LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101719\
Data File : BG043269.D
Acq On : 17 Oct 2019 19:39
Operator : JU
Sample : K5266-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190883-FIELD-BLANK

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	3.130	3	7	15	rBV2	126508	230418	5.69%	0.895%
2	3.206	15	20	35	rVB	715086	1051146	25.95%	4.083%
3	3.629	88	92	100	rVB	30244	45453	1.12%	0.177%
4	5.615	422	430	442	rBV	517429	913328	22.54%	3.548%
5	7.213	691	702	713	rBV	371317	750898	18.54%	2.917%
6	7.577	756	764	776	rBV	798581	1439361	35.53%	5.591%
7	8.036	835	842	851	rBV	185369	329296	8.13%	1.279%
8	8.365	888	898	909	rBV	570154	1046858	25.84%	4.066%
9	9.199	1032	1040	1060	rBV	443530	884638	21.84%	3.436%
10	10.844	1307	1320	1331	rBV	228111	451773	11.15%	1.755%
11	13.288	1729	1736	1750	rBV	1417003	2292884	56.60%	8.906%
12	14.111	1870	1876	1886	rBV	232875	375369	9.27%	1.458%
13	14.663	1963	1970	1985	rBV	418793	711943	17.57%	2.765%
14	16.155	2215	2224	2242	rBV	1309458	2205421	54.44%	8.566%
15	16.808	2331	2335	2343	rBV3	26651	50837	1.25%	0.197%
16	17.413	2431	2438	2446	rBV	512459	838317	20.69%	3.256%
17	18.171	2563	2567	2577	rBV	63578	109400	2.70%	0.425%
18	18.300	2584	2589	2604	rBV	332352	539582	13.32%	2.096%
19	19.722	2825	2831	2840	rBV	33419	64110	1.58%	0.249%
20	20.022	2876	2882	2896	rBV	2955969	4051193	100.00%	15.736%
21	20.703	2990	2998	3004	rBV	405224	804793	19.87%	3.126%
22	20.815	3013	3017	3023	rVB4	34723	57287	1.41%	0.223%
23	21.320	3099	3103	3113	rBV5	110461	237468	5.86%	0.922%
24	21.408	3114	3118	3124	rVB	45582	74133	1.83%	0.288%
25	21.684	3158	3165	3175	rBV	584355	1011331	24.96%	3.928%
26	21.796	3180	3184	3191	rBV2	76141	135074	3.33%	0.525%
27	22.477	3296	3300	3305	rBV4	36725	53517	1.32%	0.208%
28	23.153	3407	3415	3432	rVB2	993726	2058105	50.80%	7.994%
29	23.365	3443	3451	3462	rVB	768409	1515795	37.42%	5.888%
30	23.976	3550	3555	3561	rVB4	50328	103954	2.57%	0.404%
31	24.904	3702	3713	3729	rBV2	384905	1197776	29.57%	4.652%
32	26.050	3900	3908	3918	rVB4	37890	113410	2.80%	0.441%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101719\
Data File : BG043269.D
Acq On : 17 Oct 2019 19:39
Operator : JU
Sample : K5266-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20190883-FIELD-BLANK

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

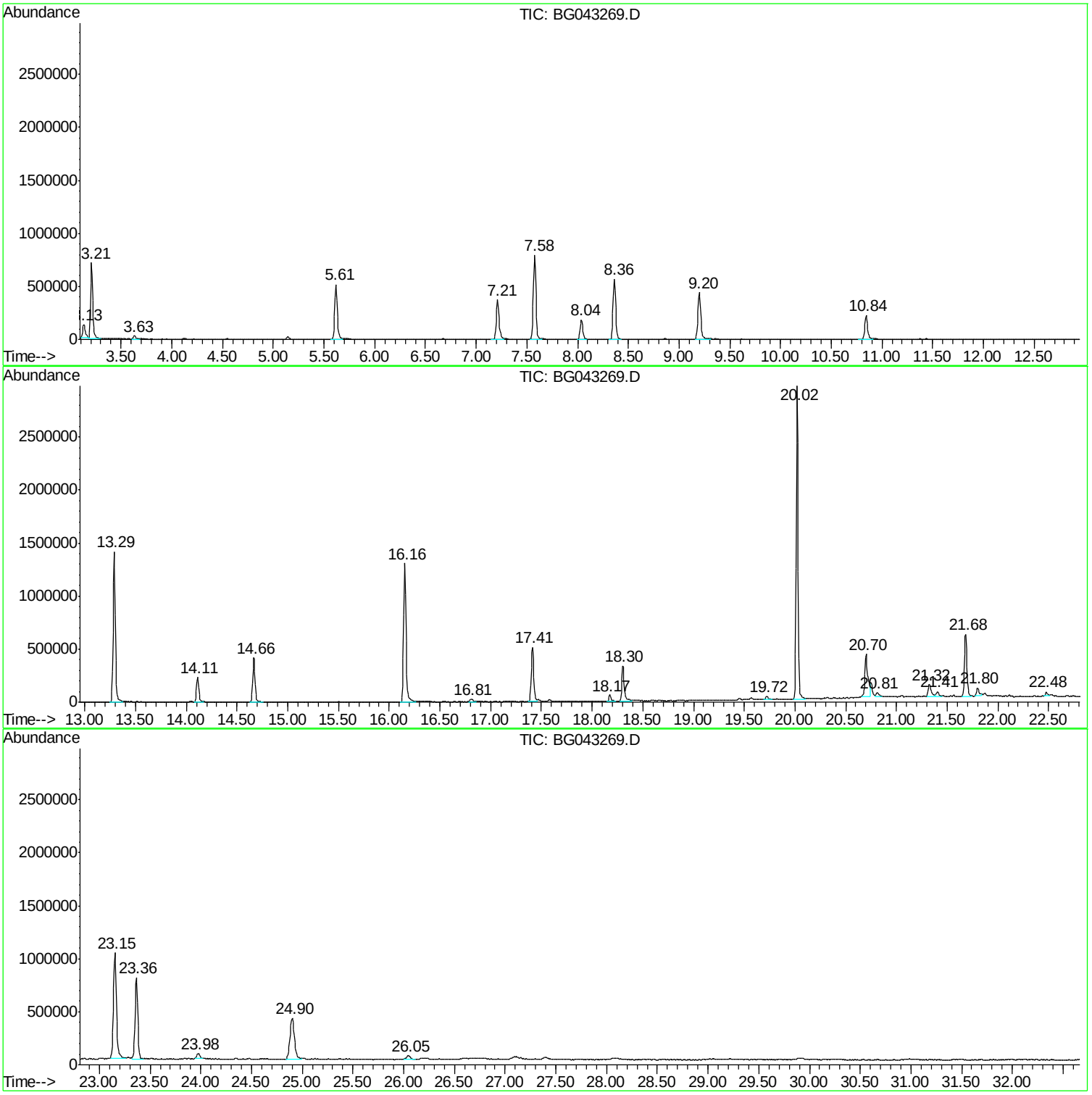
Sum of corrected areas: 25744868

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101719\
Data File : BG043269.D
Acq On : 17 Oct 2019 19:39
Operator : JU
Sample : K5266-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20190883-FIELD-BLANK

