LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043360.D
Acq On : 28 Oct 2019 21:30
Operator : JU
Sample : K5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 161-16-(0-1)

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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	3.193	14	18	26	rVB	46658	62926	2.05%	0.392%
2	5.132	342	348	360	rBV	50260	83618	2.72%	0.520%
3	5.613	422	430	445	rBV	571968	1001704	32.64%	6.232%
4	7.212	694	702	716	rBV	622483	1186456	38.66%	7.382%
5	7.564	755	762	776	rBV	612834	1126544	36.71%	7.009%
6	8.022	833	840	848	rBV	139354	244519	7.97%	1.521%
7	8.345	888	895	910	rVB	426017	785505	25.60%	4.887%
8	9.186	1030	1038	1047	rBV	322079	638721	20.81%	3.974%
9	10.831	1309	1318	1328	rBV	144910	300601	9.80%	1.870%
10	13.275	1727	1734	1747	rBV	994641	1650100	53.77%	10.267%
11	14.103	1869	1875	1886	rBV	63324	121691	3.97%	0.757%
12	14.650	1961	1968	1984	rBV	311280	518624	16.90%	3.227%
13	16.142	2215	2222	2239	rBV	1033609	1789463	58.31%	11.134%
14	17.394	2428	2435	2450	rBV2	395654	709883	23.13%	4.417%
15	18.287	2582	2587	2592	rBV6	24548	46736	1.52%	0.291%
16	19.450	2777	2785	2791	rBV	33366	64963	2.12%	0.404%
17	19.808	2842	2846	2853	rVB2	35525	53591	1.75%	0.333%
18	20.002	2873	2879	2900	rBV	2138242	3068643	100.00%	19.092%
19	21.307	3097	3101	3111	rBV6	42933	106920	3.48%	0.665%
20	21.659	3154	3161	3179	rBV	447841	903592	29.45%	5.622%
21	21.847	3189	3193	3198	rVB2	53566	72706	2.37%	0.452%
22	22.447	3291	3295	3300	rBV	62861	104569	3.41%	0.651%
23	23.140	3404	3413	3422	rVB2	70495	138263	4.51%	0.860%
24	23.328	3438	3445	3453	rVB2	43812	82007	2.67%	0.510%
25	23.933	3542	3548	3556	rVB4	54934	123611	4.03%	0.769%
26	24.861	3695	3706	3722	rBV2	331672	1004140	32.72%	6.248%
27	25.990	3887	3898	3906	rBV7	26935	82541	2.69%	0.514%

