LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099943.D
Acq On : 29 Oct 2017 5:08
Operator : SJ/JU
Sample : I6059-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 101817-TIDO-F-D-S

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	4.998	493	495	512	rBV	76260	109307	3.71%	0.643%
2	5.410	562	565	585	rBV	636103	807975	27.43%	4.755%
3	6.428	735	738	754	rBV	493660	624980	21.22%	3.678%
4	6.557	757	760	768	rVB	1661262	1503033	51.03%	8.845%
5	6.786	796	799	809	rBV	626304	565405	19.20%	3.327%
6	6.939	821	825	837	rBV	2180994	2091260	71.00%	12.306%
7	7.357	892	896	899	rBV	1493418	1518538	51.56%	8.936%
8	8.069	1013	1017	1020	rBV	856641	757661	25.72%	4.458%
9	8.628	1109	1112	1121	rBV	105721	94886	3.22%	0.558%
10	9.145	1195	1200	1203	rBV	3127416	2945260	100.00%	17.331%
11	9.539	1264	1267	1275	rBV	132279	105445	3.58%	0.620%
12	9.822	1307	1315	1319	rBV	891111	776418	26.36%	4.569%
13	9.857	1319	1321	1327	rVB	36799	32028	1.09%	0.188%
14	10.492	1426	1429	1433	rVB	72925	51813	1.76%	0.305%
15	10.533	1433	1436	1440	rBV	408829	341353	11.59%	2.009%
16	10.616	1447	1450	1464	rBV	876467	818522	27.79%	4.817%
17	11.316	1565	1569	1572	rBV	660069	598364	20.32%	3.521%
18	11.339	1572	1573	1578	rVB	51086	32206	1.09%	0.190%
19	12.704	1801	1805	1808	rBV	199473	166188	5.64%	0.978%
20	12.774	1814	1817	1821	rVB2	35157	34148	1.16%	0.201%
21	12.898	1833	1838	1841	rBV	2059619	1899598	64.50%	11.178%
22	13.404	1921	1924	1928	rBV	127370	104205	3.54%	0.613%
23	13.774	1984	1987	1995	rBV	46637	50434	1.71%	0.297%
24	13.962	2015	2019	2026	rBV	540158	494599	16.79%	2.910%
25	15.421	2263	2267	2277	rVB	350144	470129	15.96%	2.766%

Sum of corrected areas: 16993755

LSC Report - Integrated Chromatogram

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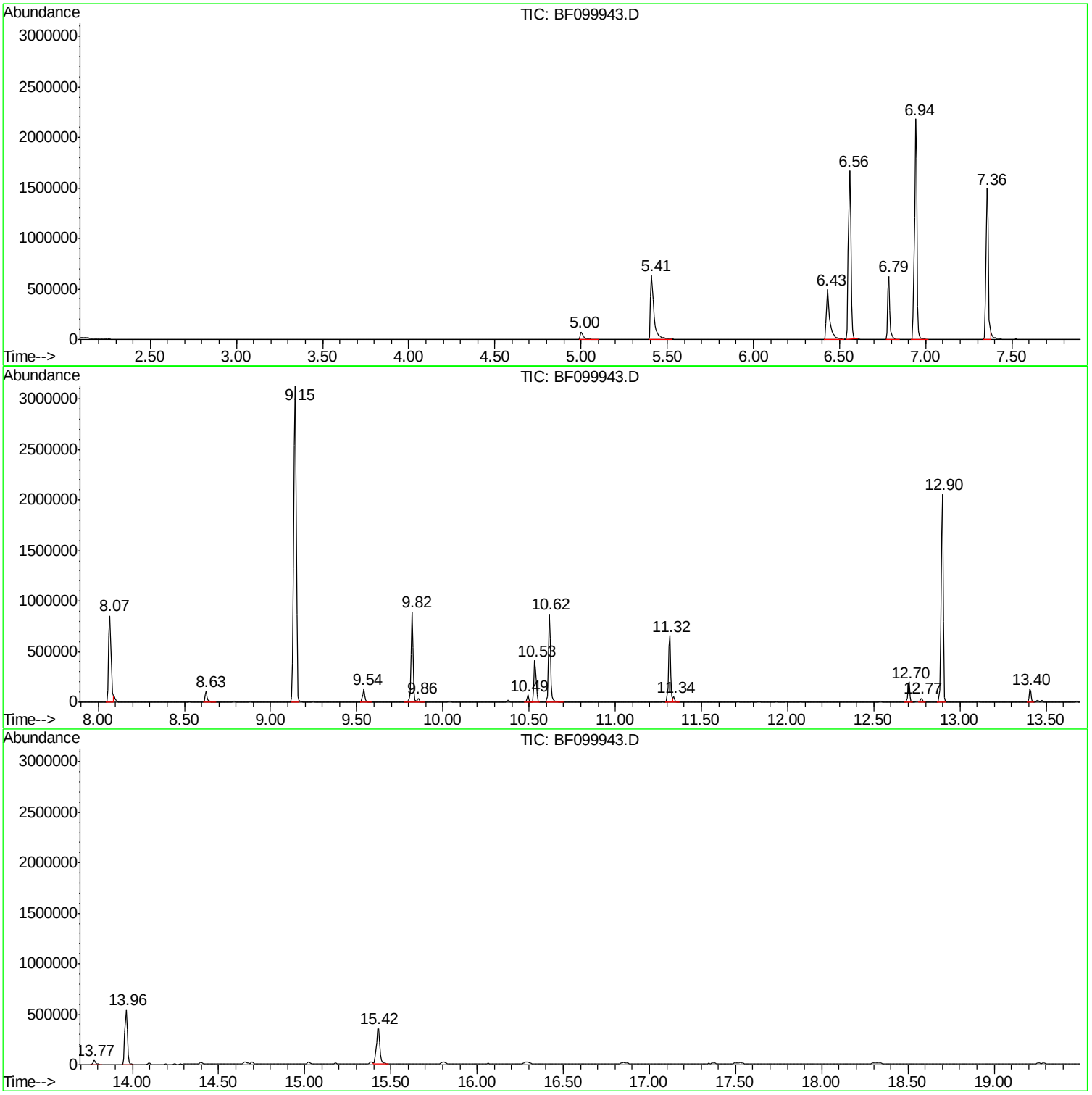
Operator : SJ/JU
Sample : I6059-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 101817-TIDO-F-D-S

