LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG082316\
Data File : BG023854.D
Acq On : 23 Aug 2016 15:39
Operator : UM/SJ
Sample : H4528-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : VITALEFILL-MCMPH3-3

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_G\Methods\8270-BG080116.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	2.967	17	22	40	rVB	4857604	7577932	100.00%	14.537%
2	3.232	61	67	75	rBV	49345	76257	1.01%	0.146%
3	5.153	387	394	405	rBV	717724	1147573	15.14%	2.201%
4	5.628	467	475	487	rBV	2055712	3500027	46.19%	6.714%
5	6.245	575	580	589	rVB	50380	79146	1.04%	0.152%
6	7.250	744	751	763	rBV	2177991	3868901	51.05%	7.422%
7	7.620	805	814	830	rBV	2103894	3723408	49.13%	7.143%
8	8.090	887	894	902	rBV	386579	670288	8.85%	1.286%
9	8.413	942	949	961	rBV	1492082	2615917	34.52%	5.018%
10	9.271	1087	1095	1105	rBV	1305326	2399354	31.66%	4.603%
11	10.921	1366	1376	1387	rBV	530227	995586	13.14%	1.910%
12	13.377	1786	1794	1805	rBV	3244198	5027086	66.34%	9.644%
13	14.205	1928	1935	1942	rBV	707534	1034966	13.66%	1.985%
14	14.763	2022	2030	2040	rBV2	861593	1373505	18.13%	2.635%
15	15.586	2165	2170	2176	rVB	62589	82758	1.09%	0.159%
16	16.261	2279	2285	2296	rBV	2788777	4375350	57.74%	8.393%
17	16.449	2313	2317	2325	rBV	81649	138431	1.83%	0.266%
18	17.530	2493	2501	2515	rBV2	1069419	1748439	23.07%	3.354%
19	18.399	2644	2649	2655	rBV2	162160	256717	3.39%	0.492%
20	19.668	2862	2865	2869	rBV2	76469	95183	1.26%	0.183%
21	20.138	2939	2945	2953	rBV	5481032	7297504	96.30%	13.999%
22	21.448	3163	3168	3176	rBV7	79775	228488	3.02%	0.438%
23	21.842	3229	3235	3243	rBV2	1150239	1947792	25.70%	3.737%
24	25.225	3801	3811	3823	rVB2	632157	1867946	24.65%	3.583%

Sum of corrected areas: 52128554

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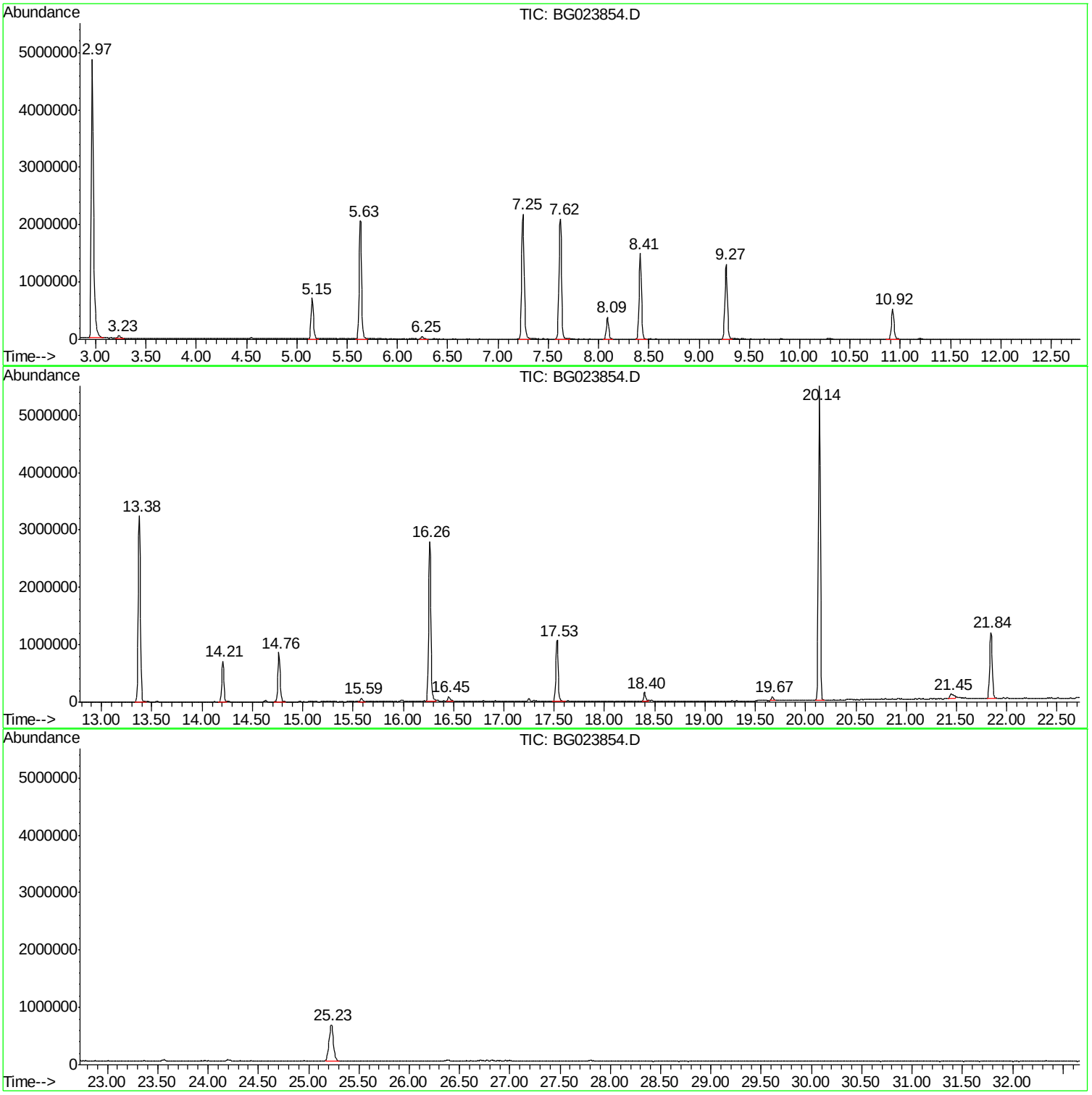
Instrument :
BNA_G
ClientSampleId :
VITALEFILL-MCMPH3-3