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101719\
Data File : BG043269.D
Acq On : 17 Oct 2019 19:39
Operator : JU
Sample : K5266-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190883-FIELD-BLANK

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

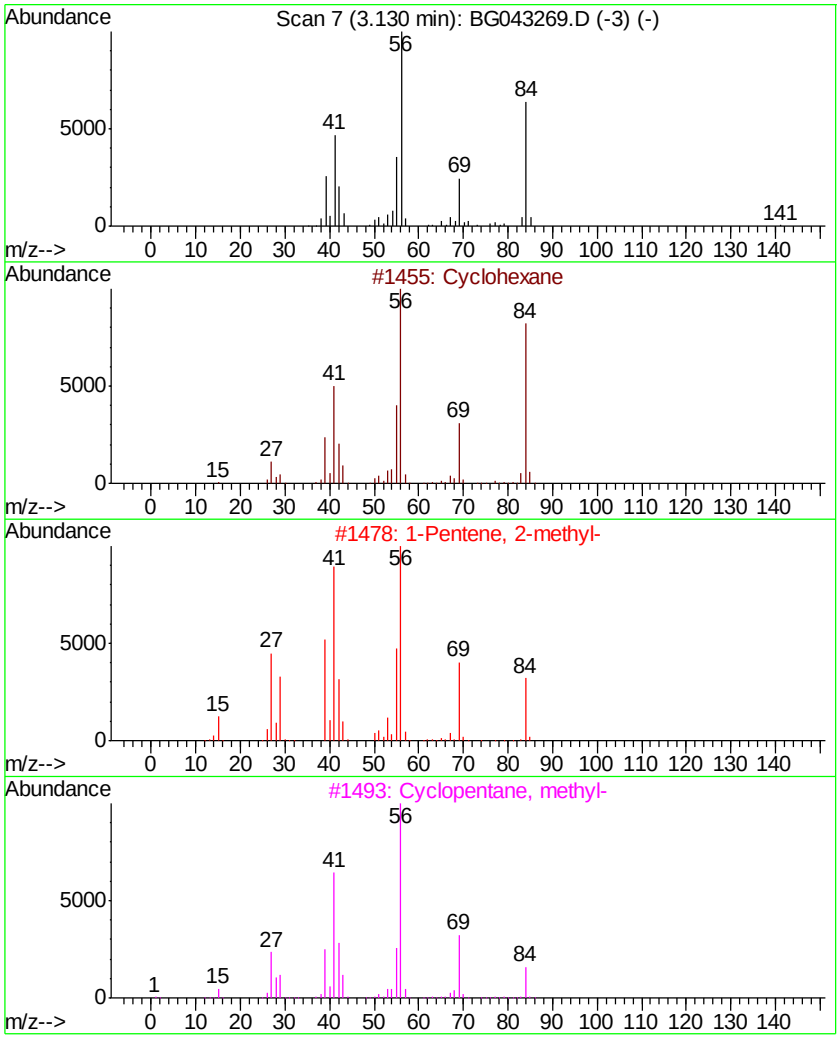
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

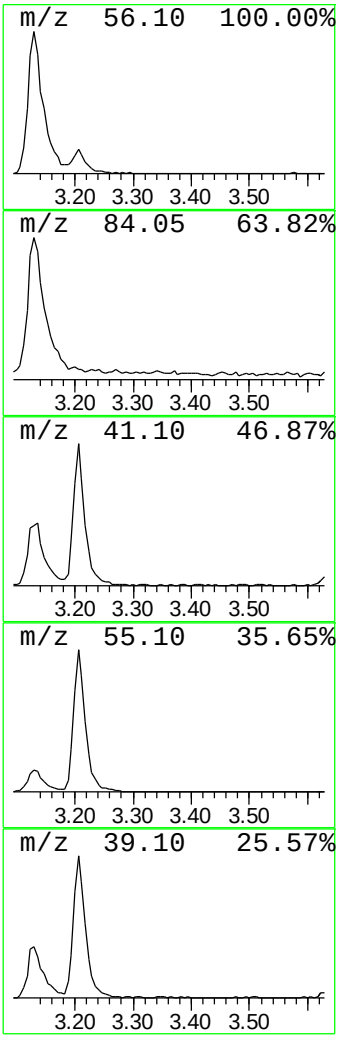
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	13.99 ng	230418	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	94
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	78
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	50
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	47
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	45





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101719\
Data File : BG043269.D
Acq On : 17 Oct 2019 19:39
Operator : JU
Sample : K5266-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190883-FIELD-BLANK

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

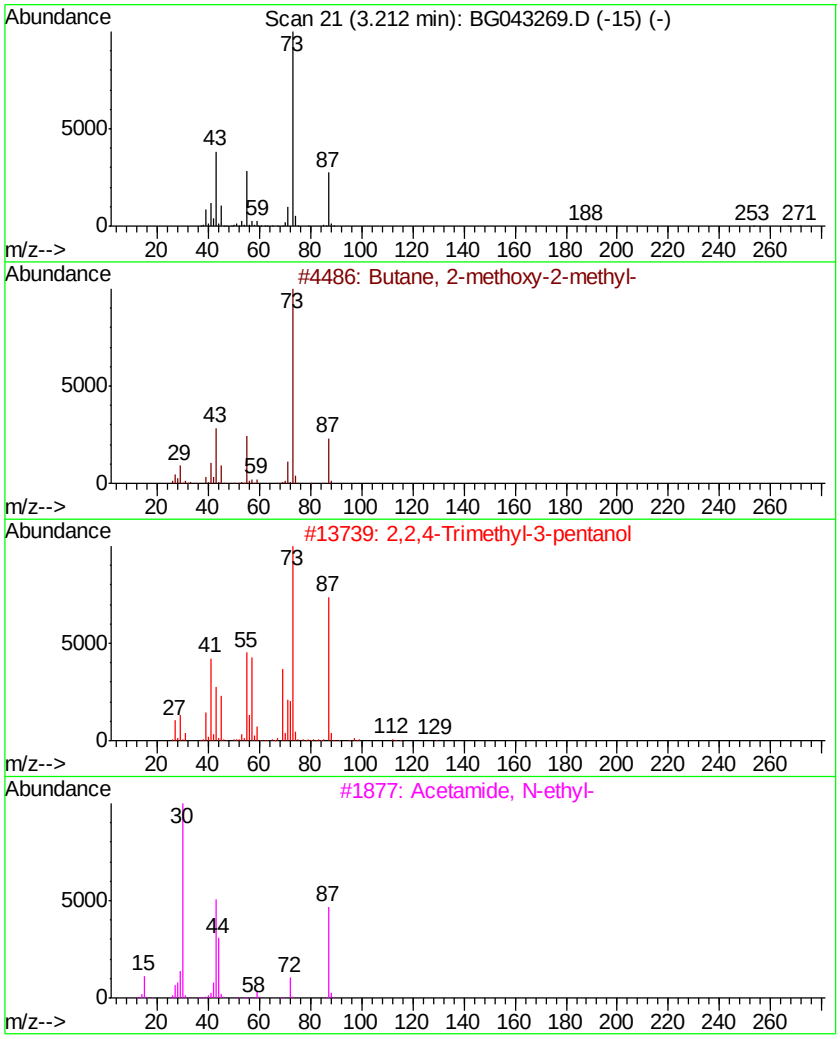
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

