LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100219\
Data File : BG042992.D
Acq On : 2 Oct 2019 19:44
Operator : JU
Sample : K5154-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106D

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-BG092519.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	3.182	8	16	24	rBV2	229011	595509	10.10%	2.020%
2	3.264	24	30	44	rVB	414329	792947	13.45%	2.690%
3	5.655	427	437	448	rBV	984043	1623400	27.53%	5.507%
4	7.242	699	707	719	rBV	716498	1323901	22.45%	4.491%
5	7.606	761	769	778	rBV	1279897	2284388	38.74%	7.750%
6	8.070	840	848	856	rBV	259297	445820	7.56%	1.512%
7	8.393	895	903	916	rBV	950490	1709490	28.99%	5.799%
8	9.228	1034	1045	1056	rBV	779942	1446903	24.54%	4.908%
9	10.873	1317	1325	1334	rBV	305656	573126	9.72%	1.944%
10	11.778	1471	1479	1488	rBV	136687	278579	4.72%	0.945%
11	13.317	1733	1741	1753	rBV	2249471	3496727	59.29%	11.862%
12	14.134	1874	1880	1886	rBV	100135	156952	2.66%	0.532%
13	14.686	1964	1974	1983	rBV	526344	852601	14.46%	2.892%
14	16.172	2219	2227	2241	rBV	2116192	3207652	54.39%	10.882%
15	17.430	2435	2441	2454	rBV2	695012	1056587	17.92%	3.584%
16	18.317	2586	2592	2602	rBV2	161601	243182	4.12%	0.825%
17	19.586	2804	2808	2812	rBV5	44268	63187	1.07%	0.214%
18	20.038	2879	2885	2893	rBV	4422707	5897174	100.00%	20.005%
19	21.355	3104	3109	3124	rBV5	75333	260490	4.42%	0.884%
20	21.701	3161	3168	3175	rBV	723791	1234062	20.93%	4.186%
21	22.506	3301	3305	3310	rBV3	48724	78356	1.33%	0.266%
22	23.205	3418	3424	3431	rVB2	72898	135910	2.30%	0.461%
23	24.010	3556	3561	3570	rVB2	74753	156971	2.66%	0.533%
24	24.927	3706	3717	3732	rBV	442651	1442920	24.47%	4.895%
25	26.108	3913	3918	3926	rVB6	47156	120958	2.05%	0.410%