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.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 G\DATA\BG082316\
Data File : BG023854.D
Acq On : 23 Aug 2016 15:39
Operator : UM/SJ
Sample : H4528-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : VITALEFILL-MCMPH3-3

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

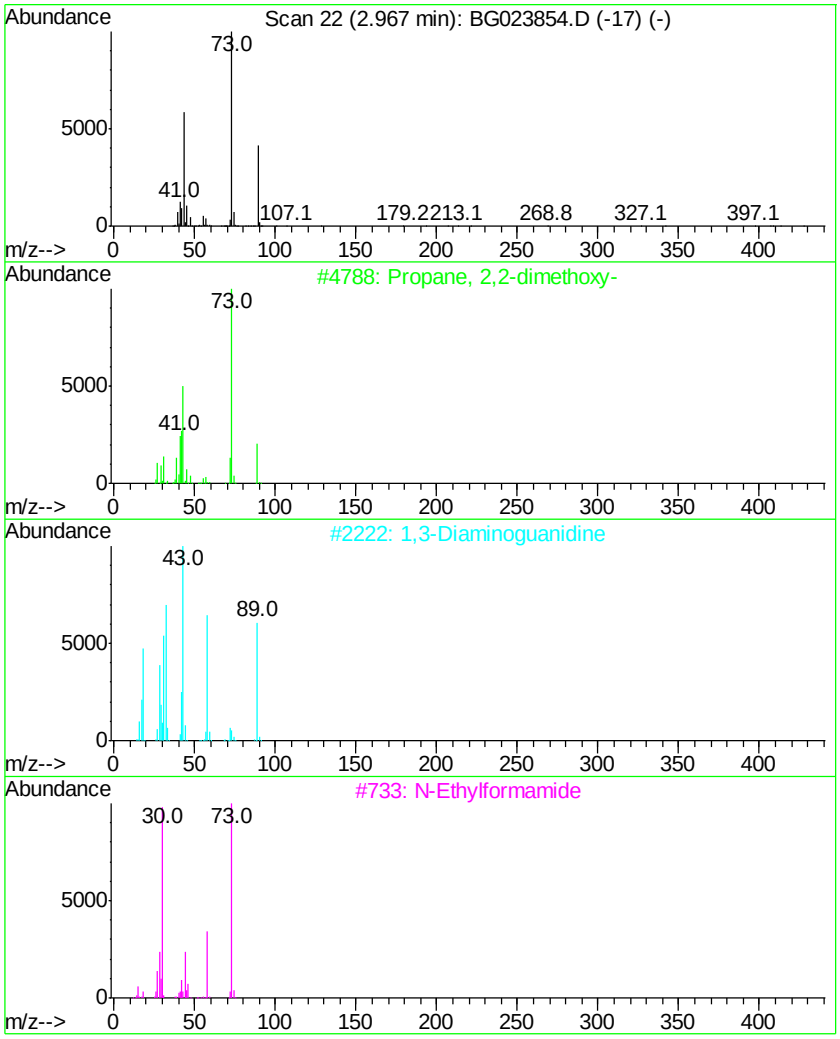
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

