LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111519\
Data File : BG043671.D
Acq On : 16 Nov 2019 4:18
Operator : JU
Sample : K5840-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PHIPPS-BH-SW-03

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	3.154	6	11	22	rVB	68792	106129	4.76%	0.715%
2	5.093	335	341	351	rBV	159877	243428	10.91%	1.640%
3	5.587	419	425	437	rBV	212257	375754	16.85%	2.532%
4	7.197	690	699	714	rBV	322699	653012	29.28%	4.401%
5	7.537	750	757	771	rBV	292366	542422	24.32%	3.655%
6	7.990	828	834	848	rBV	80868	147573	6.62%	0.994%
7	8.319	882	890	900	rBV	288464	520839	23.35%	3.510%
8	9.159	1025	1033	1048	rBV	193201	411536	18.45%	2.773%
9	10.798	1304	1312	1332	rBV	98461	204968	9.19%	1.381%
10	13.248	1722	1729	1744	rBV	693027	1176256	52.74%	7.927%
11	14.077	1865	1870	1880	rBV	27085	54864	2.46%	0.370%
12	14.623	1957	1963	1975	rBV	190400	327007	14.66%	2.204%
13	16.121	2213	2218	2230	rBV	116305	240324	10.78%	1.620%
14	17.373	2424	2431	2444	rBV	232078	413942	18.56%	2.789%
15	19.982	2869	2875	2888	rBV	1473473	2047317	91.80%	13.797%
16	21.080	3043	3062	3073	rBV5	182885	949135	42.56%	6.396%
17	21.268	3085	3094	3105	rBV8	96434	348261	15.62%	2.347%
18	21.456	3111	3126	3131	rBV5	527195	2230283	100.00%	15.030%
19	21.633	3153	3156	3166	rVB	271324	513917	23.04%	3.463%
20	23.278	3431	3436	3444	rVB	72437	134443	6.03%	0.906%
21	23.877	3536	3538	3547	rVB7	16337	27044	1.21%	0.182%
22	24.811	3688	3697	3713	rVB3	191805	606932	27.21%	4.090%
23	25.904	3866	3883	3899	rBV4	165399	934473	41.90%	6.297%
24	28.607	4322	4343	4359	rBV9	220281	1629451	73.06%	10.981%

Sum of corrected areas: 14839310

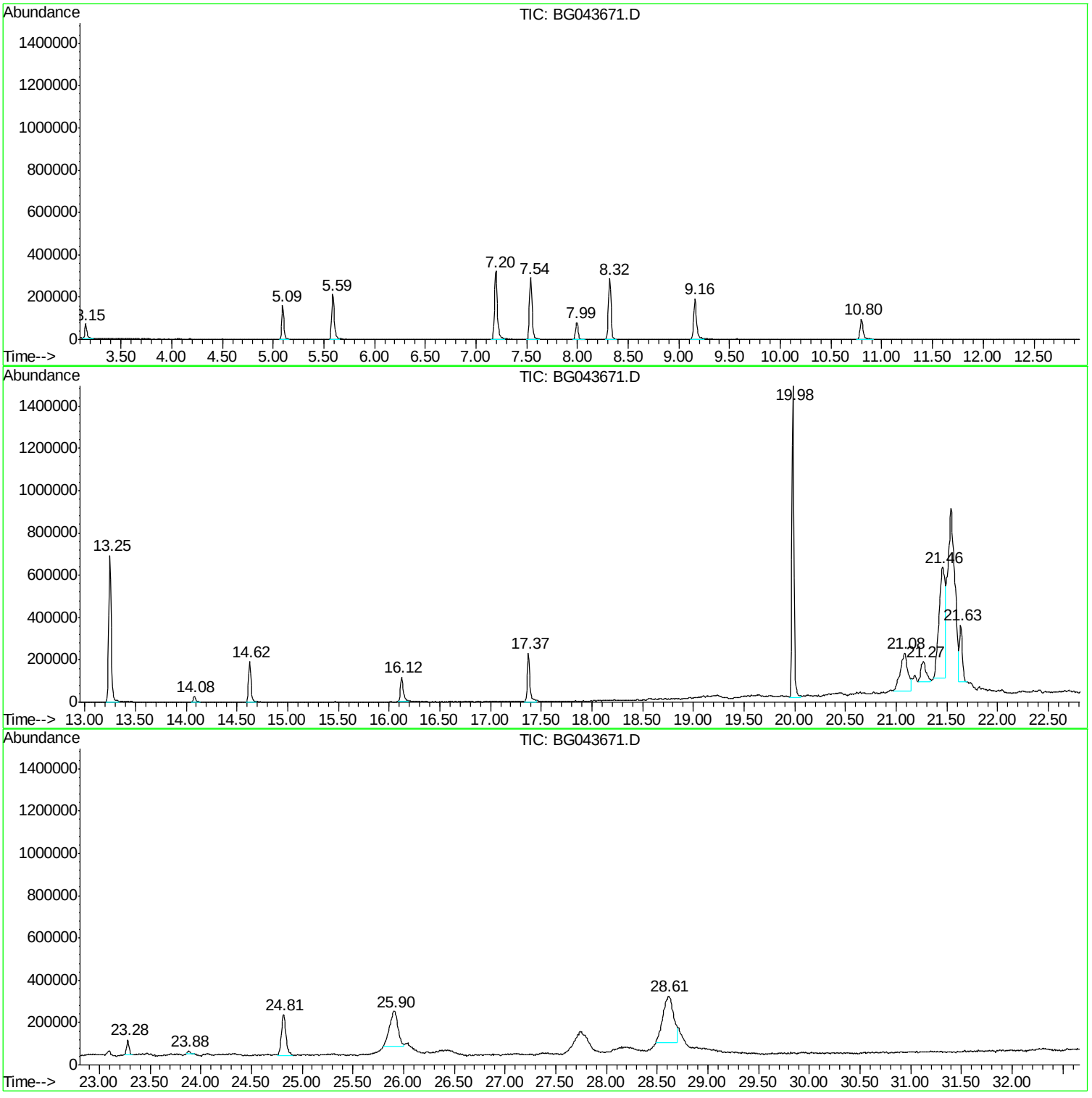
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111519\
Data File : BG043671.D
Acq On : 16 Nov 2019 4:18
Operator : JU
Sample : K5840-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PHIPPS-BH-SW-03