Sum of corrected areas: 29477792

LSC Report - Integrated Chromatogram

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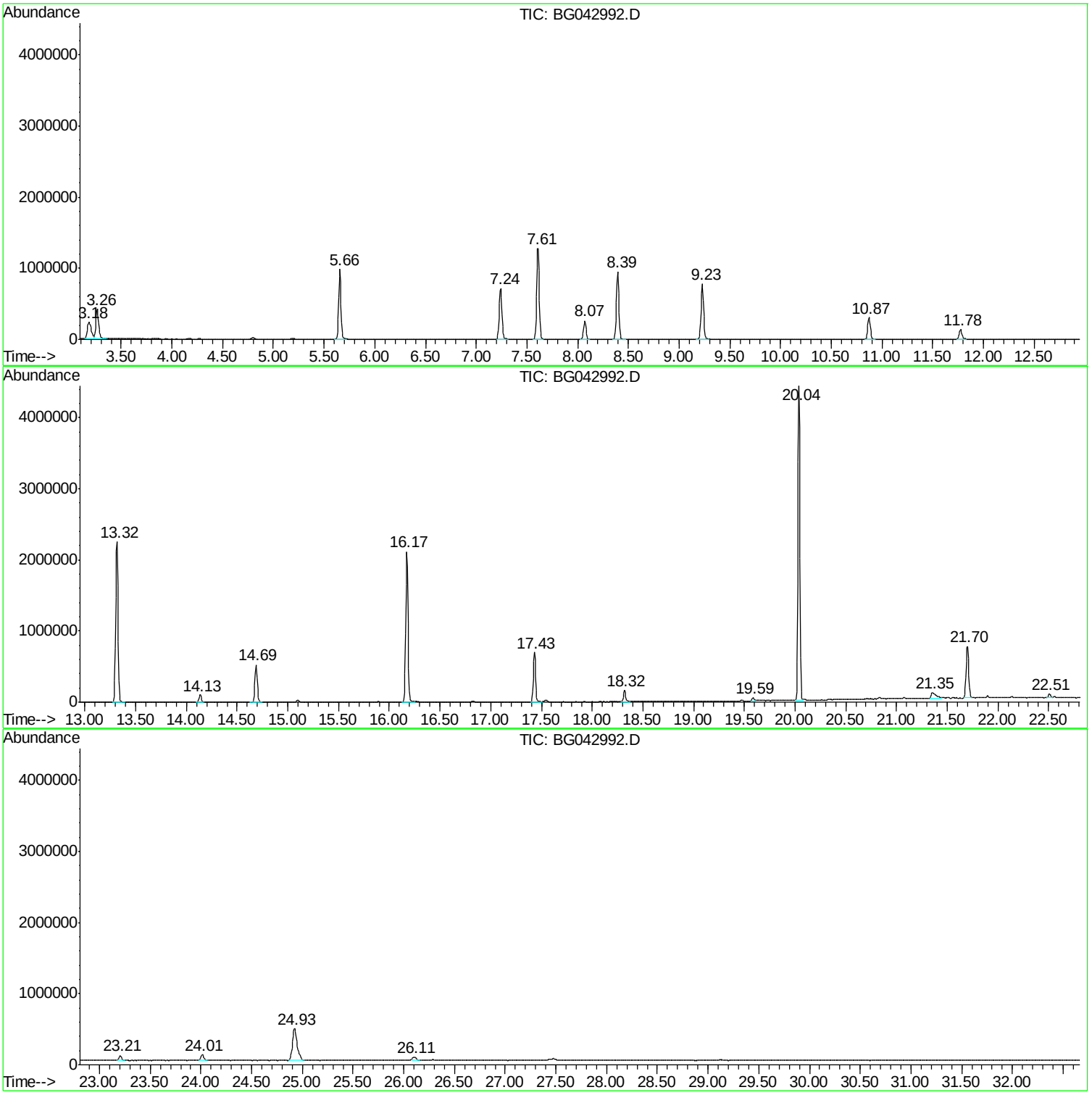
Acq On : 2 Oct 2019 19:44
Operator : JU
Sample : K5154-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100219\
Data File : BG042992.D
Acq On : 2 Oct 2019 19:44
Operator : JU
Sample : K5154-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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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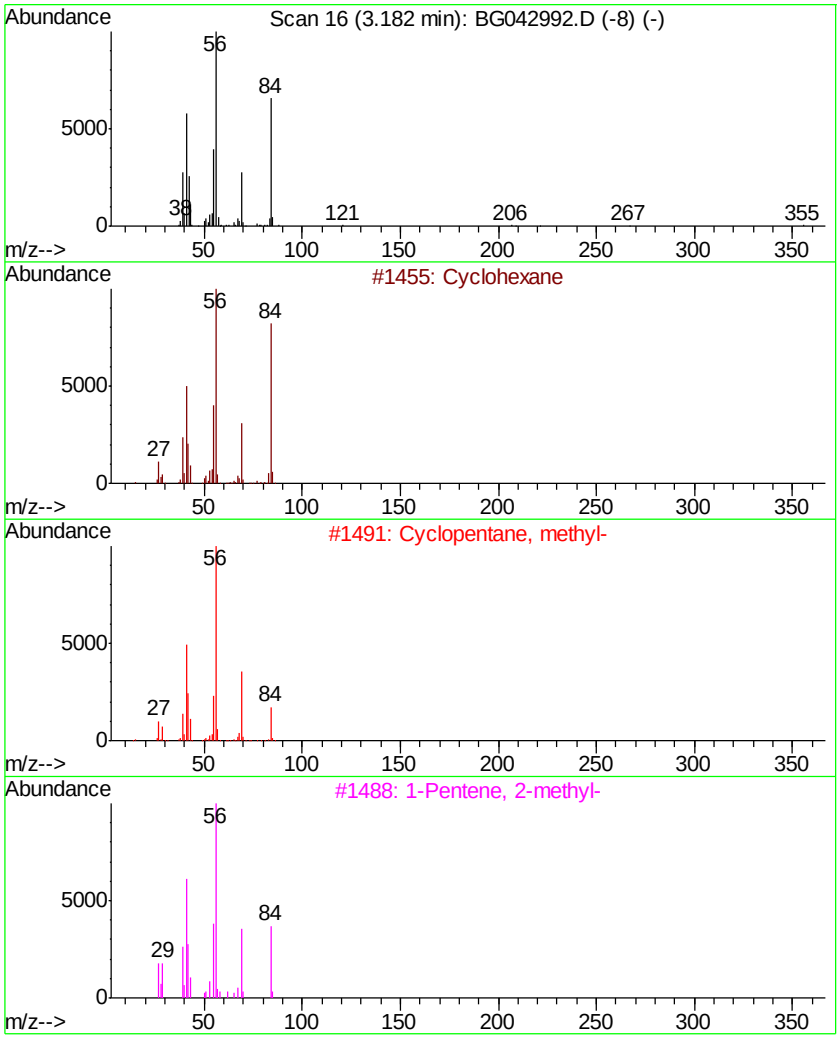
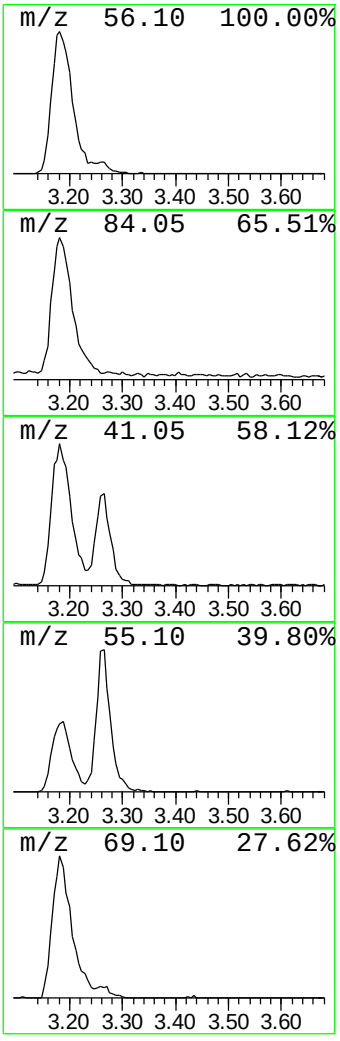
Peak Number 1 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	26.72 ng	595509	1,4-Dichlorobenzene-d4	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	94
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	72
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	56
4	1-Hexene	84	C6H12	000592-41-6	50
5	Cyclobutane	56	C4H8	000287-23-0	43





