LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100419\
Data File : BG043042.D
Acq On : 5 Oct 2019 00:01
Operator : JU
Sample : K5154-15
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105S

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	3.176	7	15	23	rBV	206762	531705	10.38%	1.724%
2	3.252	23	28	45	rVB	662853	1191253	23.26%	3.863%
3	5.385	385	391	398	rBV2	55653	97063	1.89%	0.315%
4	5.649	427	436	449	rBV	730849	1259887	24.60%	4.085%
5	7.236	697	706	719	rBV2	515273	1045986	20.42%	3.392%
6	7.600	759	768	780	rBV	1176726	2033071	39.69%	6.592%
7	8.064	839	847	854	rBV	262585	465505	9.09%	1.509%
8	8.387	894	902	911	rBV	812275	1399744	27.33%	4.539%
9	9.222	1036	1044	1056	rBV	705276	1254528	24.49%	4.068%
10	10.867	1316	1324	1332	rBV	337662	616871	12.04%	2.000%
11	13.305	1732	1739	1749	rBV	1921145	2957247	57.73%	9.589%
12	14.128	1873	1879	1889	rBV	325037	488171	9.53%	1.583%
13	14.680	1966	1973	1988	rVB2	568232	943703	18.42%	3.060%
14	15.091	2037	2043	2047	rBV4	32445	52223	1.02%	0.169%
15	15.250	2063	2070	2076	rBV2	50015	153102	2.99%	0.496%
16	16.166	2219	2226	2236	rBV	1835664	2827533	55.20%	9.168%
17	16.360	2255	2259	2266	rVB4	35085	55980	1.09%	0.182%
18	17.424	2434	2440	2446	rBV2	729517	1089511	21.27%	3.533%
19	18.323	2586	2593	2608	rBV	848877	1333049	26.02%	4.322%
20	19.586	2804	2808	2819	rBV	298817	442777	8.64%	1.436%
21	19.850	2849	2853	2859	rVB	193639	272890	5.33%	0.885%
22	20.032	2878	2884	2891	rBV	3640783	5122306	100.00%	16.609%
23	21.337	3102	3106	3117	rBV	393537	639793	12.49%	2.074%
24	21.695	3160	3167	3176	rVB	820177	1386137	27.06%	4.494%
25	21.889	3196	3200	3206	rVB	81230	110417	2.16%	0.358%
26	22.500	3299	3304	3309	rBV2	102242	174925	3.41%	0.567%
27	23.188	3416	3421	3430	rVB	151705	291465	5.69%	0.945%
28	23.992	3552	3558	3567	rVB2	171183	370844	7.24%	1.202%
29	24.915	3704	3715	3729	rBV2	544153	1872709	36.56%	6.072%
30	26.078	3905	3913	3924	rVB3	122070	360974	7.05%	1.170%

Sum of corrected areas: 30841369

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100419\
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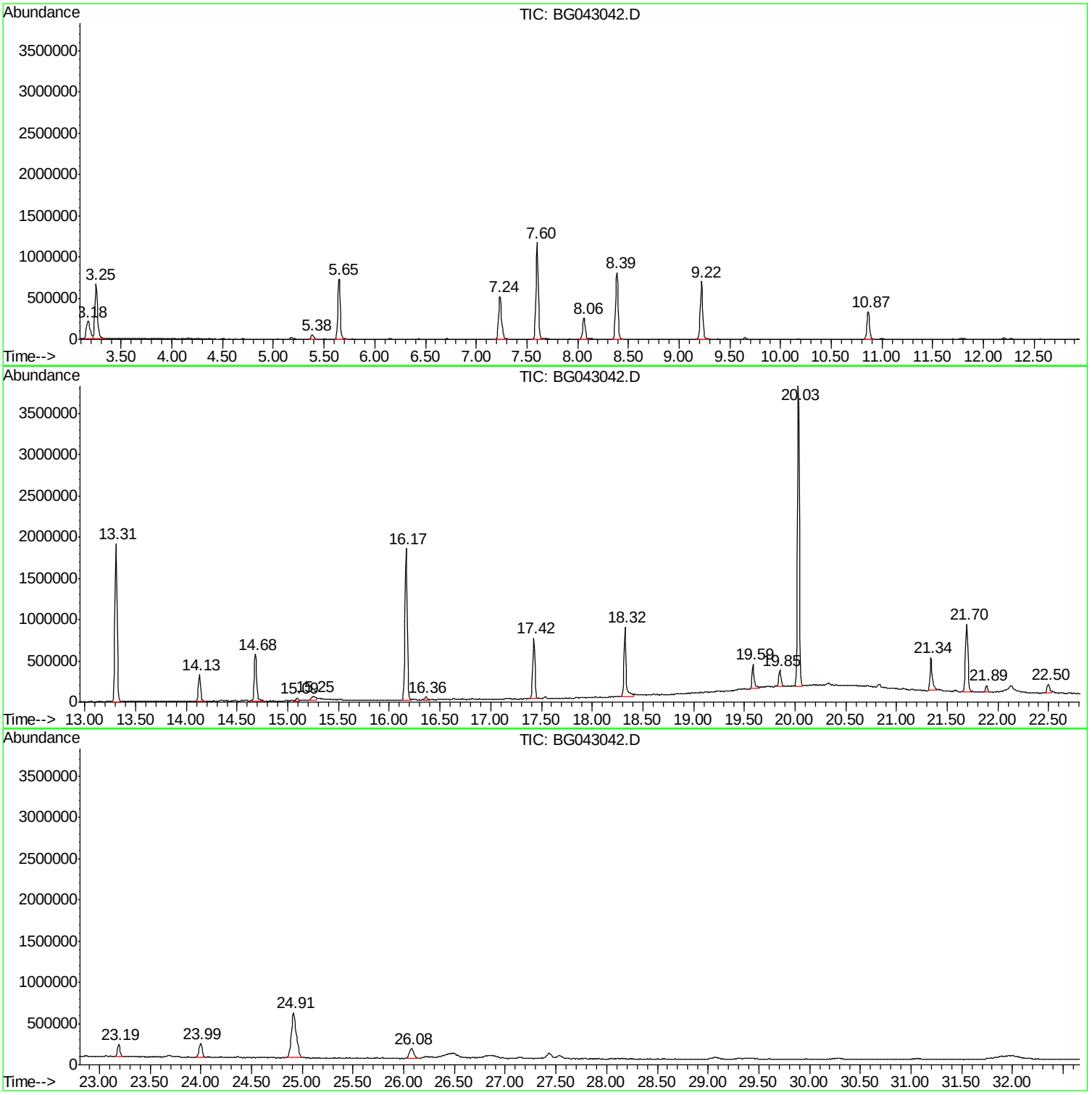
Acq On : 5 Oct 2019 00:01
Operator : JU
Sample : K5154-15
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105S

