LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG100719\
Data File : BG043080.D
Acq On : 7 Oct 2019 23:00
Operator : JU
Sample : PB123704BL
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB123704BL

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	3.164	8	13	22	rBV	252407	478091	8.28%	1.843%
2	3.240	22	26	42	rVB	608020	849125	14.70%	3.273%
3	4.568	246	252	261	rBV	78703	120285	2.08%	0.464%
4	5.167	348	354	360	rBV	81189	123950	2.15%	0.478%
5	5.637	426	434	446	rBV	671837	1107786	19.18%	4.269%
6	7.229	694	705	716	rBV	498633	929461	16.10%	3.582%
7	7.594	760	767	776	rBV	968054	1695857	29.37%	6.536%
8	8.058	839	846	854	rBV	191629	328588	5.69%	1.266%
9	8.381	893	901	911	rBV	679860	1206967	20.90%	4.652%
10	9.215	1035	1043	1052	rBV	571043	1057815	18.32%	4.077%
11	10.860	1314	1323	1333	rBV	239756	452745	7.84%	1.745%
12	13.305	1731	1739	1750	rBV	1754263	2800920	48.50%	10.795%
13	14.127	1872	1879	1885	rBV	114957	177040	3.07%	0.682%
14	14.679	1965	1973	1984	rBV2	460848	758539	13.14%	2.923%
15	16.166	2218	2226	2240	rBV	1914247	2972336	51.47%	11.455%
16	17.423	2432	2440	2449	rBV2	655810	1045320	18.10%	4.029%
17	18.310	2586	2591	2601	rBV4	71595	169684	2.94%	0.654%
18	20.032	2877	2884	2895	rBV	4239232	5774768	100.00%	22.256%
19	20.332	2929	2935	2944	rBV2	52478	63159	1.09%	0.243%
20	20.825	3015	3019	3023	rBV	82412	98719	1.71%	0.380%
21	21.336	3101	3106	3111	rBV	96312	122755	2.13%	0.473%
22	21.689	3159	3166	3181	rVB	740595	1259048	21.80%	4.852%
23	21.883	3194	3199	3204	rVB	115745	157197	2.72%	0.606%
24	22.488	3297	3302	3308	rBV	116845	194878	3.37%	0.751%
25	23.181	3414	3420	3427	rVB2	107050	205230	3.55%	0.791%
26	23.986	3550	3557	3567	rBV3	87642	193718	3.35%	0.747%
27	24.909	3702	3714	3726	rBV2	413840	1389101	24.05%	5.354%
28	26.066	3903	3911	3919	rVB6	52746	146642	2.54%	0.565%
29	26.748	4022	4027	4034	rVB10	28215	67519	1.17%	0.260%

Sum of corrected areas: 25947243

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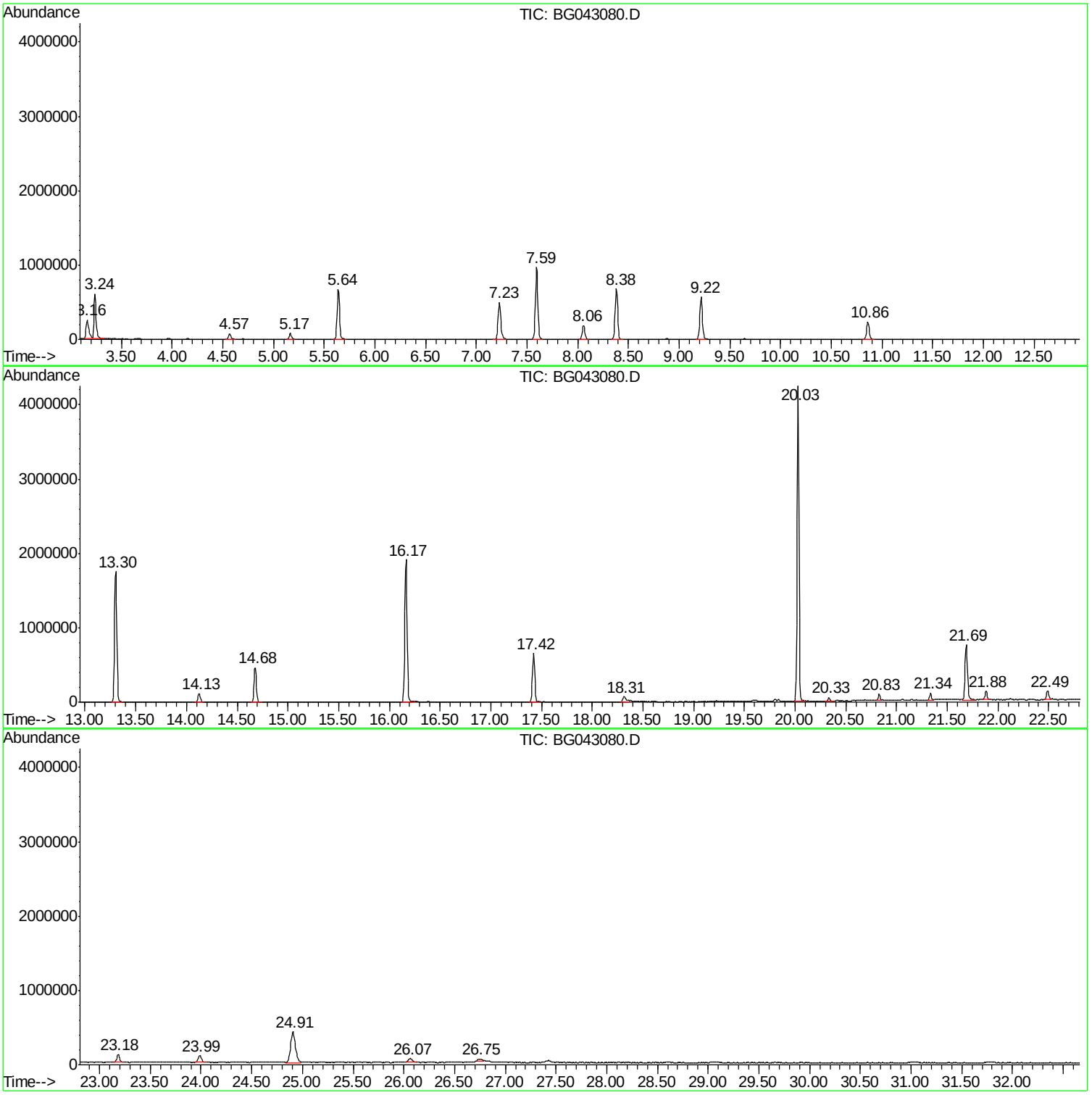
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB123704BL