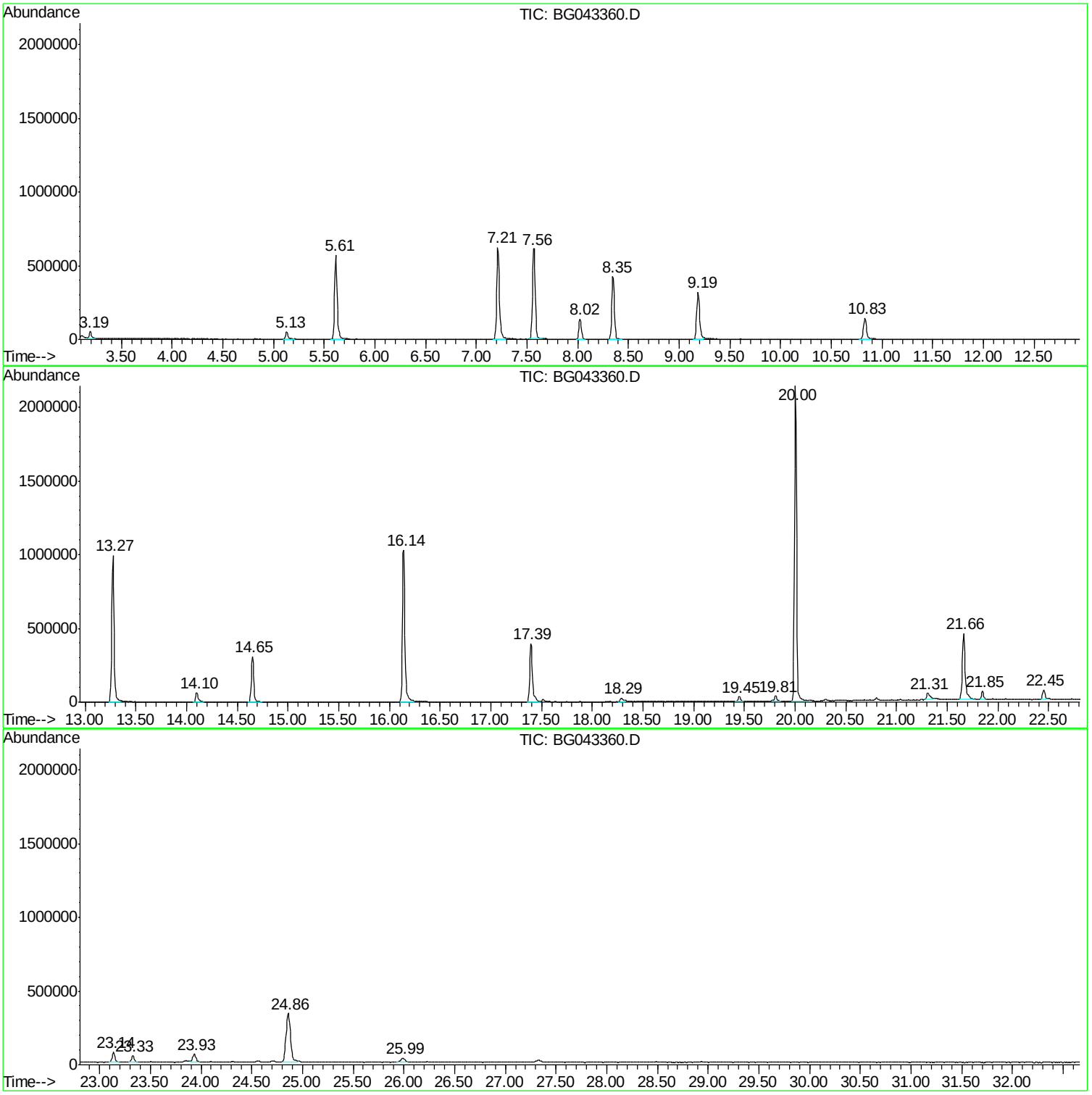
Sum of corrected areas: 16072637

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043360.D
Acq On : 28 Oct 2019 21:30
Operator : JU
Sample : K5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
161-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043360.D
Acq On : 28 Oct 2019 21:30
Operator : JU
Sample : K5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 161-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

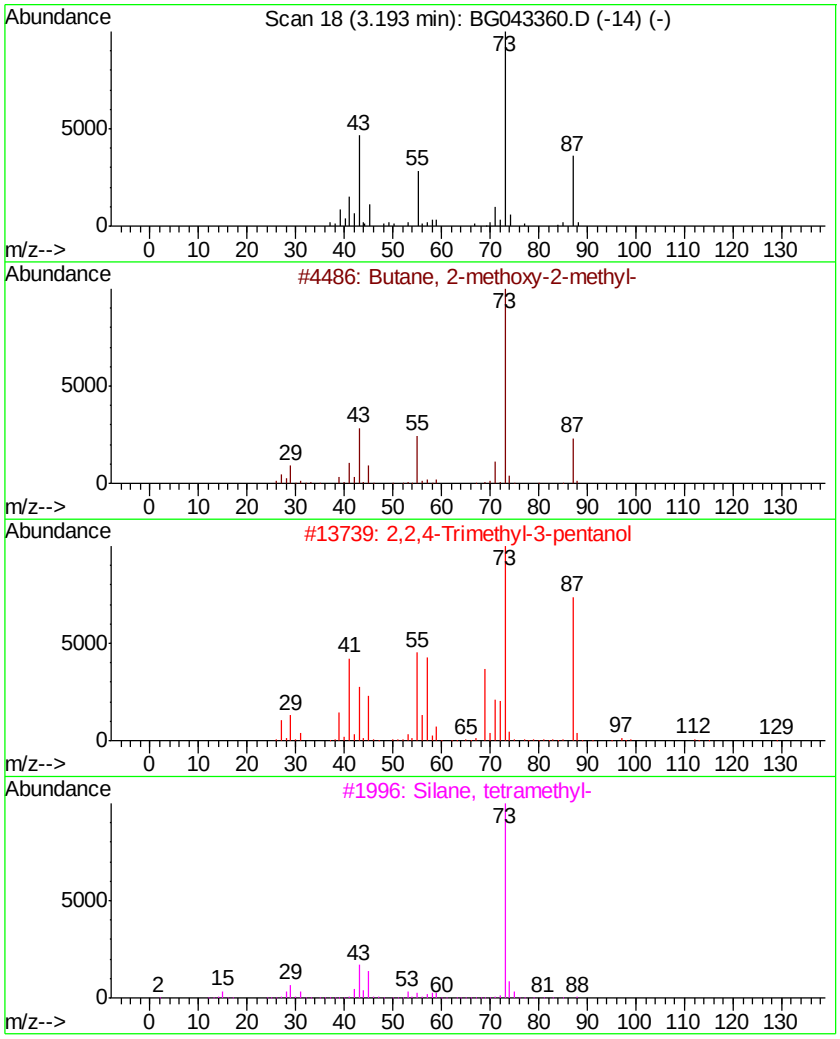
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