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

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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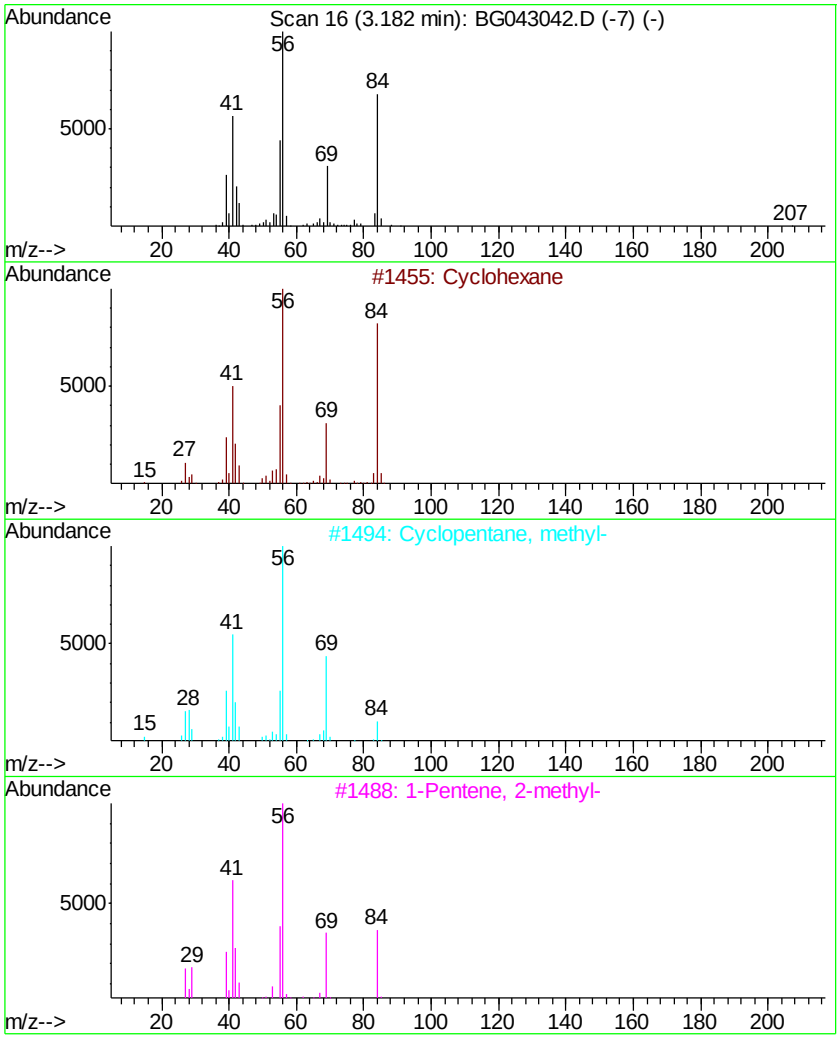
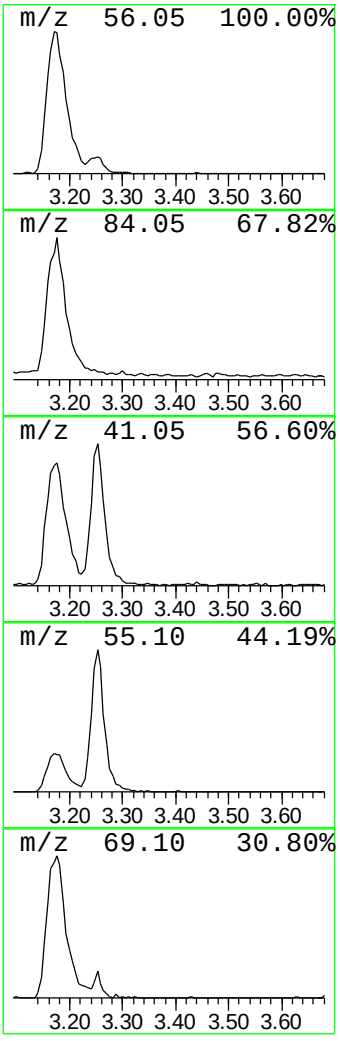
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	22.84 ng	531705	1,4-Dichlorobenzene-d4	8.06

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	59
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	56
4	1-Hexene	84	C6H12	000592-41-6	53
5	1-Butanol	74	C4H10O	000071-36-3	47





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : MW-105S

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

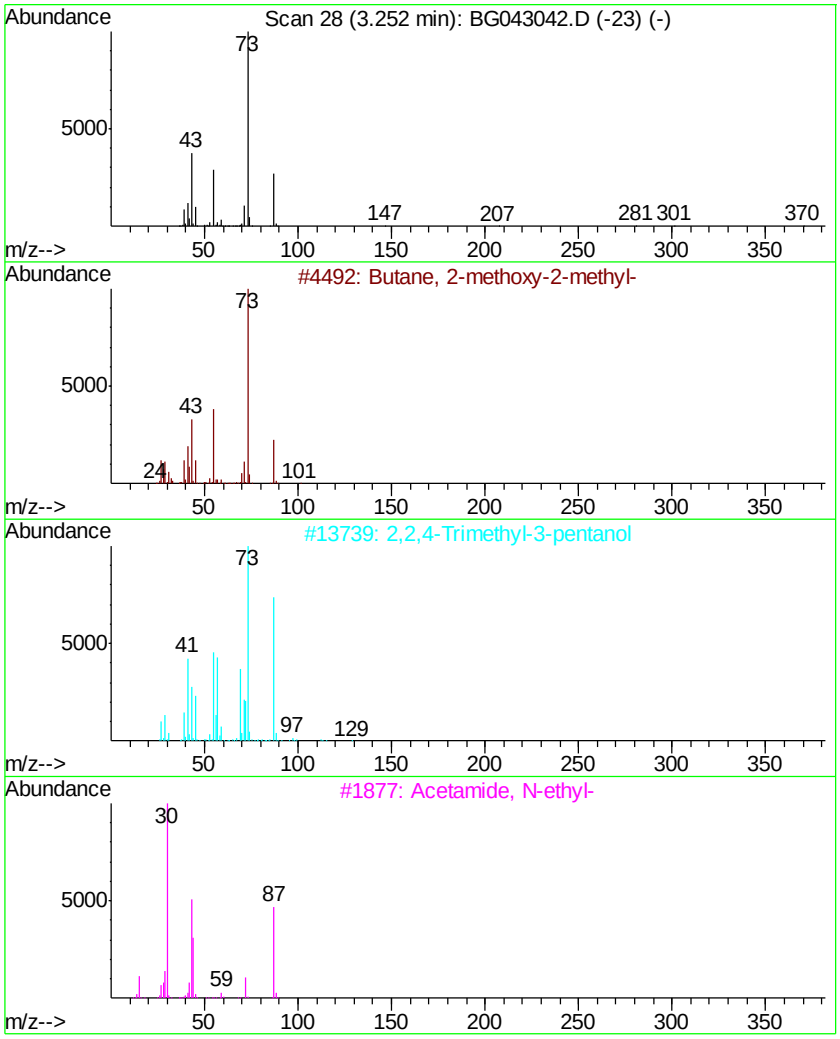
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

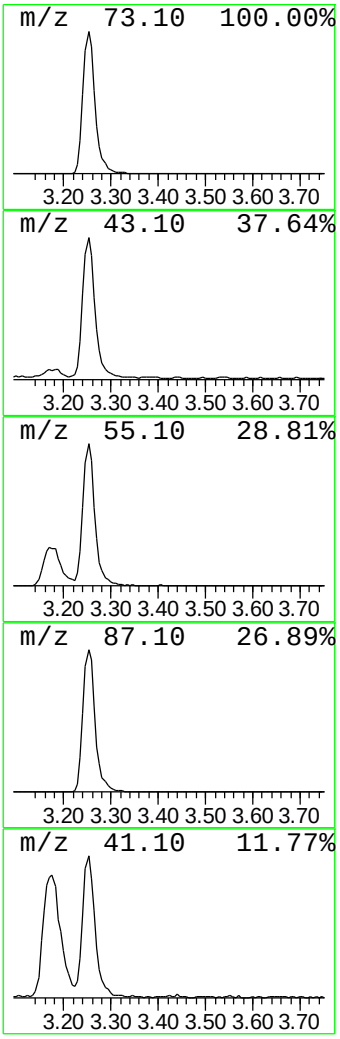
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.25	51.18 ng	1191250	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	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Library Search Compound Report

