1512530	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5	1-Aminoindan	133	C9H11N	034698-41-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099946.D
Acq On : 29 Oct 2017 6:32
Operator : SJ/JU
Sample : I6100-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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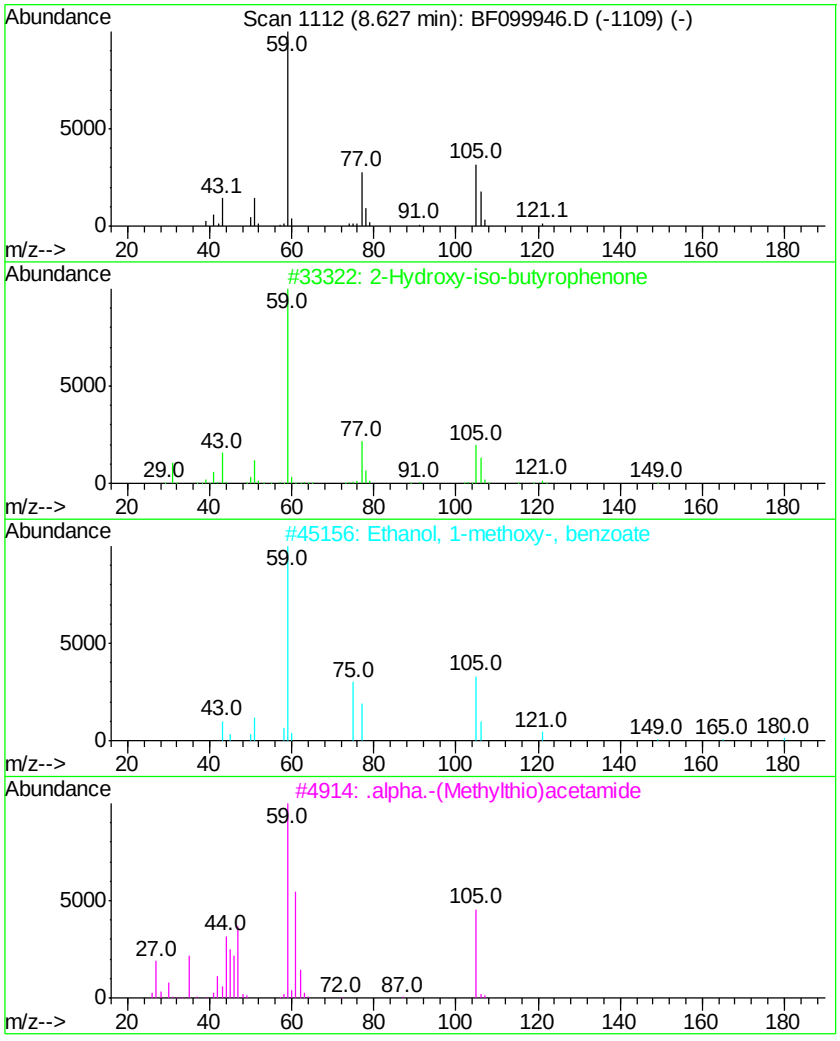
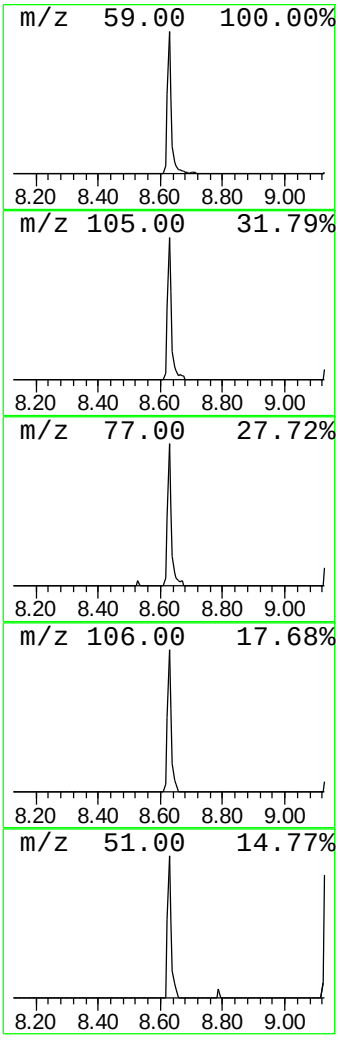
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.63	2.03 ng	82695	Naphthalene-d8	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	86
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	64
3	.alpha.-(Methylthio)acetamide	105	C3H7NOS	022551-24-2	7
4	Formamide, N-methyl-	59	C2H5NO	000123-39-7	7
5	Guanidine	59	CH5N3	000113-00-8	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099946.D