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099943.D
Acq On : 29 Oct 2017 5:08
Operator : SJ/JU
Sample : I6059-02
Misc :
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Instrument : BNA_F
ClientSampleId : 101817-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

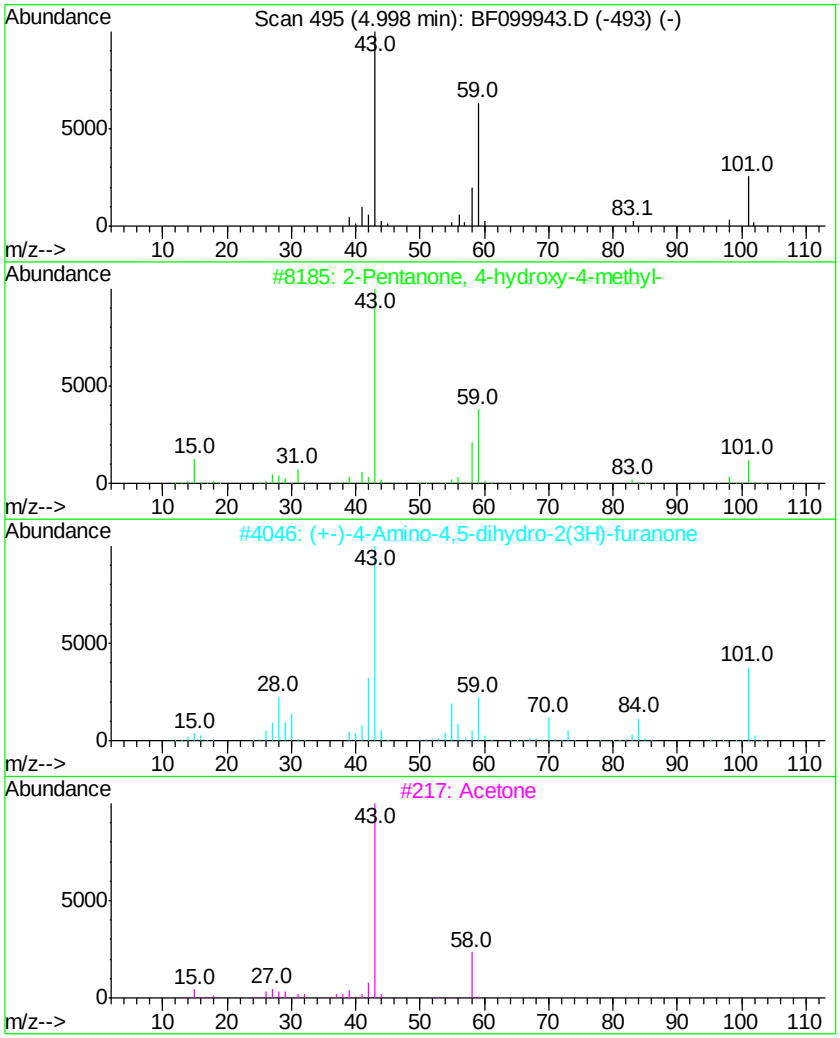
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

