LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023434.D
Acq On : 3 Aug 2016 20:42
Operator : UM/SJ
Sample : H4287-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-60-7.0-8.0

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_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	2.991	22	26	41	rVB	3179469	4513059	45.42%	7.740%
2	5.183	392	399	409	rBV	529892	834106	8.39%	1.431%
3	5.658	473	480	491	rBV	2103843	3442707	34.65%	5.905%
4	7.274	748	755	767	rBV	2223450	3930487	39.56%	6.741%
5	7.644	810	818	829	rBV	2082980	3710667	37.35%	6.364%
6	8.120	891	899	906	rBV	351578	630083	6.34%	1.081%
7	8.443	946	954	962	rBV	1521720	2599057	26.16%	4.458%
8	9.295	1091	1099	1109	rBV	1351145	2443939	24.60%	4.192%
9	10.951	1373	1381	1389	rBV	528606	942265	9.48%	1.616%
10	13.395	1787	1797	1811	rBV	3471619	5685830	57.22%	9.752%
11	14.223	1931	1938	1946	rBV	1500143	2229737	22.44%	3.824%
12	14.781	2027	2033	2041	rBV2	958679	1515219	15.25%	2.599%
13	15.604	2168	2173	2178	rVB4	70103	100690	1.01%	0.173%
14	16.279	2281	2288	2298	rBV	3720284	5784845	58.22%	9.921%
15	16.467	2316	2320	2324	rBV	80096	121860	1.23%	0.209%
16	17.542	2495	2503	2510	rBV2	1431680	2256314	22.71%	3.870%
17	17.901	2559	2564	2575	rBV	444334	782843	7.88%	1.343%
18	18.412	2646	2651	2662	rBV	511688	797641	8.03%	1.368%
19	19.269	2792	2797	2804	rBV4	75762	162353	1.63%	0.278%
20	19.681	2863	2867	2878	rBV	449771	654588	6.59%	1.123%
21	20.151	2941	2947	2955	rBV	7427743	9936025	100.00%	17.041%
22	21.467	3166	3171	3184	rBV5	97997	276087	2.78%	0.474%
23	21.854	3230	3237	3253	rBV2	1472365	2602898	26.20%	4.464%
24	25.232	3803	3812	3825	rVB2	812034	2352994	23.68%	4.036%