Acq On : 29 Oct 2017 6:32
Operator : SJ/JU
Sample : I6100-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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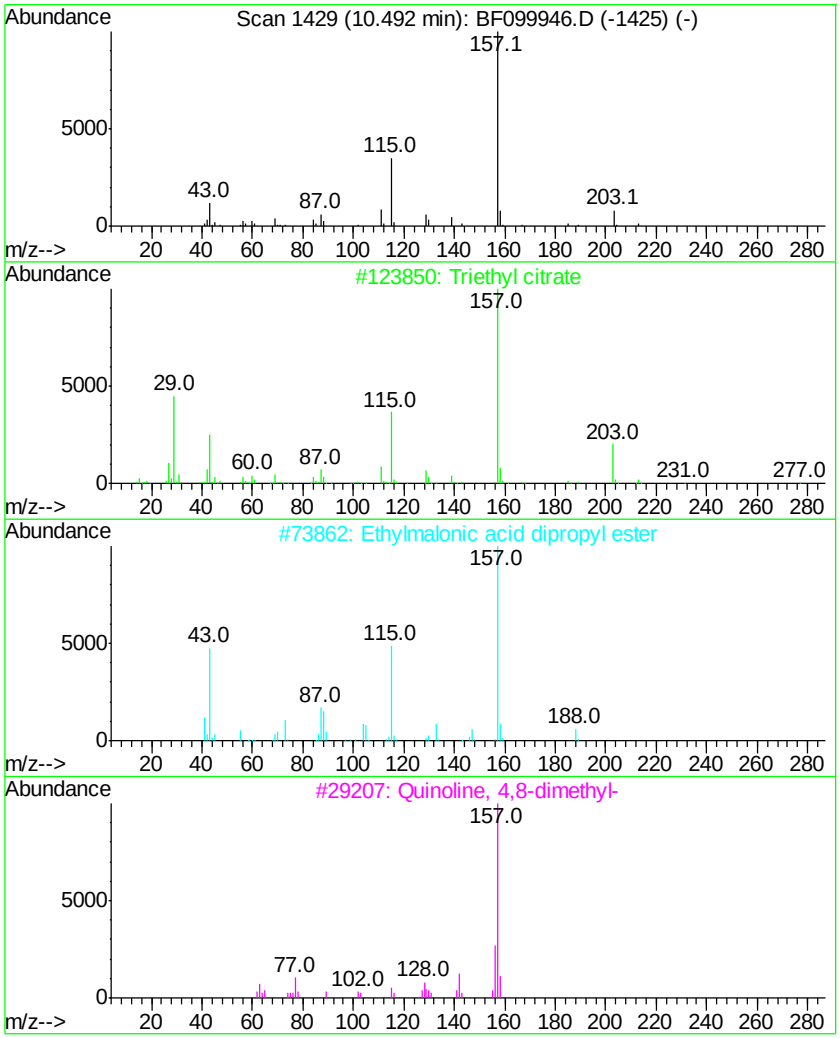
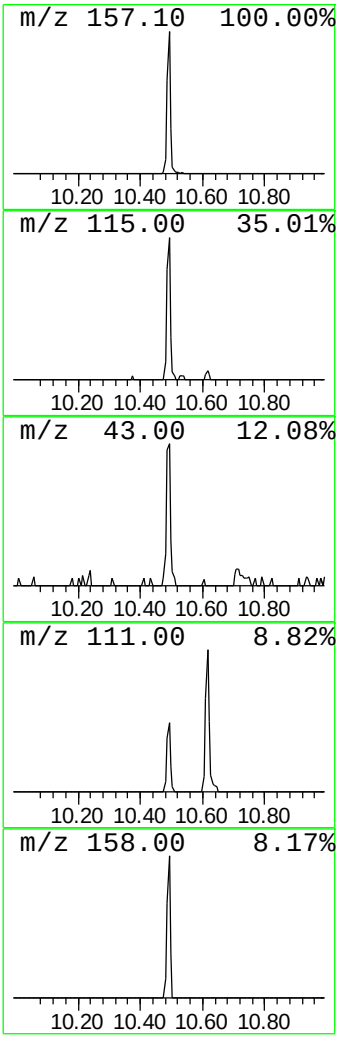
Peak Number 5 Triethyl citrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.49	2.23 ng	89353	Acenaphthene-d10	9.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	83
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	50
3	Quinoline, 4,8-dimethyl-	157	C11H11N	013362-80-6	42
4	Quinoline, 2,4-dimethyl-	157	C11H11N	001198-37-4	38
5	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-80-2	36





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Data File : BF099946.D