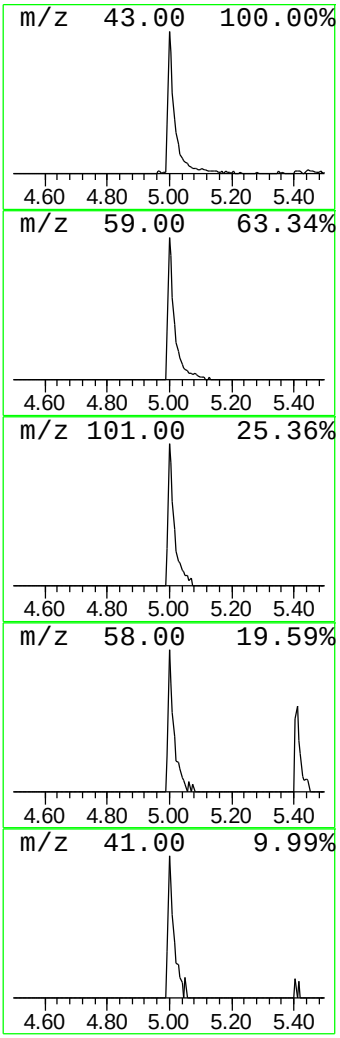
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	3.87 ng	109307	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	53
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3	Acetone	58	C3H6O	000067-64-1	22
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Data File : BF099943.D
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Operator : SJ/JU
Sample : I6059-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 101817-TIDO-F-D-S

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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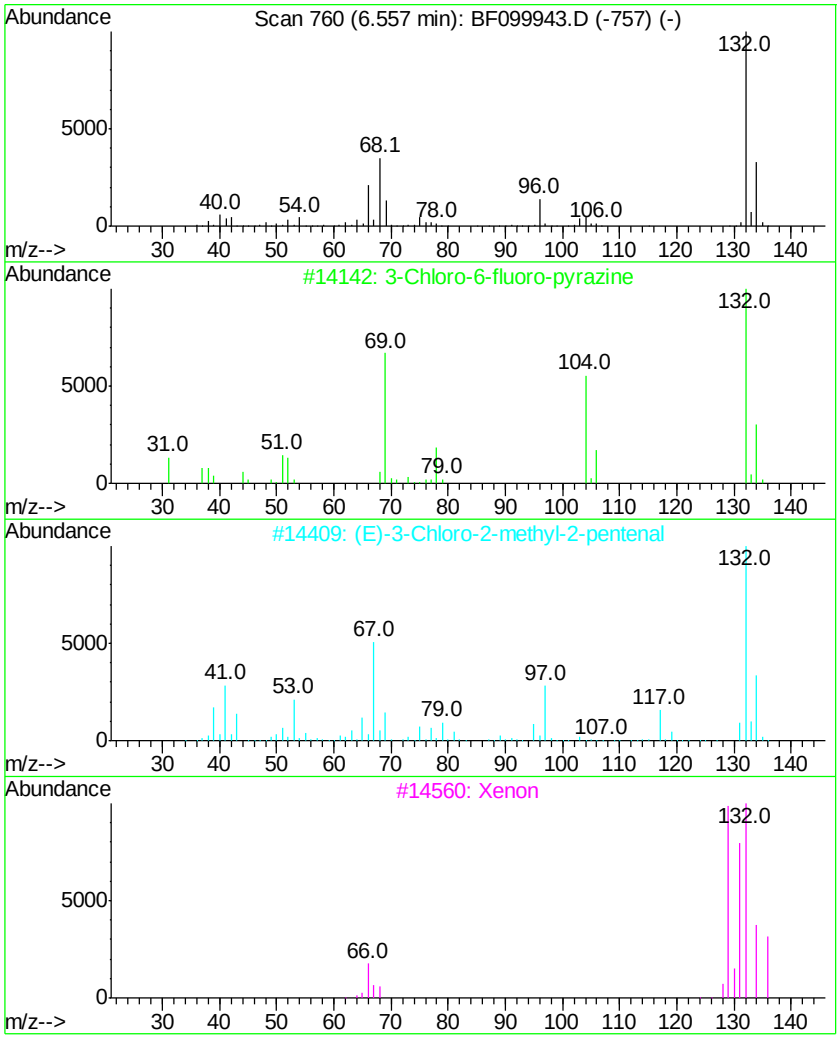
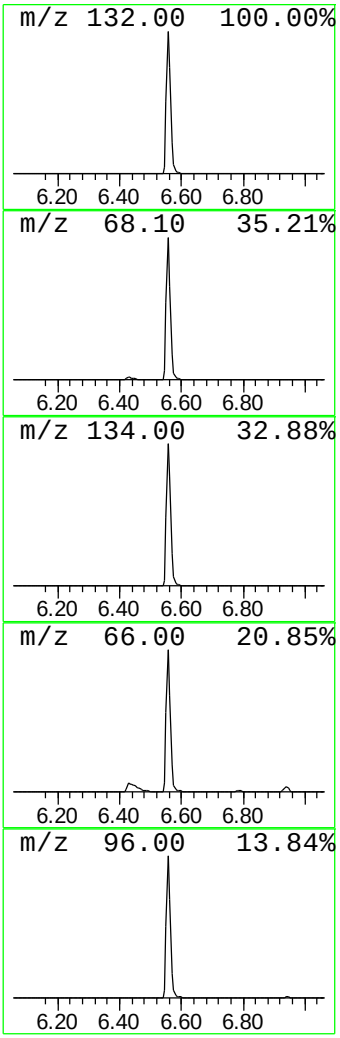
Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	53.17 ng	1503030	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	25
3	Xenon	132	Xe	007440-63-3	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099943.D
Acq On : 29 Oct 2017 5:08
Operator : SJ/JU
Sample : I6059-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 101817-TIDO-F-D-S