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\BG111519\
Data File : BG043671.D
Acq On : 16 Nov 2019 4:18
Operator : JU
Sample : K5840-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PHIPPS-BH-SW-03

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

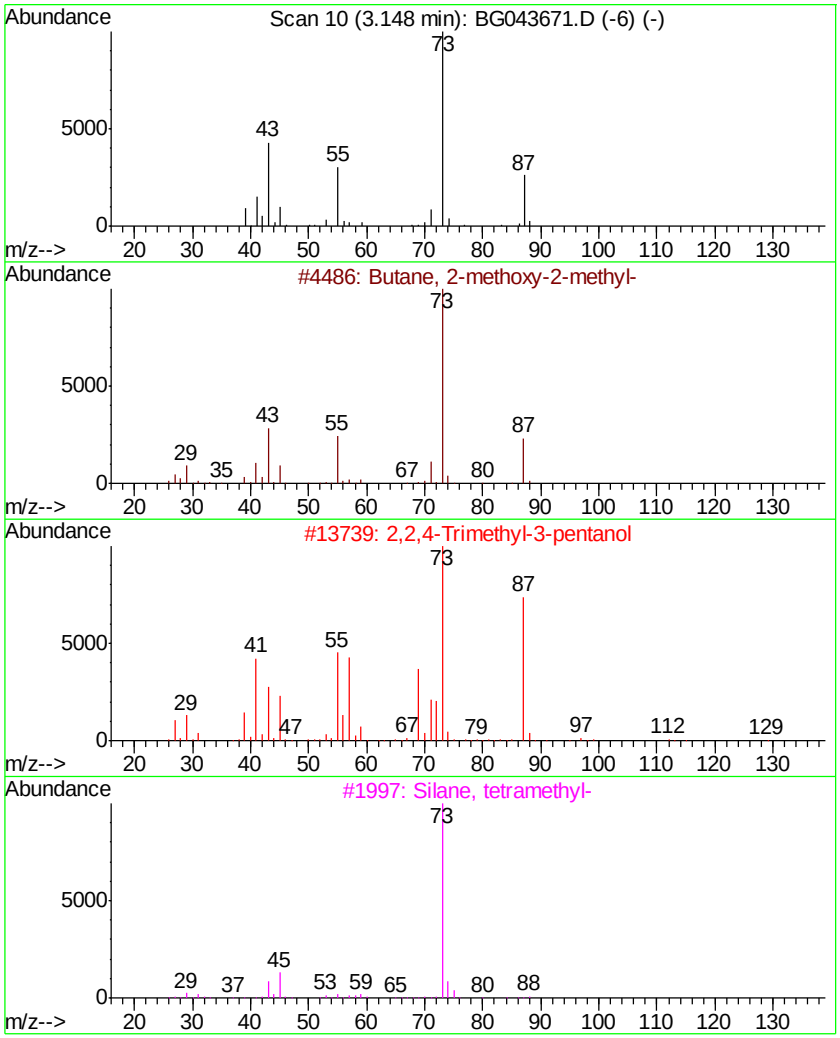
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

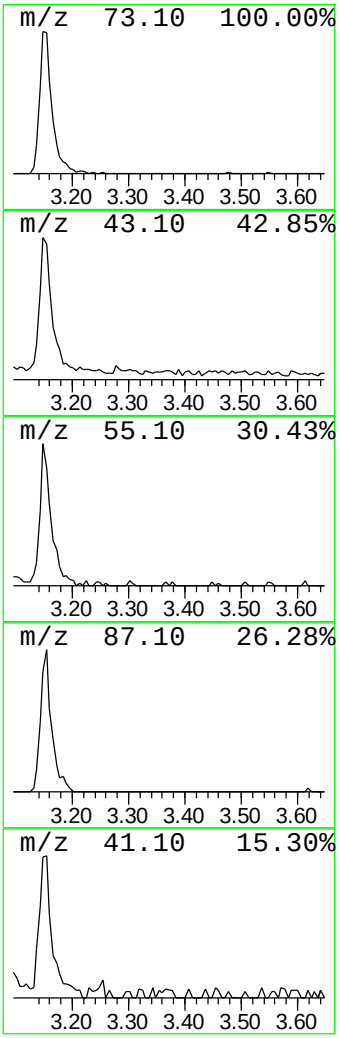
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	14.38 ng	106129	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111519\
Data File : BG043671.D
Acq On : 16 Nov 2019 4:18
Operator : JU
Sample : K5840-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PHIPPS-BH-SW-03