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Data File : BG042992.D
Acq On : 2 Oct 2019 19:44
Operator : JU
Sample : K5154-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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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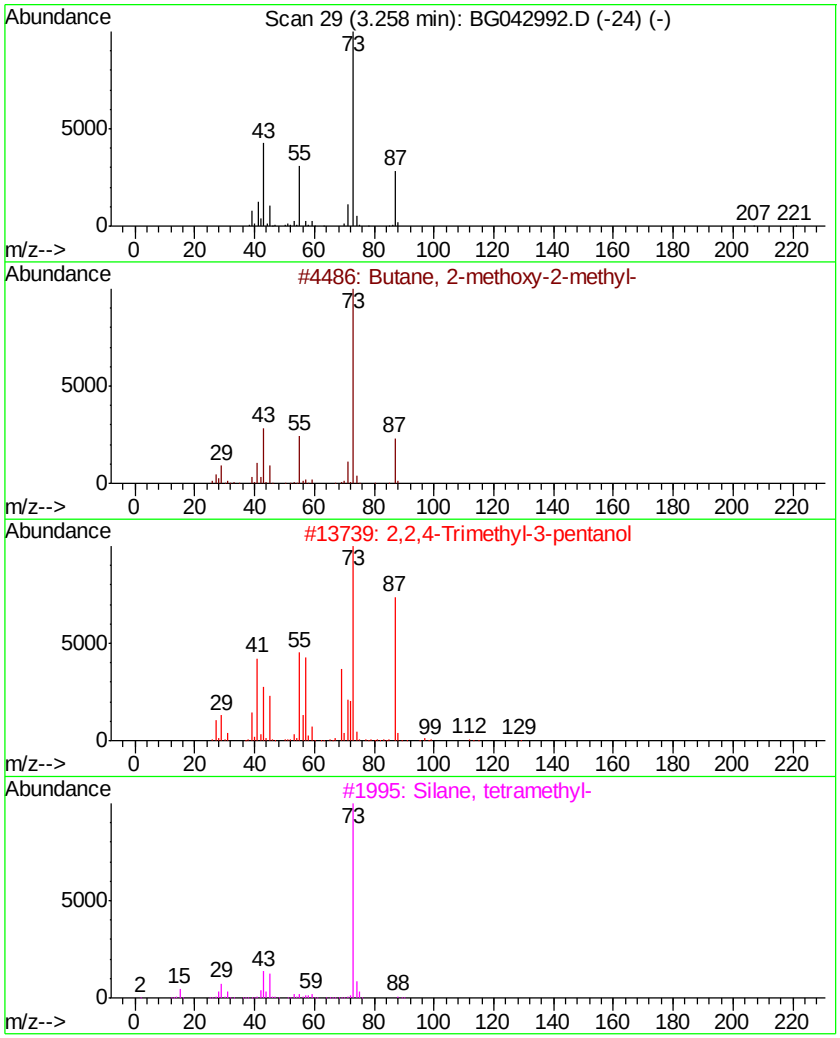
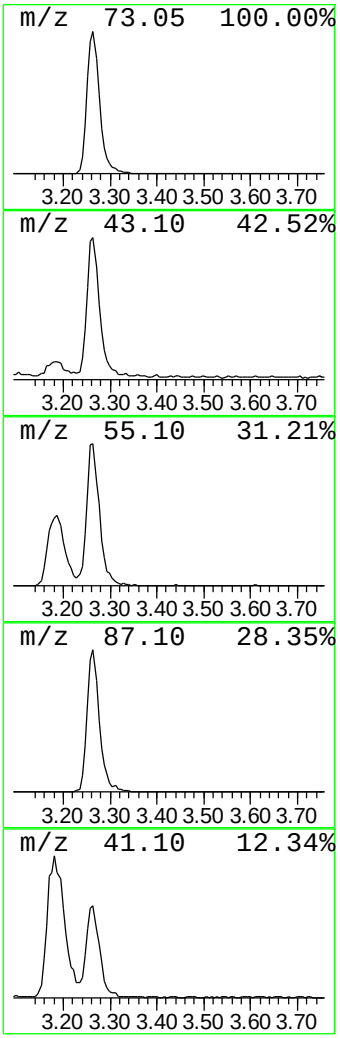
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.26	35.57 ng	792947	1,4-Dichlorobenzene-d4	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100219\
Data File : BG042992.D
Acq On : 2 Oct 2019 19:44
Operator : JU
Sample : K5154-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