Acq On : 29 Oct 2017 6:32
Operator : SJ/JU
Sample : I6100-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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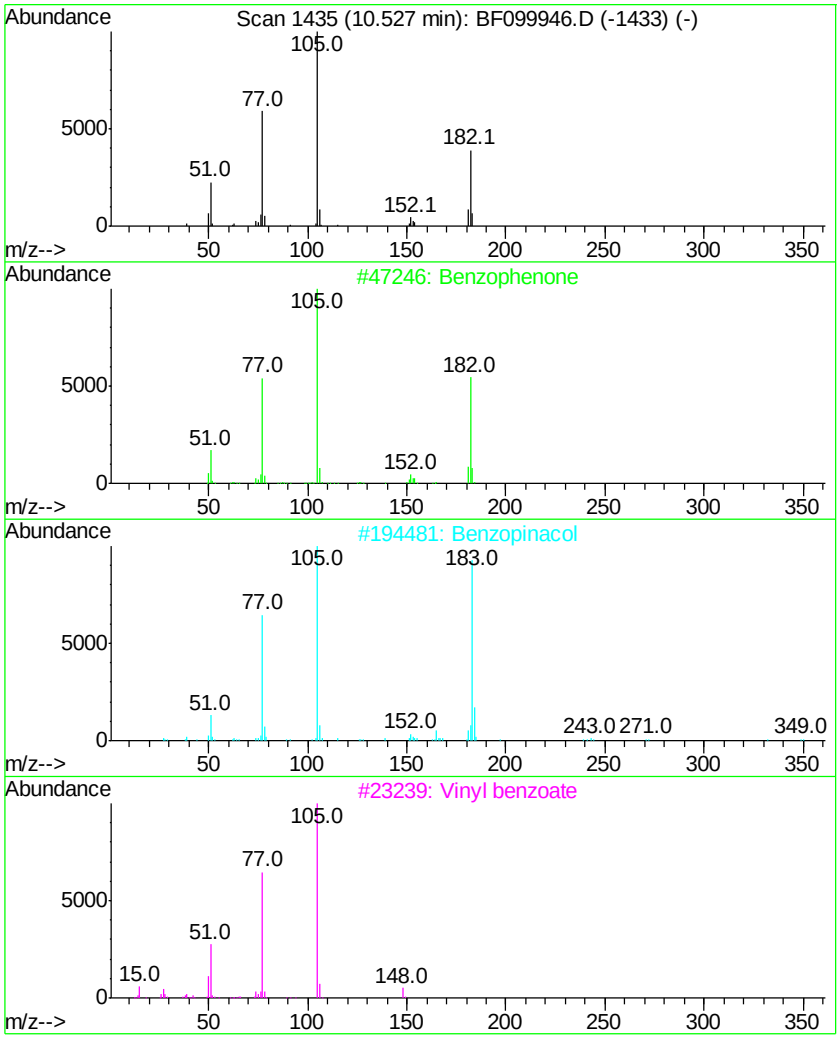
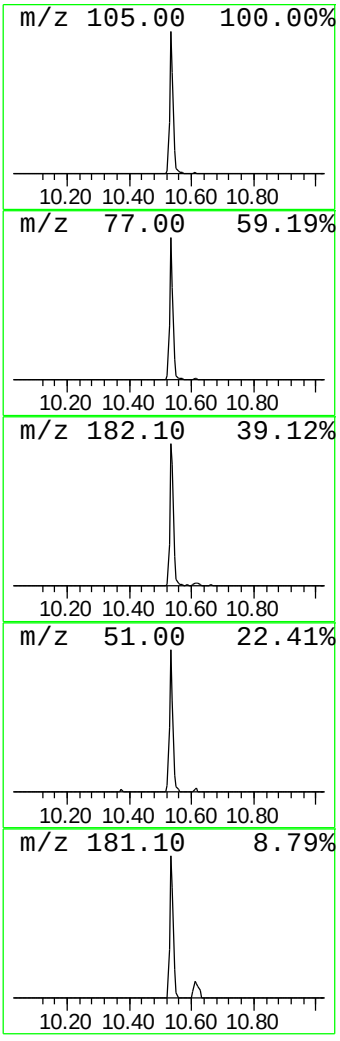
Peak Number 6 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	6.87 ng	274842	Acenaphthene-d10	9.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzopinacol	366	C26H22O2	000464-72-2	50
3	Vinyl benzoate	148	C9H8O2	000769-78-8	43
4	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	43
5	S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	43





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ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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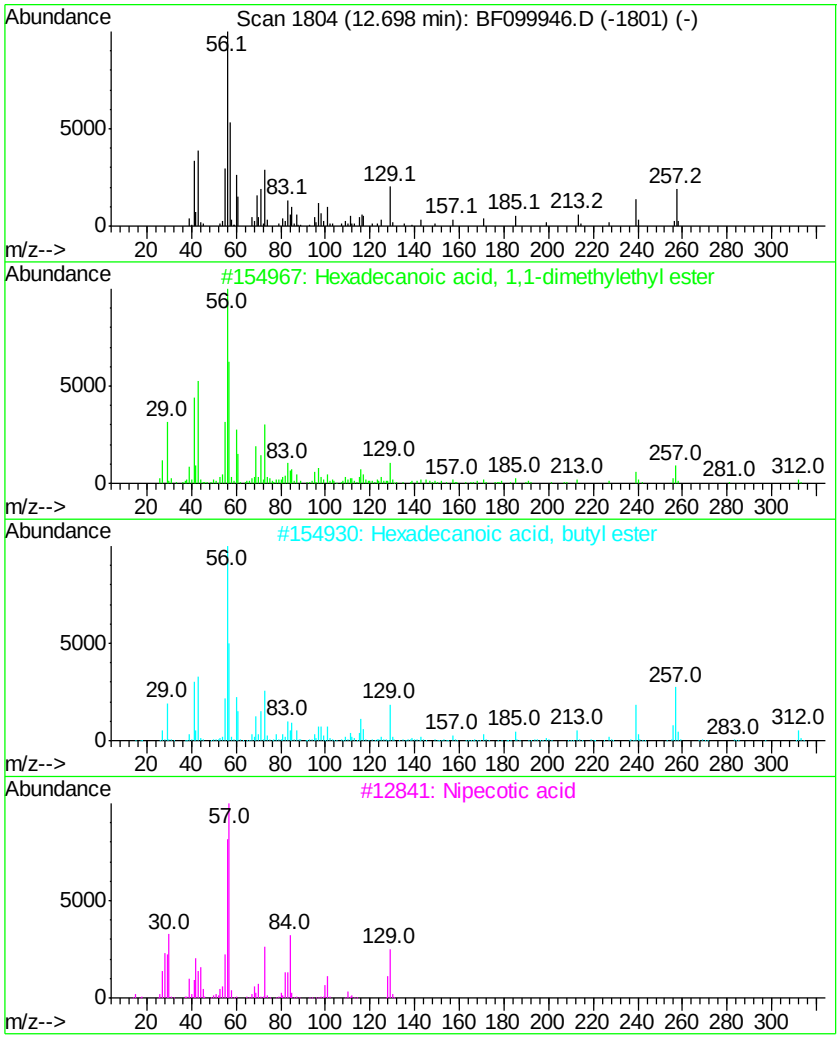