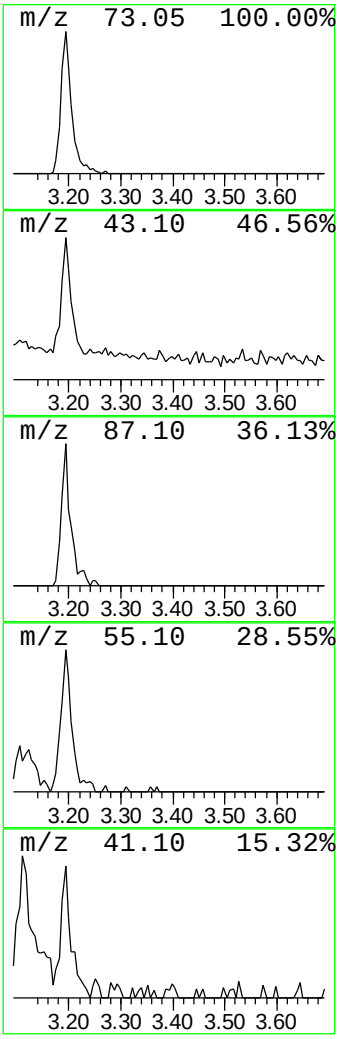
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	5.15 ng	62926	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	38
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043360.D
Acq On : 28 Oct 2019 21:30
Operator : JU
Sample : K5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 161-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

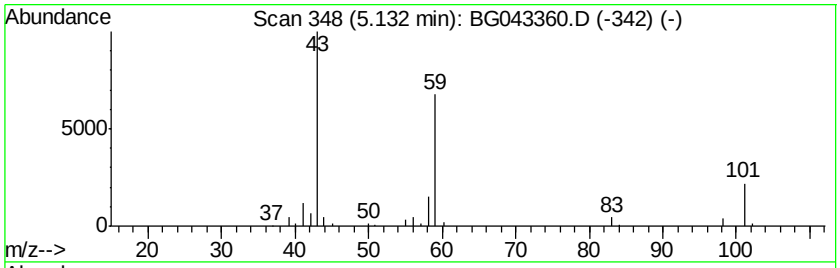
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

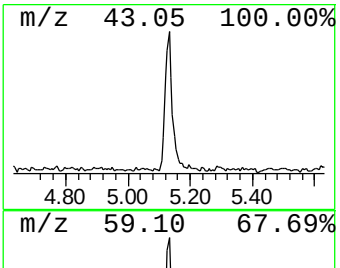
****

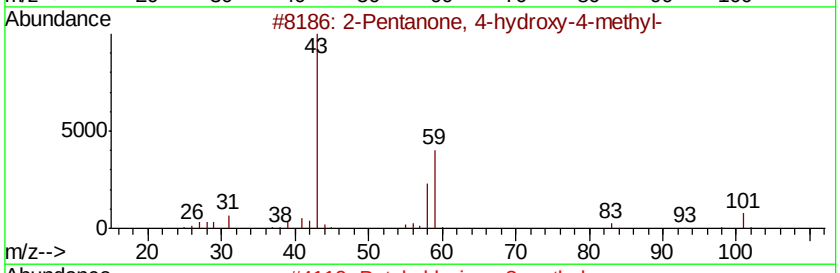
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

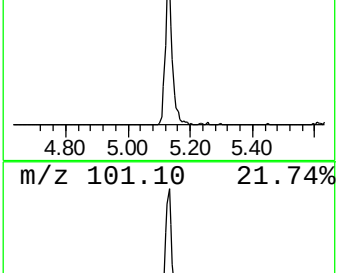
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	6.84 ng	83618	1,4-Dichlorobenzene-d4	8.02

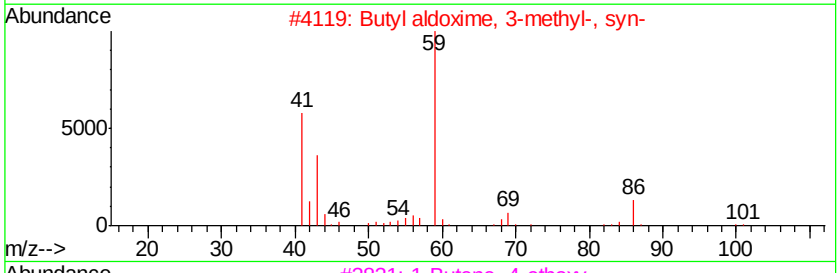
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
3	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9

