LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012119\
Data File : BG039232.D
Acq On : 21 Jan 2019 14:03
Operator : JU/SJ
Sample : K1205-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C-1

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-BG010919.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	3.125	3	6	14	rVB	9898	13431	1.09%	0.215%
2	5.094	335	341	351	rBV	14509	23644	1.93%	0.379%
3	5.564	414	421	431	rBV	257341	421532	34.34%	6.750%
4	7.174	687	695	705	rBV	278767	498654	40.62%	7.985%
5	7.538	748	757	767	rBV	268002	460564	37.52%	7.375%
6	8.008	830	837	847	rBB	47617	78442	6.39%	1.256%
7	8.331	883	892	900	rBB	190920	335945	27.37%	5.380%
8	9.189	1030	1038	1049	rBV	158757	293243	23.89%	4.696%
9	10.822	1308	1316	1328	rBV	61629	110728	9.02%	1.773%
10	13.267	1725	1732	1747	rVB	455298	707809	57.66%	11.335%
11	14.101	1868	1874	1880	rBV	23936	37880	3.09%	0.607%
12	14.647	1960	1967	1975	rBV2	112751	185180	15.08%	2.965%
13	16.140	2215	2221	2238	rBV2	460306	712900	58.07%	11.416%
14	17.397	2429	2435	2447	rBV2	164039	251469	20.48%	4.027%
15	18.261	2577	2582	2592	rBV2	11347	18242	1.49%	0.292%
16	20.000	2872	2878	2885	rBV	926338	1227584	100.00%	19.658%
17	21.269	3088	3094	3105	rBV2	52625	88199	7.18%	1.412%
18	21.668	3155	3162	3171	rBV	180202	291777	23.77%	4.672%
19	21.804	3178	3185	3190	rBV2	10801	17625	1.44%	0.282%
20	22.409	3282	3288	3293	rBV2	13138	22474	1.83%	0.360%
21	23.102	3400	3406	3413	rVB3	25327	44789	3.65%	0.717%
22	23.895	3534	3541	3549	rBV3	15180	34301	2.79%	0.549%
23	24.847	3693	3703	3707	rBV5	11357	29158	2.38%	0.467%
24	24.929	3707	3717	3729	rVB	95355	279762	22.79%	4.480%
25	25.969	3883	3894	3902	rBV6	8995	29444	2.40%	0.472%
26	26.110	3912	3918	3927	rBV9	4326	13115	1.07%	0.210%
27	27.309	4113	4122	4134	rBV8	4902	16778	1.37%	0.269%