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

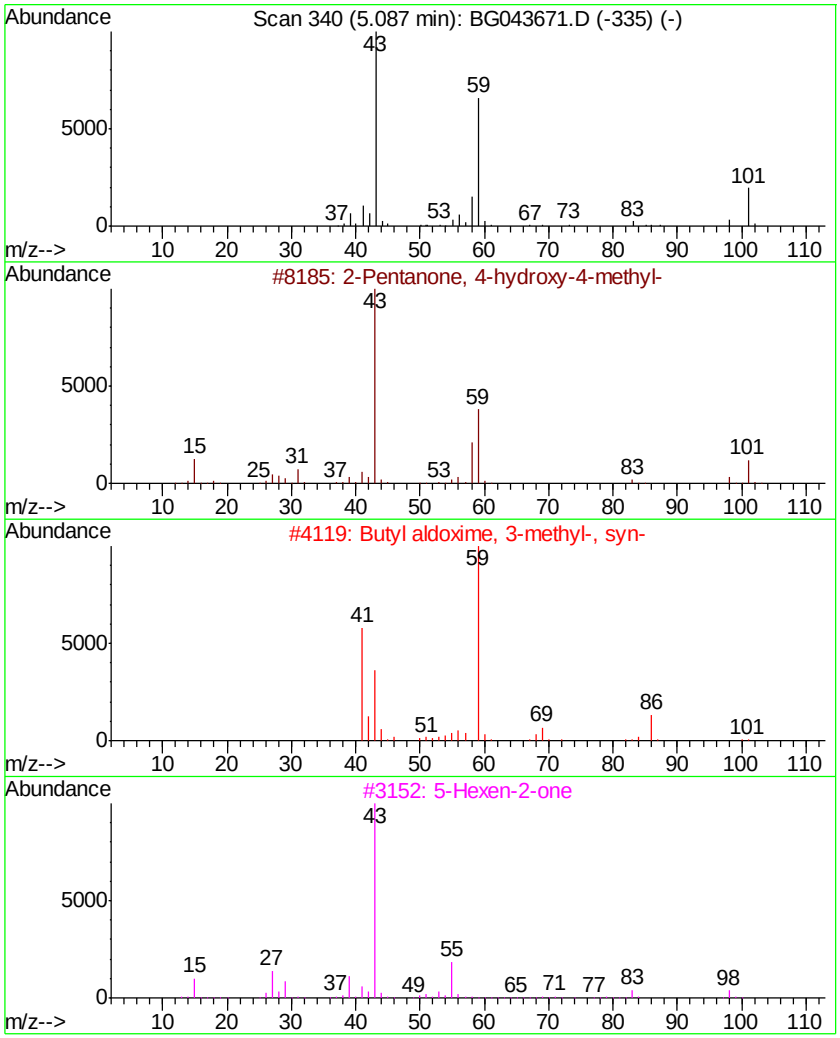
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

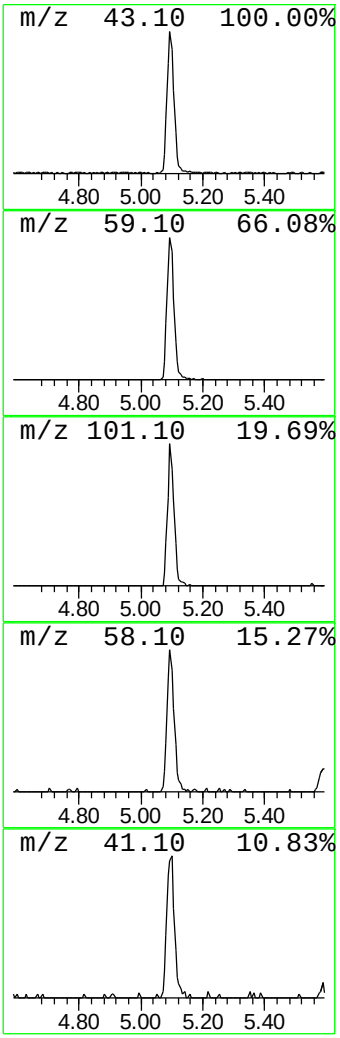
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	32.99 ng	243428	1,4-Dichlorobenzene-d4	8.00

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	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	9
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9





Library Search Compound Report

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Data File : BG043671.D
Acq On : 16 Nov 2019 4:18
Operator : JU
Sample : K5840-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PHIPPS-BH-SW-03