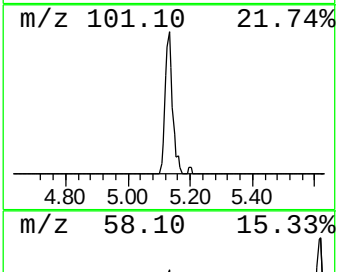


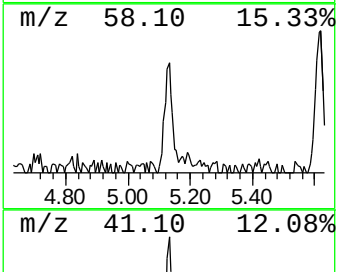


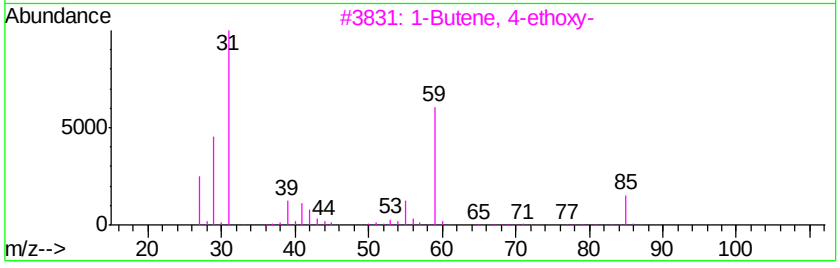


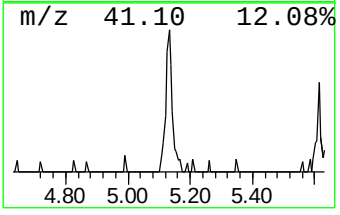












Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043360.D
Acq On : 28 Oct 2019 21:30
Operator : JU
Sample : K5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 161-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

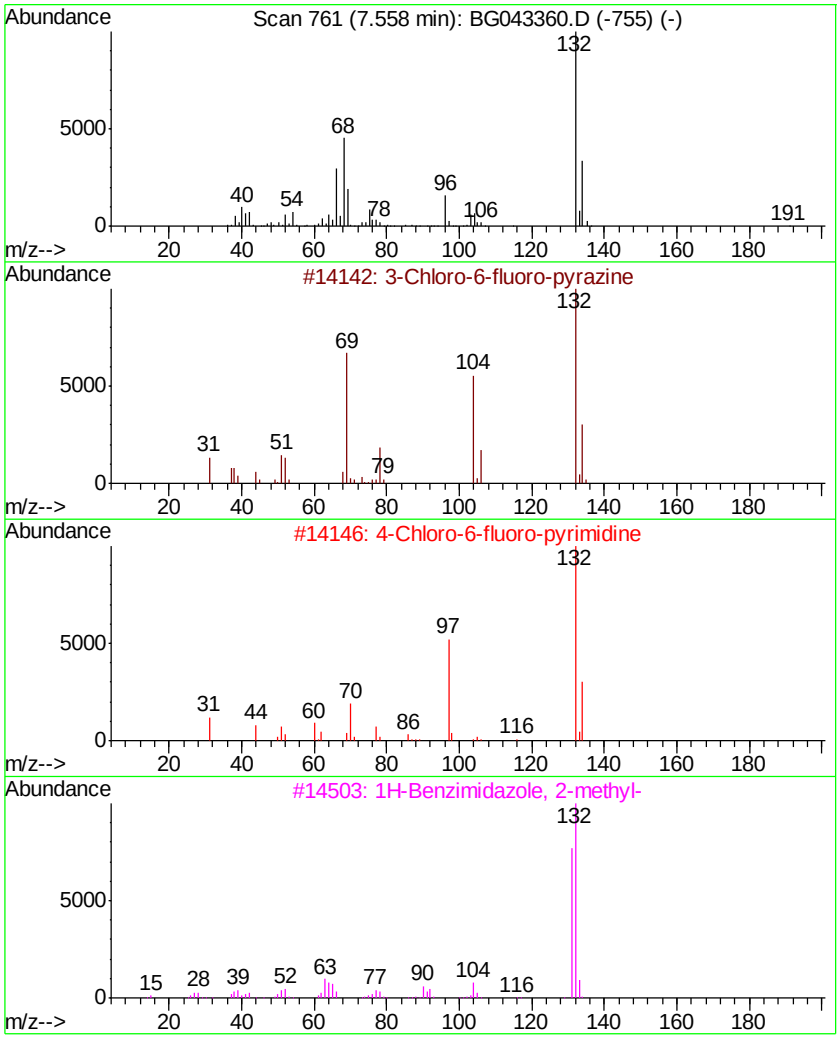
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

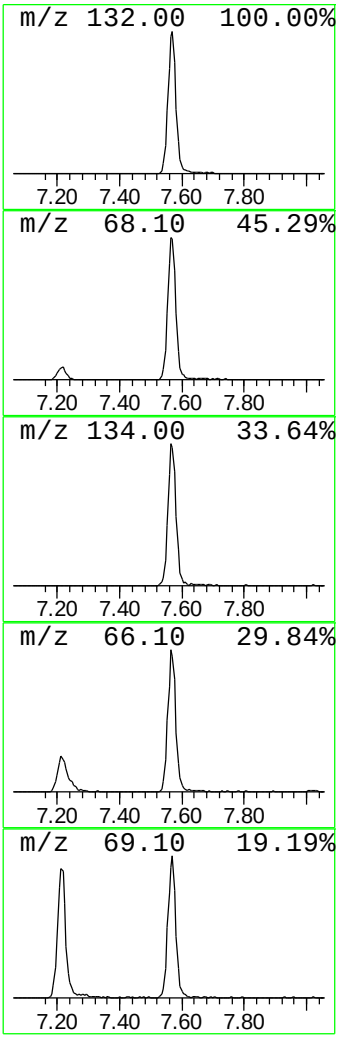
****

Peak Number 3 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	92.14 ng	1126540	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	22
5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043360.D
Acq On : 28 Oct 2019 21:30
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Sample : K5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 161-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