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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Data File : BG043080.D
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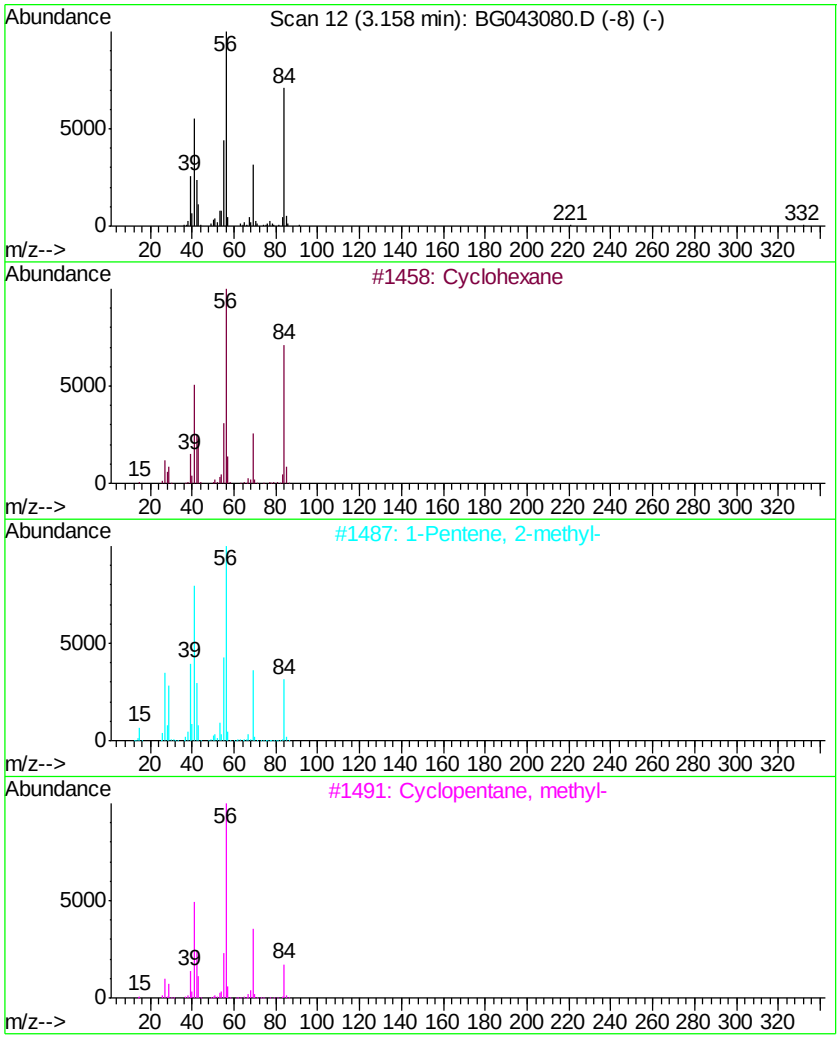
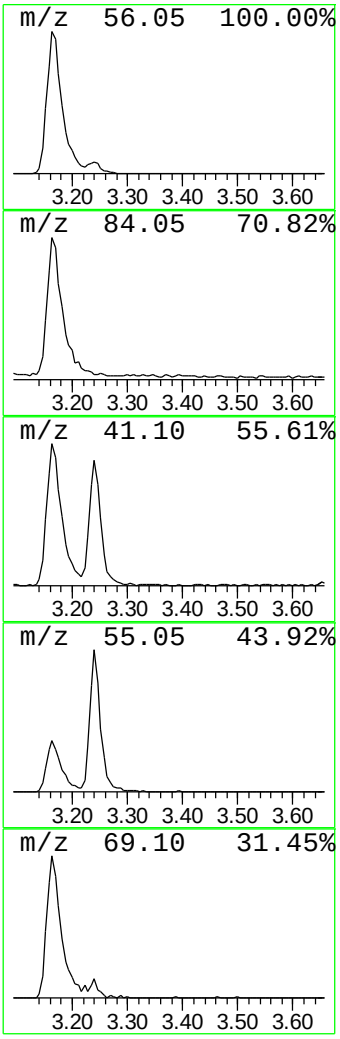
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.16	29.10 ng	478091	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	91
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	80
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	72
4	Cyanic acid, 2-methylpropyl ester	99	C5H9NO	001768-25-8	64
5	1-Hexene	84	C6H12	000592-41-6	53





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Instrument : BNA_G
ClientSampleId : PB123704BL

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

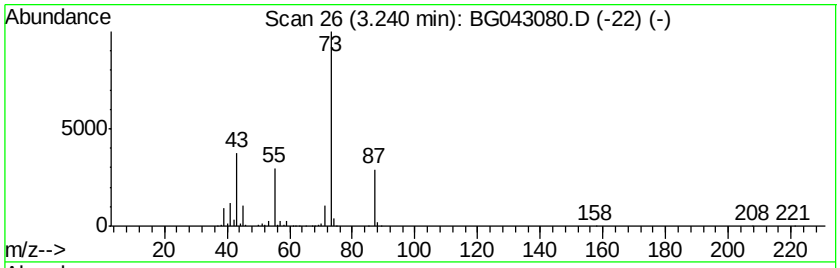
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

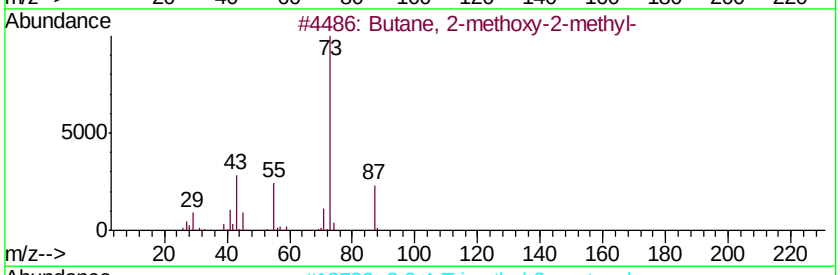
****

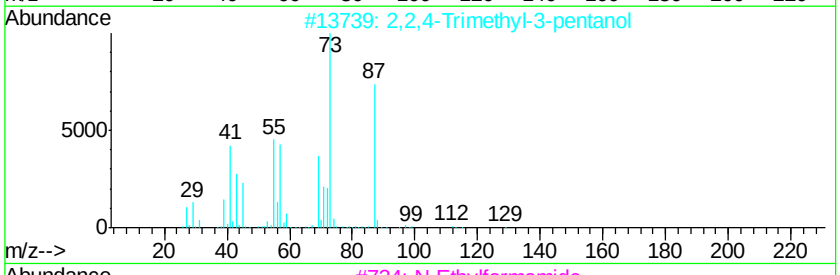
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

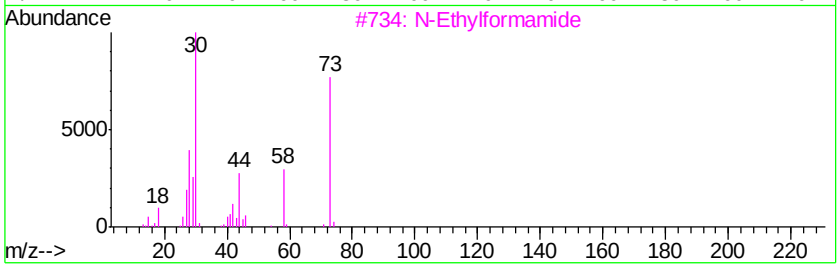
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.24	51.68 ng	849125	1,4-Dichlorobenzene-d4	8.06