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
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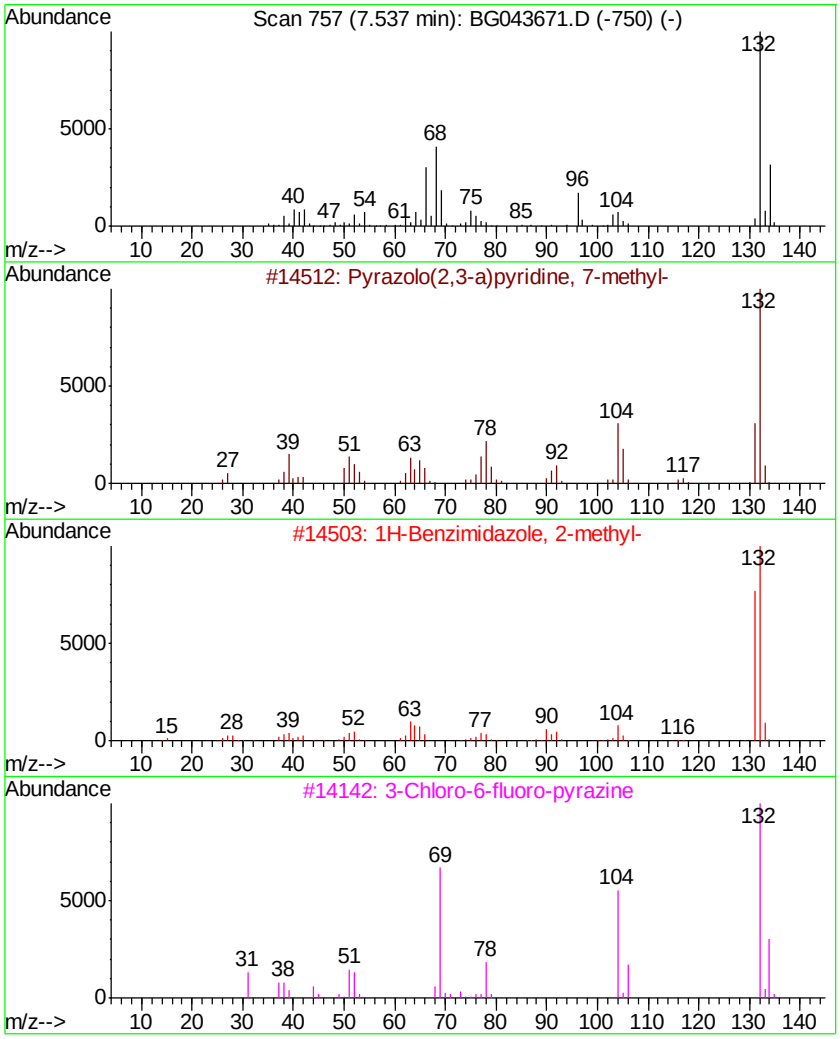
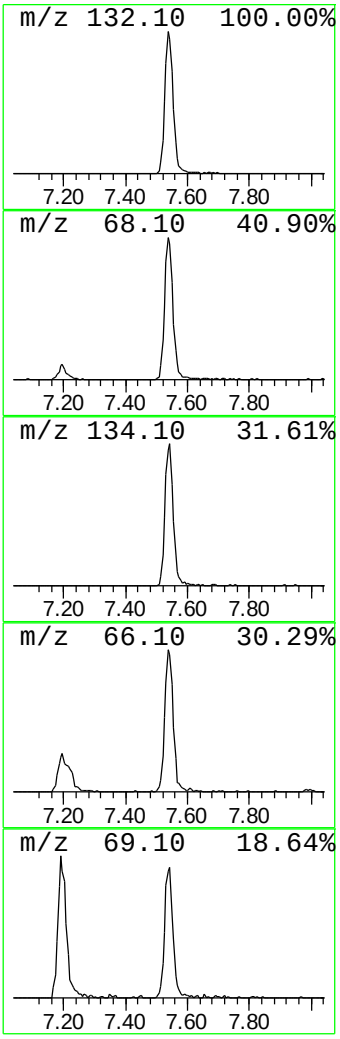
Peak Number 3 unknown7.54 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	73.51 ng	542422	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	12





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Data File : BG043671.D
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Operator : JU
Sample : K5840-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PHIPPS-BH-SW-03

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

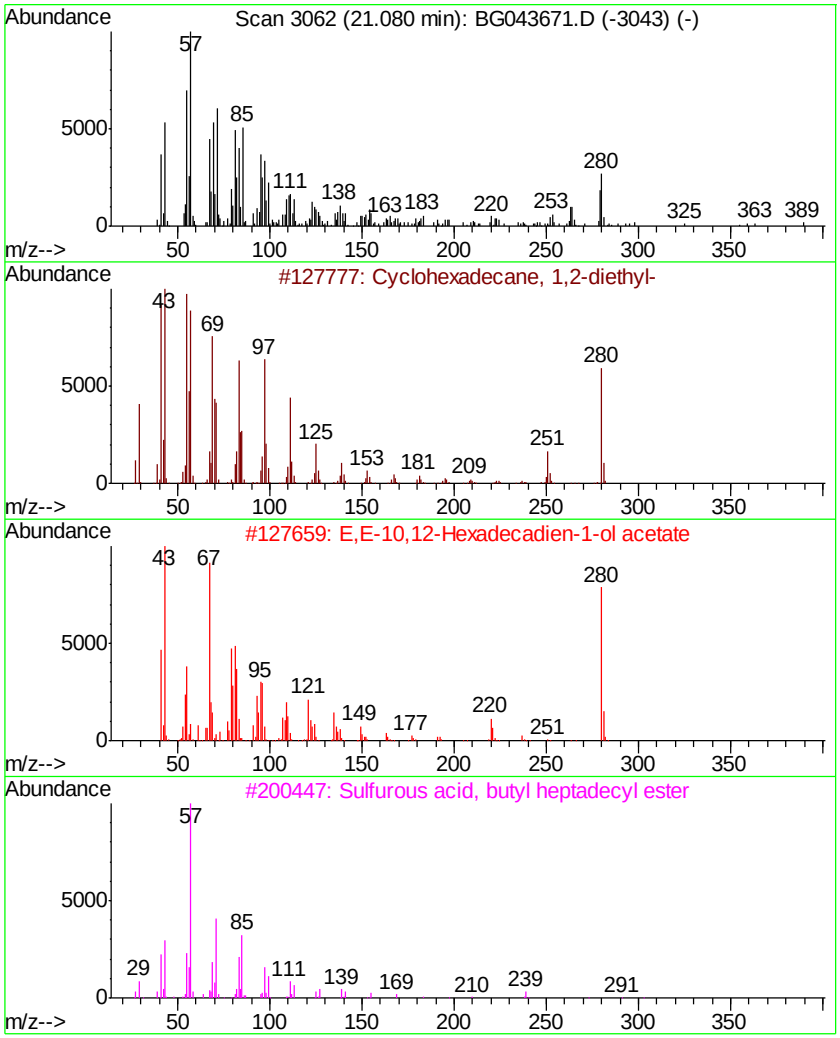
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