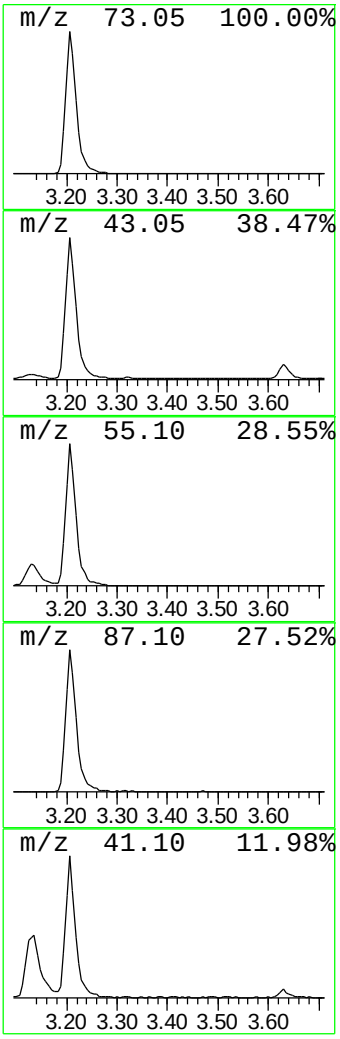
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	63.84 ng	1051150	1,4-Dichlorobenzene-d4	8.04

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	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101719\
Data File : BG043269.D
Acq On : 17 Oct 2019 19:39
Operator : JU
Sample : K5266-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190883-FIELD-BLANK

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

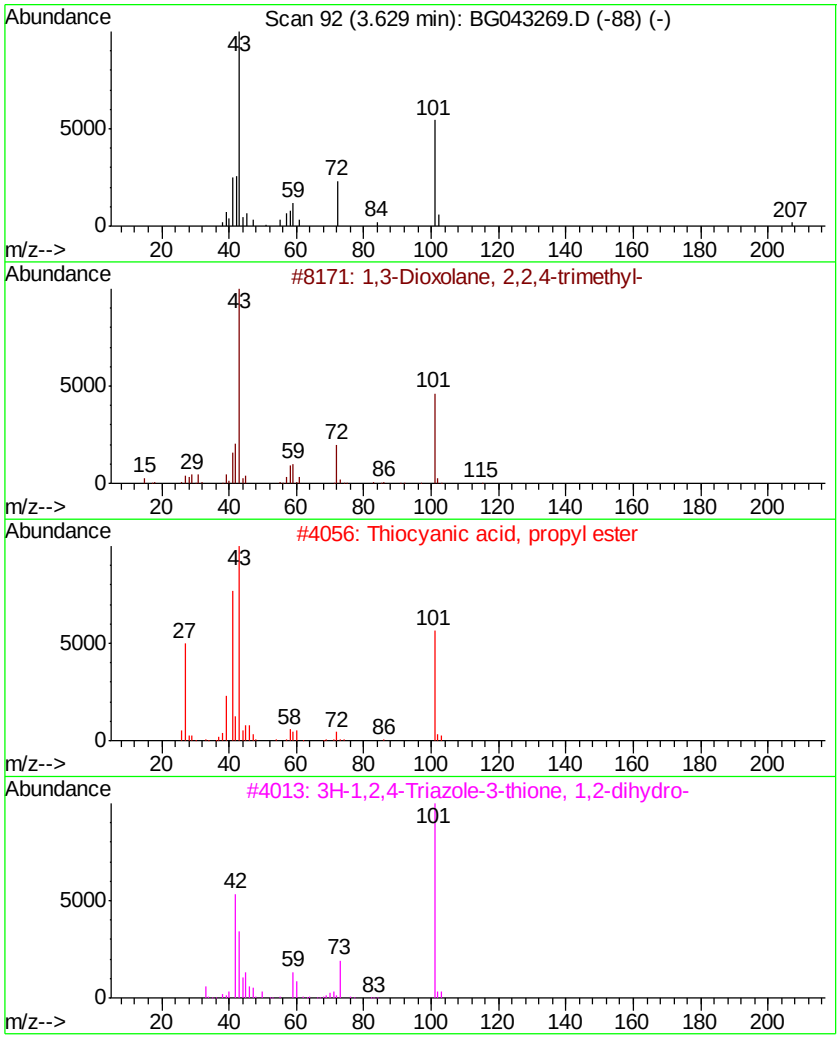
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

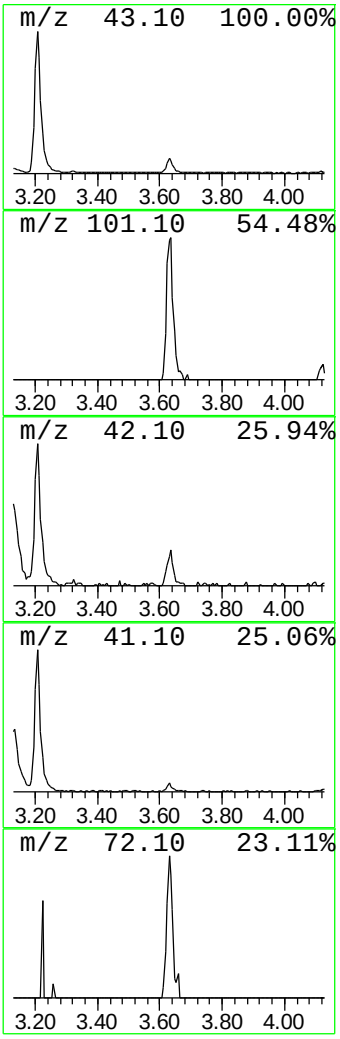
****

Peak Number 3 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.63	2.76 ng	45453	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	78
2	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	53
3	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	47
4	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	40
5	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	38