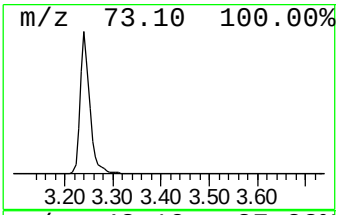
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9

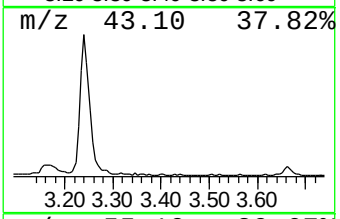


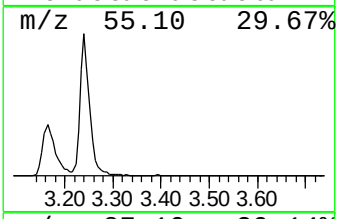


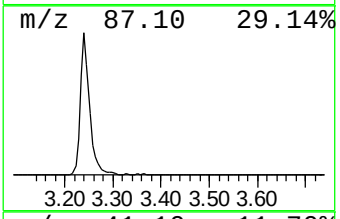


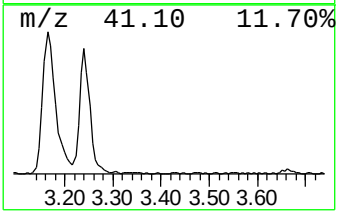












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Data File : BG043080.D
Acq On : 7 Oct 2019 23:00
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Sample : PB123704BL
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB123704BL

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

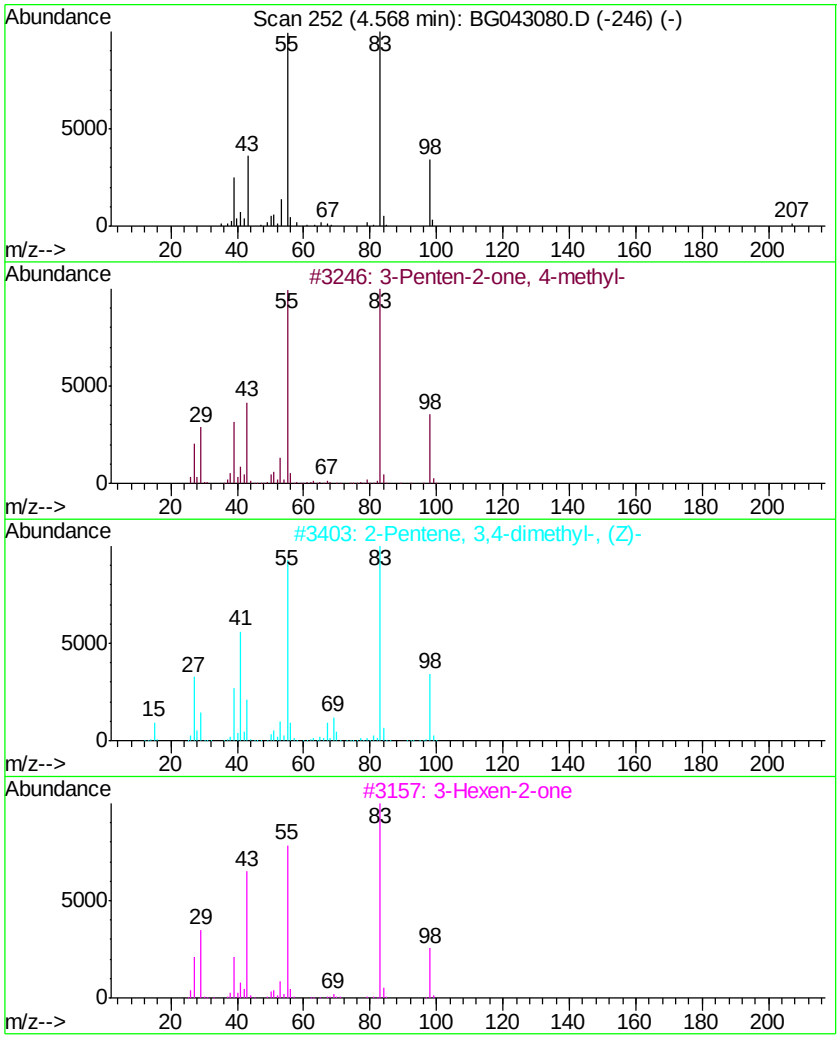
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

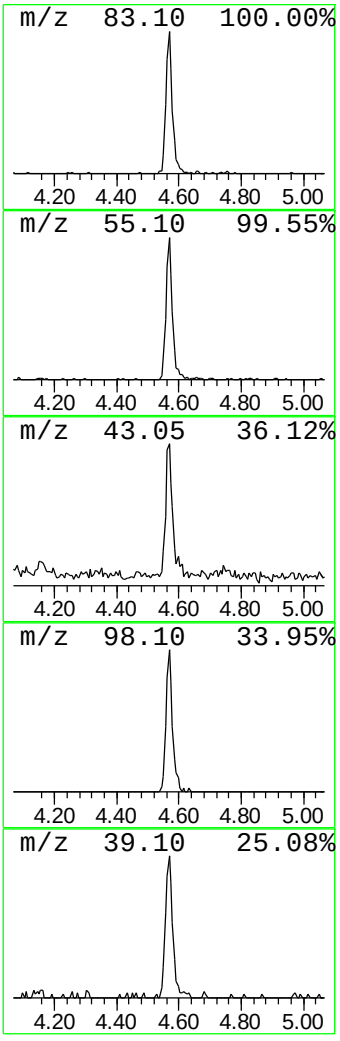
****

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	7.32 ng	120285	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
3	3-Hexen-2-one	98	C6H10O	000763-93-9	86
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86





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Instrument : BNA_G
ClientSampleId : PB123704BL