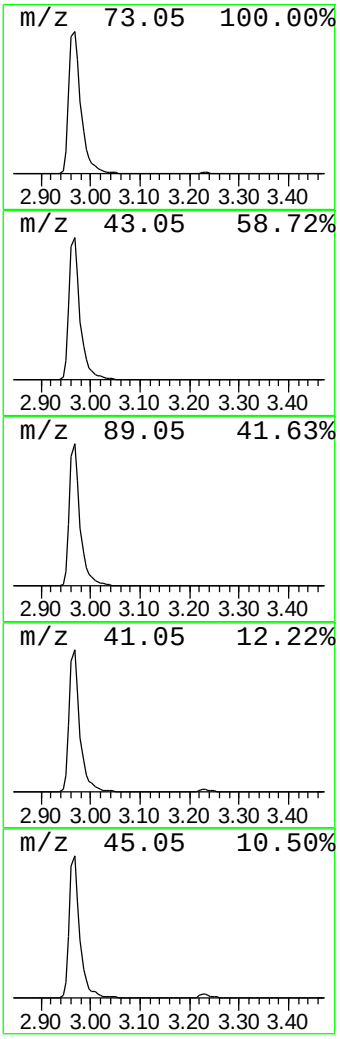
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.97	226.11 ng	7577930	1,4-Dichlorobenzene-d4	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	64
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	9





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Operator : UM/SJ
Sample : H4528-12
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ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : VITALEFILL-MCMPH3-3

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.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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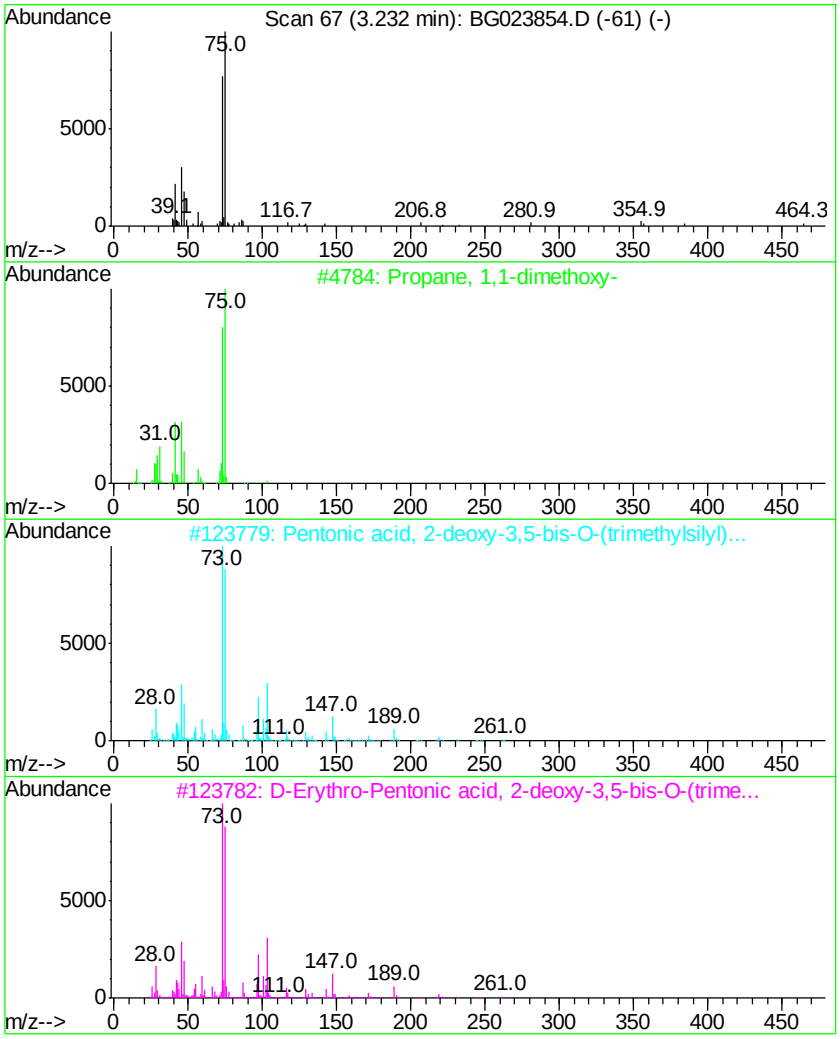
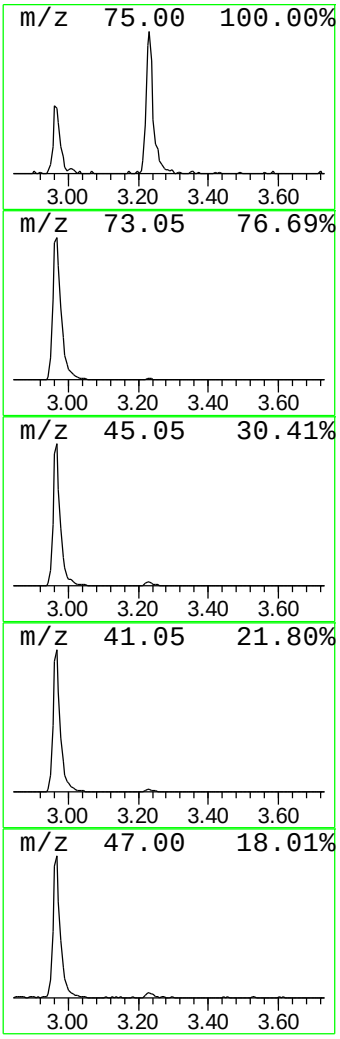
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	2.28 ng	76257	1,4-Dichlorobenzene-d4	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	Pentonic acid, 2-deoxy-3,5-bis-O...	276	C11H24O4Si2	074742-34-0	40
3	D-Erythro-Pentonic acid, 2-deoxy...	276	C11H24O4Si2	010589-33-0	40
4	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	38
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG082316\
Data File : BG023854.D
Acq On : 23 Aug 2016 15:39
Operator : UM/SJ
Sample : H4528-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : VITALEFILL-MCMPH3-3