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101719\
Data File : BG043269.D
Acq On : 17 Oct 2019 19:39
Operator : JU
Sample : K5266-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190883-FIELD-BLANK

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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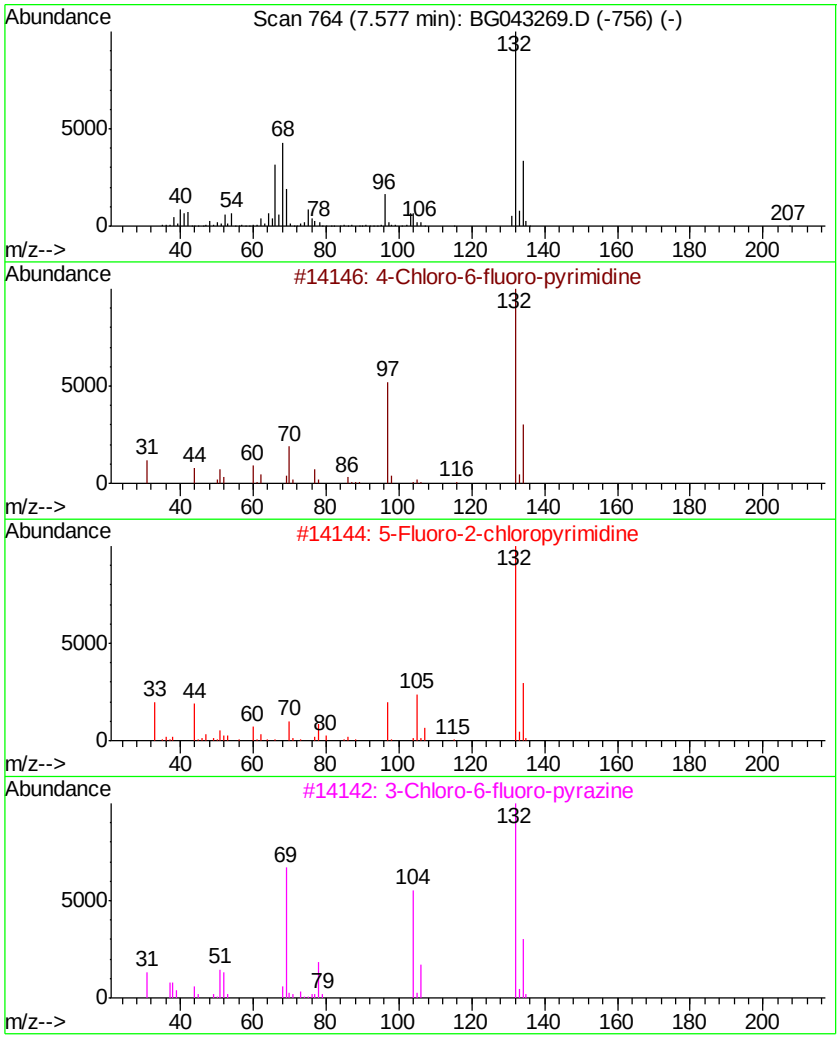
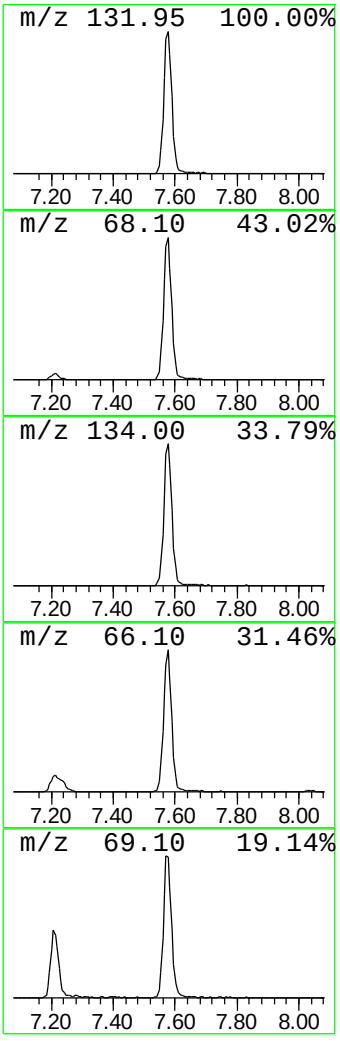
****

Peak Number 4 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	87.42 ng	1439360	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101719\
Data File : BG043269.D
Acq On : 17 Oct 2019 19:39
Operator : JU
Sample : K5266-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190883-FIELD-BLANK

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

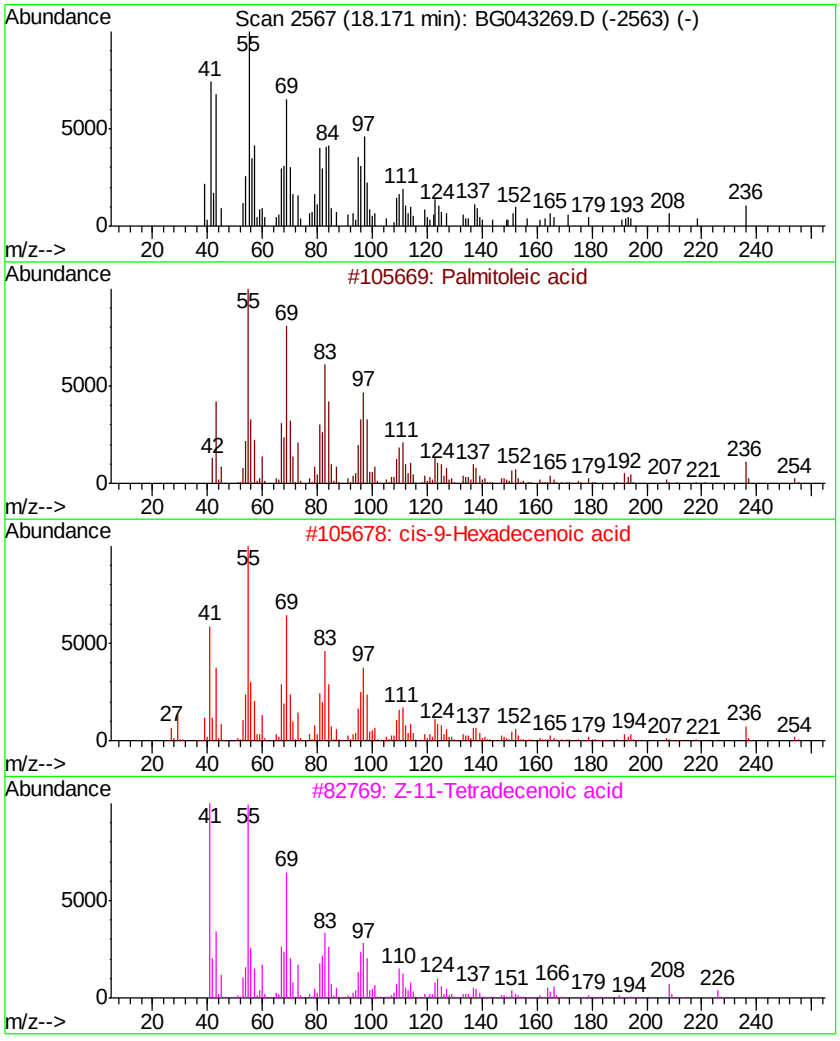
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