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Sample : K5154-15
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105S

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

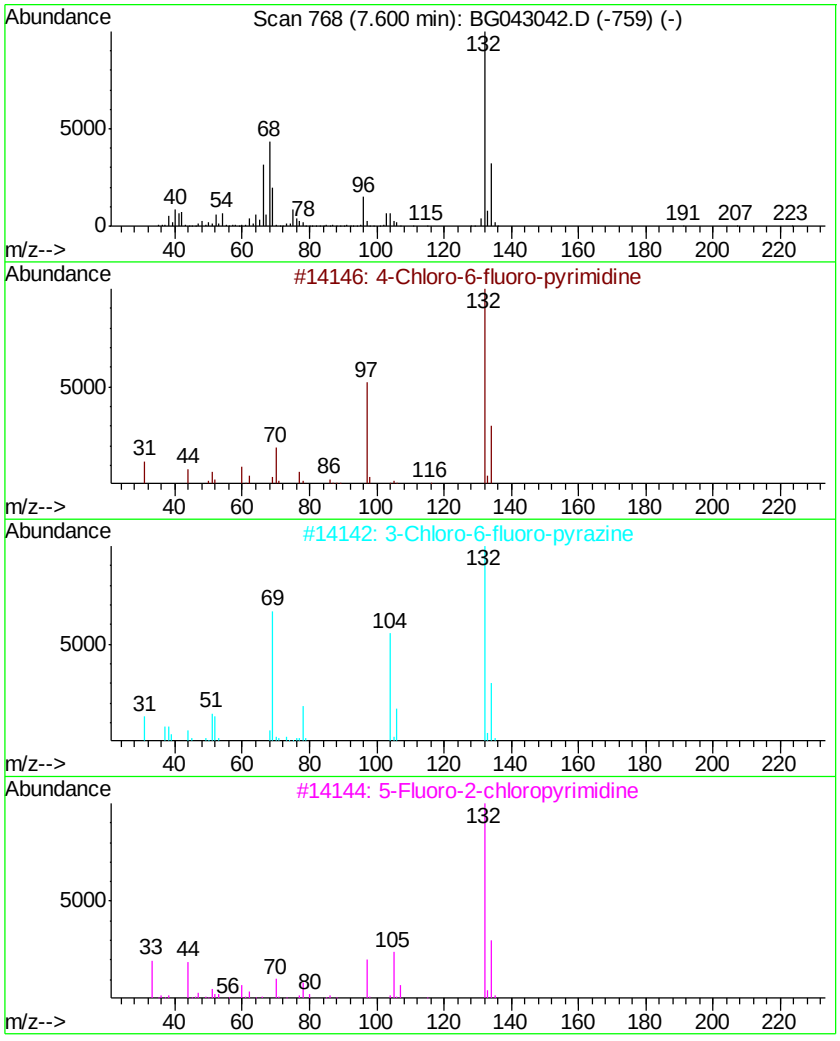
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

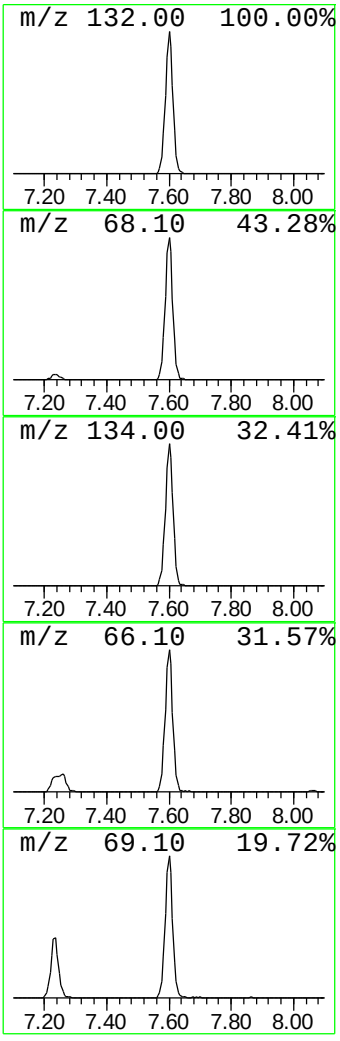
****

Peak Number 4 unknown7.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	87.35 ng	2033070	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105S

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

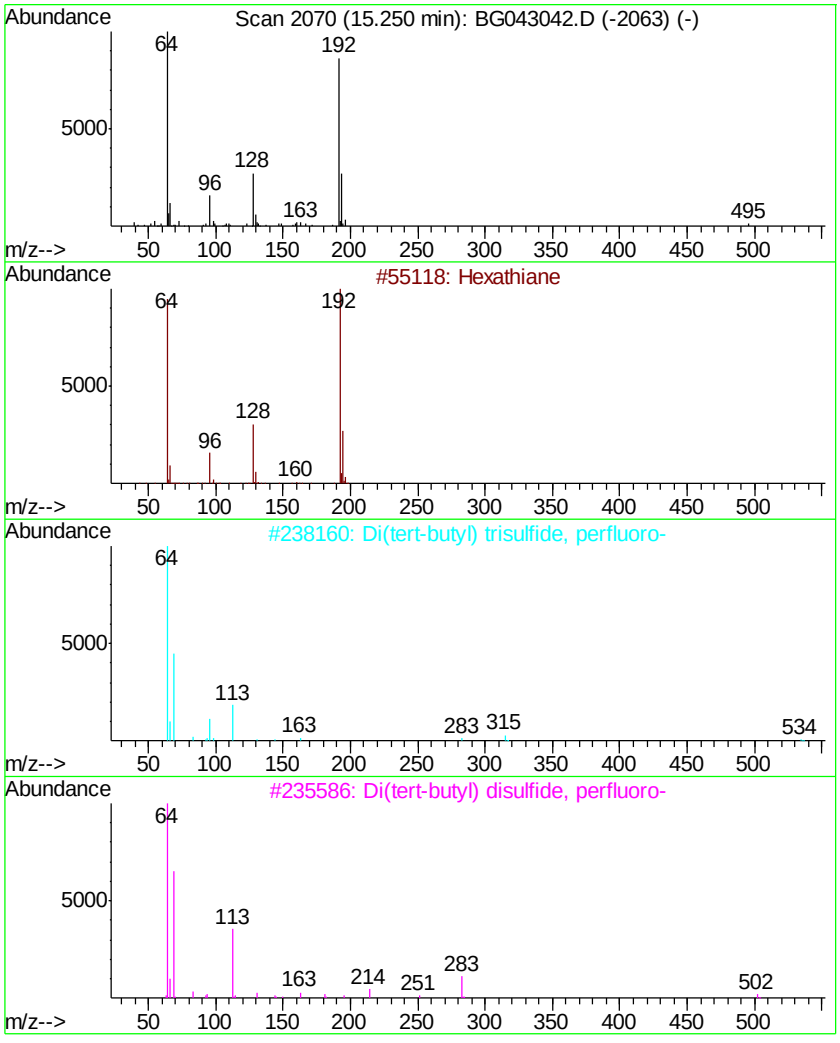
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