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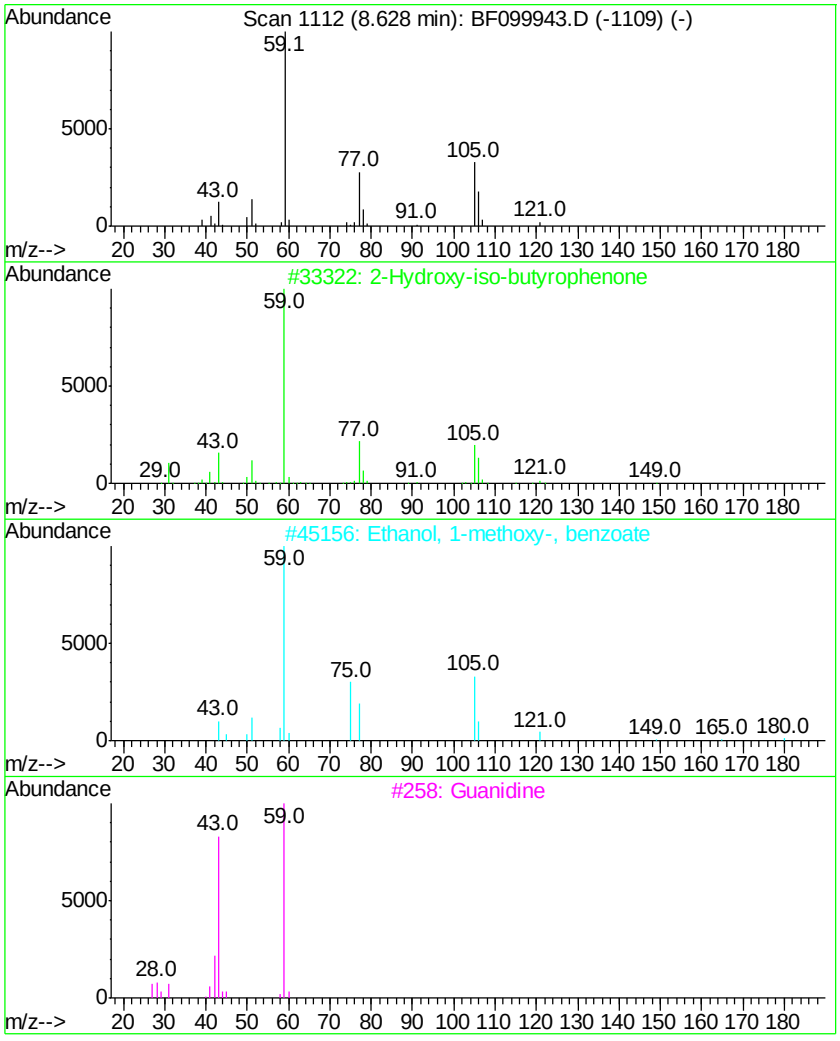
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