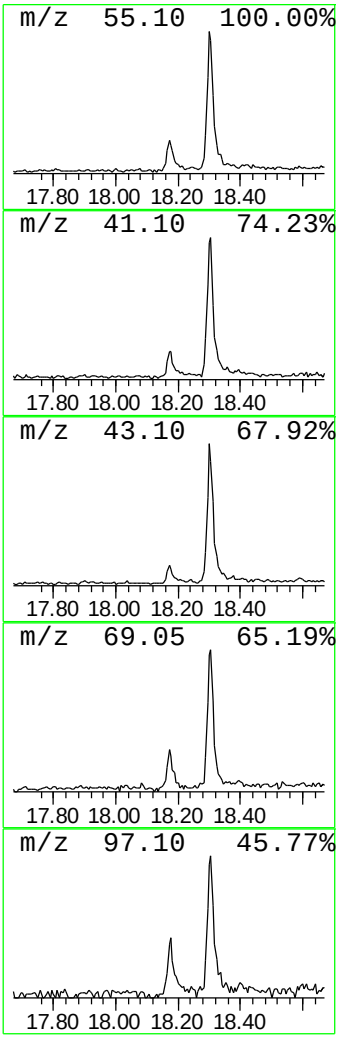
****

Peak Number 6 Palmitoleic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.17	2.61 ng	109400	Phenanthrene-d10	17.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palmitoleic acid	254	C16H30O2	000373-49-9	90
2	cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	87
3	Z-11-Tetradecenoic acid	226	C14H26O2	1000130-83-3	72
4	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	68
5	1,2-Cyclooctanedione	140	C8H12O2	003008-37-5	53





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Data File : BG043269.D
Acq On : 17 Oct 2019 19:39
Operator : JU
Sample : K5266-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190883-FIELD-BLANK

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

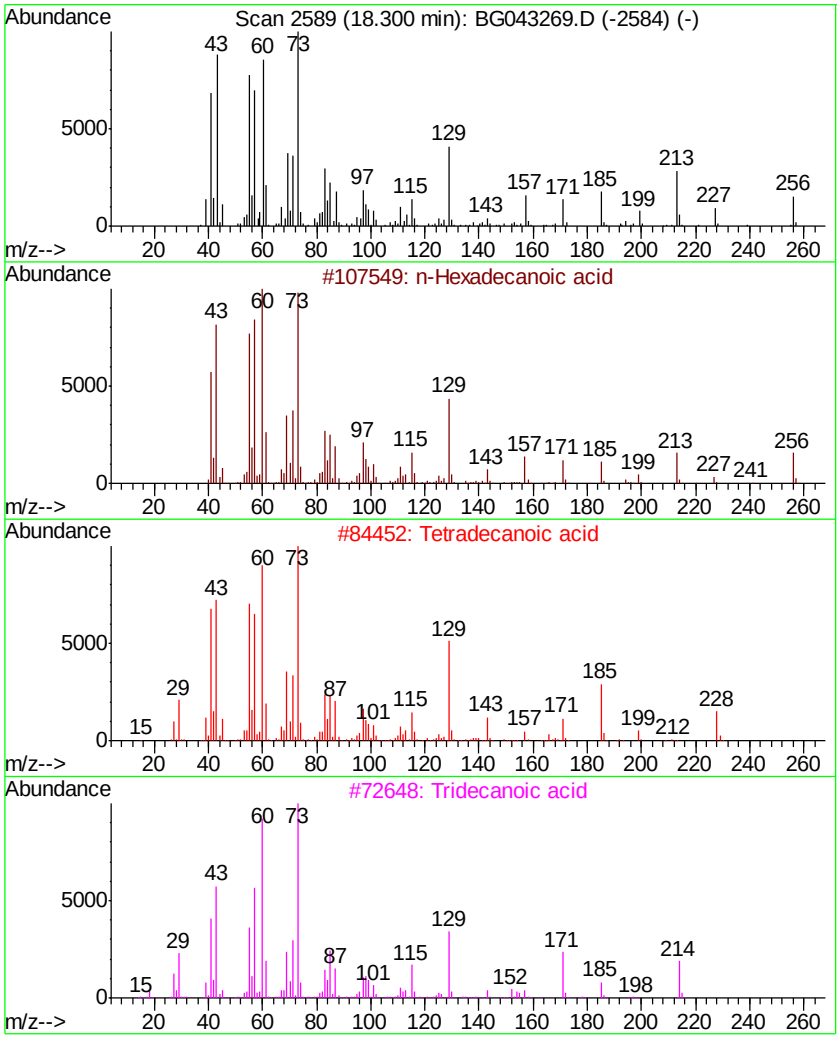
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

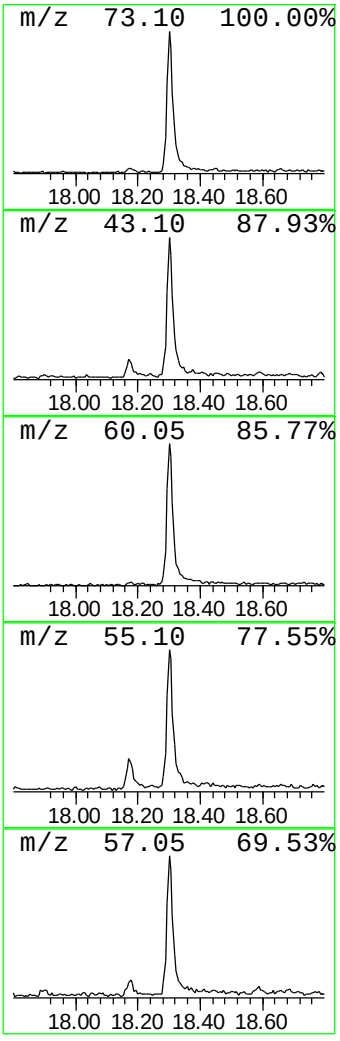
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	12.87 ng	539582	Phenanthrene-d10	17.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





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Data File : BG043269.D
Acq On : 17 Oct 2019 19:39
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Sample : K5266-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190883-FIELD-BLANK