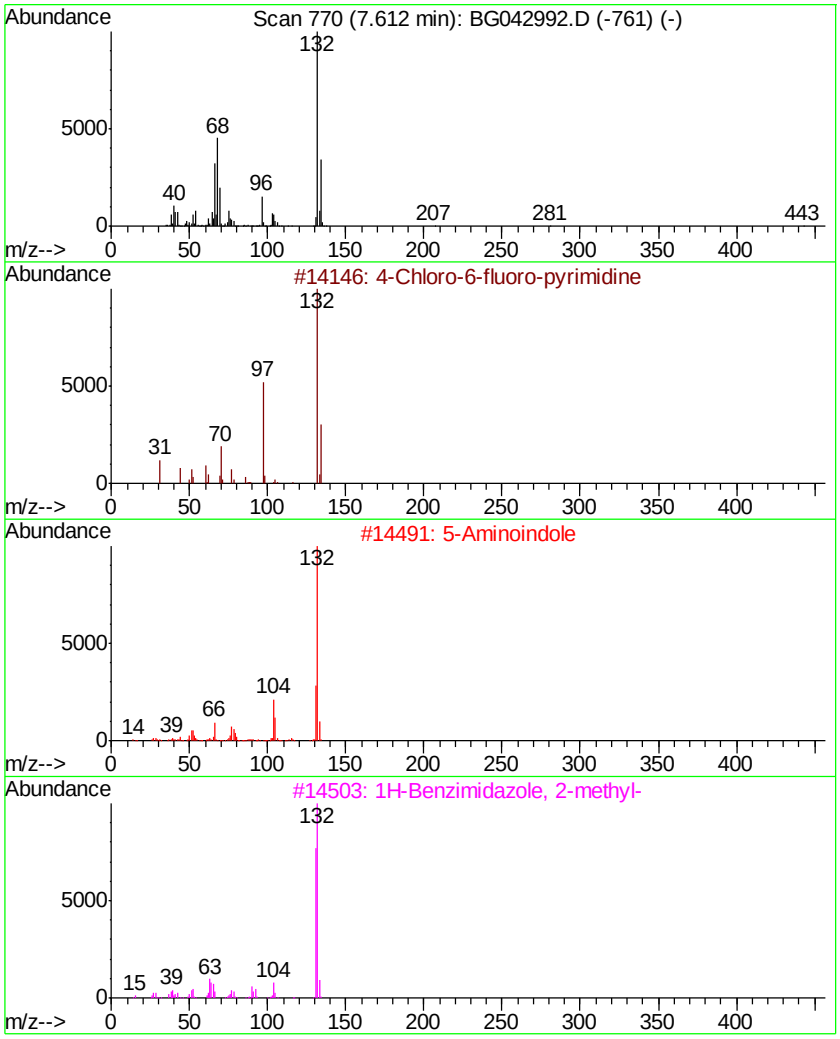
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

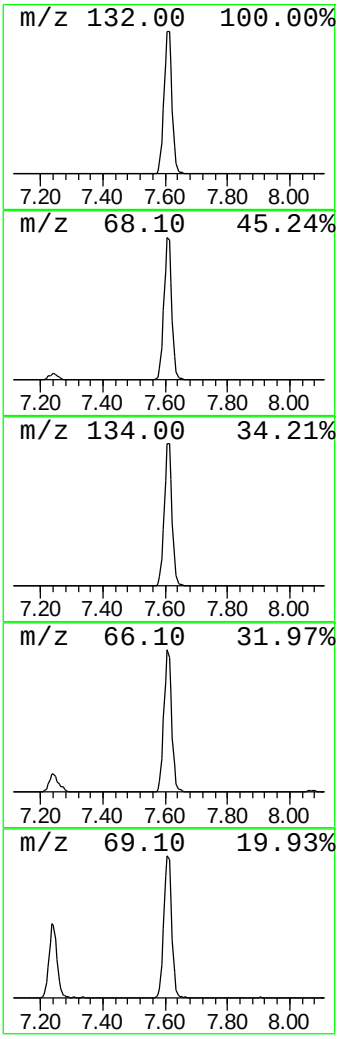
****

Peak Number 3 unknown7.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.61	102.48 ng	2284390	1,4-Dichlorobenzene-d4	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	22
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16