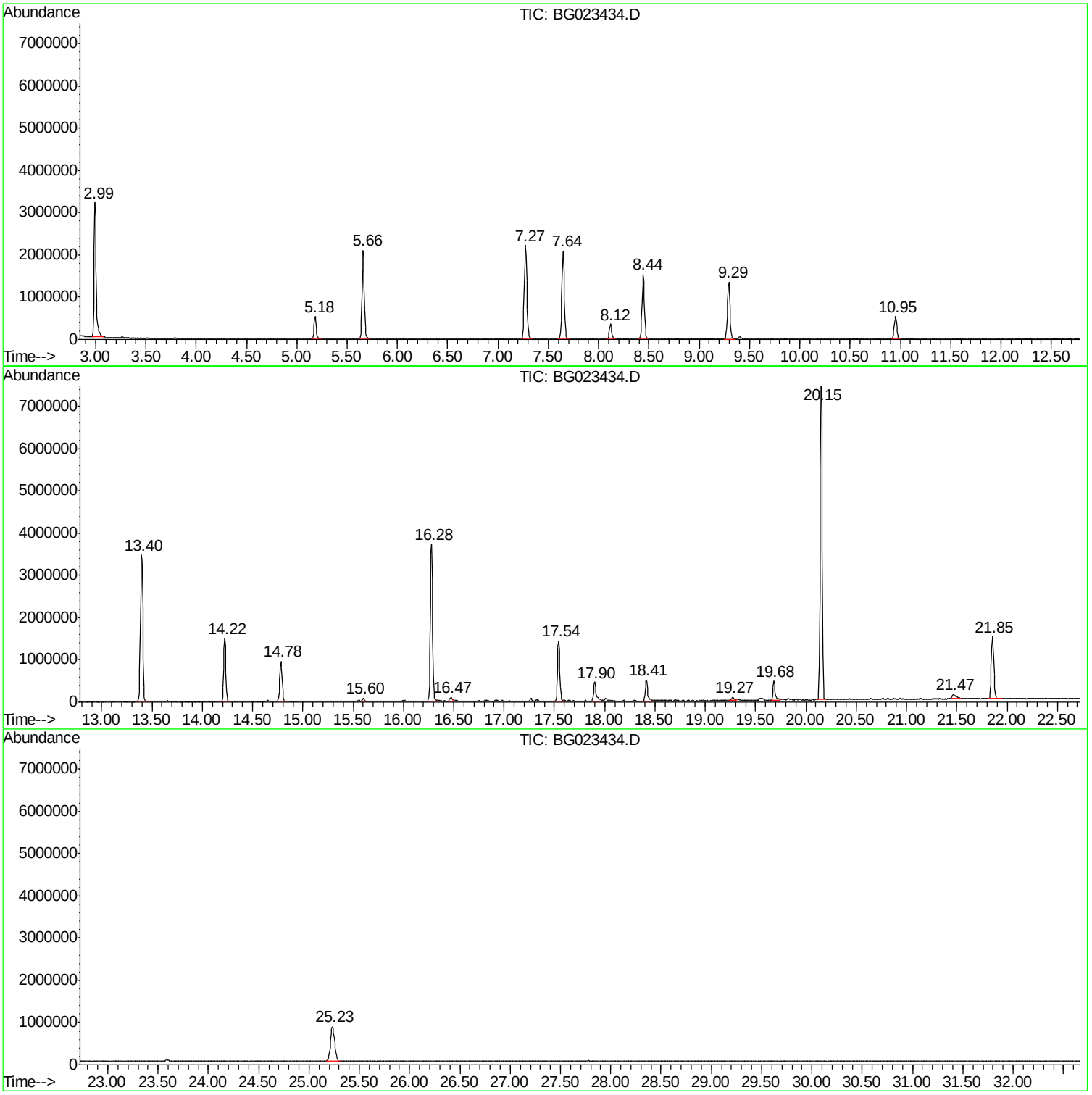
Sum of corrected areas: 58306294

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023434.D
Acq On : 3 Aug 2016 20:42
Operator : UM/SJ
Sample : H4287-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-60-7.0-8.0

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023434.D
Acq On : 3 Aug 2016 20:42
Operator : UM/SJ
Sample : H4287-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-60-7.0-8.0

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

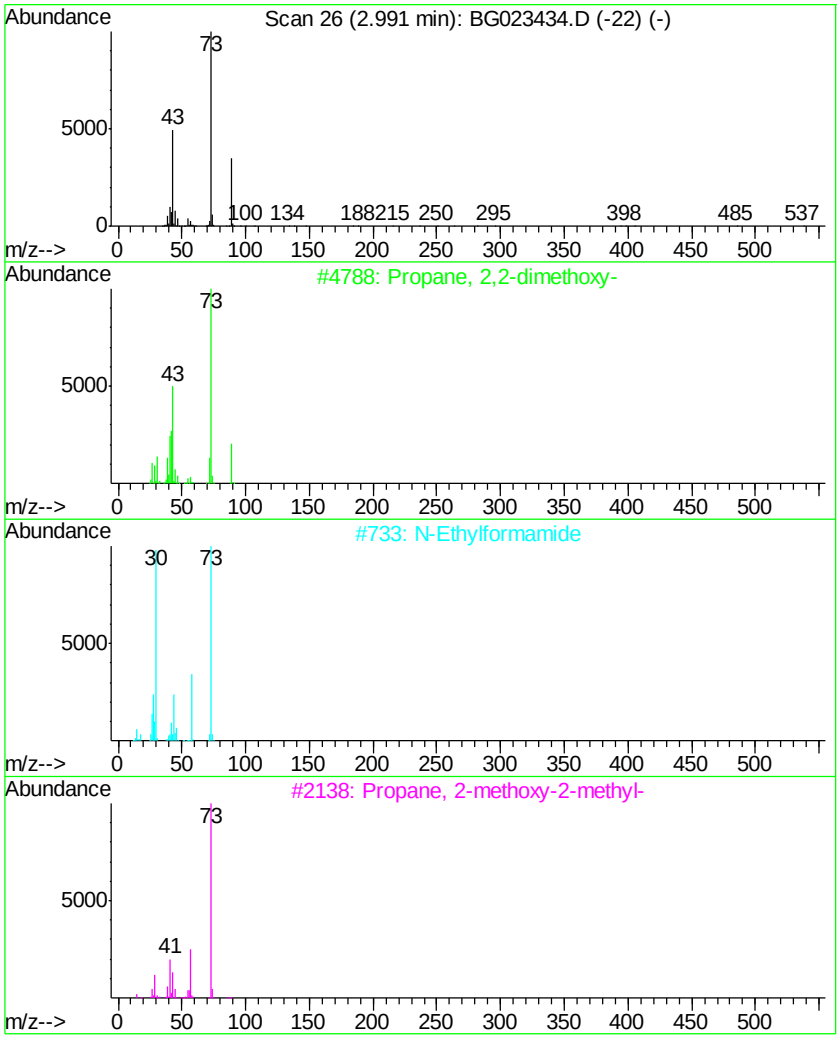
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