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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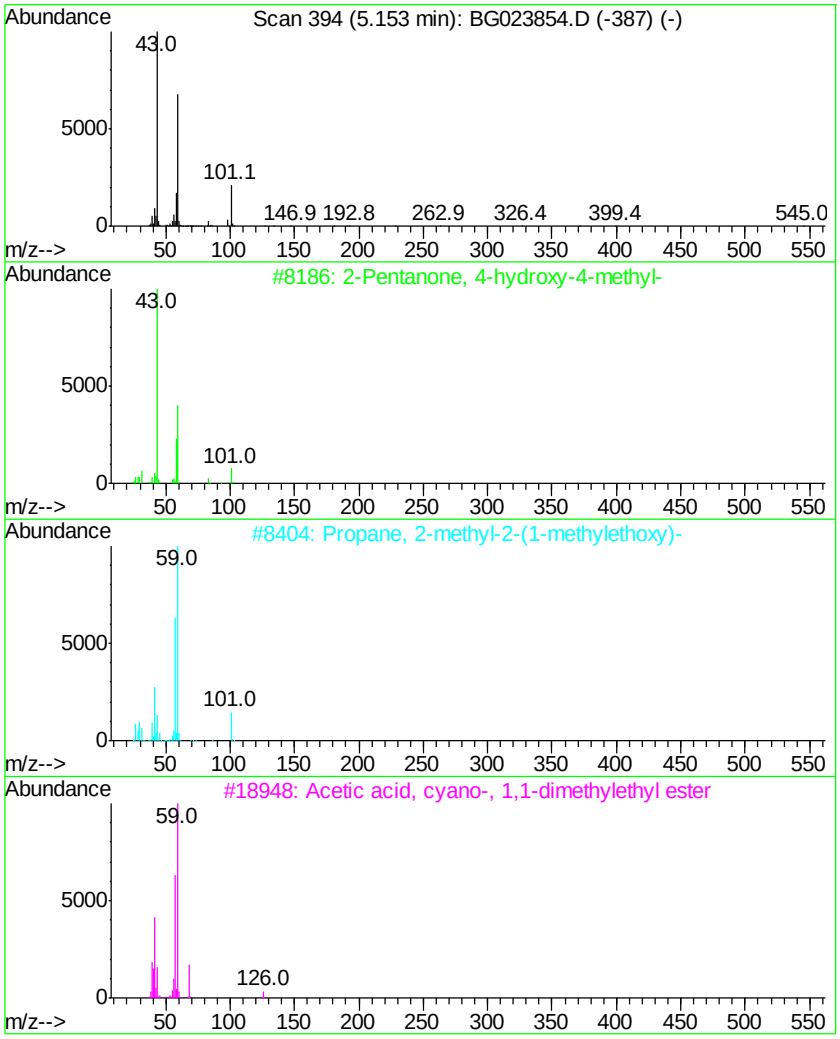
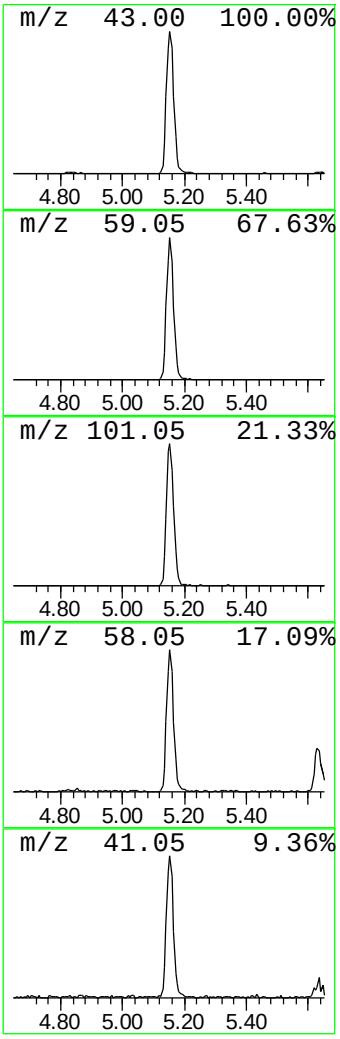
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	34.24 ng	1147570	1,4-Dichlorobenzene-d4	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	Acetone	58	C3H6O	000067-64-1	10