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Data File : BG042992.D
Acq On : 2 Oct 2019 19:44
Operator : JU
Sample : K5154-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

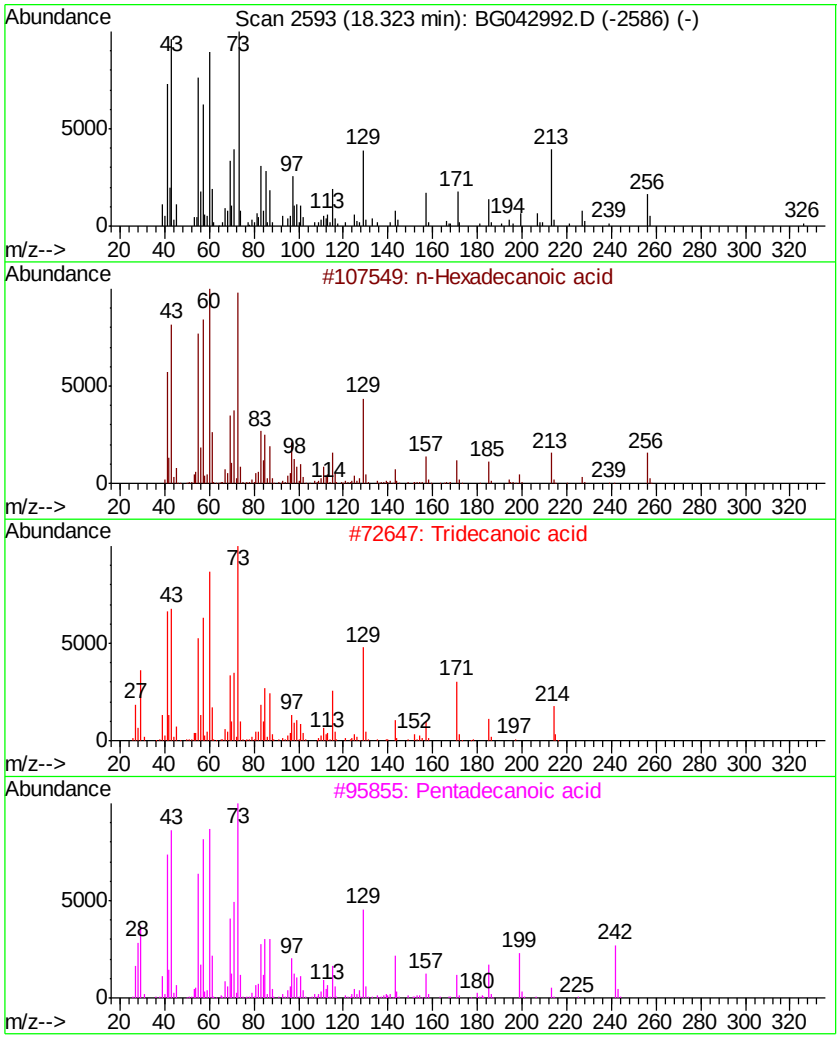
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

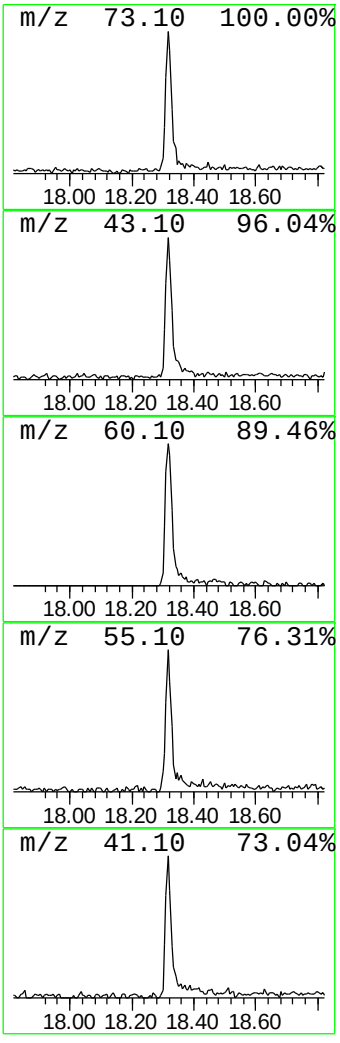
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	4.60 ng	243182	Phenanthrene-d10	17.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Nonanoic acid	158	C9H18O2	000112-05-0	30
5	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	18