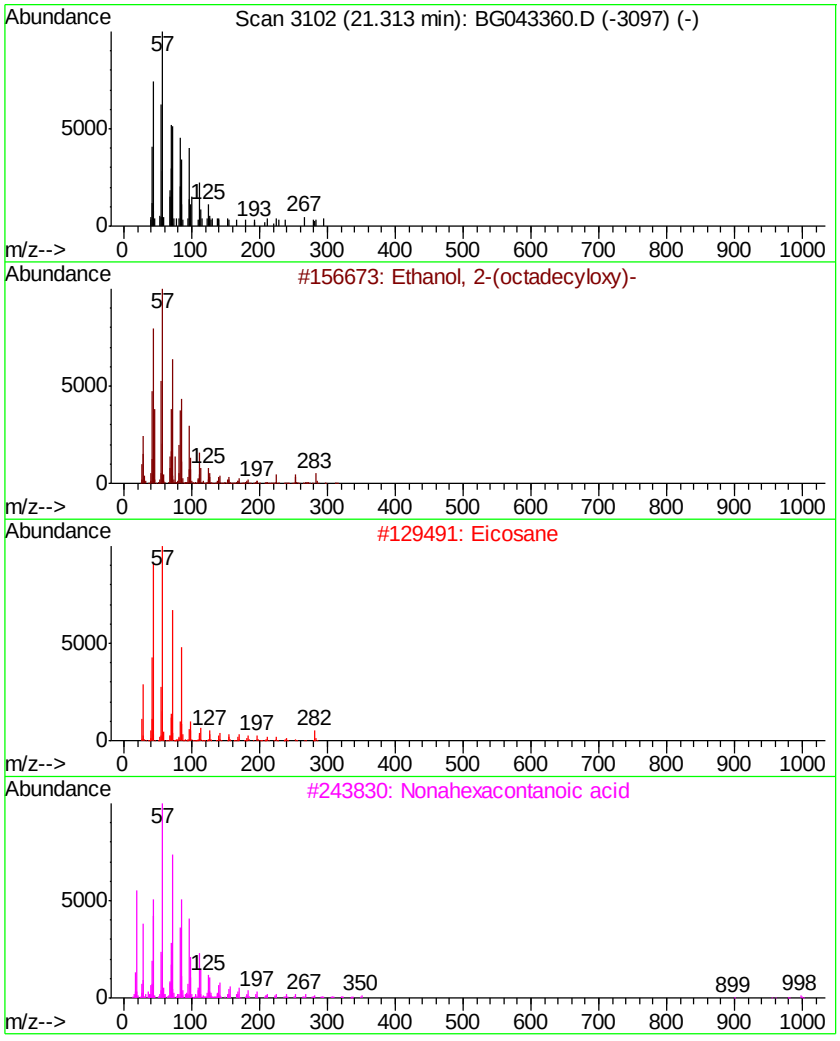
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

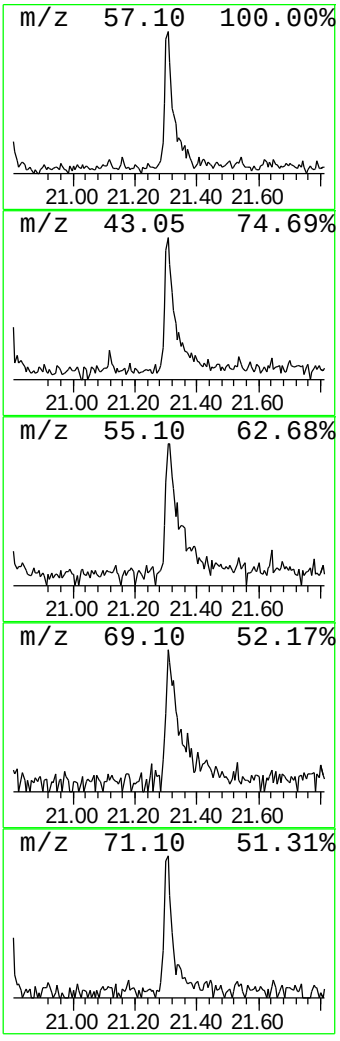
****

Peak Number 5 Ethanol, 2-(octadecyloxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	2.37 ng	106920	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	91
2	Eicosane	282	C20H42	000112-95-8	89
3	Nonahexacontanoic acid	999	C69H138O2	040710-32-5	87
4	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	87
5	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043360.D
Acq On : 28 Oct 2019 21:30
Operator : JU
Sample : K5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 161-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