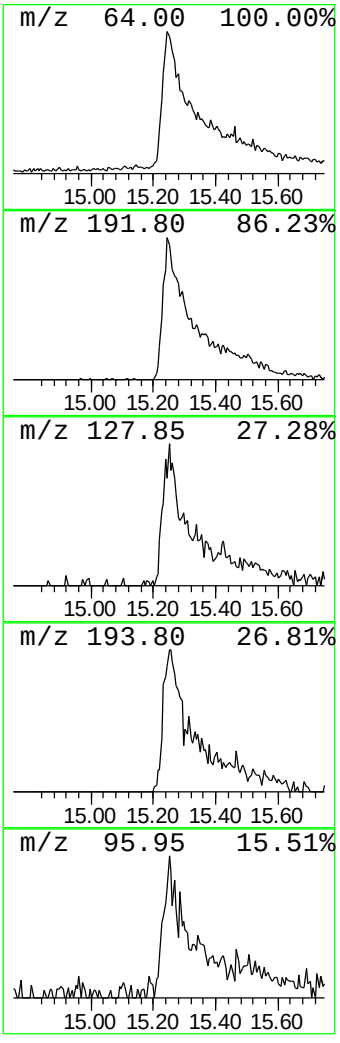
****

Peak Number 6 Hexathiane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	3.24 ng	153102	Acenaphthene-d10	14.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiane	192	S6	013798-23-7	94
2	Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	53
3	Di(tert-butyl) disulfide, perflu...	502	C8F18S2	034880-30-3	36
4	2-Chloro-7-methoxynaphthalene	192	C11H9ClO	067061-67-0	36
5	tert-Butyl isopropyl disulfide, ...	452	C7F16S2	1000226-69-7	36





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Sample : K5154-15
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105S

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

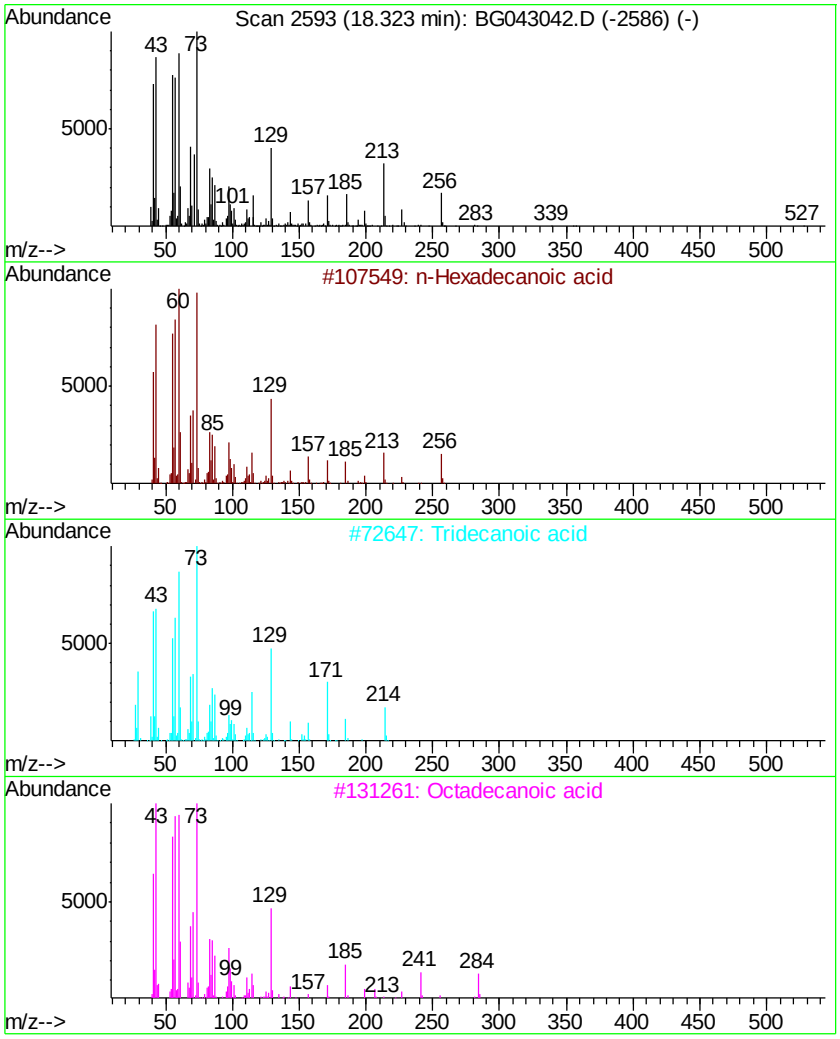
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

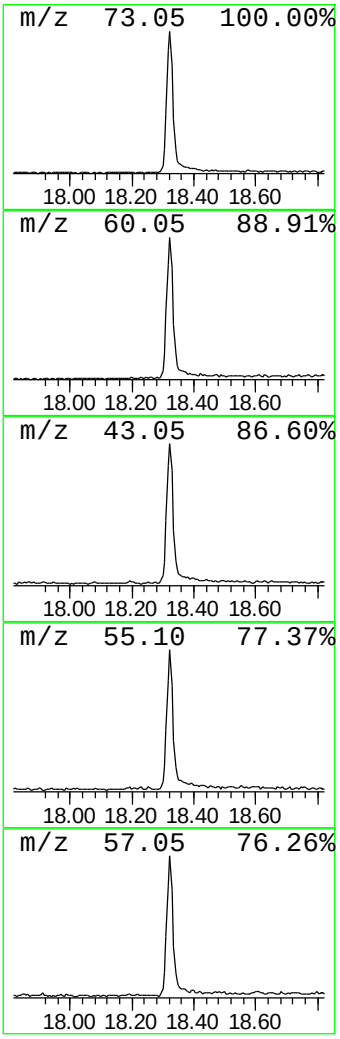
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	24.47 ng	1333050	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	97
3	Octadecanoic acid	284	C18H36O2	000057-11-4	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105S

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

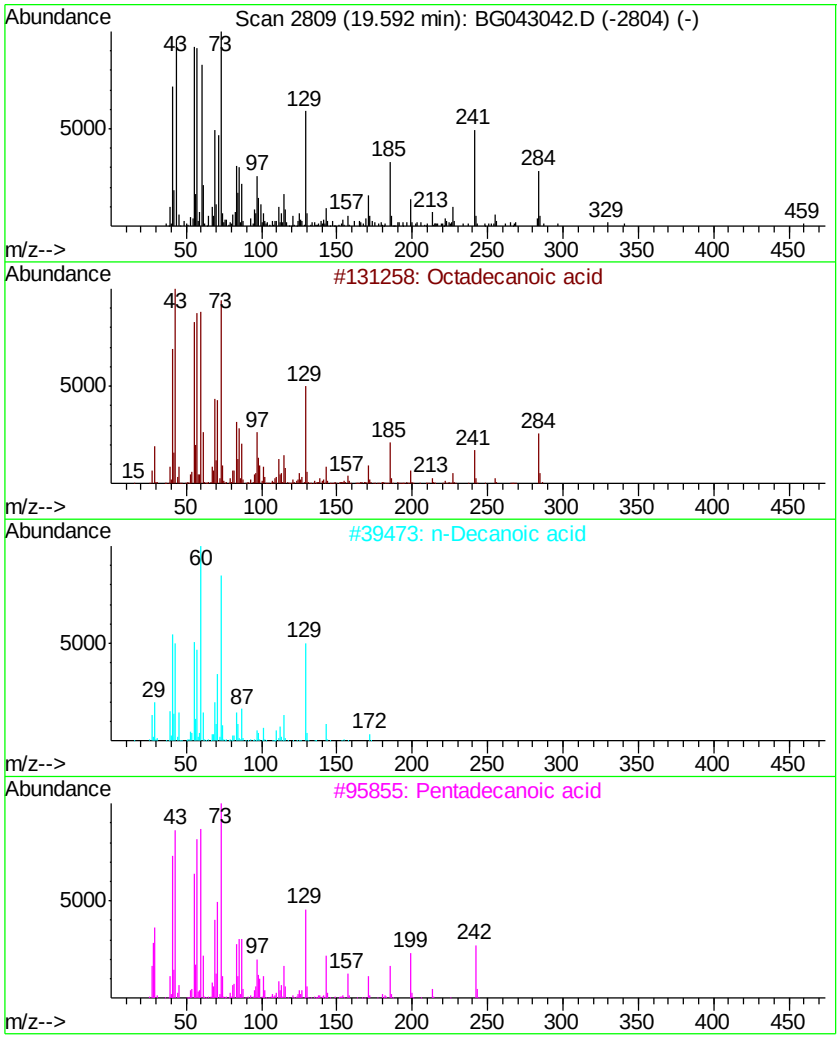
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