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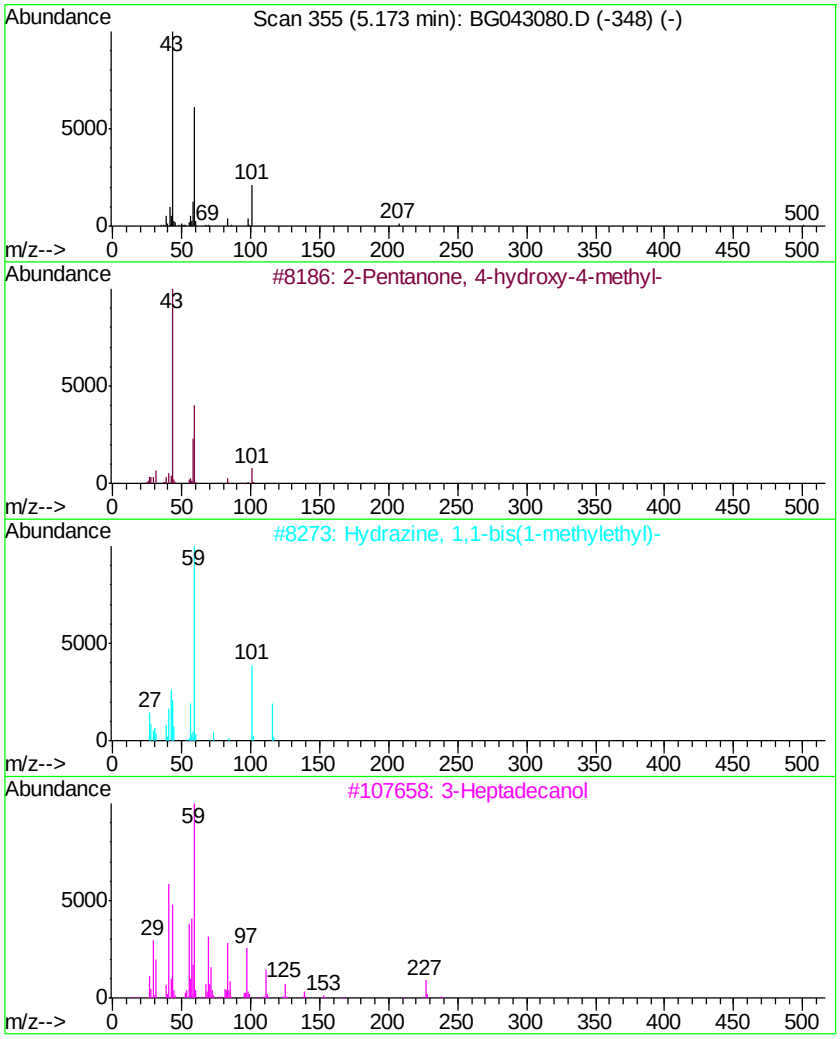
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

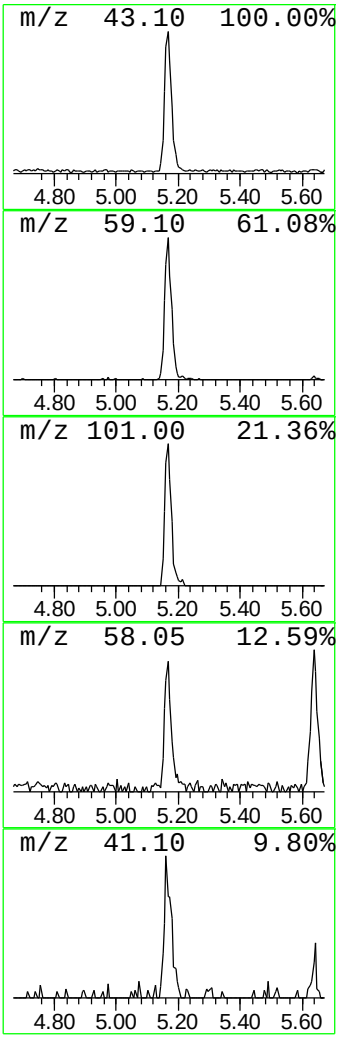
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	7.54 ng	123950	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	47
3	3-Heptadecanol	256	C17H36O	084534-30-5	25
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17





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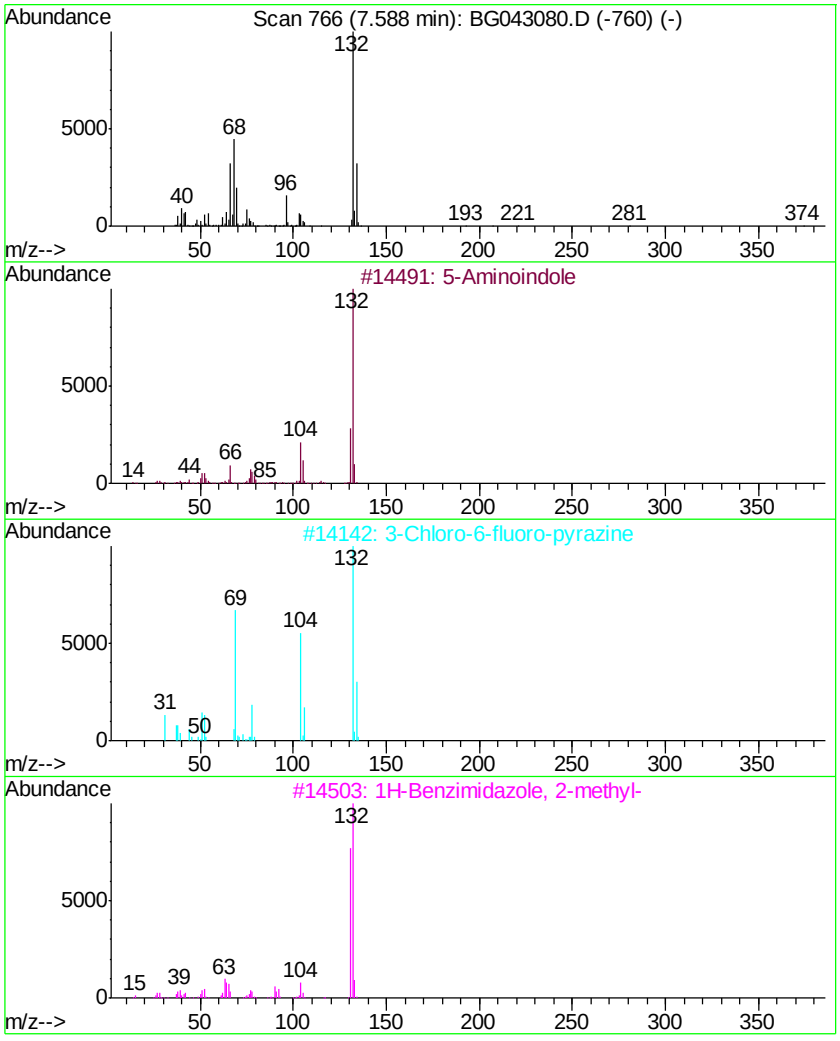
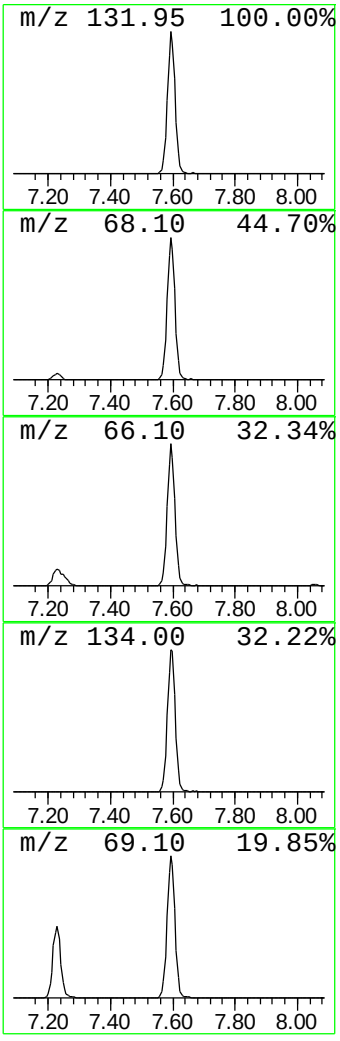
****