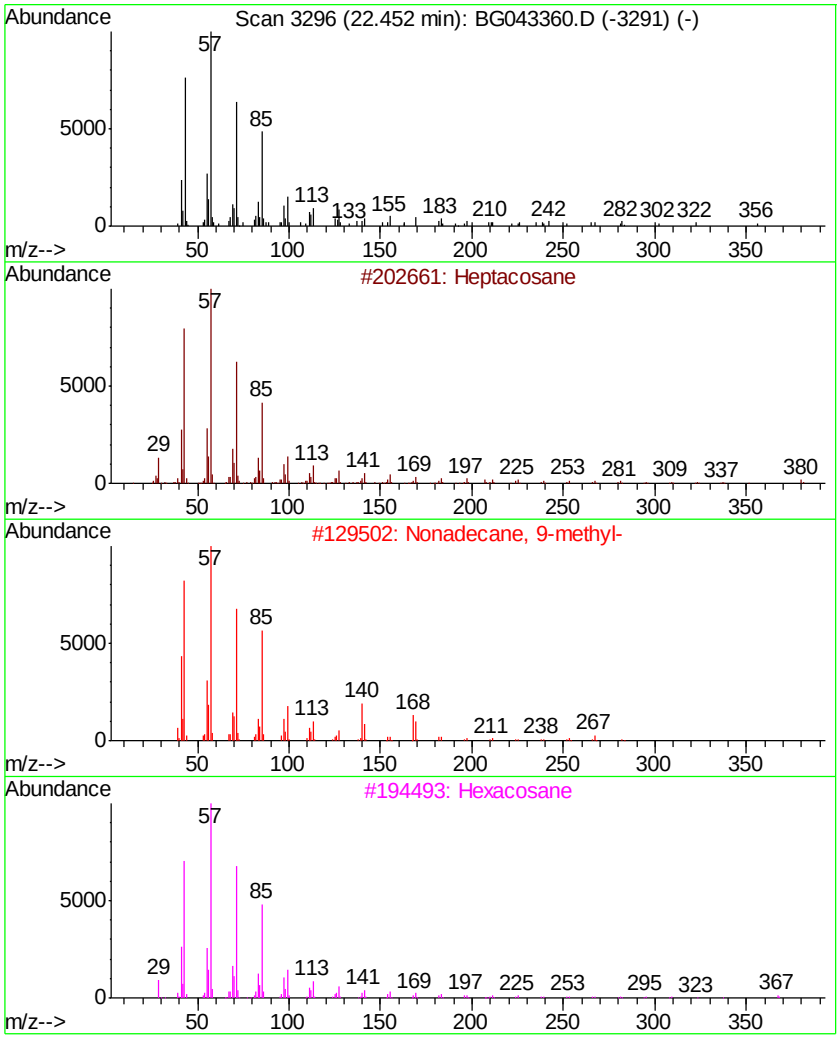
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

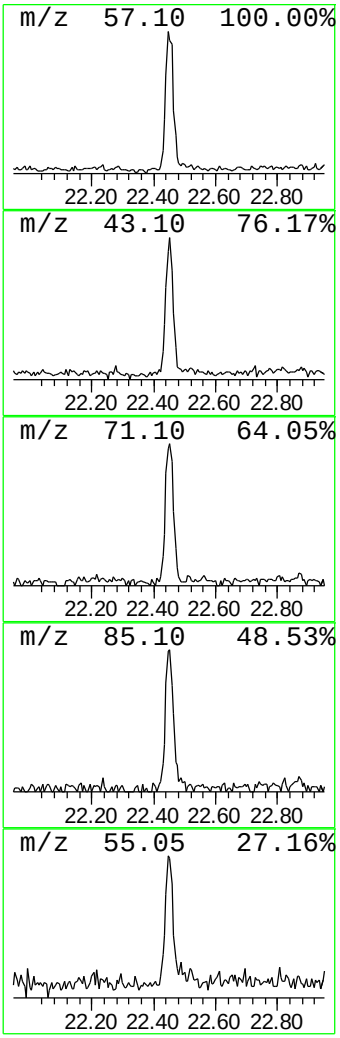
****

Peak Number 6 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.45	2.31 ng	104569	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Octadecane	254	C18H38	000593-45-3	90
5	Hentriacontane	437	C31H64	000630-04-6	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043360.D
Acq On : 28 Oct 2019 21:30
Operator : JU
Sample : K5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 161-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