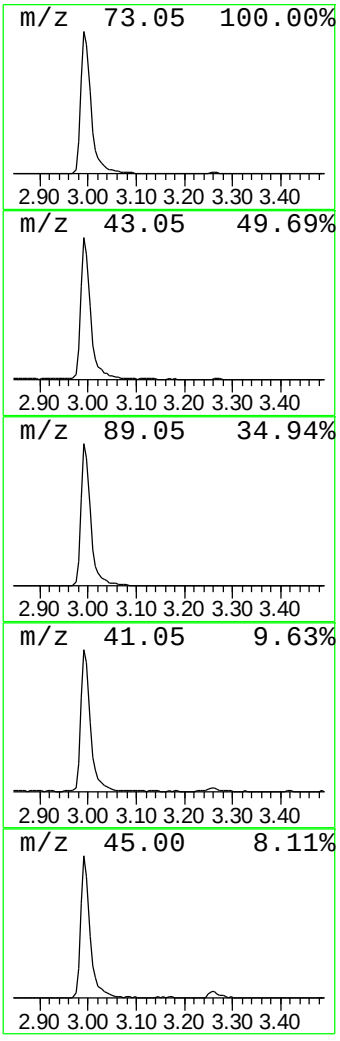
****

Peak Number 1 unknown2.99 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	143.25 ng	4513060	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023434.D
Acq On : 3 Aug 2016 20:42
Operator : UM/SJ
Sample : H4287-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-60-7.0-8.0

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

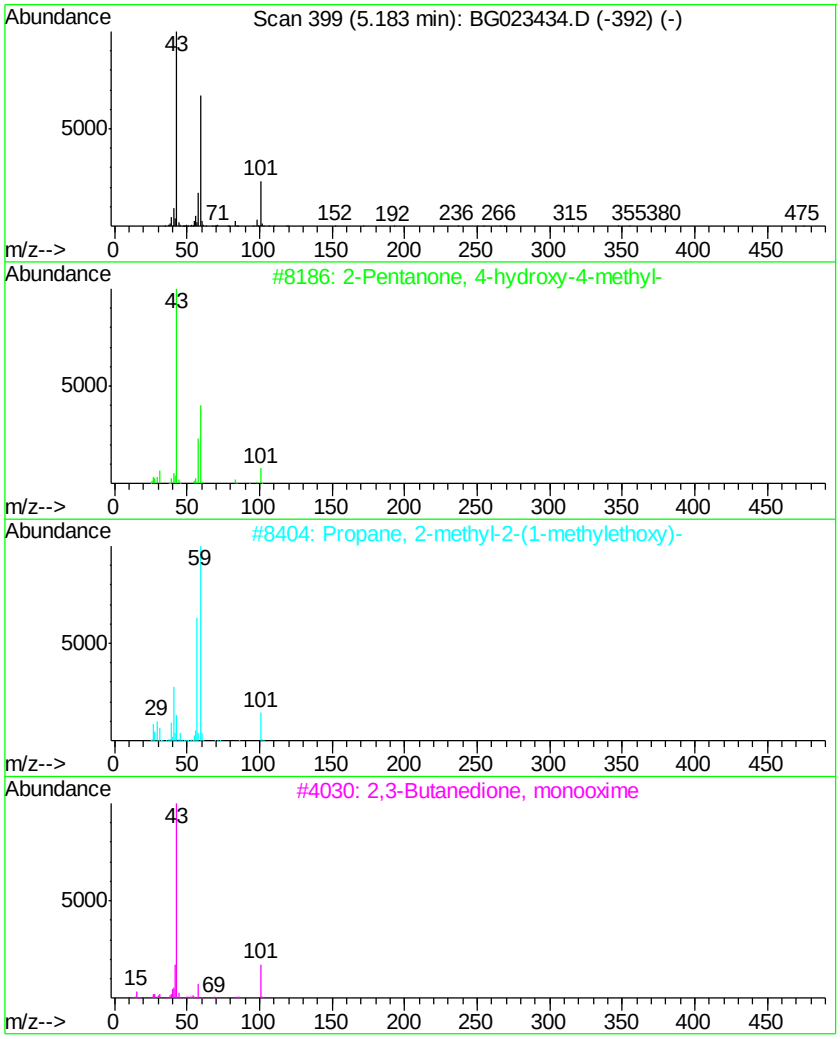
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