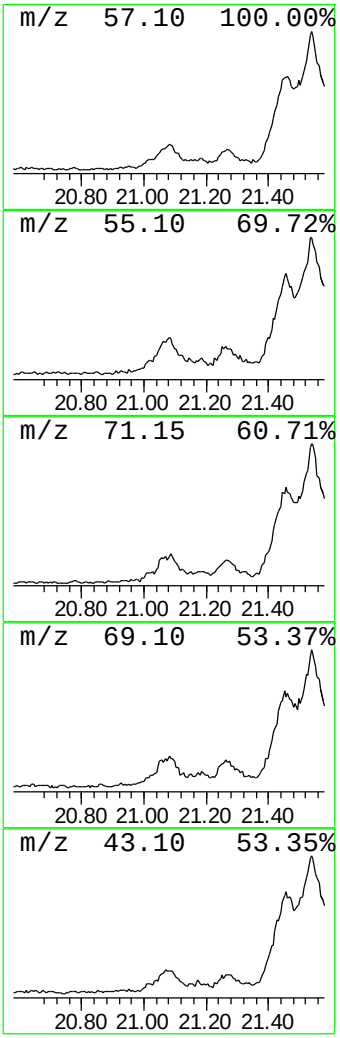
****

Peak Number 5 Cyclohexadecane, 1,2-diethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.08	36.94 ng	949135	Chrysene-d12	21.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	78
2	E,E-10,12-Hexadecadien-1-ol acetate	280	C18H32O2	1000130-87-6	53
3	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	53
4	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	50
5	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	49





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111519\
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Sample : K5840-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PHIPPS-BH-SW-03

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

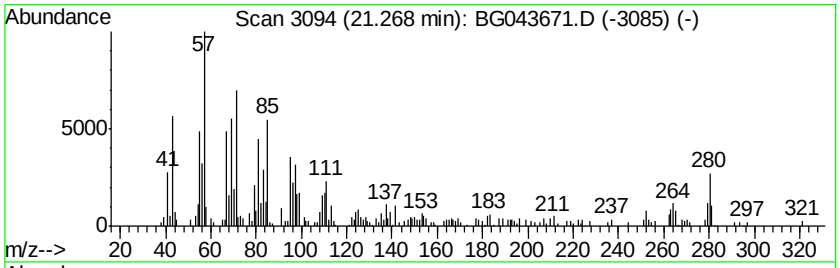
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

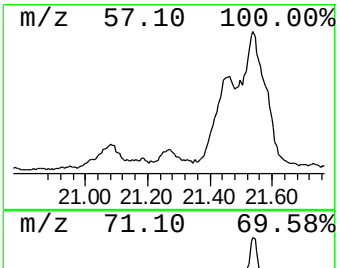
****

Peak Number 6 unknown21.27 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.27	13.55 ng	348261	Chrysene-d12	21.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	43
2	Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	43
3	Nonadecane	268	C19H40	000629-92-5	42
4	Octadecane	254	C18H38	000593-45-3	38
5	7-Oxabicyclo[4.1.0]heptane, 1,5-...	126	C8H14O	162239-52-3	38





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Sample : K5840-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PHIPPS-BH-SW-03

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

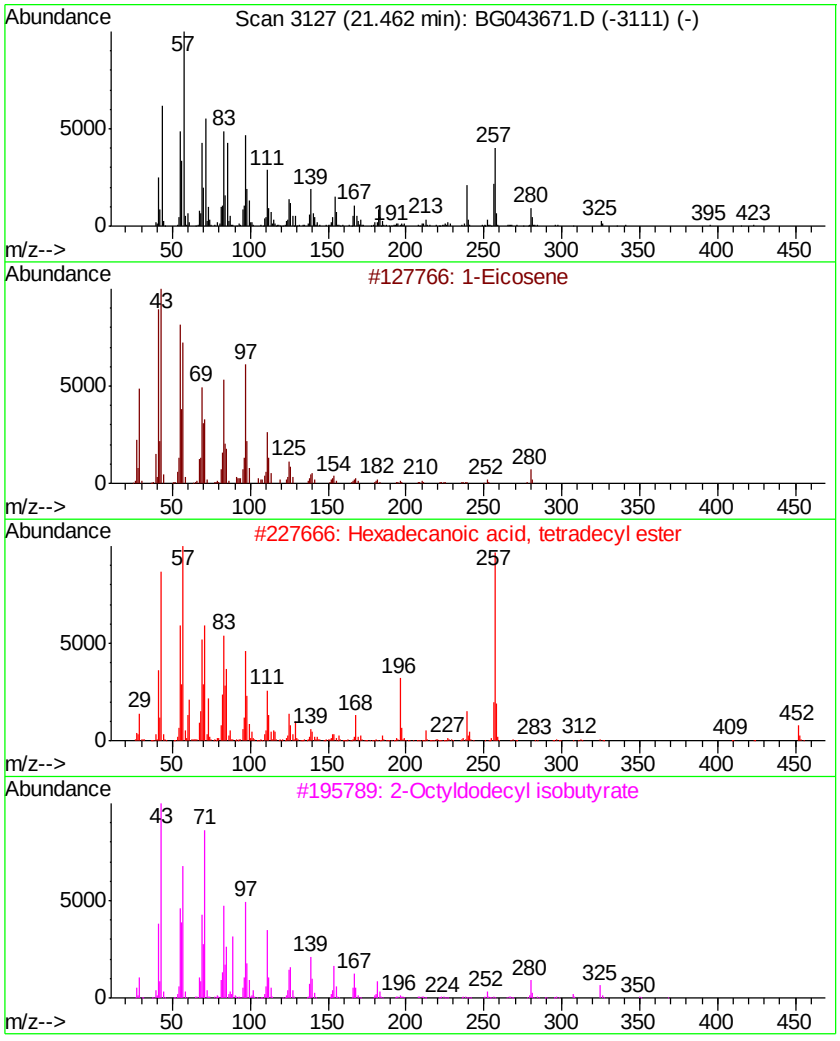
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