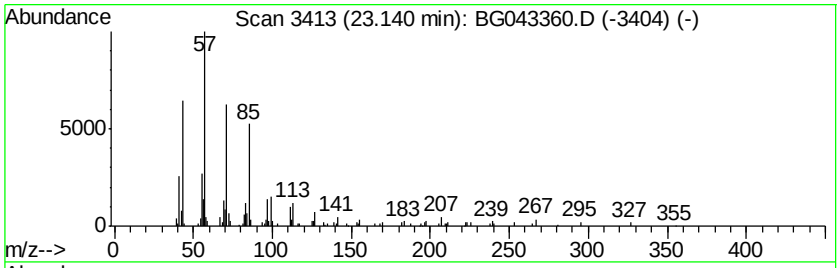
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

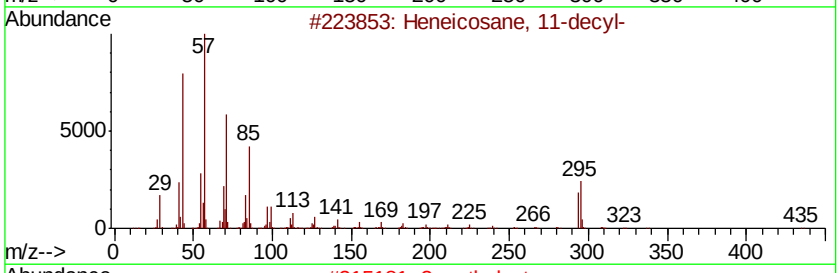
****

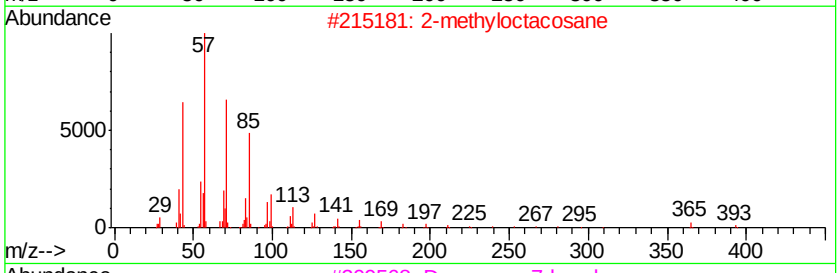
Peak Number 7 Heneicosane, 11-decyl- Concentration Rank 5

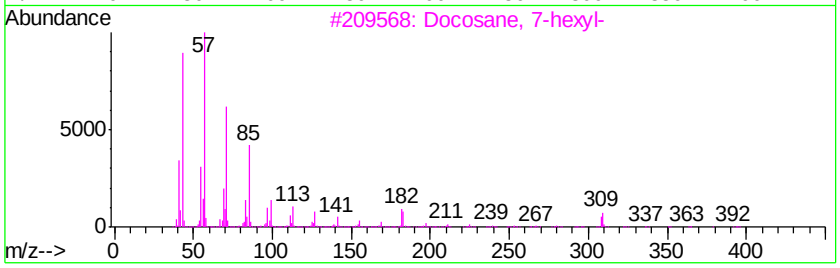
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.14	3.06 ng	138263	Chrysene-d12	21.66

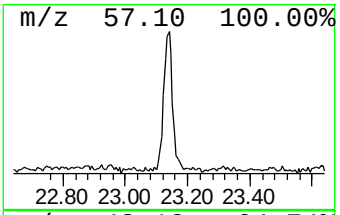
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Docosane, 7-hexyl-	394	C28H58	055373-86-9	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87

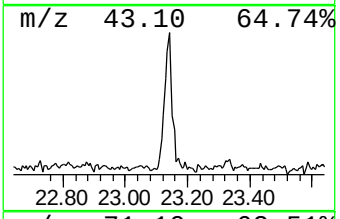


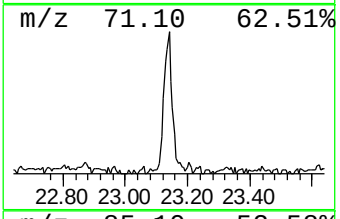


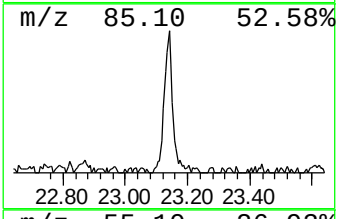


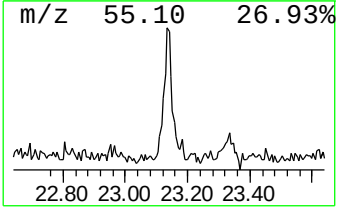












Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043360.D
Acq On : 28 Oct 2019 21:30
Operator : JU
Sample : K5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 161-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