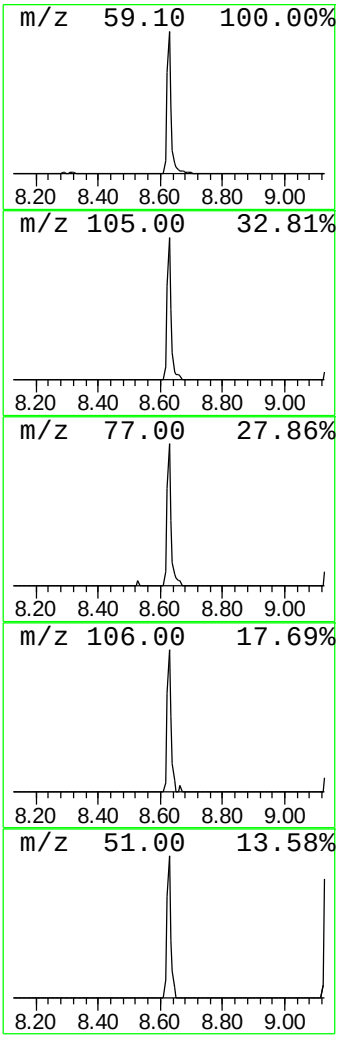
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.63	2.50 ng	94886	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	50
3	Guanidine	59	CH5N3	000113-00-8	7
4	Formamide, N-methyl-	59	C2H5NO	000123-39-7	5
5	Acetamide	59	C2H5NO	000060-35-5	5





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099943.D
Acq On : 29 Oct 2017 5:08
Operator : SJ/JU
Sample : I6059-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 101817-TIDO-F-D-S

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

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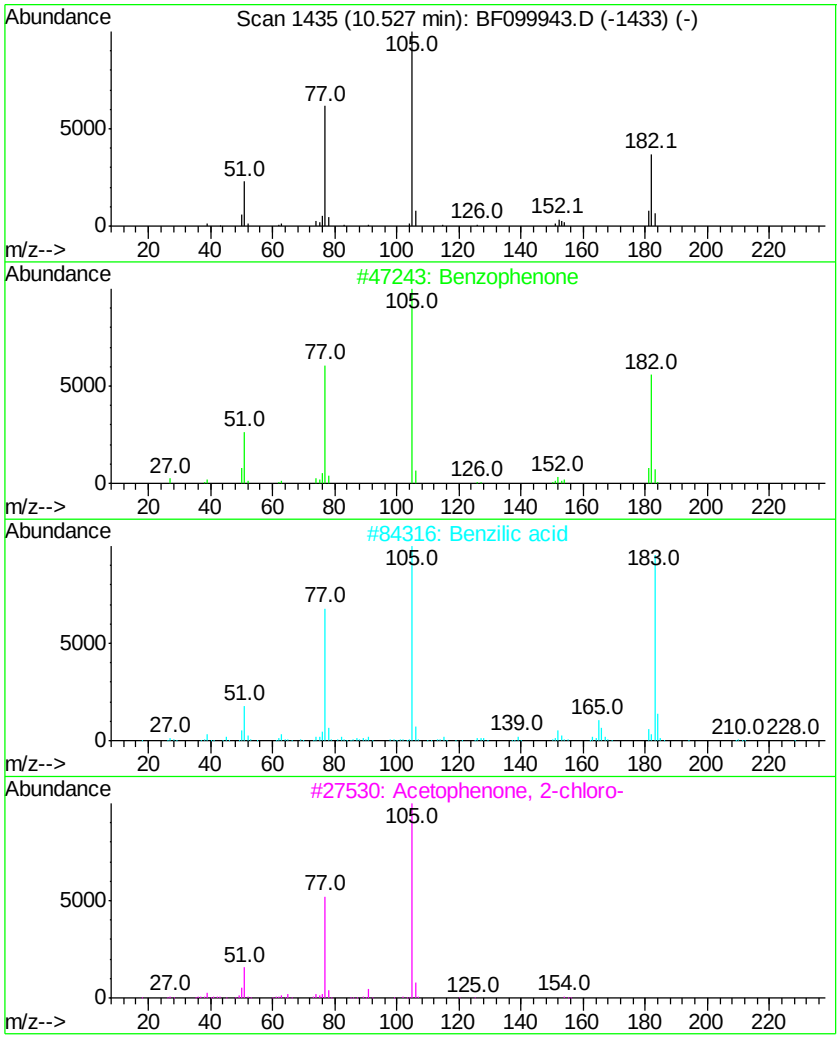
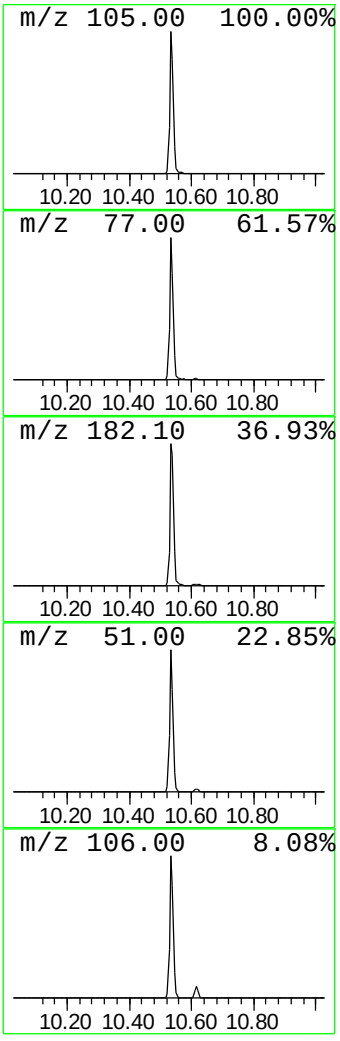
Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	8.79 ng	341353	Acenaphthene-d10	9.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzilic acid	228	C14H12O3	000076-93-7	50
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	43
5	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099943.D
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Operator : SJ/JU
Sample : I6059-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 101817-TIDO-F-D-S