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Operator : UM/SJ
Sample : H4528-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : VITALEFILL-MCMPH3-3

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

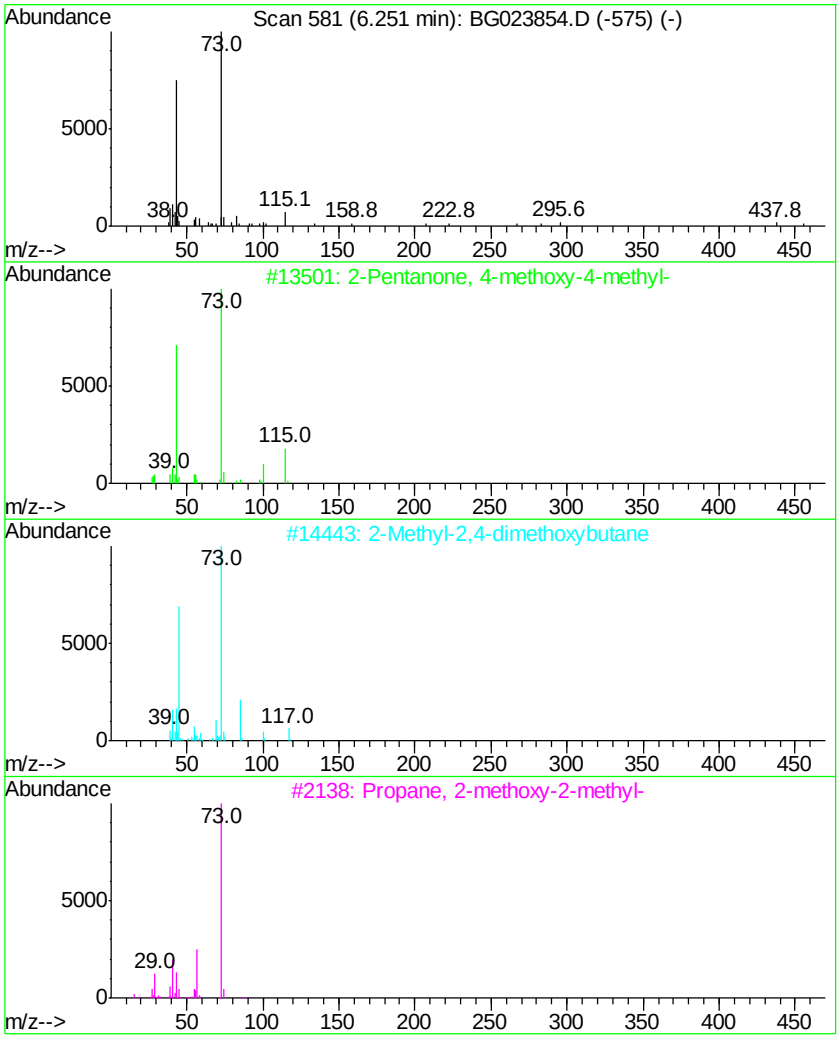
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

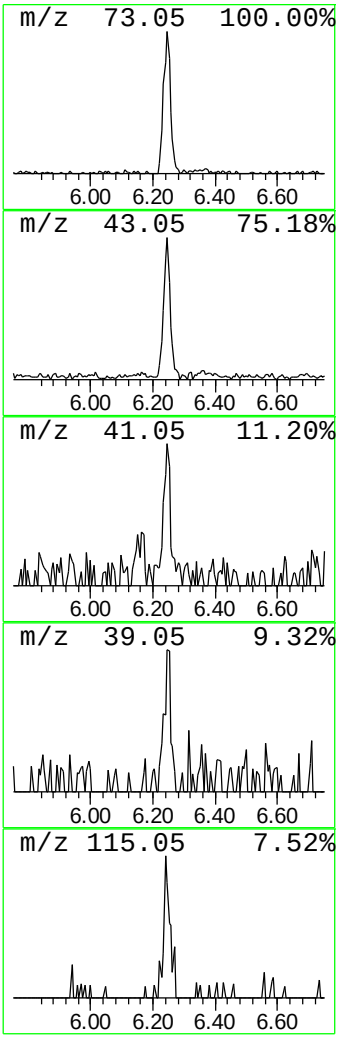
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.25	2.36 ng	79146	1,4-Dichlorobenzene-d4	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	50
2	2-Methyl-2,4-dimethoxybutane	132	C7H16O2	039836-89-0	17
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	10
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
5	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG082316\
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Sample : H4528-12
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ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : VITALEFILL-MCMPH3-3