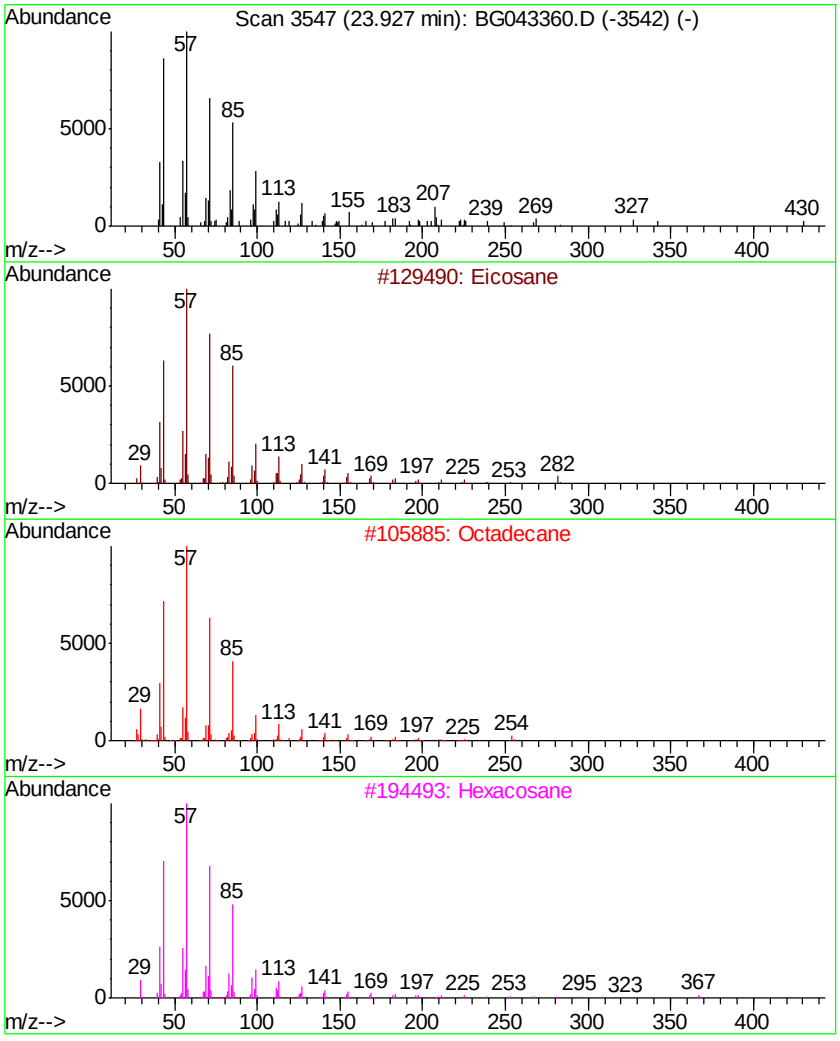
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

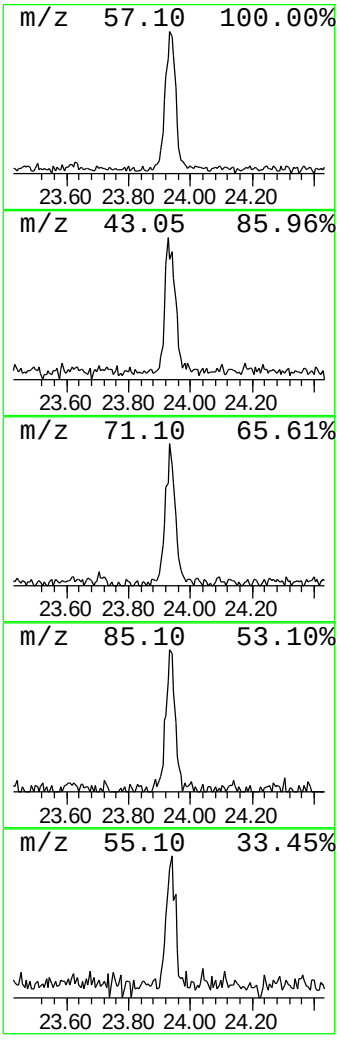
****

Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.93	2.46 ng	123611	Perylene-d12	24.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Octadecane	254	C18H38	000593-45-3	96
3	Hexacosane	366	C26H54	000630-01-3	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Tetratetracontane	619	C44H90	007098-22-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG102819\
Data File : BG043360.D
Acq On : 28 Oct 2019 21:30
Operator : JU
Sample : K5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 161-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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
Butane, 2-methoxy...	3.19	5.2	ng	62926	1	8.02	244519	20.0
2-Pentanone, 4-hy...	5.13	6.8	ng	83618	1	8.02	244519	20.0
unknown7.56	7.56	92.1	ng	1126540	1	8.02	244519	20.0
Ethanol, 2-(octad...	21.31	2.4	ng	106920	5	21.66	903592	20.0
Heptacosane	22.45	2.3	ng	104569	5	21.66	903592	20.0
Heneicosane, 11-d...	23.14	3.1	ng	138263	5	21.66	903592	20.0
Eicosane	23.93	2.5	ng	123611	6	24.86	1004140	20.0