Peak Number 5 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	103.22 ng	1695860	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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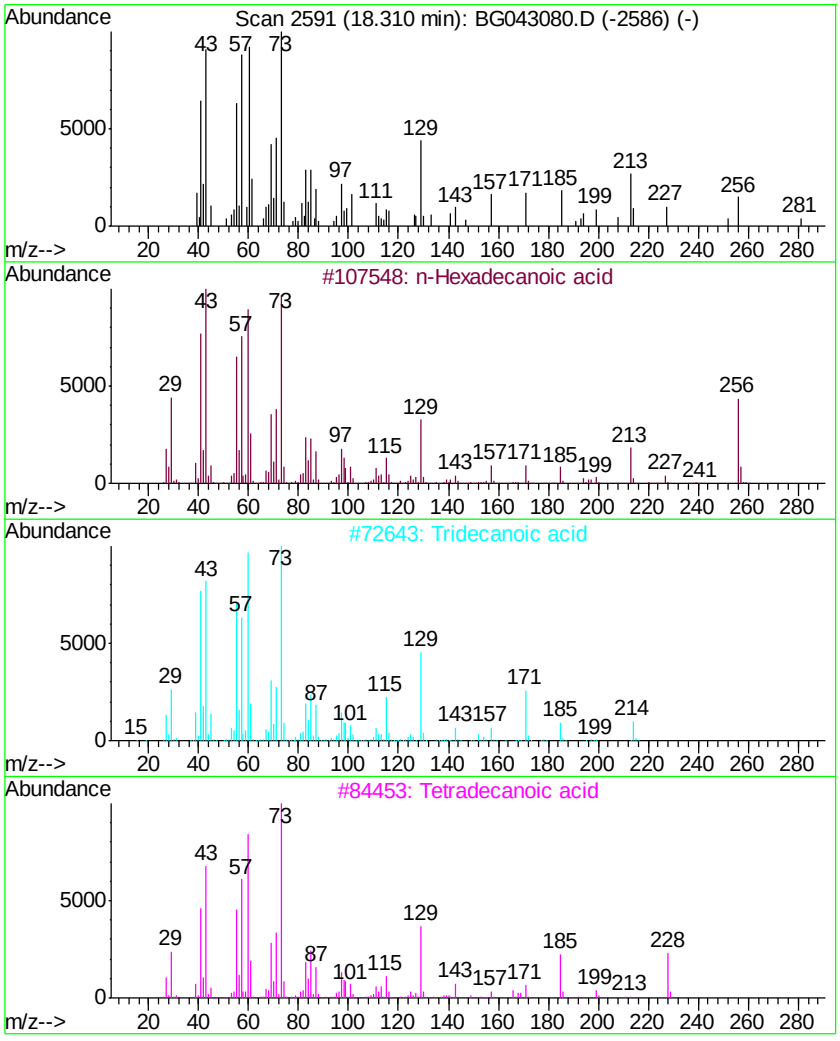
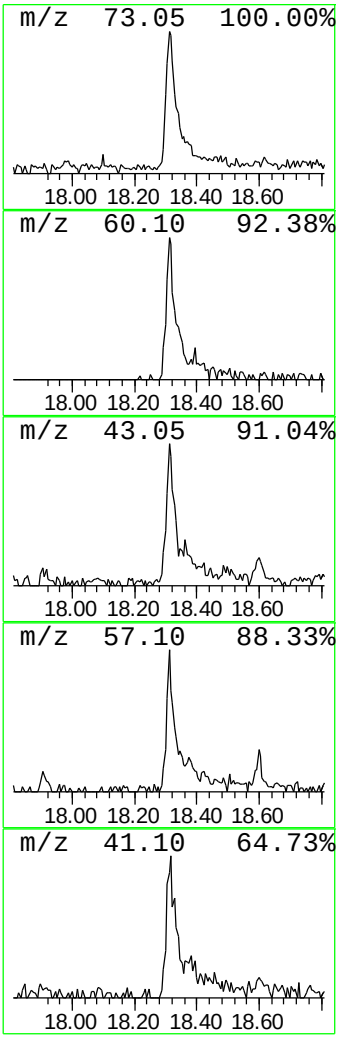
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.31	3.25 ng	169684	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25





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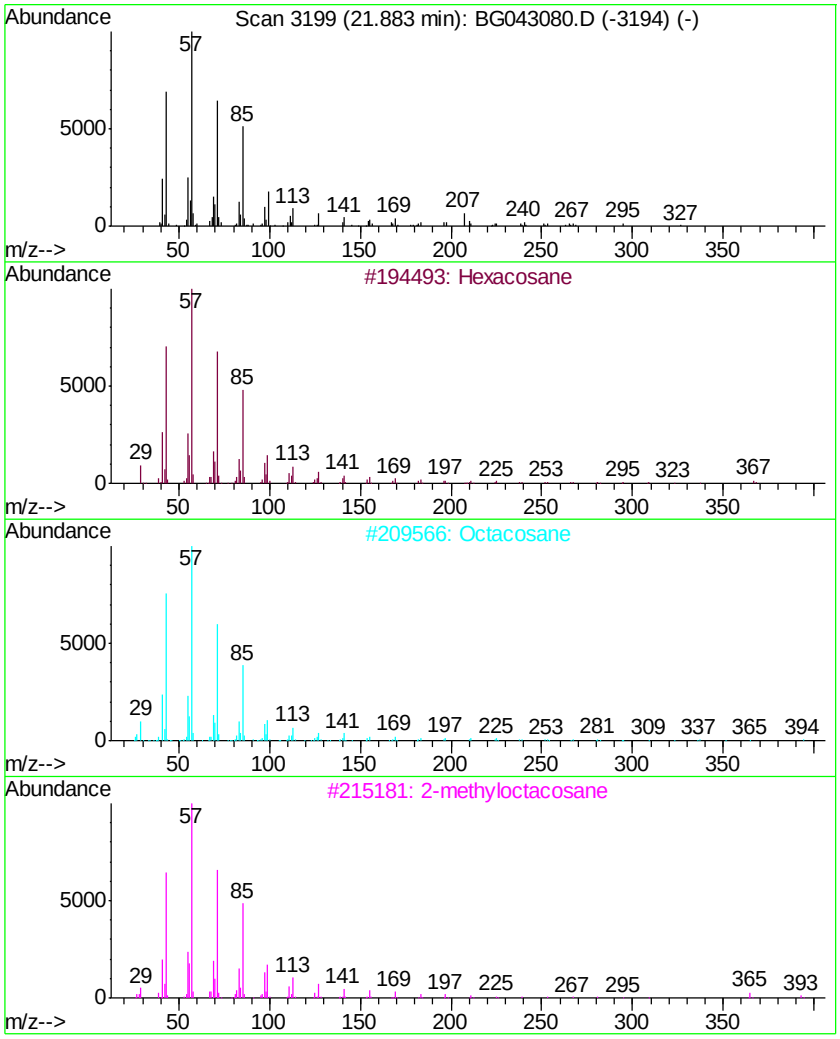
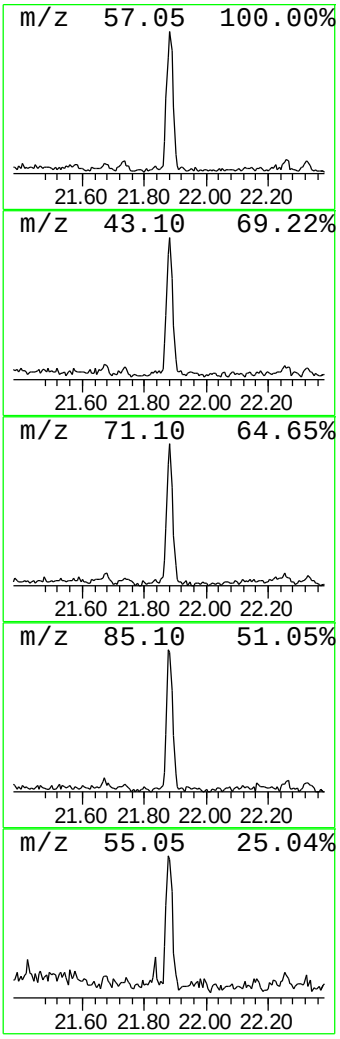
****