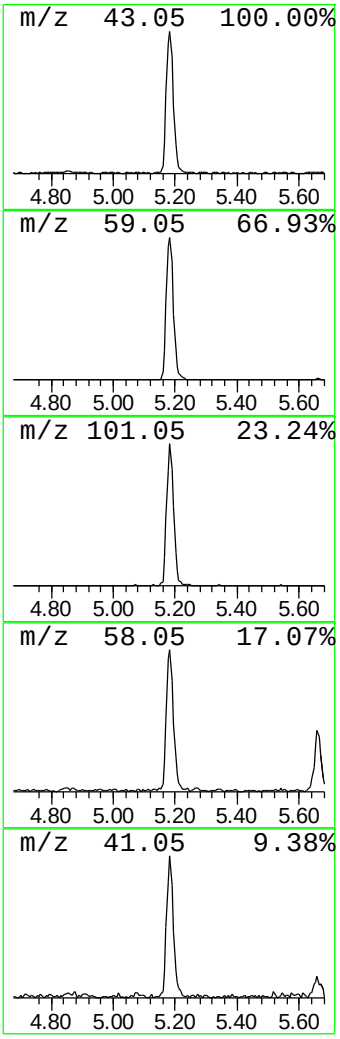
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	26.48 ng	834106	1,4-Dichlorobenzene-d4	8.12

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	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023434.D
Acq On : 3 Aug 2016 20:42
Operator : UM/SJ
Sample : H4287-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-60-7.0-8.0

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

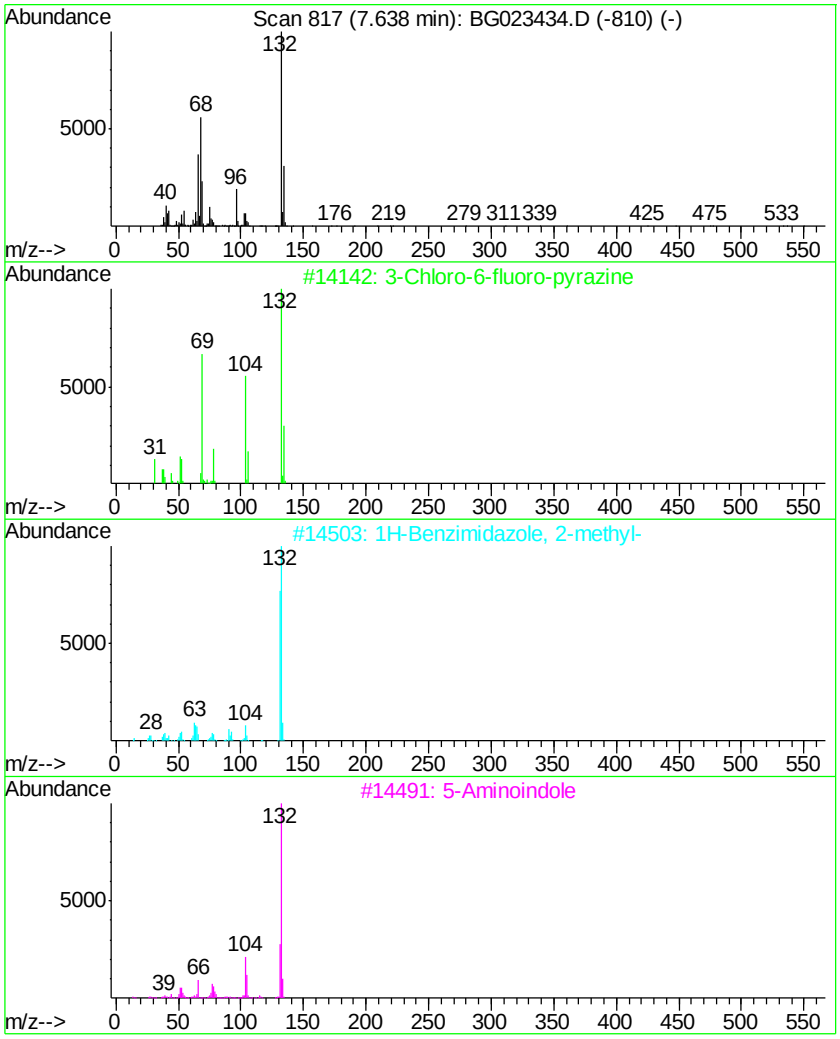
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

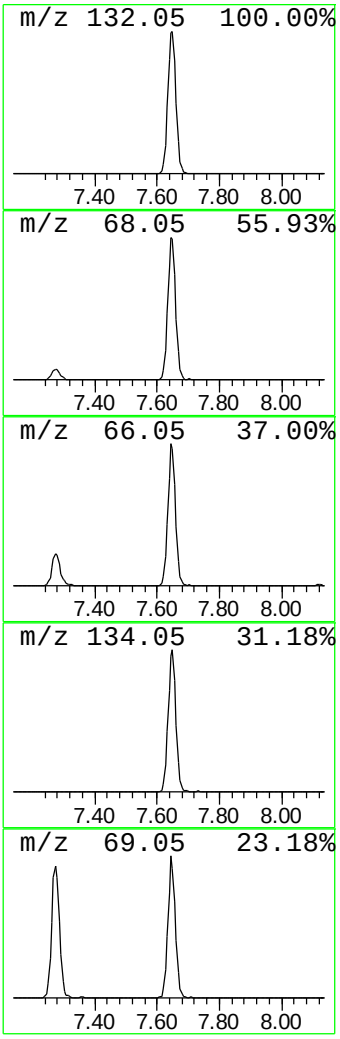
****

Peak Number 3 unknown7.64 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	117.78 ng	3710670	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
3	5-Aminoindole	132	C8H8N2	005192-03-0	10
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023434.D
Acq On : 3 Aug 2016 20:42
Operator : UM/SJ
Sample : H4287-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-60-7.0-8.0