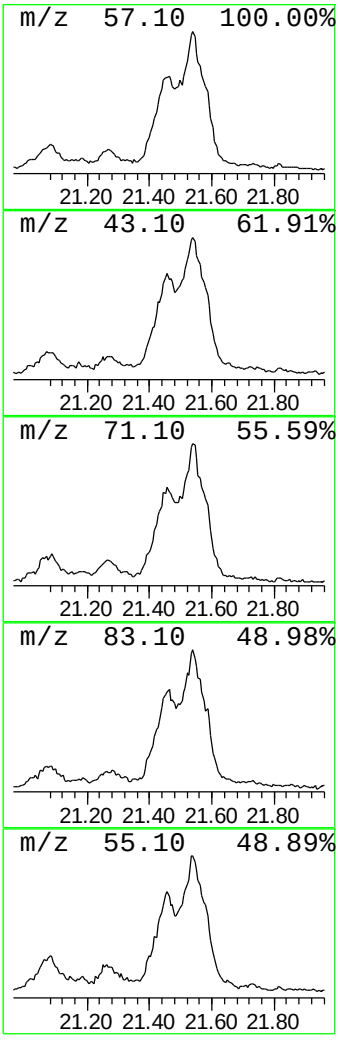
****

Peak Number 7 1-Eicosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.46	86.80 ng	2230280	Chrysene-d12	21.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosene	280	C20H40	003452-07-1	84
2	Hexadecanoic acid, tetradecyl ester	452	C30H60O2	004536-26-9	68
3	2-Octyldodecyl isobutyrate	368	C24H48O2	1000368-55-5	60
4	1-Dodecanol, 2-octyl-, acetate	340	C22H44O2	074051-84-6	60
5	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	55





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Acq On : 16 Nov 2019 4:18
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Instrument : BNA_G
ClientSampleId : PHIPPS-BH-SW-03

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

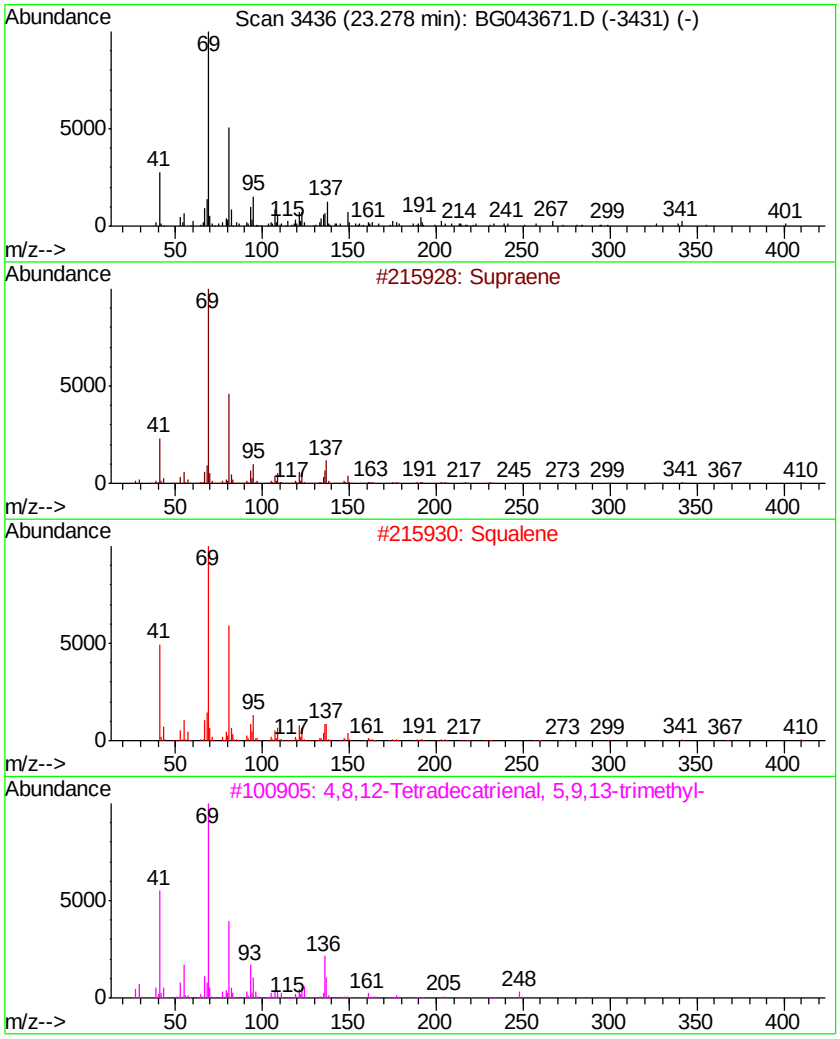
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