Library Search Compound Report

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Data File : BG042992.D
Acq On : 2 Oct 2019 19:44
Operator : JU
Sample : K5154-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

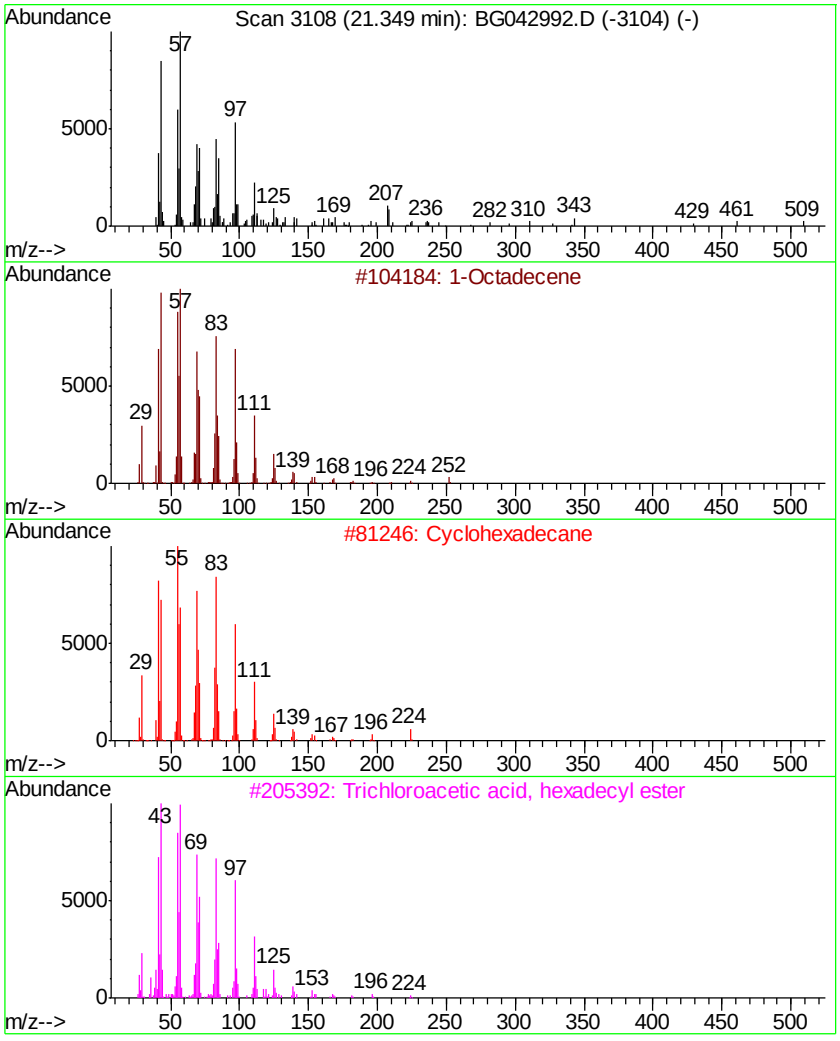
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

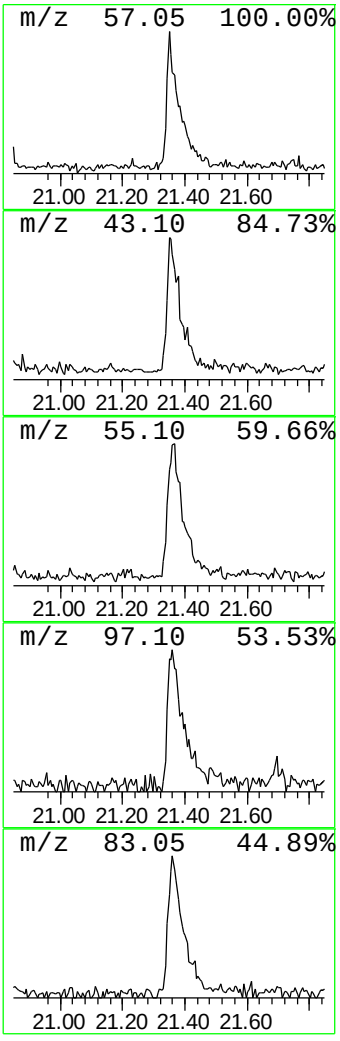
****

Peak Number 6 1-Octadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	4.22 ng	260490	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	96
2	Cyclohexadecane	224	C16H32	000295-65-8	96
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
4	E-15-Heptadecenal	252	C17H32O	1000130-97-9	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





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Data File : BG042992.D
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Operator : JU
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