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

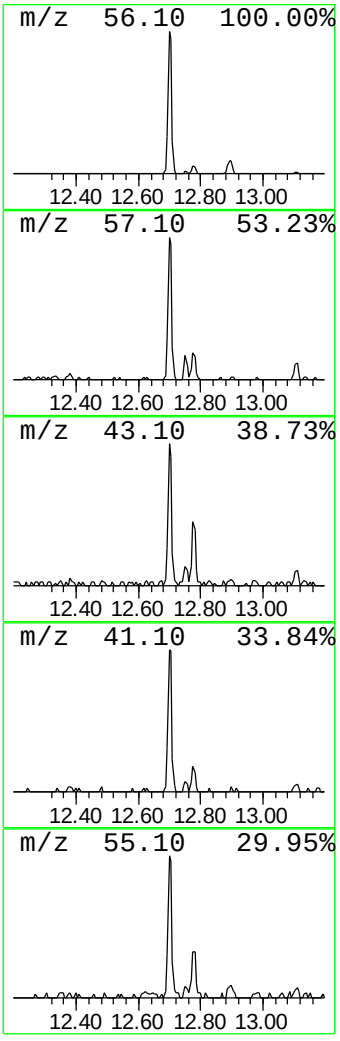
****

Peak Number 7 Hexadecanoic acid, 1,1-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	7.36 ng	194088	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	95
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3	Nipecotic acid	129	C6H11NO2	000498-95-3	47
4	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	43
5	Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	40





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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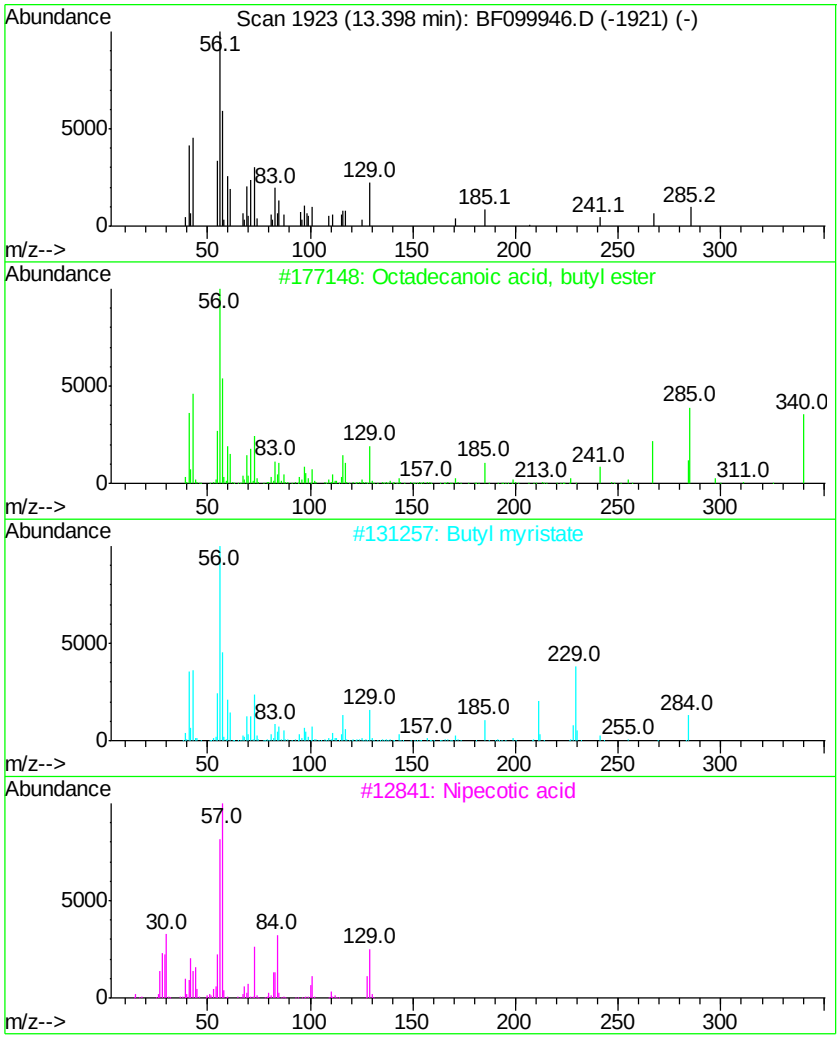
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

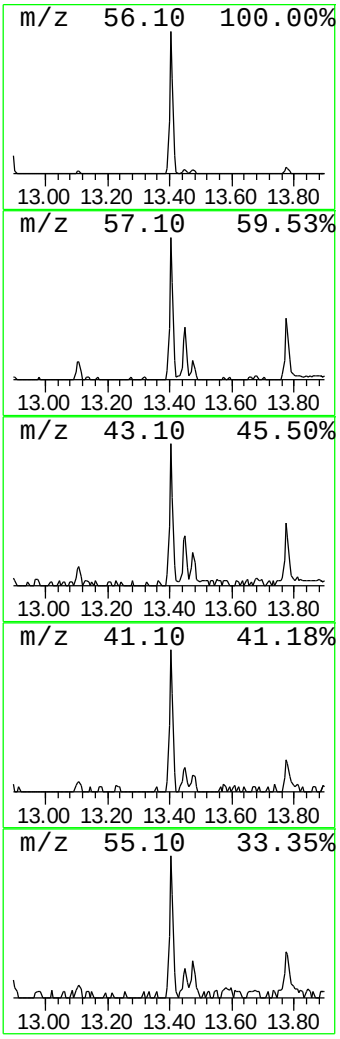
****

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	5.17 ng	136429	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	87
2	Butyl myristate	284	C18H36O2	000110-36-1	64
3	Nipecotic acid	129	C6H11NO2	000498-95-3	47
4	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	46
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35





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
2-Pentanone, 4-hy...	5.00	4.0	ng	122461	1	6.79	607219	20.0
unknown6.56	6.56	49.8	ng	1512530	1	6.79	607219	20.0
2-Hydroxy-iso-but...	8.63	2.0	ng	82695	2	8.07	814811	20.0
Triethyl citrate	10.49	2.2	ng	89353	3	9.82	800539	20.0
Benzophenone	10.53	6.9	ng	274842	3	9.82	800539	20.0
Hexadecanoic acid...	12.70	7.4	ng	194088	5	13.96	527630	20.0
Octadecanoic acid...	13.40	5.2	ng	136429	5	13.96	527630	20.0