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

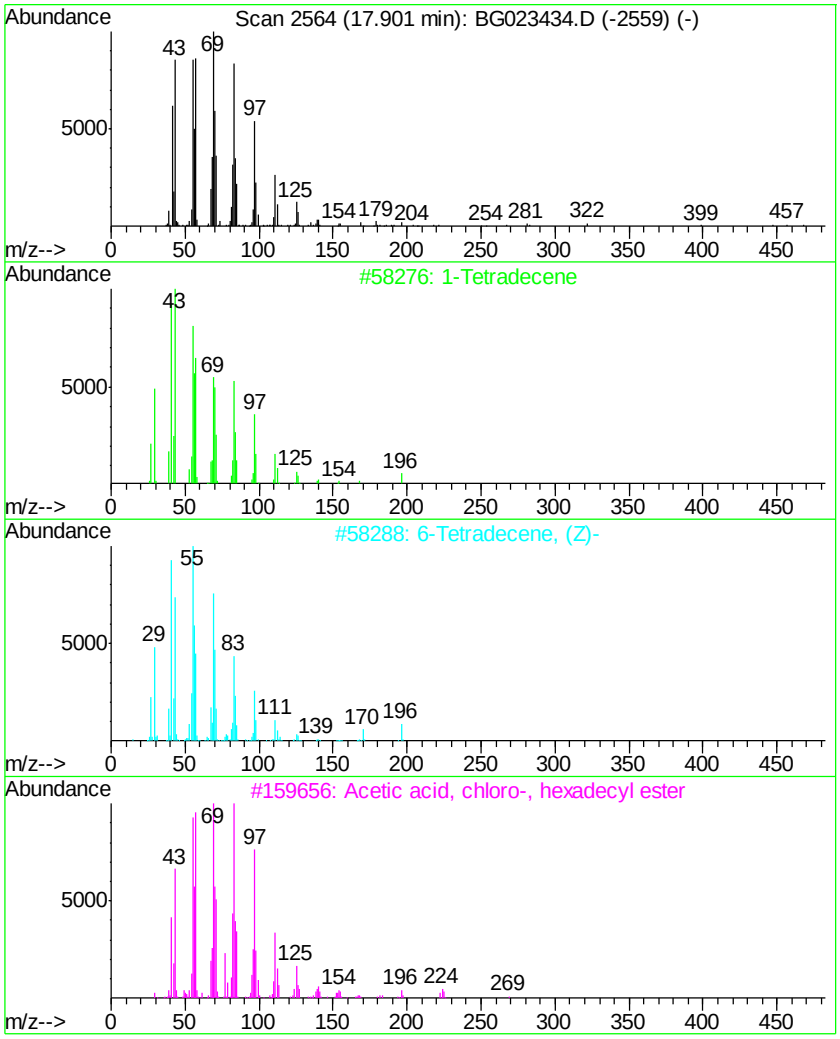
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

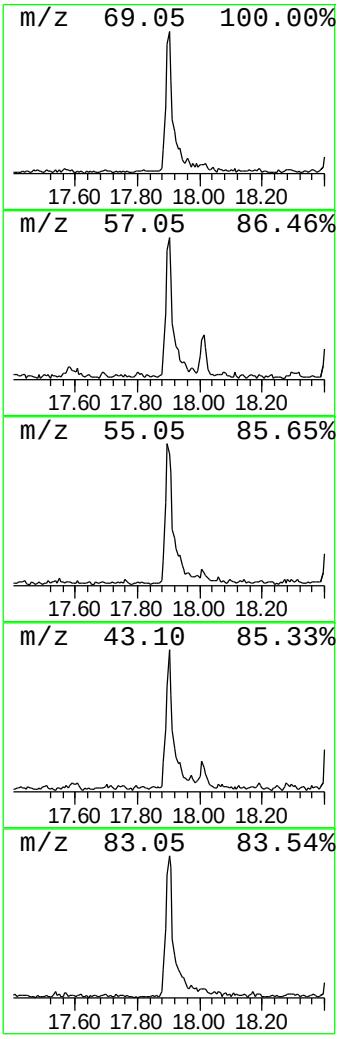
****

Peak Number 5 1-Tetradecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.90	6.94 ng	782843	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetradecene	196	C14H28	001120-36-1	98
2	6-Tetradecene, (Z)-	196	C14H28	041446-61-1	93
3	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	91
4	3-Hexadecene, (Z)-	224	C16H32	034303-81-6	91
5	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91





Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023434.D
Acq On : 3 Aug 2016 20:42
Operator : UM/SJ
Sample : H4287-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-60-7.0-8.0

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

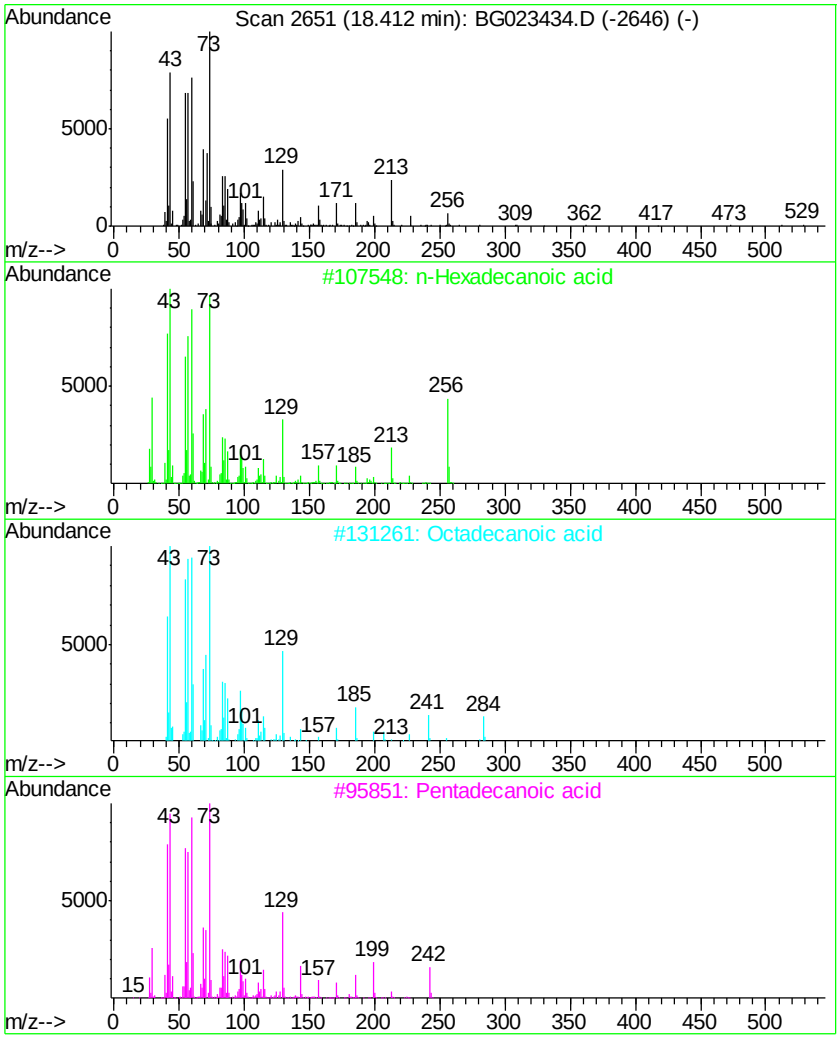
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

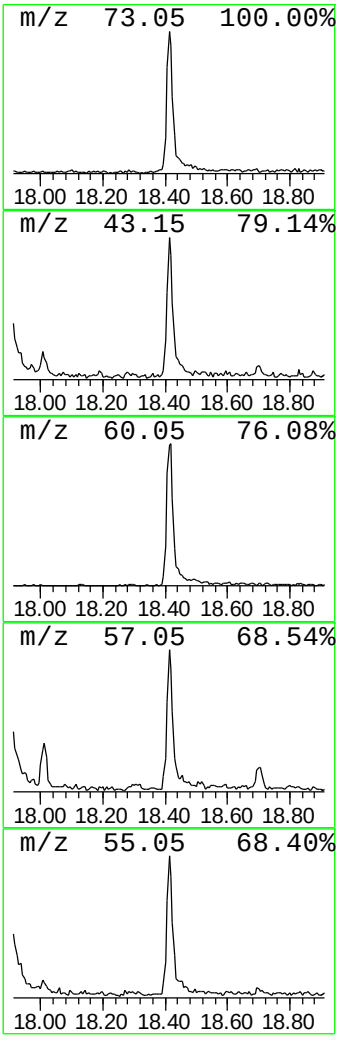
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.41	7.07 ng	797641	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72





Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023434.D
Acq On : 3 Aug 2016 20:42
Operator : UM/SJ
Sample : H4287-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-60-7.0-8.0

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

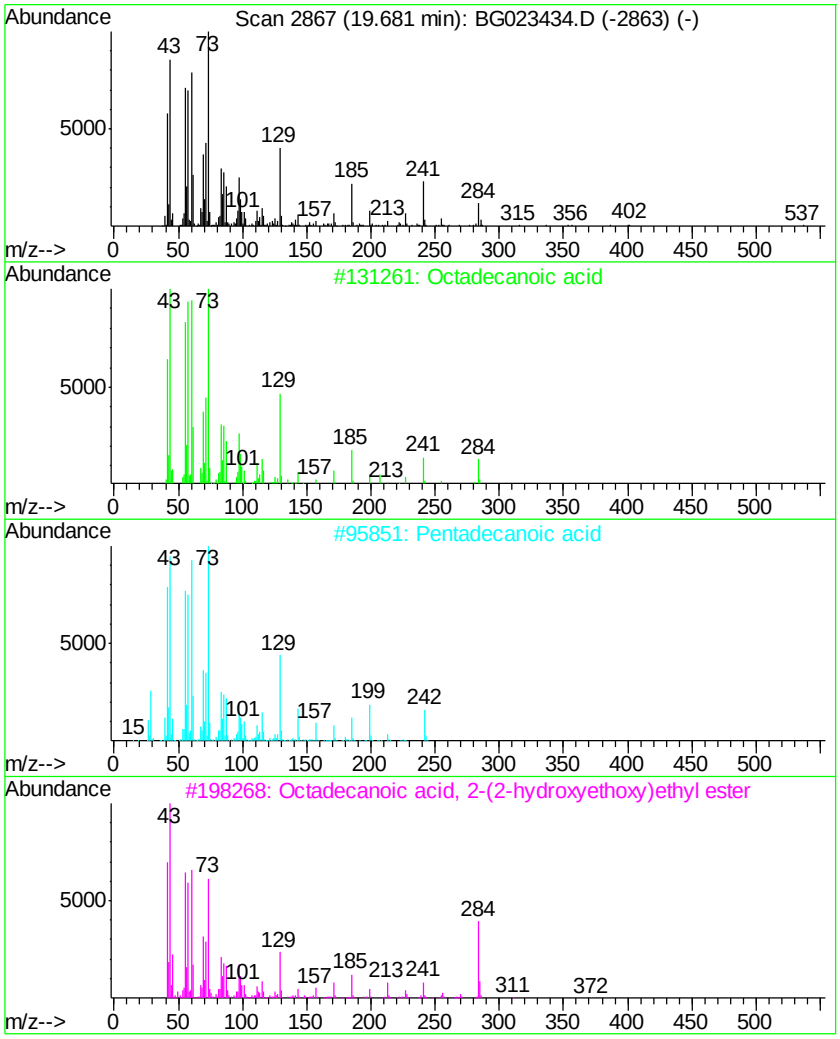
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

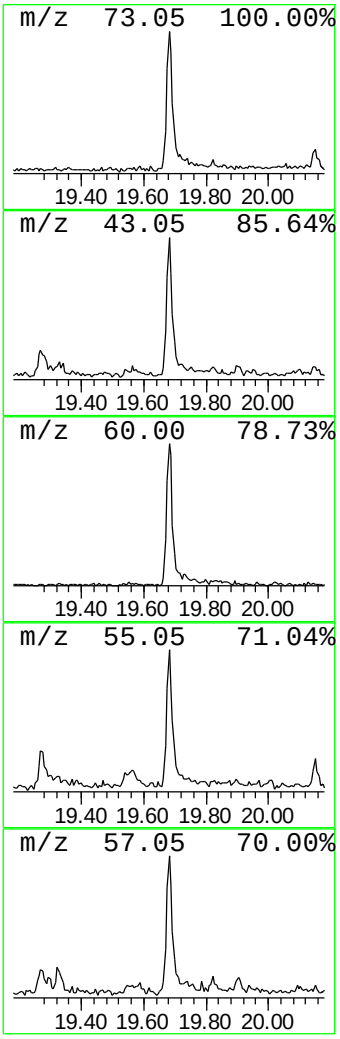
****

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.68	5.80 ng	654588	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023434.D
Acq On : 3 Aug 2016 20:42
Operator : UM/SJ
Sample : H4287-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-60-7.0-8.0