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.M
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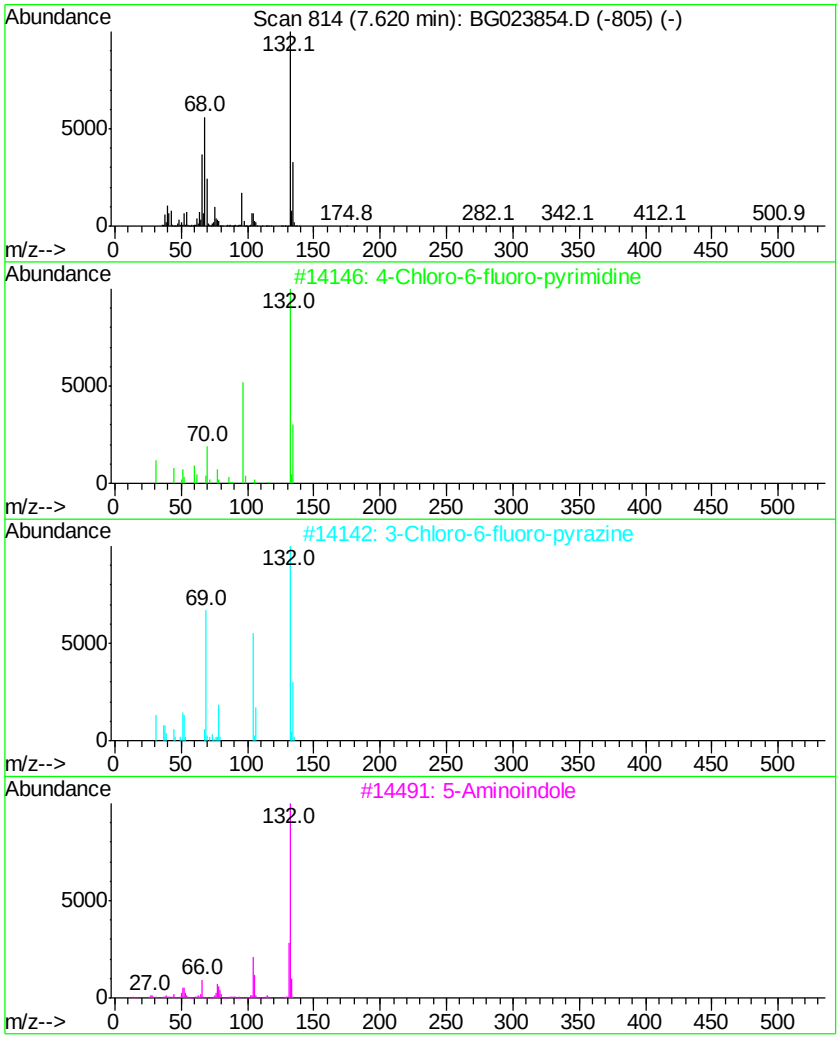
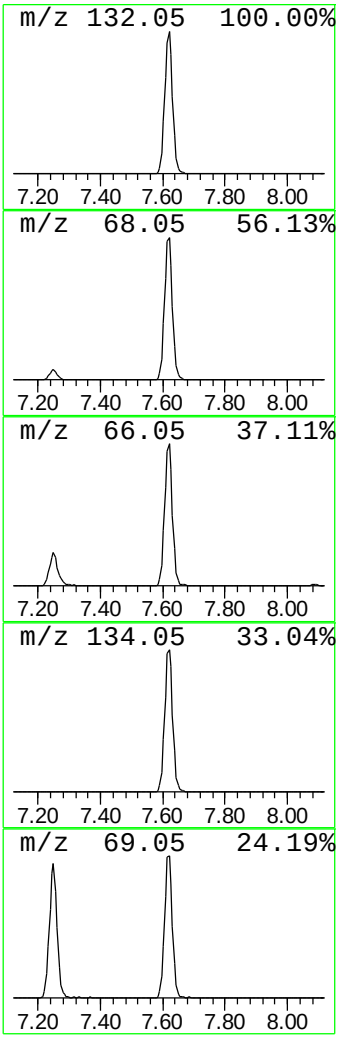
****

Peak Number 5 unknown7.62 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	111.10 ng	3723410	1,4-Dichlorobenzene-d4	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	16