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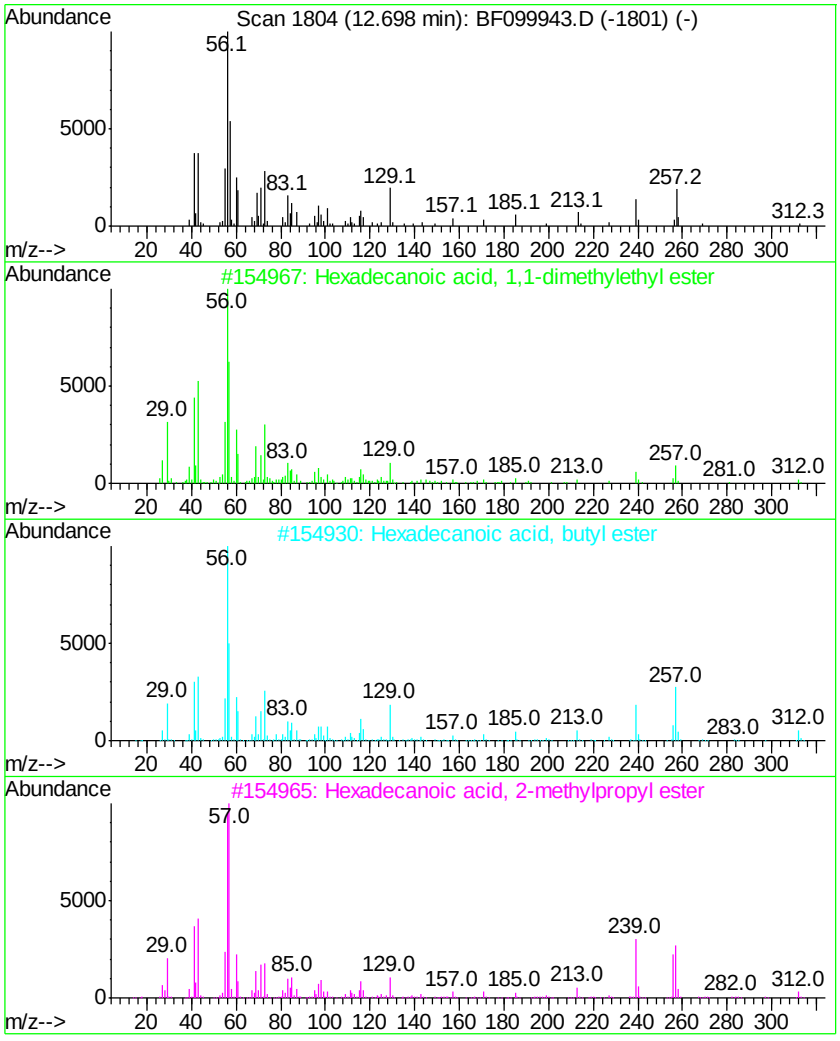
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

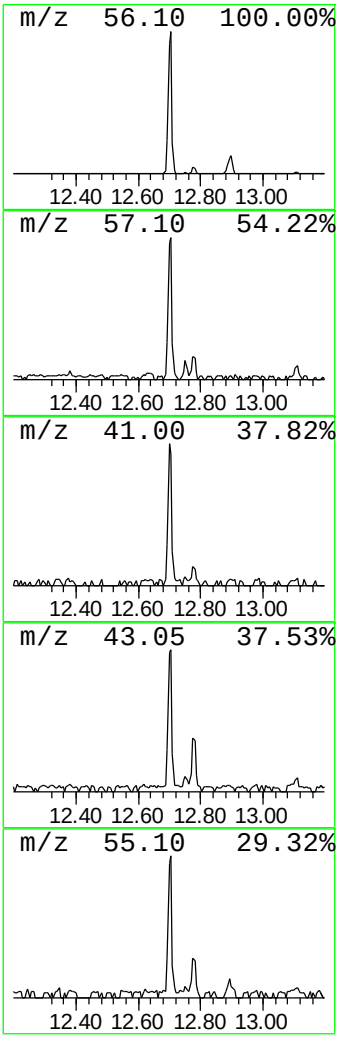
****

Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	6.72 ng	166188	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	58
4	Nipecotic acid	129	C6H11NO2	000498-95-3	47
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	27