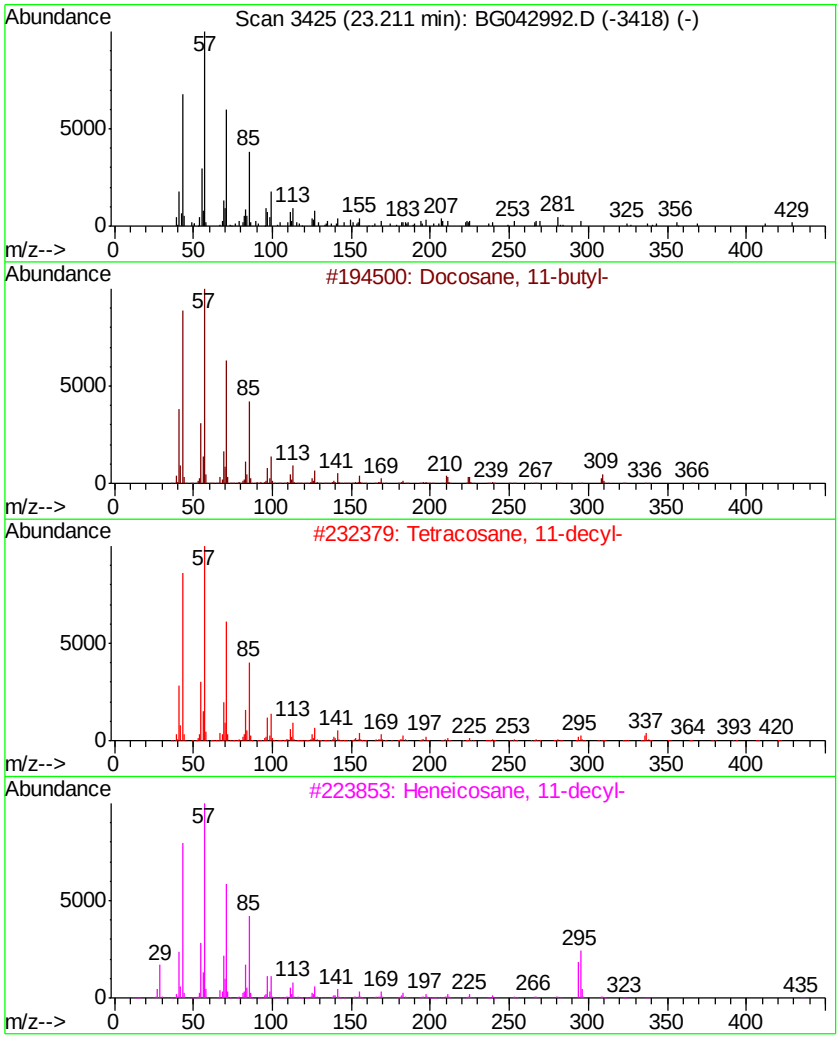
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

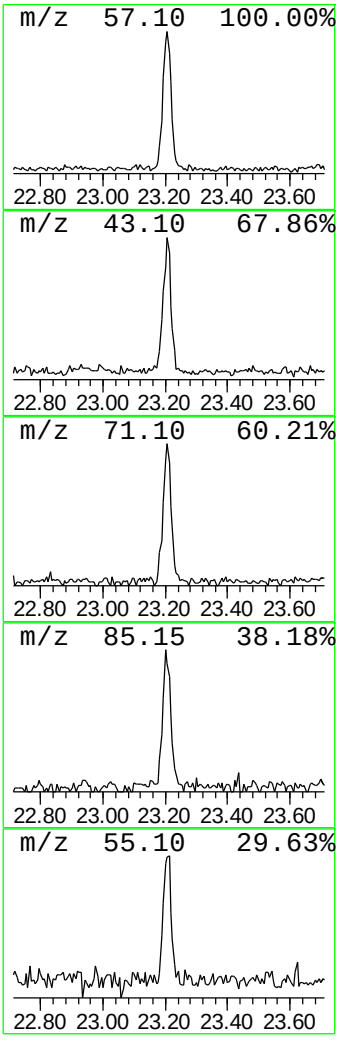
****

Peak Number 7 Docosane, 11-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.21	2.20 ng	135910	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	81
2	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	81
3	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	81
4	Tetracosane	338	C24H50	000646-31-1	74
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	74





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Instrument : BNA_G
ClientSampleId : MW-106D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