Peak Number 8 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.88	2.50 ng	157197	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Octacosane	394	C28H58	000630-02-4	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	Triacontane	422	C30H62	000638-68-6	86





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Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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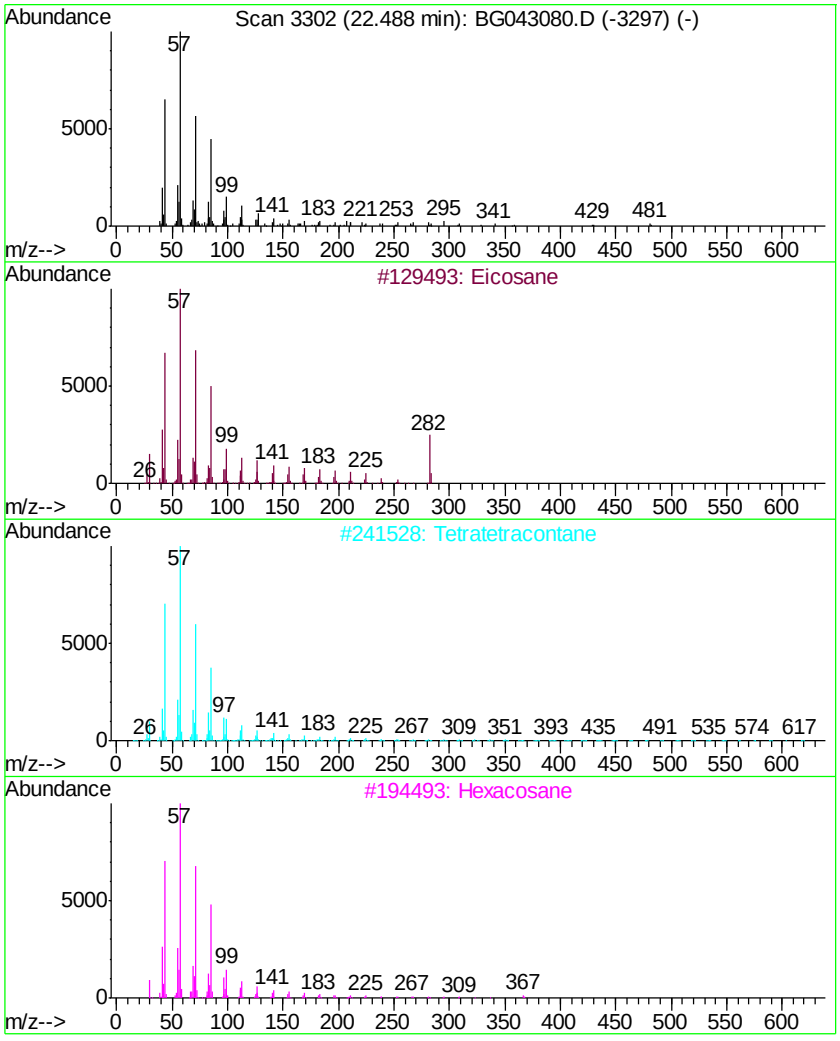
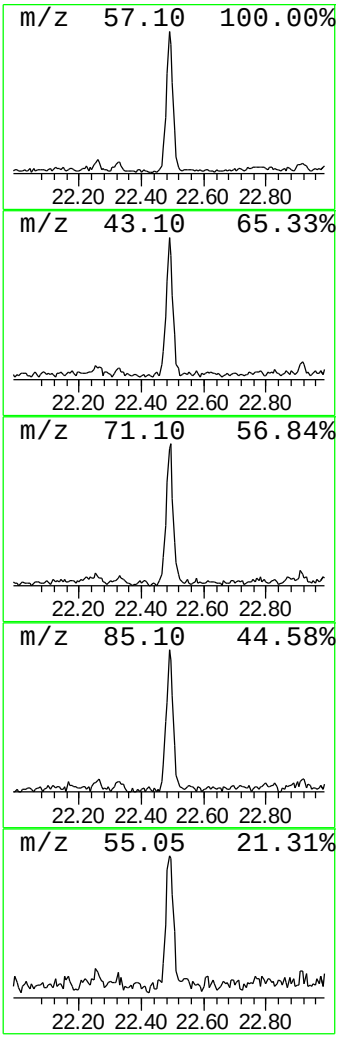
Peak Number 9 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.49	3.10 ng	194878	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Docosane	310	C22H46	000629-97-0	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG100719\
Data File : BG043080.D
Acq On : 7 Oct 2019 23:00
Operator : JU
Sample : PB123704BL
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB123704BL