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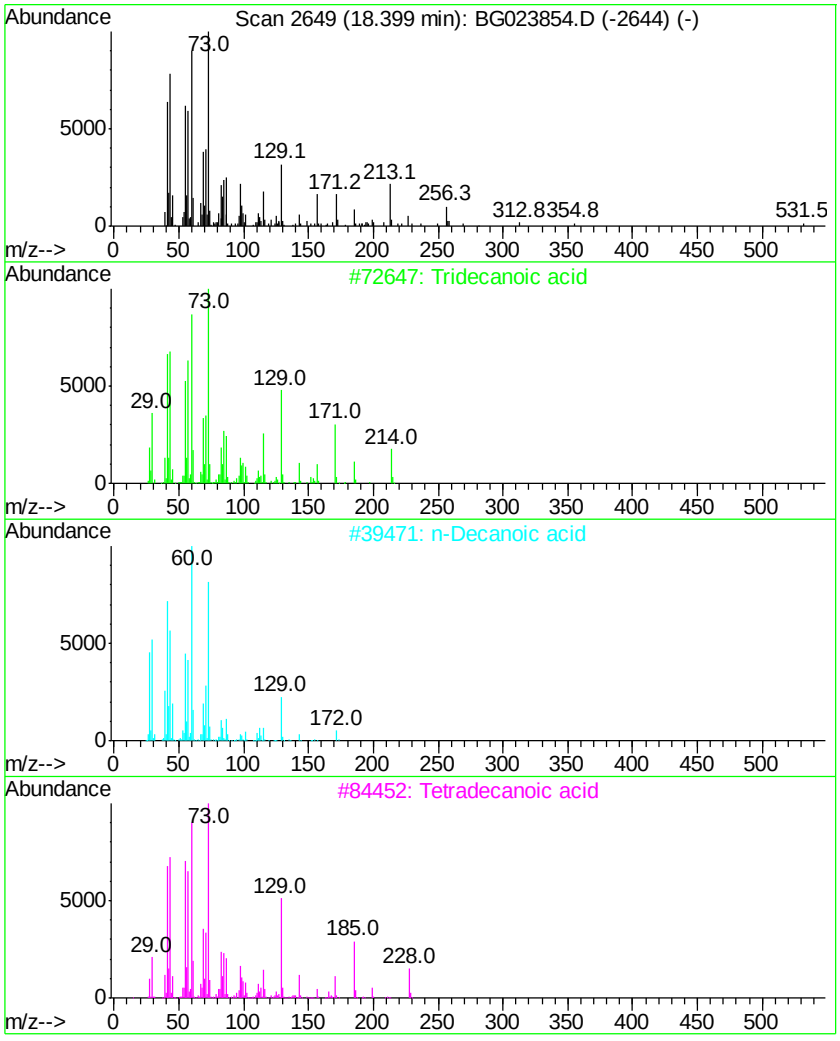
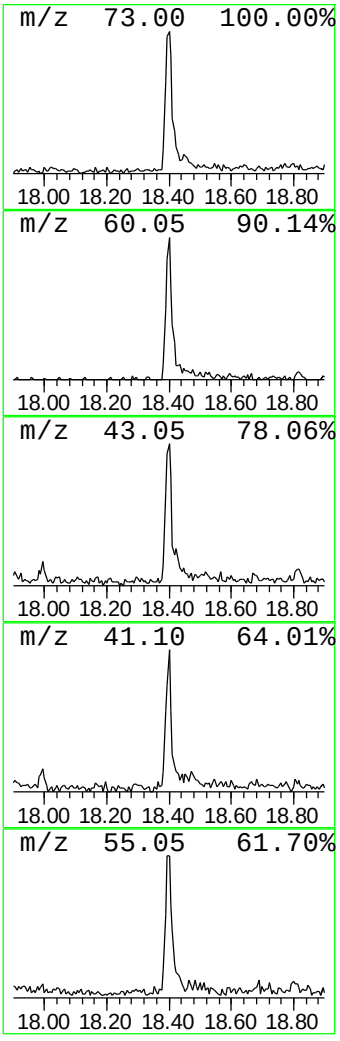
****

Peak Number 7 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.40	2.94 ng	256717	Phenanthrene-d10	17.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	92
2	n-Decanoic acid	172	C10H20O2	000334-48-5	62
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
5	Heptanoic acid	130	C7H14O2	000111-14-8	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