Sum of corrected areas: 6244669

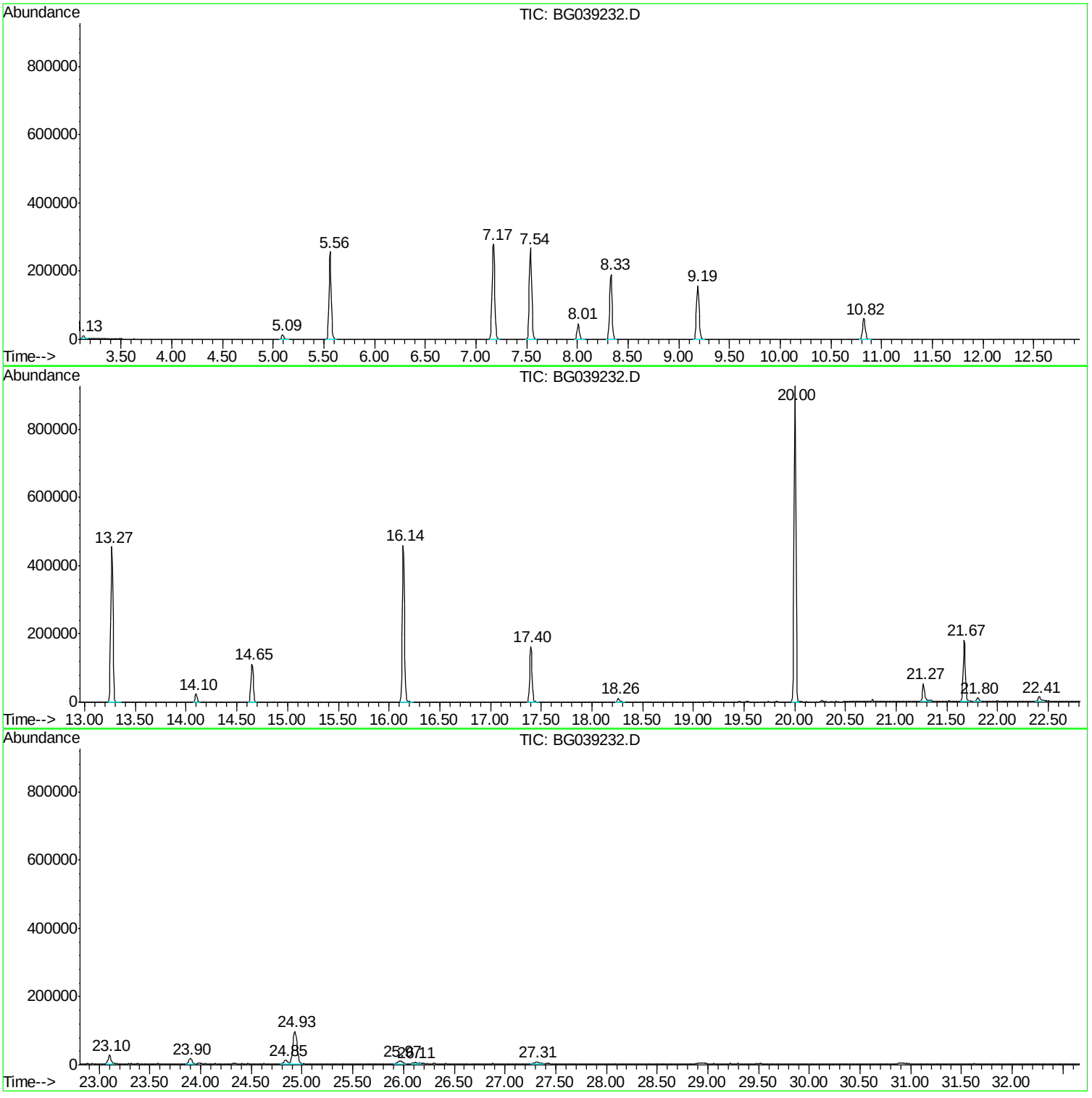
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012119\
Data File : BG039232.D
Acq On : 21 Jan 2019 14:03
Operator : JU/SJ
Sample : K1205-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.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\BG012119\
Data File : BG039232.D
Acq On : 21 Jan 2019 14:03
Operator : JU/SJ
Sample : K1205-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

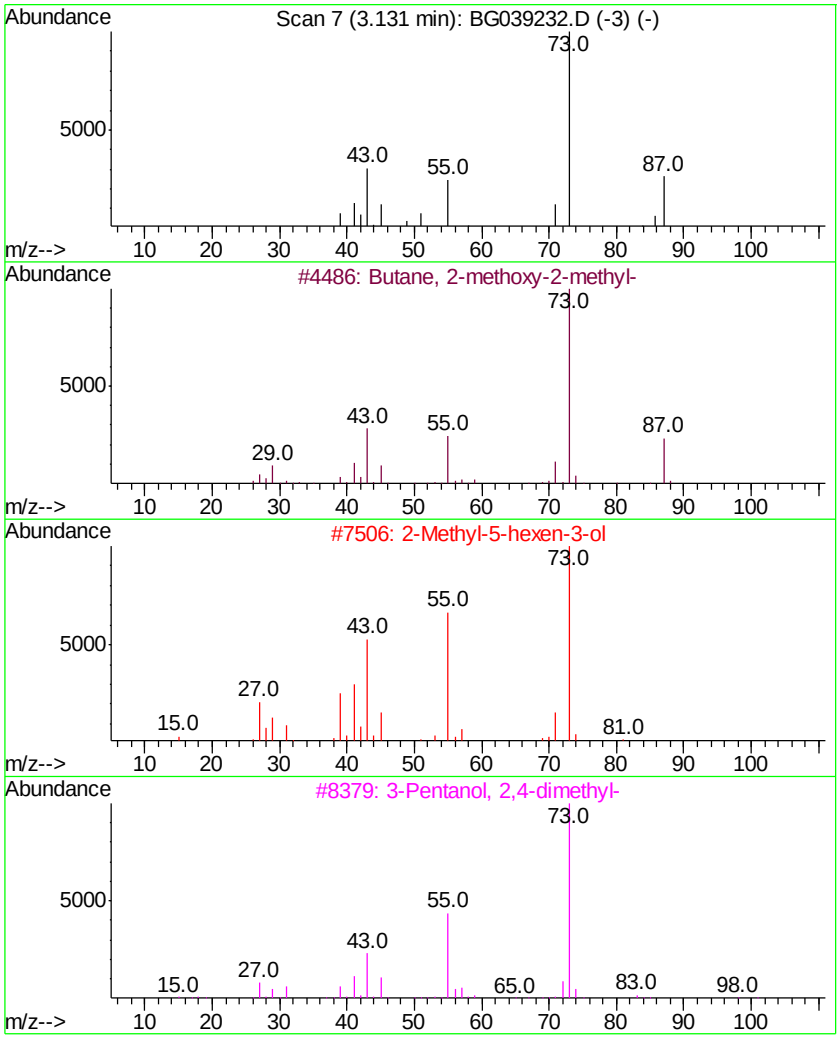
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