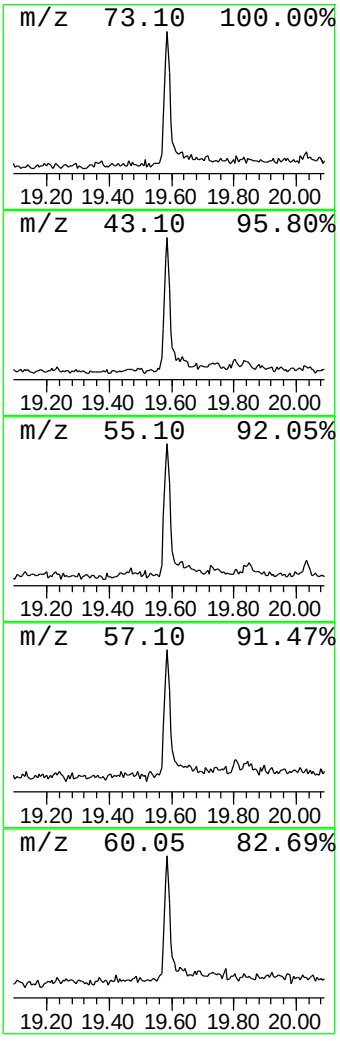
****

Peak Number 8 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.59	6.39 ng	442777	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Decanoic acid	172	C10H20O2	000334-48-5	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52





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Instrument : BNA_G
ClientSampleId : MW-105S

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

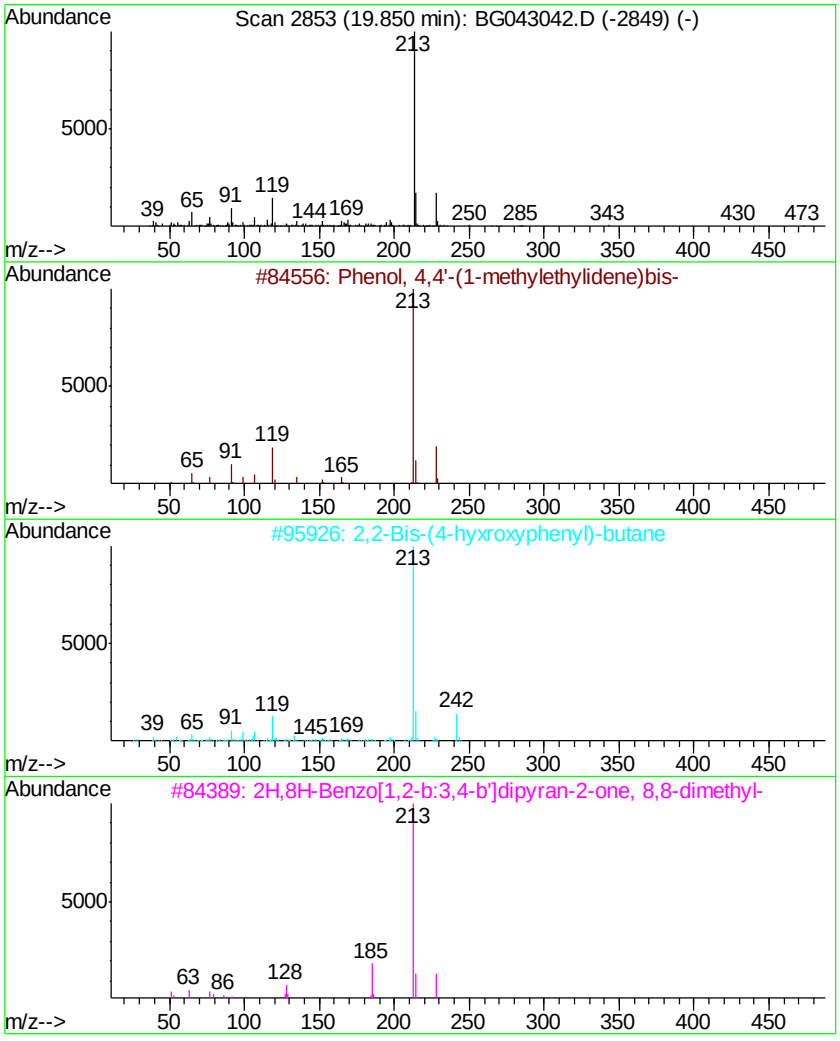
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

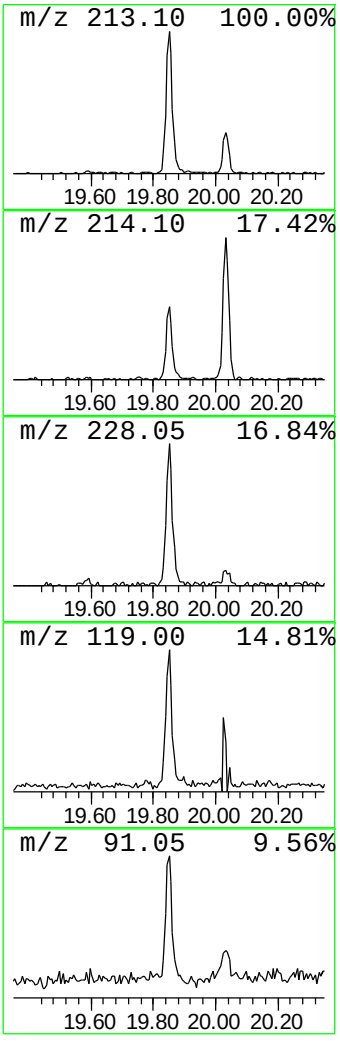
****

Peak Number 9 Phenol, 4,4'-(1-methylethyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.85	3.94 ng	272890	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	93
2	2,2-Bis-(4-hyxroxyphenyl)-butane	242	C16H18O2	000077-40-7	72
3	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	64
4	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	59
5	Diphenolic acid	286	C17H18O4	000126-00-1	59