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

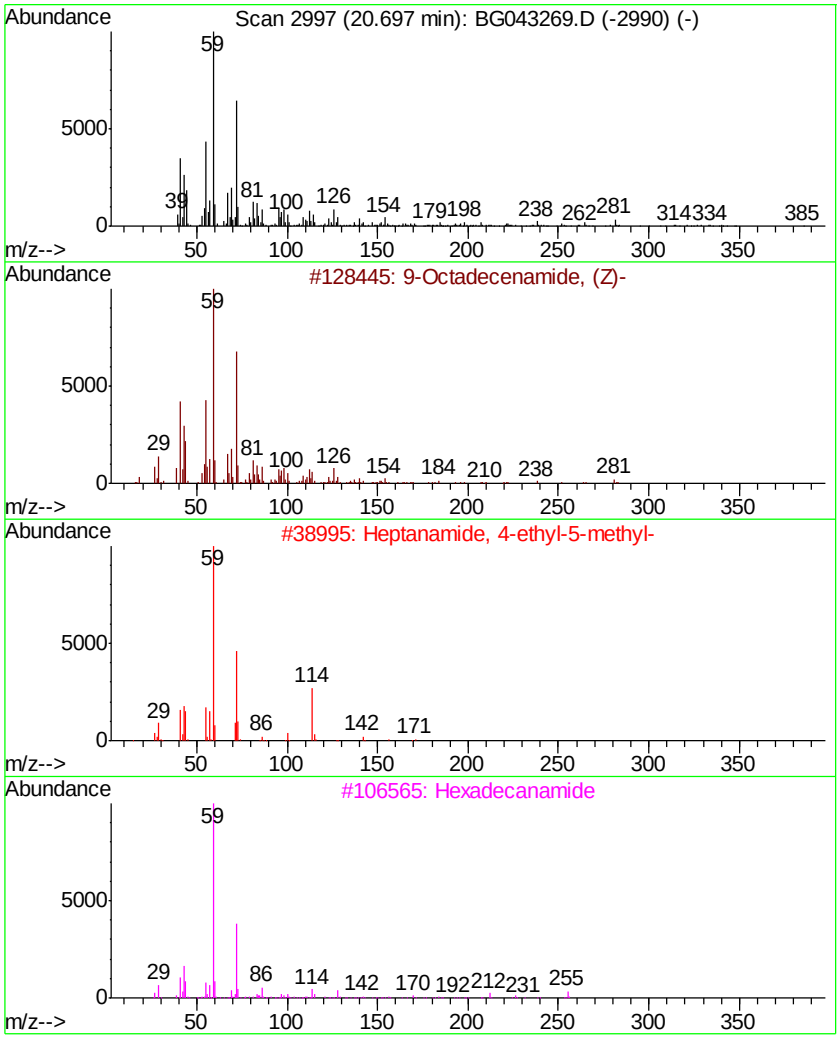
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

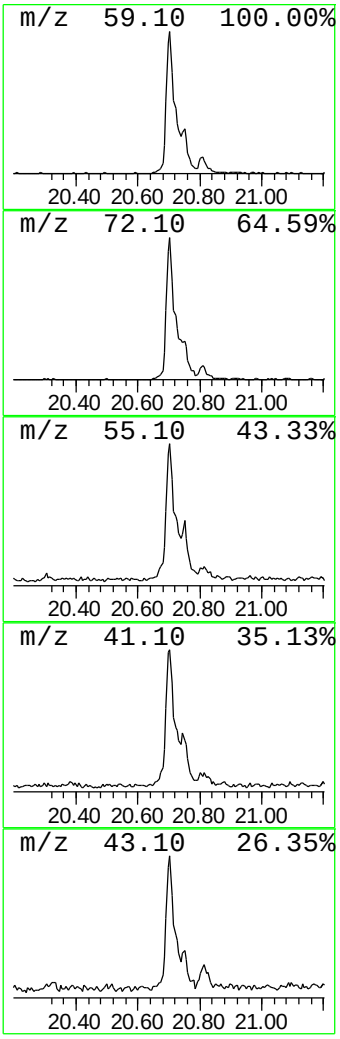
****

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.70	15.92 ng	804793	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	80
3	Hexadecanamide	255	C16H33NO	000629-54-9	64
4	Octanamide	143	C8H17NO	000629-01-6	64
5	Nonanamide	157	C9H19NO	001120-07-6	59





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Misc :
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Instrument : BNA_G
ClientSampleId : 20190883-FIELD-BLANK

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

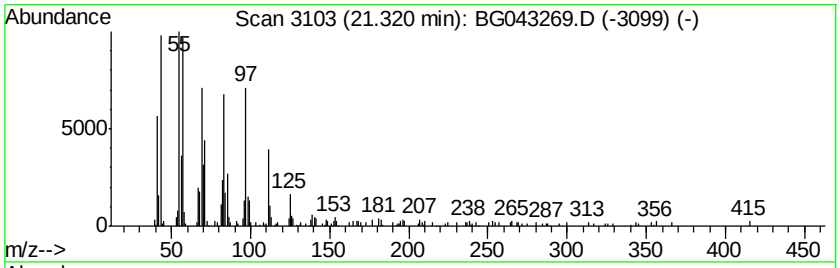
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

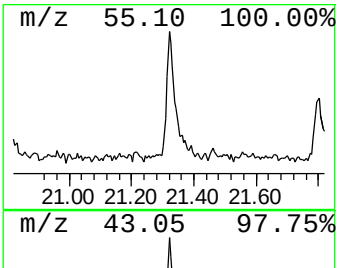
****

Peak Number 9 Heptafluorobutyric acid, he... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	4.70 ng	237468	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
2	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101719\
Data File : BG043269.D
Acq On : 17 Oct 2019 19:39
Operator : JU
Sample : K5266-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190883-FIELD-BLANK