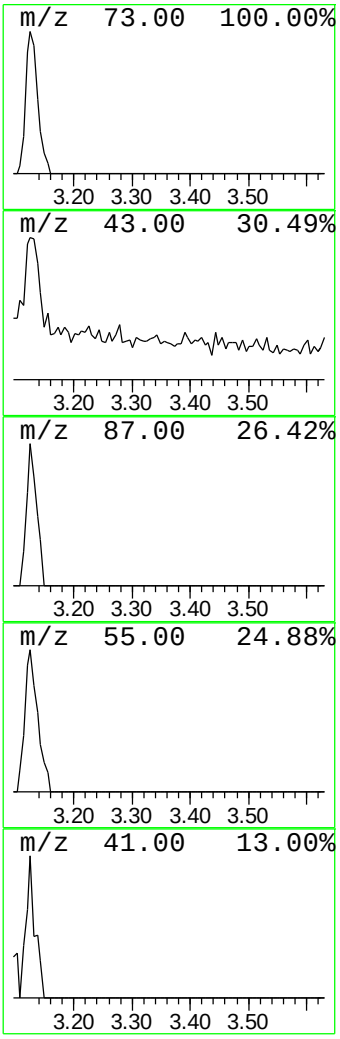
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	3.42 ng	13431	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	5
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	5





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012119\
Data File : BG039232.D
Acq On : 21 Jan 2019 14:03
Operator : JU/SJ
Sample : K1205-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

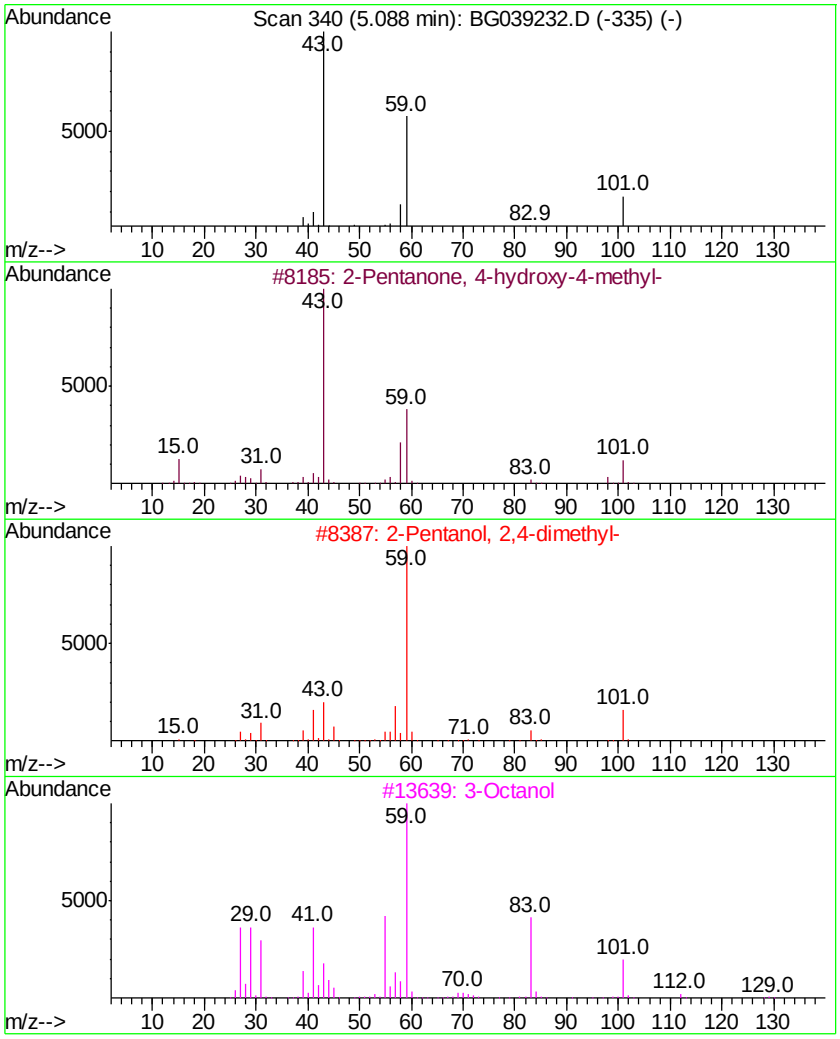
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