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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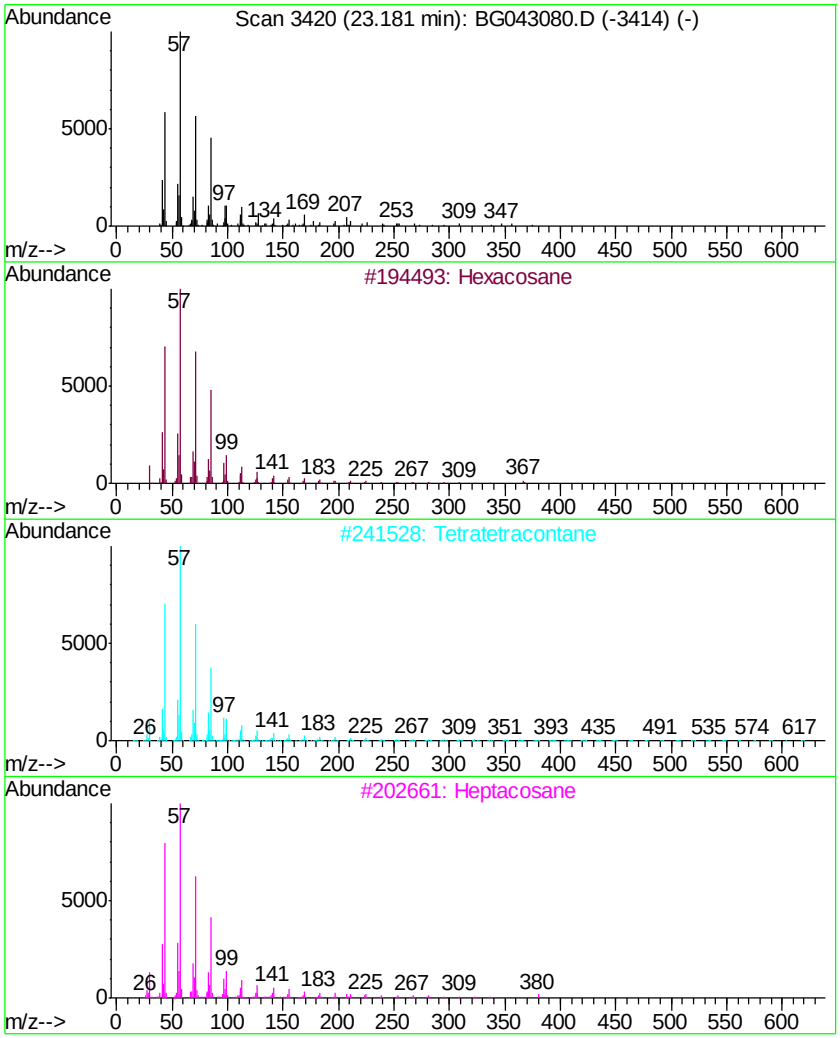
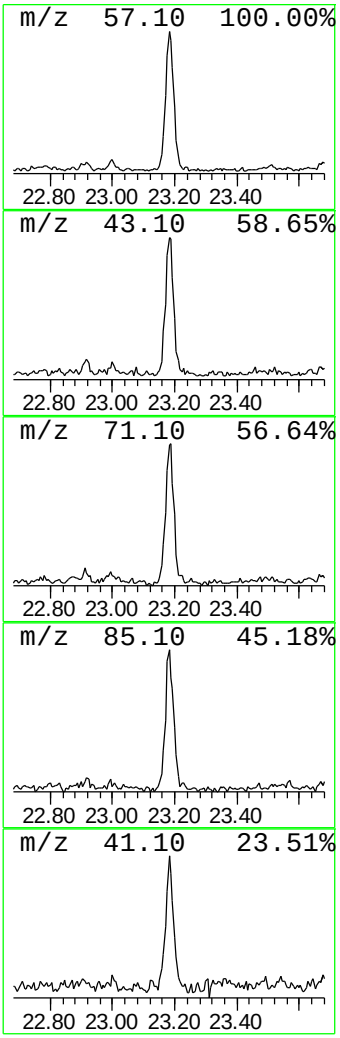
Peak Number 10 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	3.26 ng	205230	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Heptacosane	380	C27H56	000593-49-7	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Tetracosane	338	C24H50	000646-31-1	87





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Data File : BG043080.D
Acq On : 7 Oct 2019 23:00
Operator : JU
Sample : PB123704BL
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB123704BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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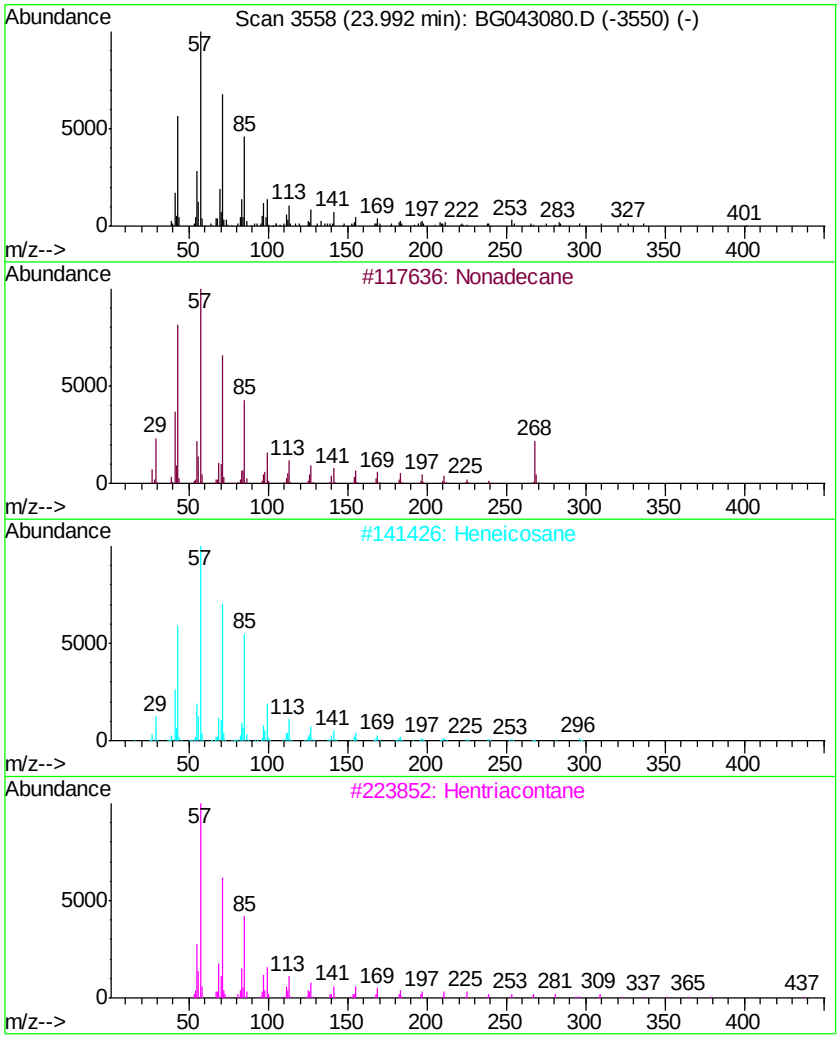
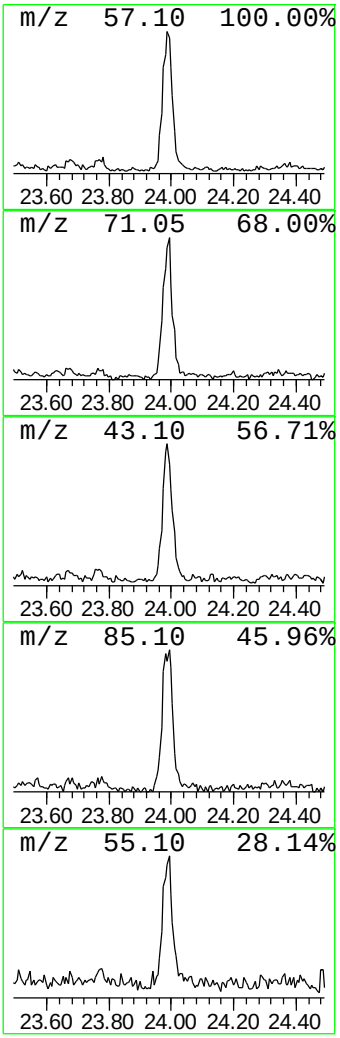
Peak Number 11 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	2.79 ng	193718	Perylene-d12	24.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Heneicosane	296	C21H44	000629-94-7	93
3	Hentriacontane	437	C31H64	000630-04-6	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Hexatriacontane	507	C36H74	000630-06-8	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG100719\
Data File : BG043080.D
Acq On : 7 Oct 2019 23:00
Operator : JU
Sample : PB123704BL
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB123704BL