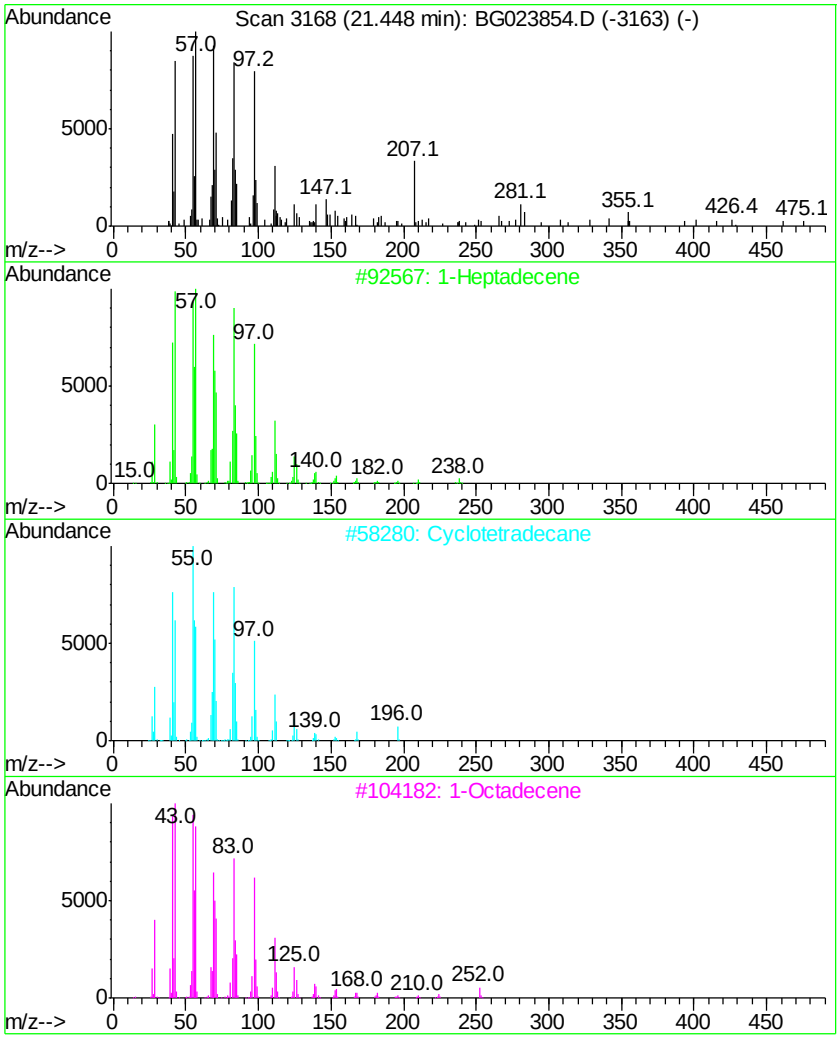
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

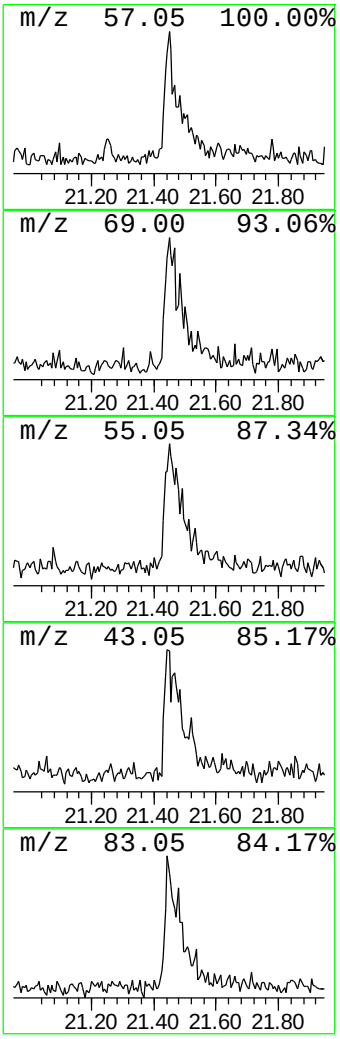
****

Peak Number 8 1-Heptadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.45	2.35 ng	228488	Chrysene-d12	21.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptadecene	238	C17H34	006765-39-5	91
2	Cyclotetradecane	196	C14H28	000295-17-0	87
3	1-Octadecene	252	C18H36	000112-88-9	83
4	E-14-Hexadecenal	238	C16H30O	330207-53-9	83
5	3-Octadecene, (E)-	252	C18H36	007206-19-1	83





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
Propane, 2,2-dime...	2.97	226.1	ng	7577930	1	8.09	670288	20.0
Propane, 1,1-dime...	3.23	2.3	ng	76257	1	8.09	670288	20.0
2-Pentanone, 4-hy...	5.15	34.2	ng	1147570	1	8.09	670288	20.0
2-Pentanone, 4-me...	6.25	2.4	ng	79146	1	8.09	670288	20.0
unknown7.62	7.62	111.1	ng	3723410	1	8.09	670288	20.0
Tridecanoic acid	18.40	2.9	ng	256717	4	17.52	1748440	20.0
1-Heptadecene	21.45	2.4	ng	228488	5	21.84	1947790	20.0