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

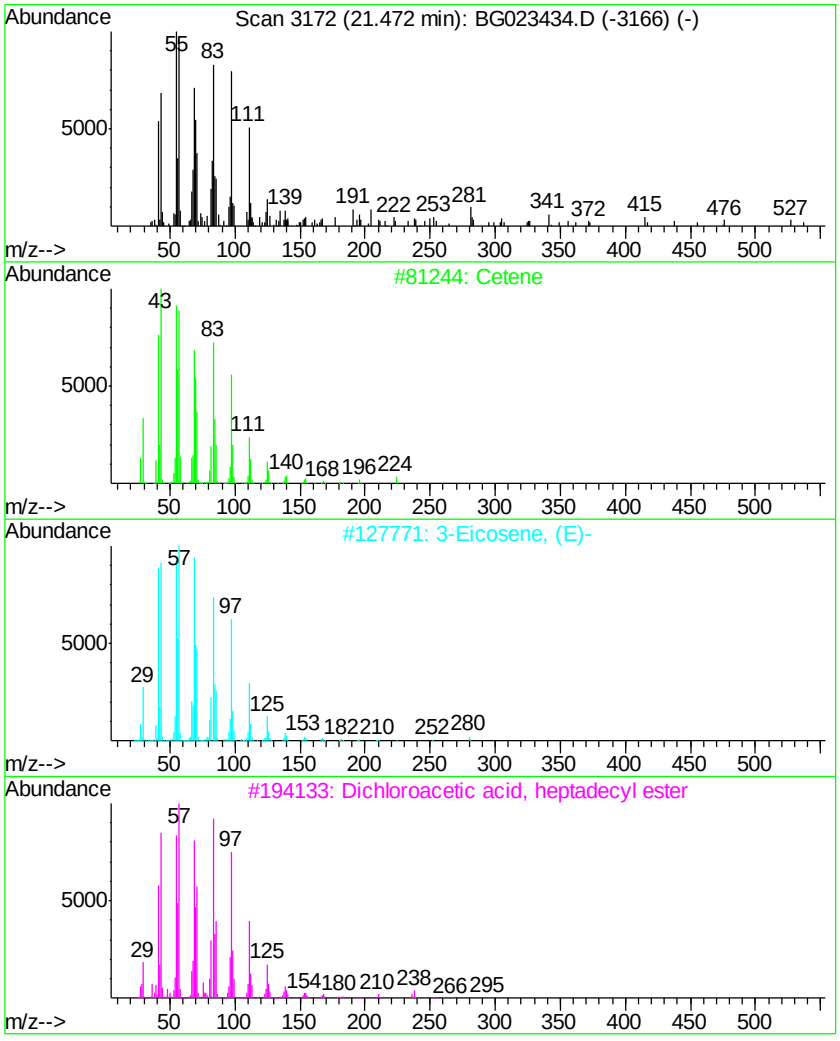
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

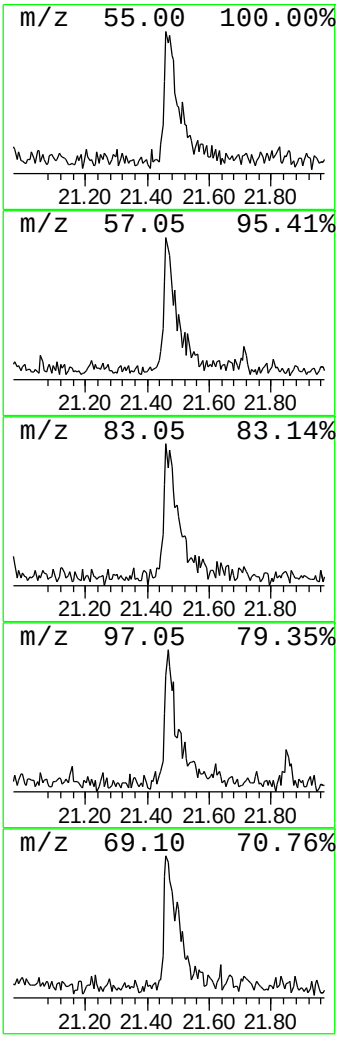
****

Peak Number 8 Cetene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.47	2.12 ng	276087	Chrysene-d12	21.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	90
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	87
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	64
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG080316\
Data File : BG023434.D
Acq On : 3 Aug 2016 20:42
Operator : UM/SJ
Sample : H4287-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-60-7.0-8.0

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown2.99	2.99	143.3	ng	4513060	1	8.12	630083	20.0
2-Pentanone, 4-hy...	5.18	26.5	ng	834106	1	8.12	630083	20.0
unknown7.64	7.64	117.8	ng	3710670	1	8.12	630083	20.0
1-Tetradecene	17.90	6.9	ng	782843	4	17.54	2256310	20.0
n-Hexadecanoic acid	18.41	7.1	ng	797641	4	17.54	2256310	20.0
Octadecanoic acid	19.68	5.8	ng	654588	4	17.54	2256310	20.0
Cetene	21.47	2.1	ng	276087	5	21.85	2602900	20.0