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Misc :
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Instrument : BNA_F
ClientSampleId : 101817-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

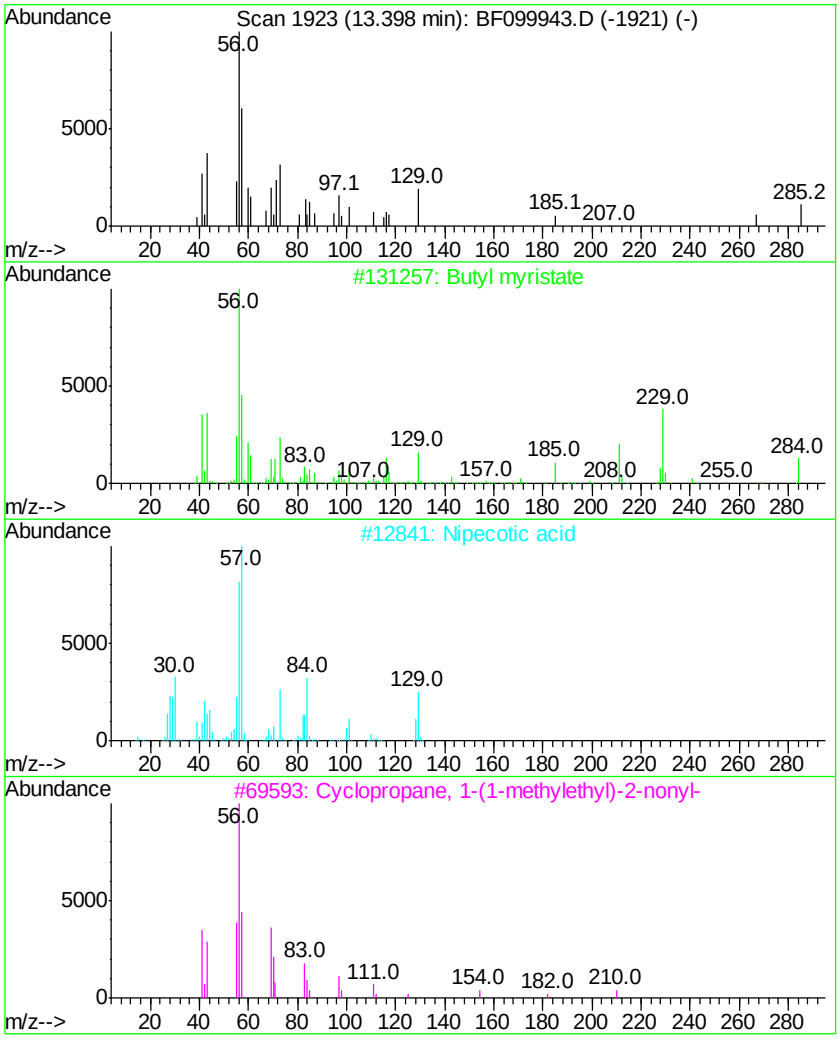
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

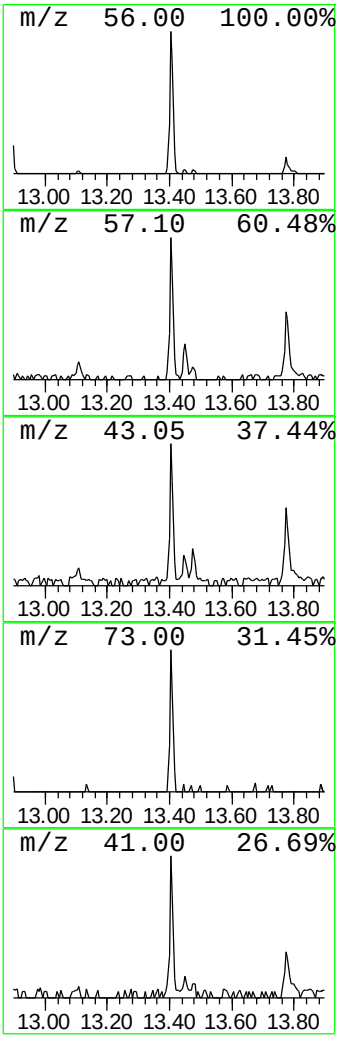
****

Peak Number 7 Butyl myristate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	4.21 ng	104205	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	64
2	Nipecotic acid	129	C6H11NO2	000498-95-3	38
3	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27