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
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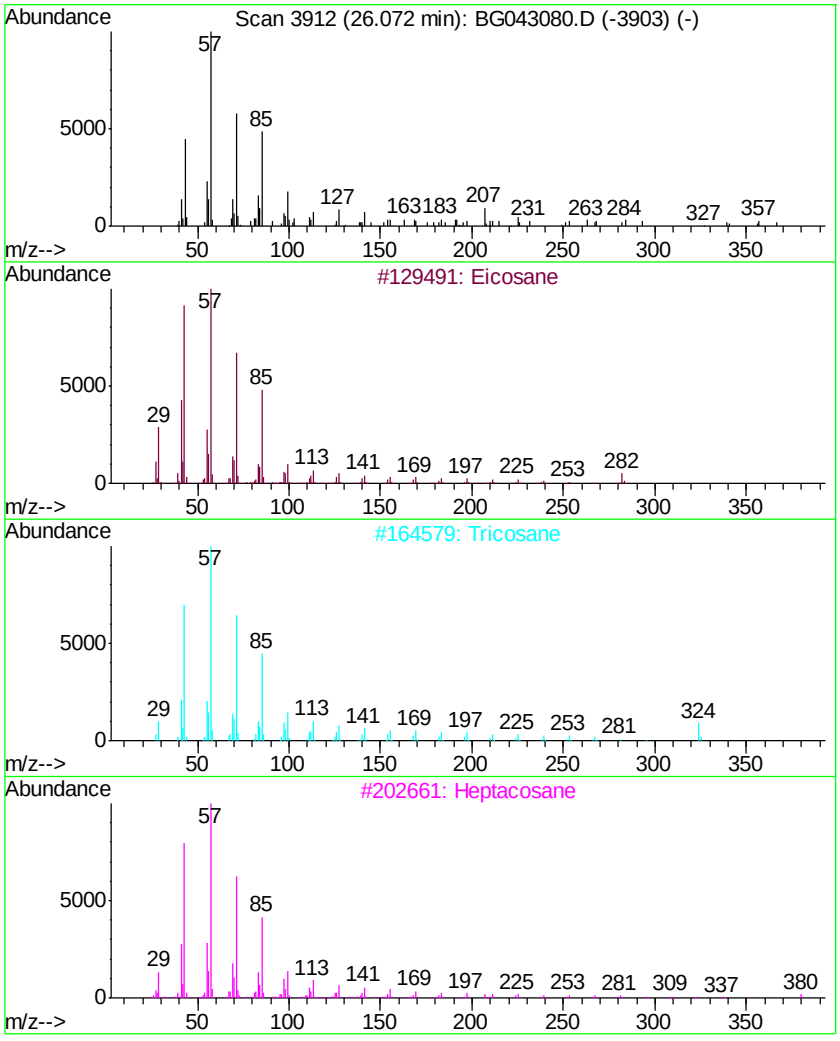
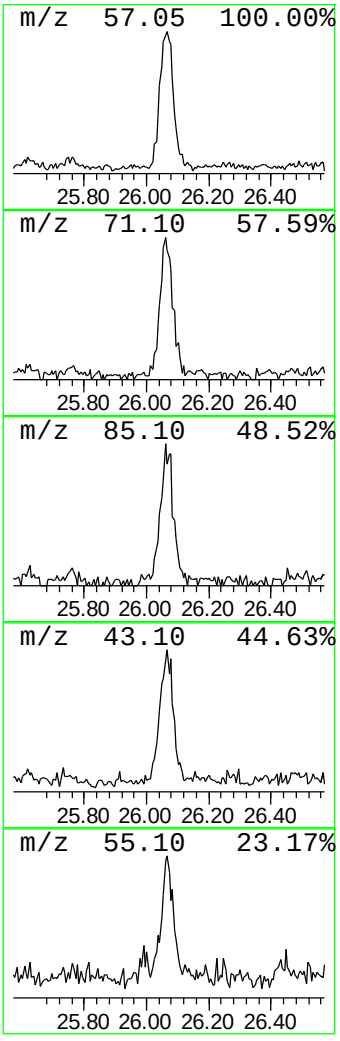
Peak Number 12 Tricosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.07	2.11 ng	146642	Perylene-d12	24.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	89
2	Tricosane	324	C23H48	000638-67-5	83
3	Heptacosane	380	C27H56	000593-49-7	80
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80
5	Hentriacontane	437	C31H64	000630-04-6	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG100719\
Data File : BG043080.D
Acq On : 7 Oct 2019 23:00
Operator : JU
Sample : PB123704BL
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB123704BL

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Pentene, 2-methyl-	3.16	29.1	ng	478091	1	8.06	328588	20.0
Butane, 2-methoxy...	3.24	51.7	ng	849125	1	8.06	328588	20.0
3-Penten-2-one, 4...	4.57	7.3	ng	120285	1	8.06	328588	20.0
2-Pentanone, 4-hy...	5.17	7.5	ng	123950	1	8.06	328588	20.0
unknown7.59	7.59	103.2	ng	1695860	1	8.06	328588	20.0
n-Hexadecanoic acid	18.31	3.3	ng	169684	4	17.42	1045320	20.0
Octacosane	21.88	2.5	ng	157197	5	21.69	1259050	20.0
Eicosane	22.49	3.1	ng	194878	5	21.69	1259050	20.0
Hexacosane	23.18	3.3	ng	205230	5	21.69	1259050	20.0
Nonadecane	23.99	2.8	ng	193718	6	24.90	1389100	20.0
Tricosane	26.07	2.1	ng	146642	6	24.90	1389100	20.0