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

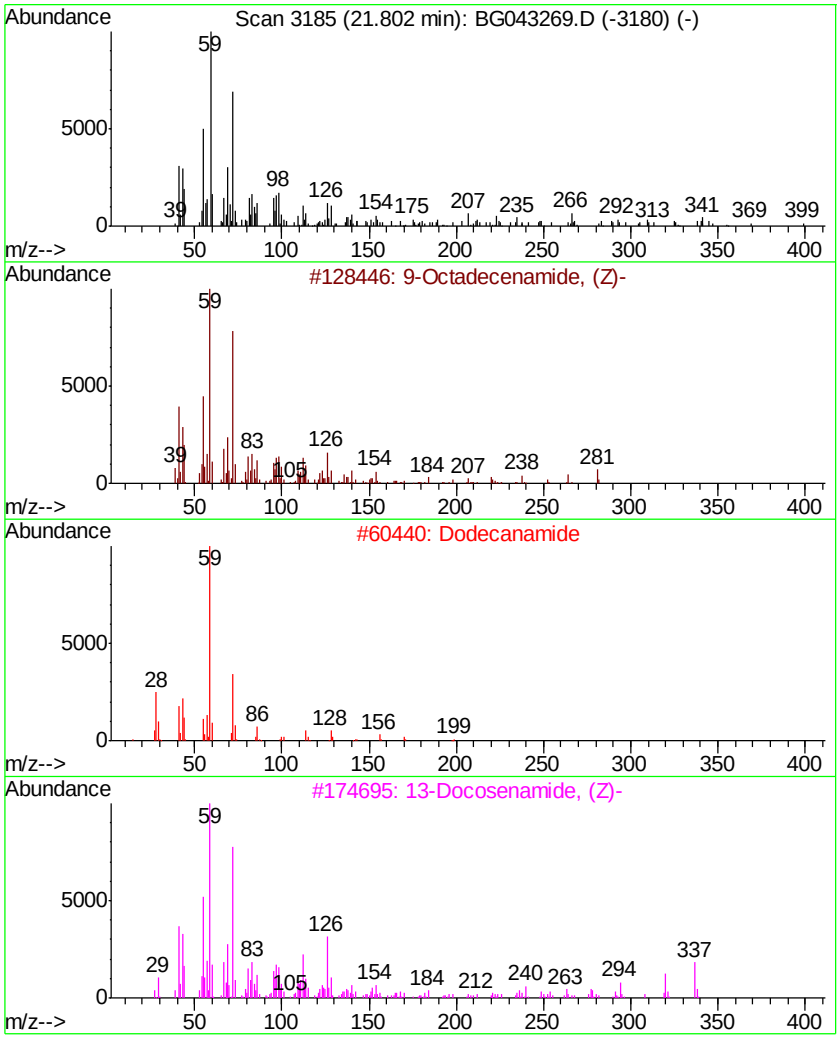
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

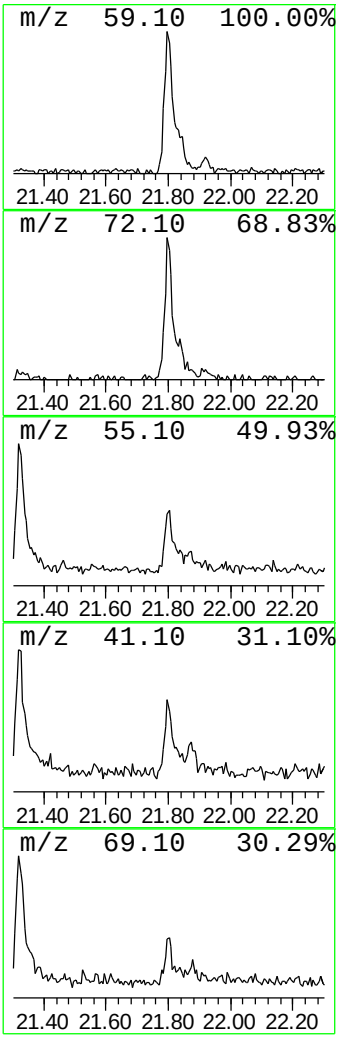
****

Peak Number 10 Dodecanamide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.80	2.67 ng	135074	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
2	Dodecanamide	199	C12H25NO	001120-16-7	60
3	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	50
4	Tetradecanamide	227	C14H29NO	000638-58-4	49
5	Nonanamide	157	C9H19NO	001120-07-6	49





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Acq On : 17 Oct 2019 19:39
Operator : JU
Sample : K5266-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190883-FIELD-BLANK

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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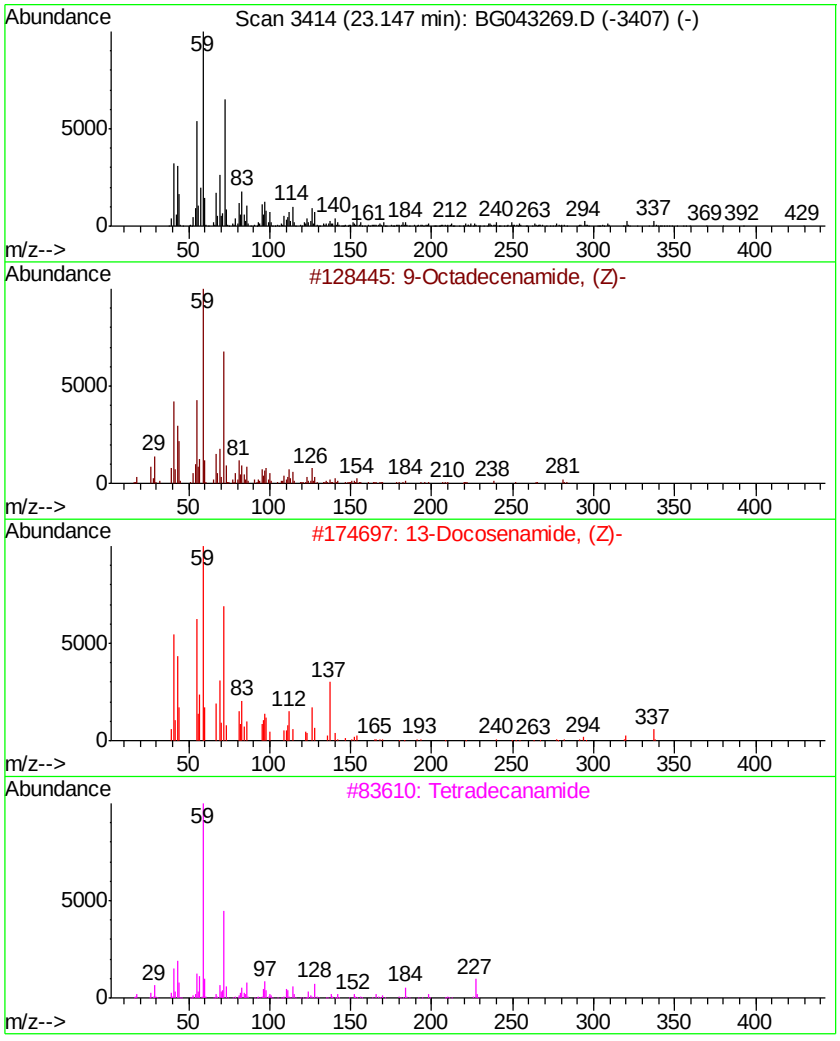
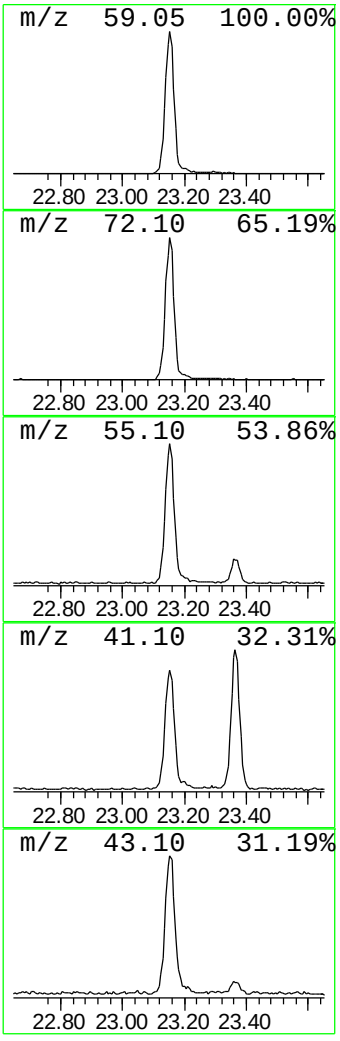
Peak Number 11 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.15	40.70 ng	2058110	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
3	Tetradecanamide	227	C14H29NO	000638-58-4	78
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59
5	Octadecanamide	283	C18H37NO	000124-26-5	59