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TIC Library : C:\Database\NIST11.L
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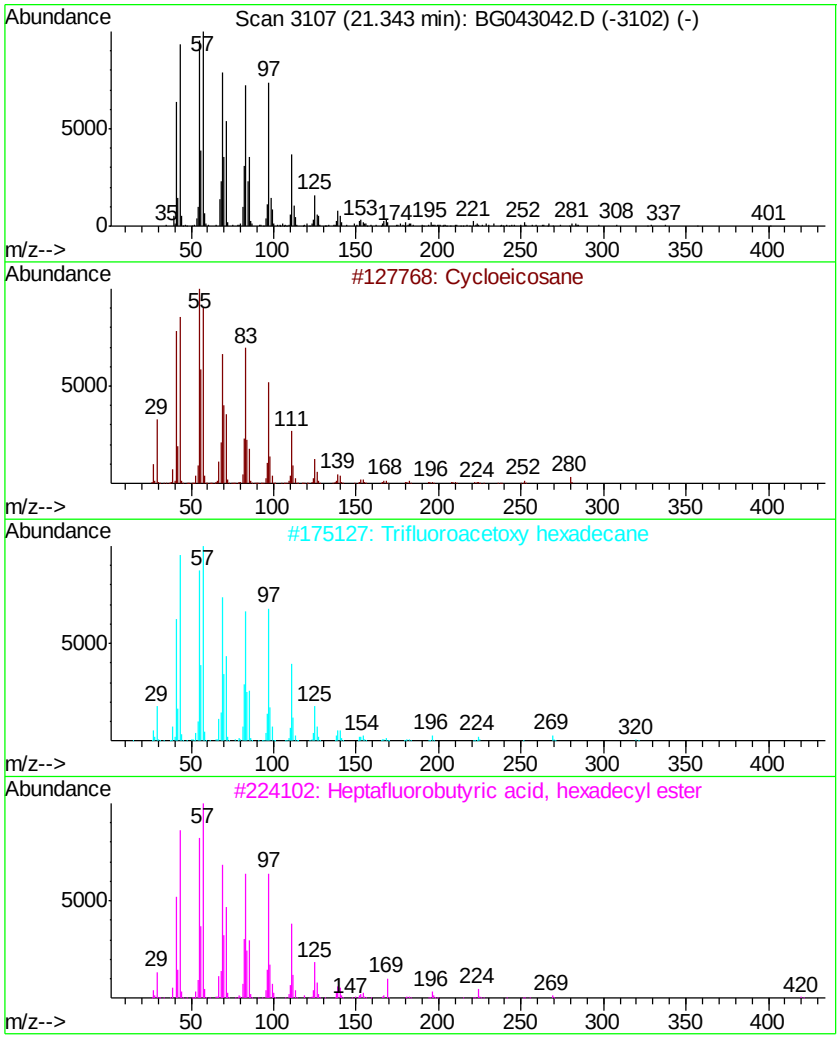
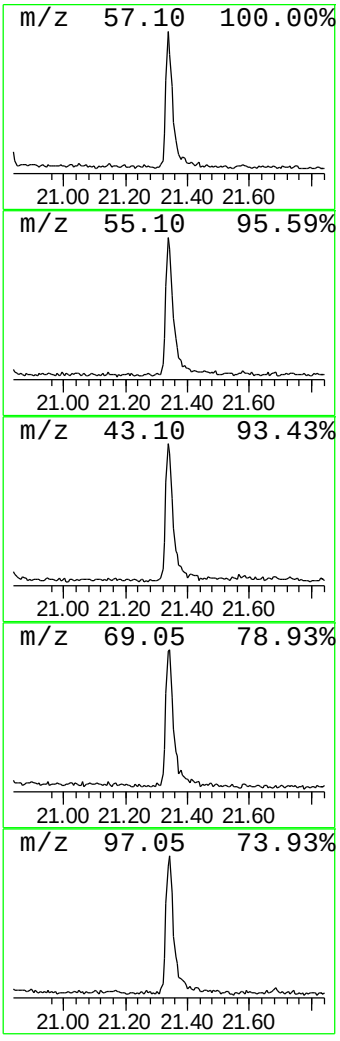
Peak Number 10 Cycloeicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.34	9.23 ng	639793	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91





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Data File : BG043042.D
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Operator : JU
Sample : K5154-15
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105S

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

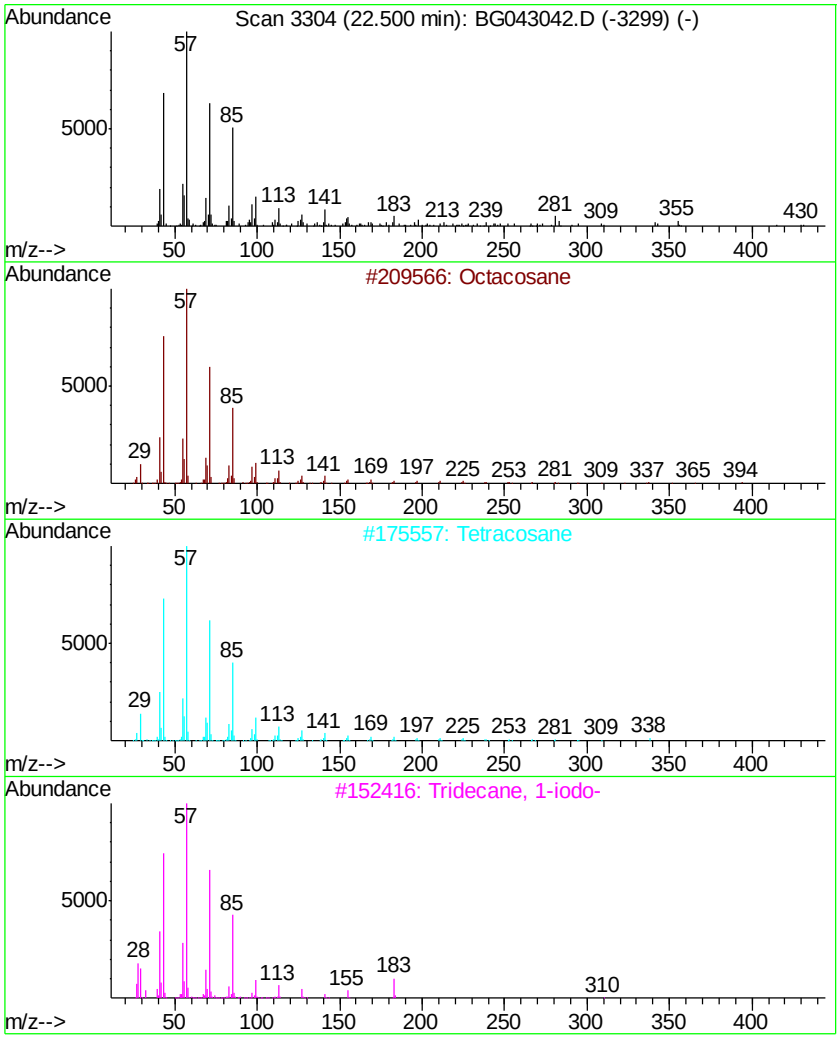
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

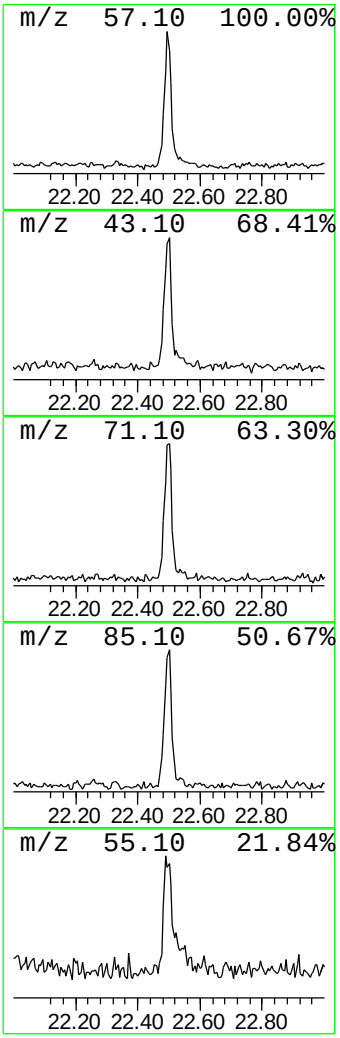
****

Peak Number 11 Tetracosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.50	2.52 ng	174925	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Tetracosane	338	C24H50	000646-31-1	86
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105S