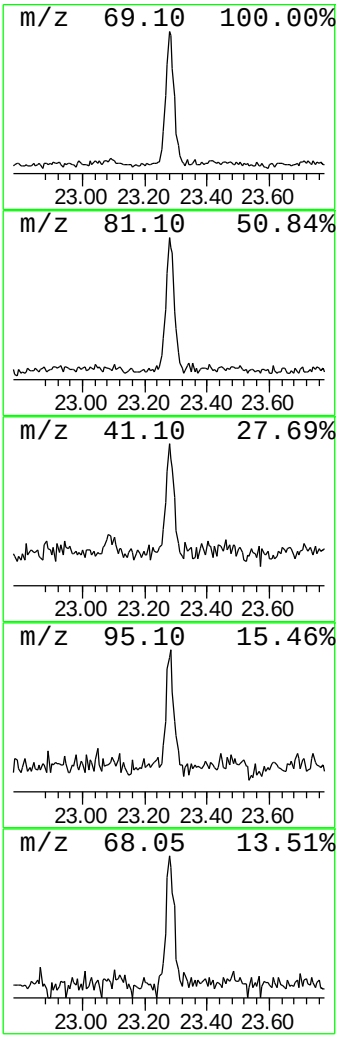
****

Peak Number 8 Supraene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.28	4.43 ng	134443	Perylene-d12	24.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	83
2	Squalene	410	C30H50	000111-02-4	80
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	64





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Misc :
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Instrument : BNA_G
ClientSampleId : PHIPPS-BH-SW-03

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

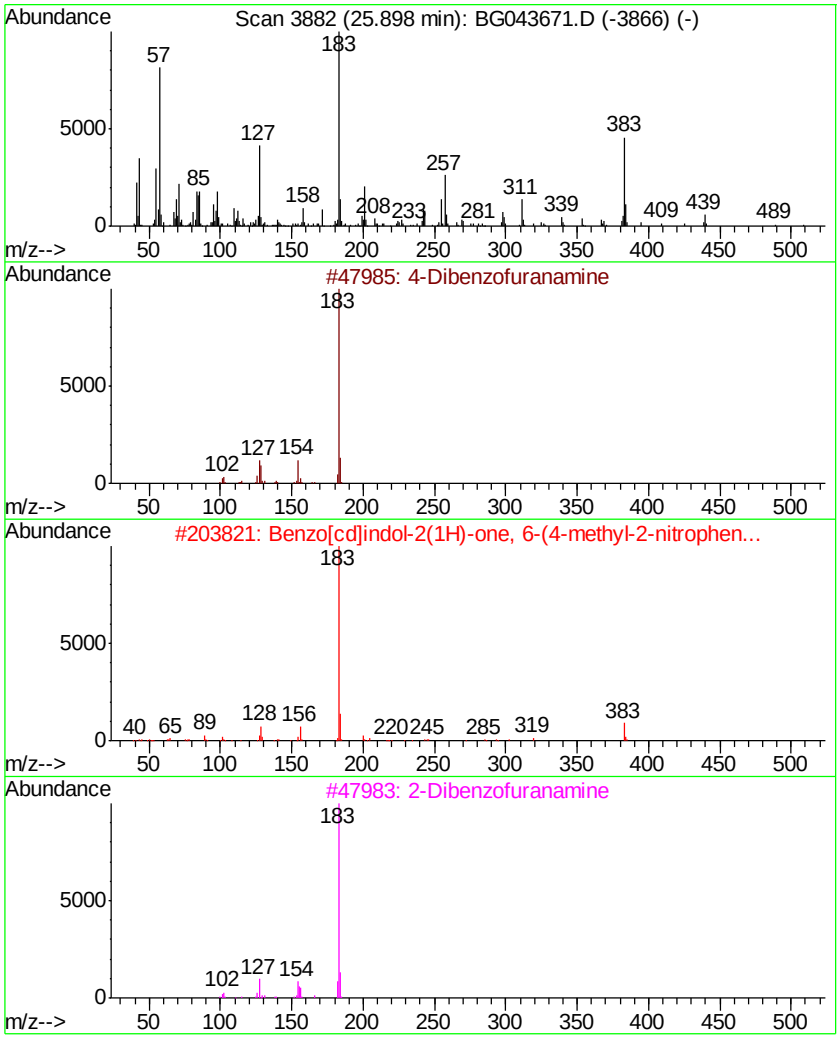
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

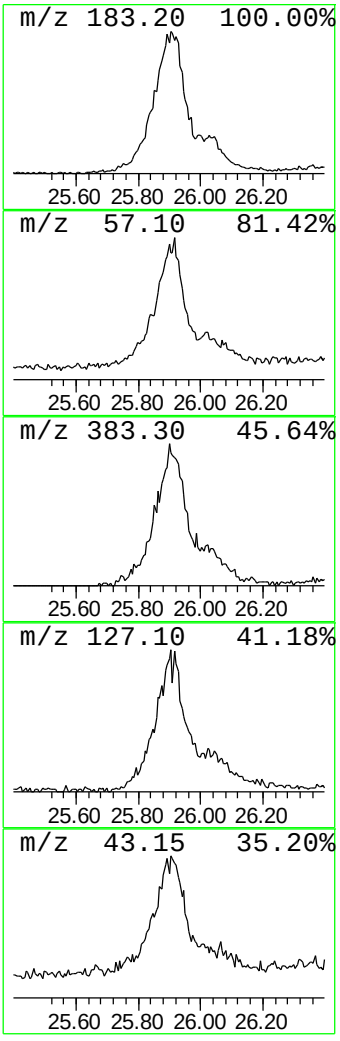
****

Peak Number 9 unknown25.90 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.90	30.79 ng	934473	Perylene-d12	24.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Dibenzofuranamine	183	C12H9NO	050548-43-1	38
2	Benzo[cd]indol-2(1H)-one, 6-(4-m...	383	C18H13N3O5S	327043-60-7	38
3	2-Dibenzofuranamine	183	C12H9NO	003693-22-9	35
4	Fumaric acid, di(2-methylpent-3-...	284	C16H28O4	1000348-77-7	35
5	Fumaric acid, isohexyl 4-octyl e...	312	C18H32O4	1000339-21-6	35