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101719\
Data File : BG043269.D
Acq On : 17 Oct 2019 19:39
Operator : JU
Sample : K5266-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190883-FIELD-BLANK

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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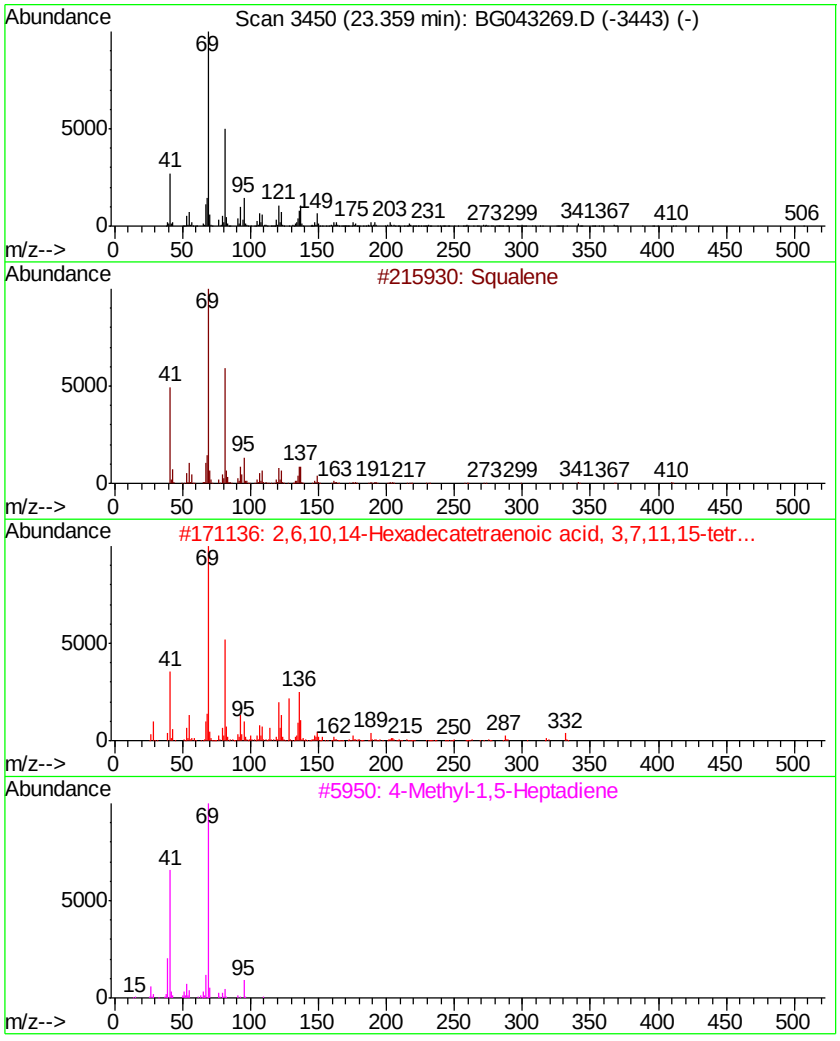
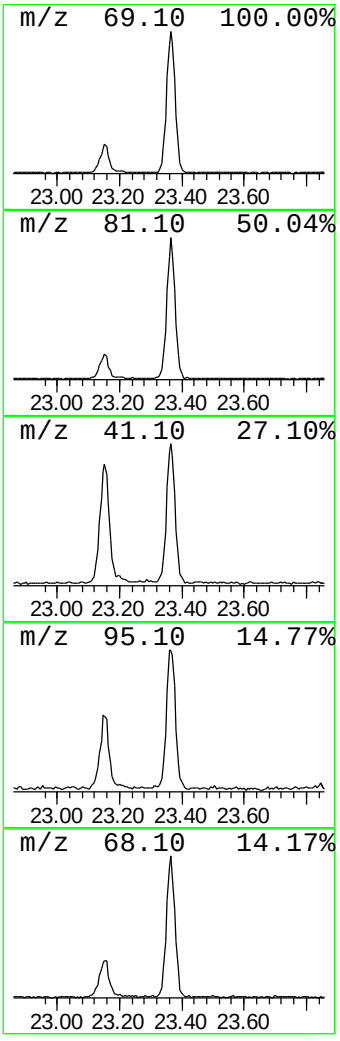
Peak Number 12 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.36	25.31 ng	1515800	Perylene-d12	24.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	99
2	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
3	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	52
4	Cyclopentane, bromo-	148	C5H9Br	000137-43-9	47
5	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG101719\
Data File : BG043269.D
Acq On : 17 Oct 2019 19:39
Operator : JU
Sample : K5266-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190883-FIELD-BLANK

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-	3.13	14.0	ng	230418	1	8.04	329296	20.0
Butane, 2-methoxy...	3.21	63.8	ng	1051150	1	8.04	329296	20.0
1,3-Dioxolane, 2,...	3.63	2.8	ng	45453	1	8.04	329296	20.0
unknown7.58	7.58	87.4	ng	1439360	1	8.04	329296	20.0
Palmitoleic acid	18.17	2.6	ng	109400	4	17.41	838317	20.0
n-Hexadecanoic acid	18.30	12.9	ng	539582	4	17.41	838317	20.0
9-Octadecenamide,...	20.70	15.9	ng	804793	5	21.68	1011330	20.0
Heptafluorobutyri...	21.32	4.7	ng	237468	5	21.68	1011330	20.0
Dodecanamide	21.80	2.7	ng	135074	5	21.68	1011330	20.0
13-Docosenamide, ...	23.15	40.7	ng	2058110	5	21.68	1011330	20.0
Squalene	23.36	25.3	ng	1515800	6	24.89	1197780	20.0