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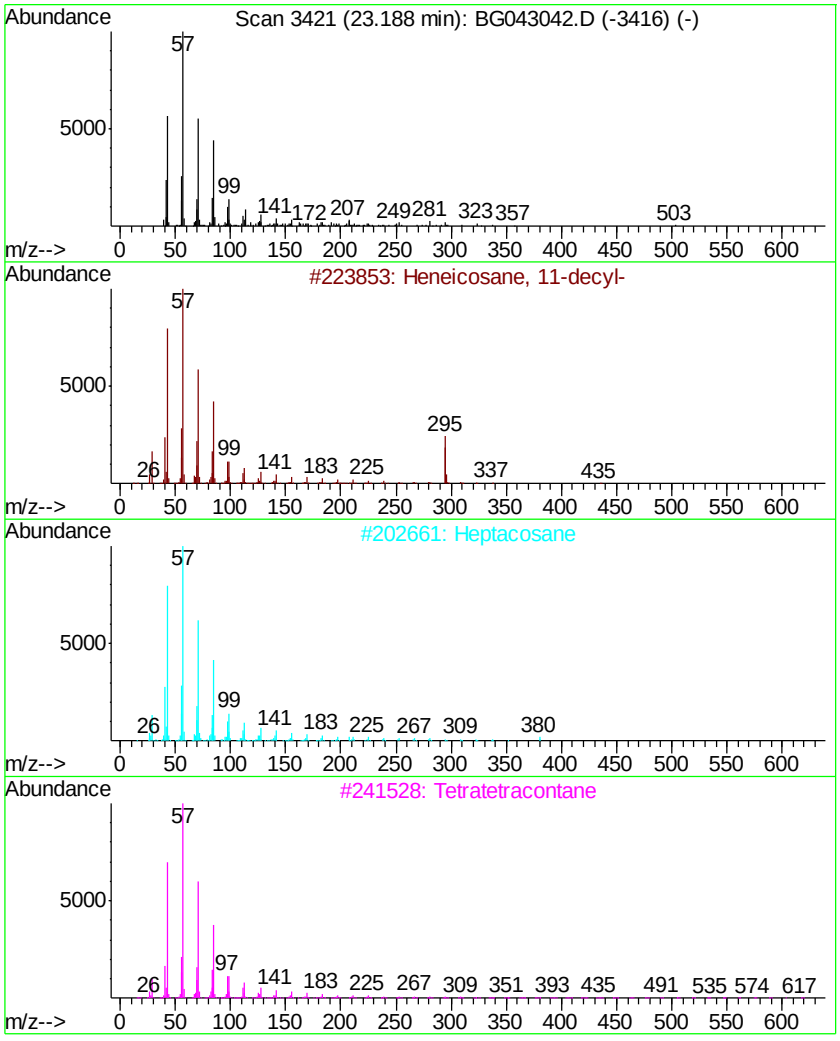
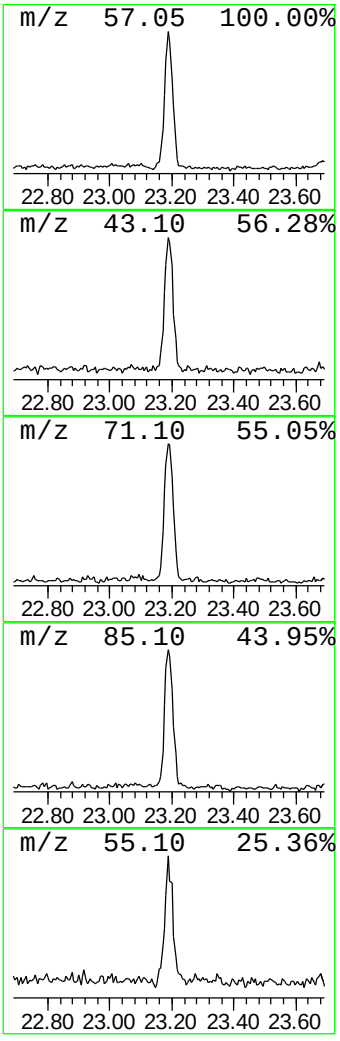
****

Peak Number 12 Heneicosane, 11-decyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	4.21 ng	291465	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	90
2	Heptacosane	380	C27H56	000593-49-7	90
3	Tetratetracontane	619	C44H90	007098-22-8	90
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Hexatriacontane	507	C36H74	000630-06-8	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100419\
Data File : BG043042.D
Acq On : 5 Oct 2019 00:01
Operator : JU
Sample : K5154-15
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105S

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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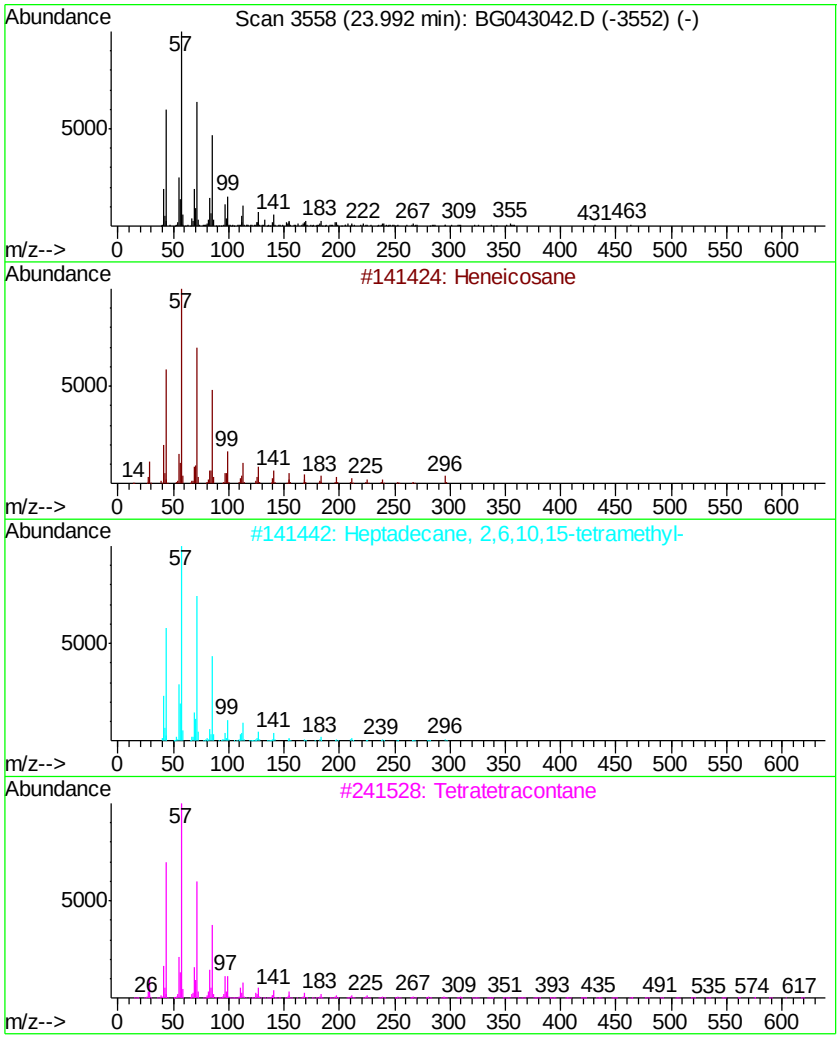
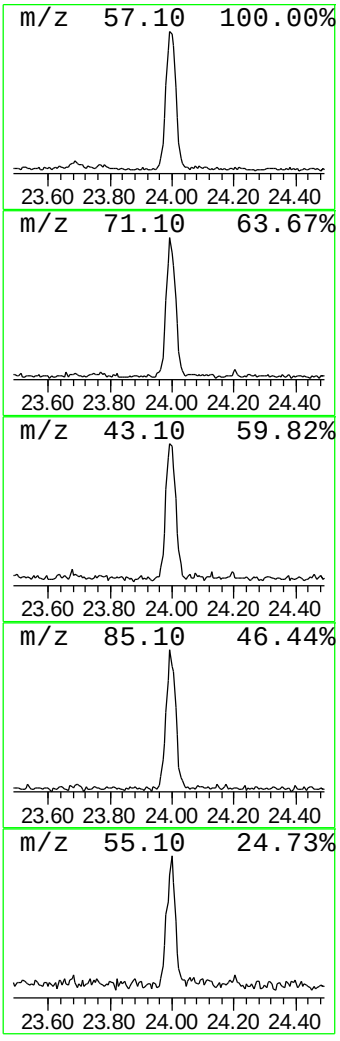
Peak Number 13 Heptadecane, 2,6,10,15-tetr... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	3.96 ng	370844	Perylene-d12	24.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
3	Tetratetracontane	619	C44H90	007098-22-8	90
4	Heptadecane	240	C17H36	000629-78-7	90
5	2-methyloctacosane	408	C29H60	1000376-72-8	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100419\
Data File : BG043042.D
Acq On : 5 Oct 2019 00:01
Operator : JU
Sample : K5154-15
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105S