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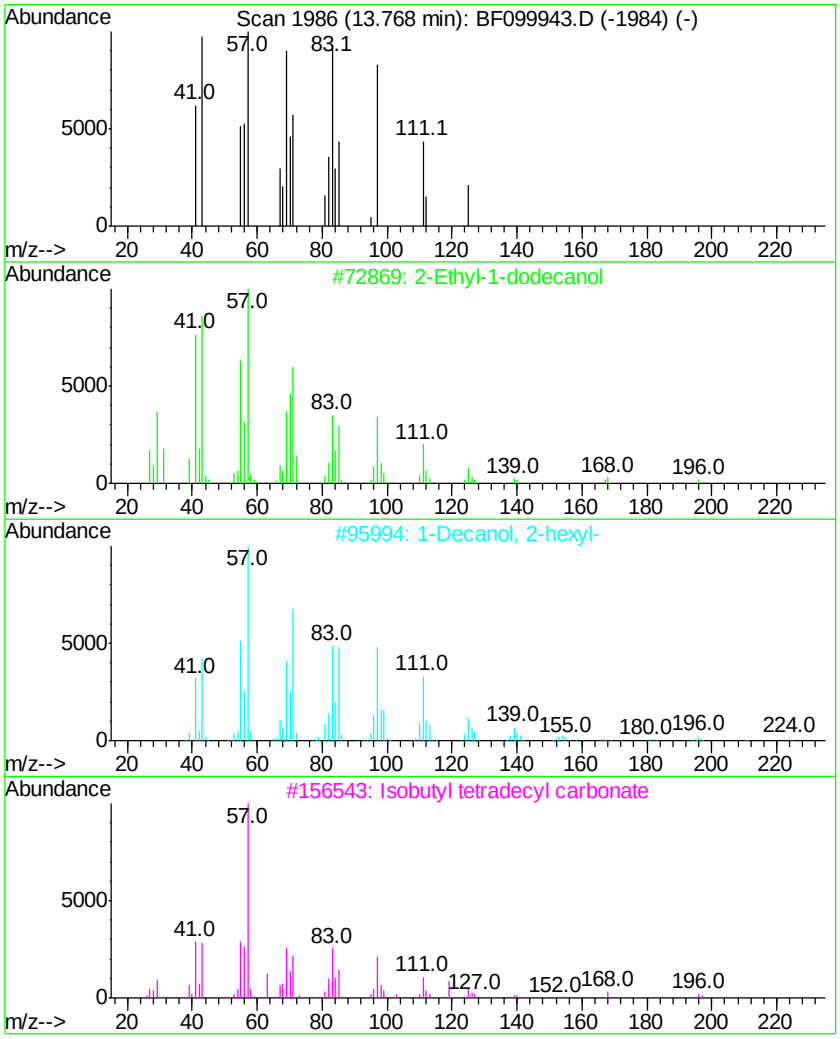
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

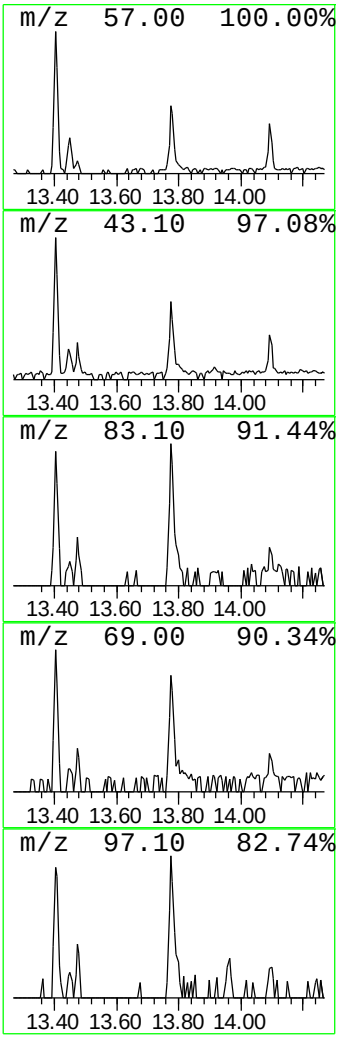
****

Peak Number 8 2-Ethyl-1-dodecanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	2.04 ng	50434	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	86
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	80
3	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	80
4	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	80
5	2-Hexyl-1-octanol	214	C14H30O	019780-79-1	80





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	3.9	ng	109307	1	6.79	565405	20.0
unknown6.56	6.56	53.2	ng	1503030	1	6.79	565405	20.0
2-Hydroxy-iso-but...	8.63	2.5	ng	94886	2	8.07	757661	20.0
Benzophenone	10.53	8.8	ng	341353	3	9.82	776418	20.0
Hexadecanoic acid...	12.70	6.7	ng	166188	5	13.96	494599	20.0
Butyl myristate	13.40	4.2	ng	104205	5	13.96	494599	20.0
2-Ethyl-1-dodecanol	13.77	2.0	ng	50434	5	13.96	494599	20.0