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PHIPPS-BH-SW-03

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

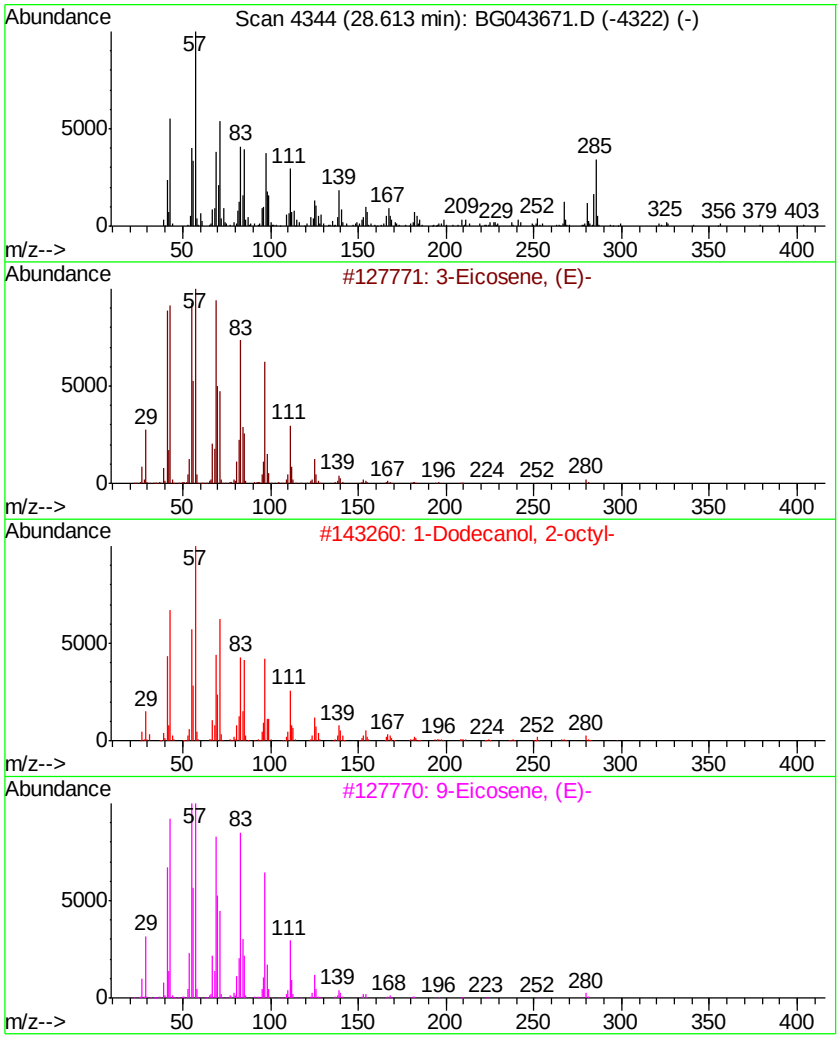
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

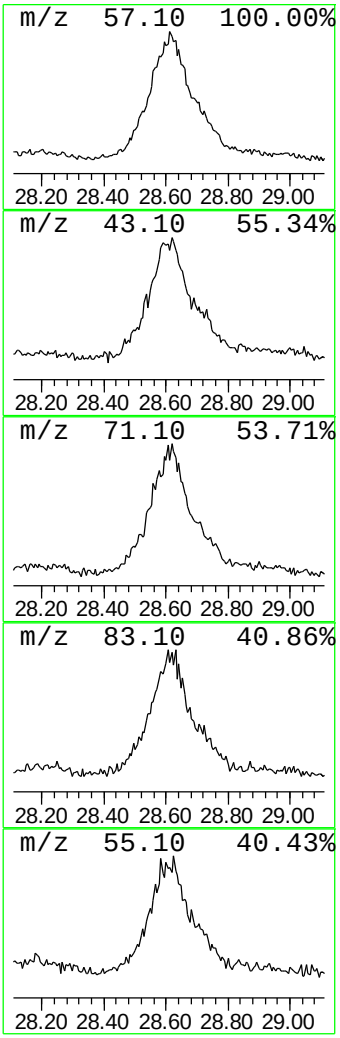
****

Peak Number 10 3-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.61	53.69 ng	1629450	Perylene-d12	24.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	89
2	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	64
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	64
4	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	64
5	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG111519\
Data File : BG043671.D
Acq On : 16 Nov 2019 4:18
Operator : JU
Sample : K5840-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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ClientSampleId : PHIPPS-BH-SW-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.15	14.4	ng	106129	1	8.00	147573	20.0
2-Pentanone, 4-hy...	5.09	33.0	ng	243428	1	8.00	147573	20.0
unknown7.54	7.54	73.5	ng	542422	1	8.00	147573	20.0
Cyclohexadecane, ...	21.08	36.9	ng	949135	5	21.64	513917	20.0
unknown21.27	21.27	13.6	ng	348261	5	21.64	513917	20.0
1-Eicosene	21.46	86.8	ng	2230280	5	21.64	513917	20.0
Supraene	23.28	4.4	ng	134443	6	24.82	606932	20.0
unknown25.90	25.90	30.8	ng	934473	6	24.82	606932	20.0
3-Eicosene, (E)-	28.61	53.7	ng	1629450	6	24.82	606932	20.0