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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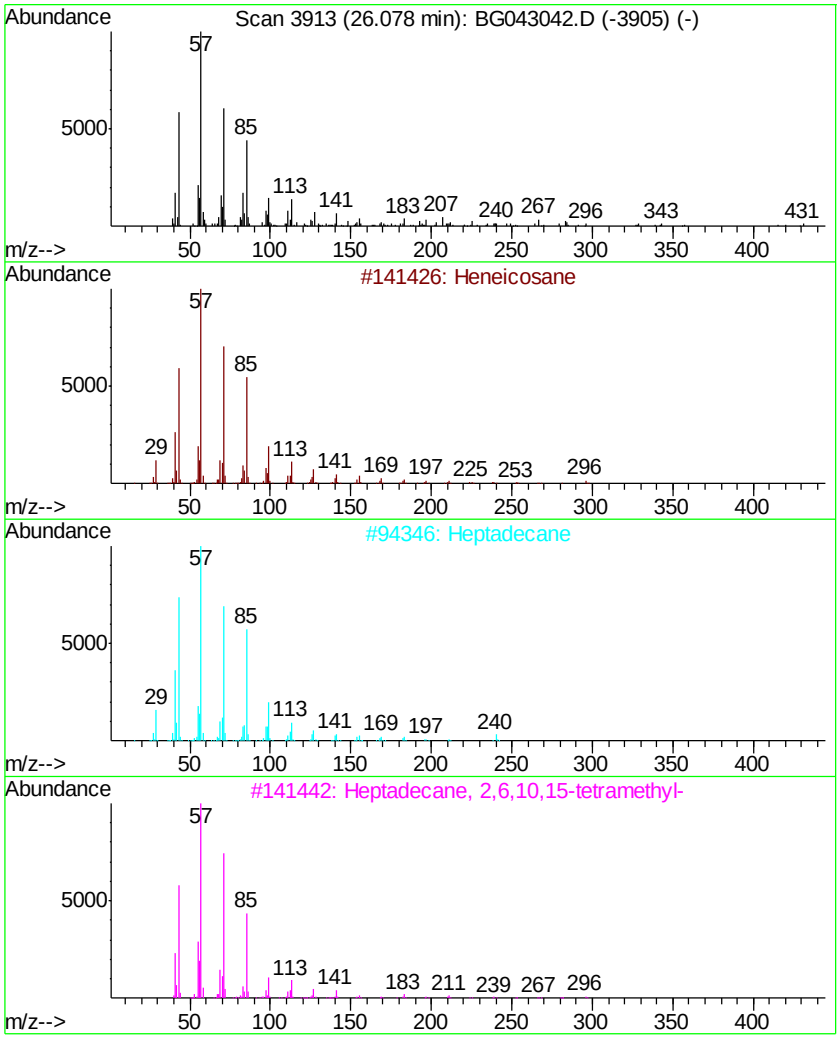
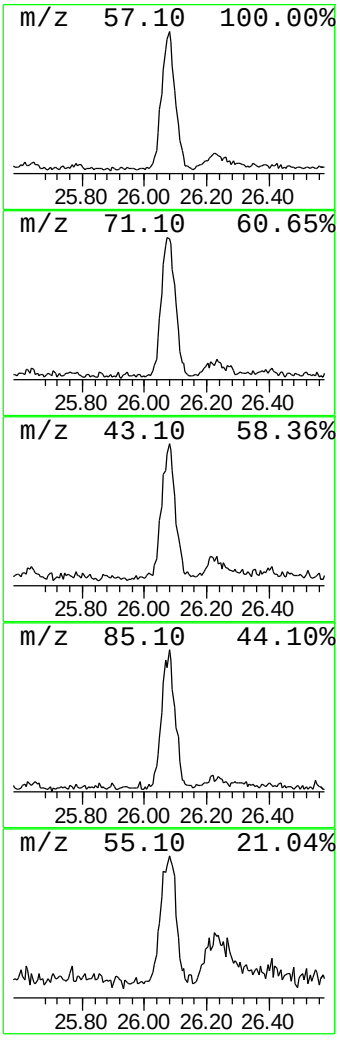
Peak Number 14 Pentadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.08	3.86 ng	360974	Perylene-d12	24.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Heptadecane	240	C17H36	000629-78-7	97
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	96
4	Pentadecane	212	C15H32	000629-62-9	94
5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG100419\
Data File : BG043042.D
Acq On : 5 Oct 2019 00:01
Operator : JU
Sample : K5154-15
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105S

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
Cyclopentane, met...	3.18	22.8	ng	531705	1	8.06	465505	20.0
Butane, 2-methoxy...	3.25	51.2	ng	1191250	1	8.06	465505	20.0
unknown7.60	7.60	87.3	ng	2033070	1	8.06	465505	20.0
Hexathiane	15.25	3.2	ng	153102	3	14.68	943703	20.0
n-Hexadecanoic acid	18.32	24.5	ng	1333050	4	17.42	1089510	20.0
Octadecanoic acid	19.59	6.4	ng	442777	5	21.70	1386140	20.0
Phenol, 4,4'-(1-m...	19.85	3.9	ng	272890	5	21.70	1386140	20.0
Cycloeicosane	21.34	9.2	ng	639793	5	21.70	1386140	20.0
Tetracosane	22.50	2.5	ng	174925	5	21.70	1386140	20.0
Heneicosane, 11-d...	23.19	4.2	ng	291465	5	21.70	1386140	20.0
Heptadecane, 2,6,...	23.99	4.0	ng	370844	6	24.91	1872710	20.0
Pentadecane	26.08	3.9	ng	360974	6	24.91	1872710	20.0