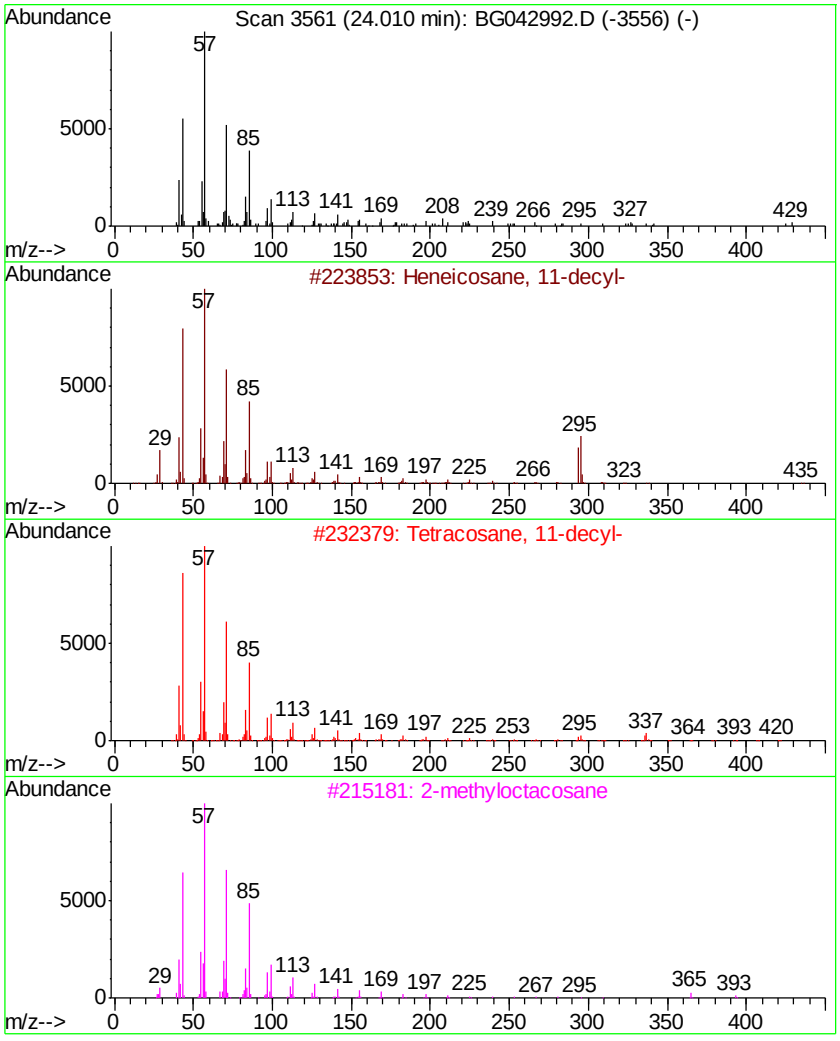
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

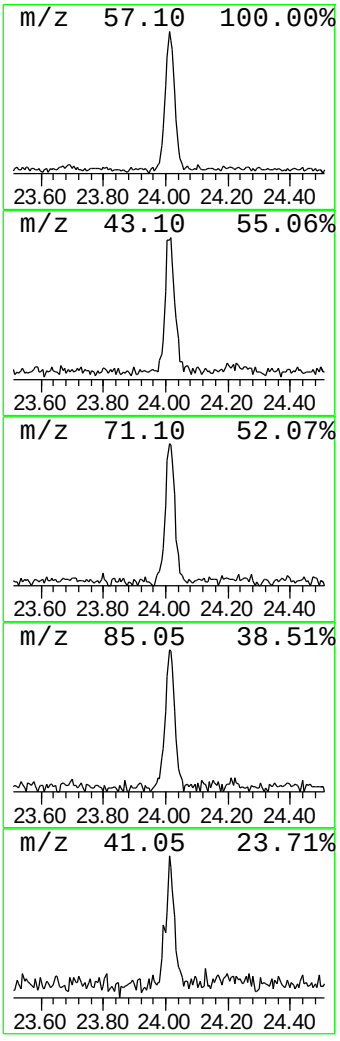
****

Peak Number 8 Heneicosane, 11-decyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.01	2.18 ng	156971	Perylene-d12	24.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	83
2	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	80
3	2-methyloctacosane	408	C29H60	1000376-72-8	80
4	Octadecane	254	C18H38	000593-45-3	80
5	Hexacosane	366	C26H54	000630-01-3	80





Tentatively Identified Compound (LSC) summary

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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
Cyclopentane, met...	3.18	26.7	ng	595509	1	8.07	445820	20.0
Butane, 2-methoxy...	3.26	35.6	ng	792947	1	8.07	445820	20.0
unknown7.61	7.61	102.5	ng	2284390	1	8.07	445820	20.0
n-Hexadecanoic acid	18.32	4.6	ng	243182	4	17.43	1056590	20.0
1-Octadecene	21.35	4.2	ng	260490	5	21.70	1234060	20.0
Docosane, 11-butyl-	23.21	2.2	ng	135910	5	21.70	1234060	20.0
Heneicosane, 11-d...	24.01	2.2	ng	156971	6	24.93	1442920	20.0