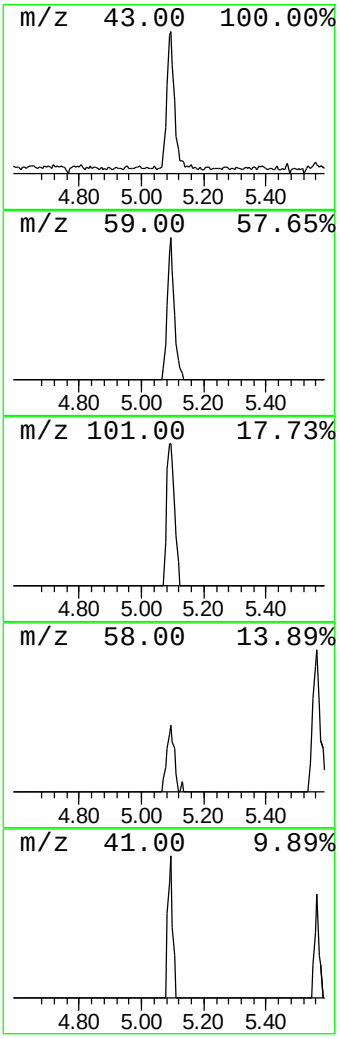
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	6.03 ng	23644	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9
3	3-Octanol	130	C8H18O	000589-98-0	9
4	Diacetamide	101	C4H7NO2	000625-77-4	7
5	3-Methylpenta-1,4-diene-3-ol	98	C6H10O	000918-86-5	7





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012119\
Data File : BG039232.D
Acq On : 21 Jan 2019 14:03
Operator : JU/SJ
Sample : K1205-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

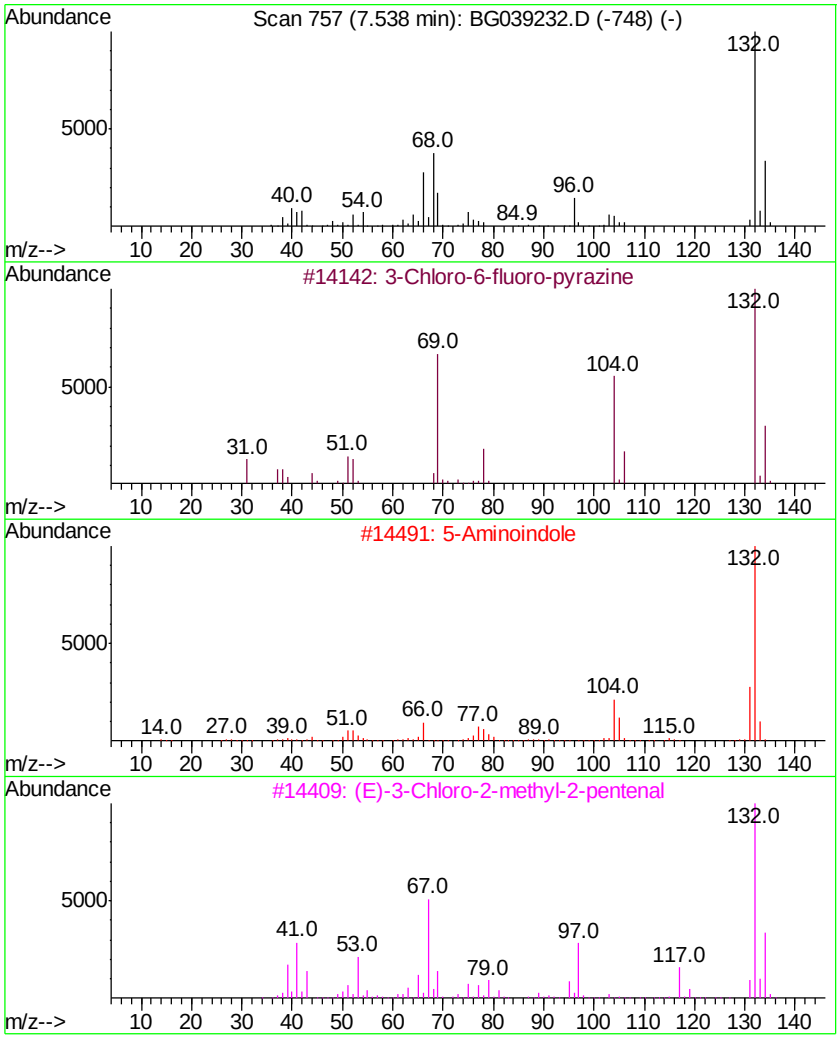
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

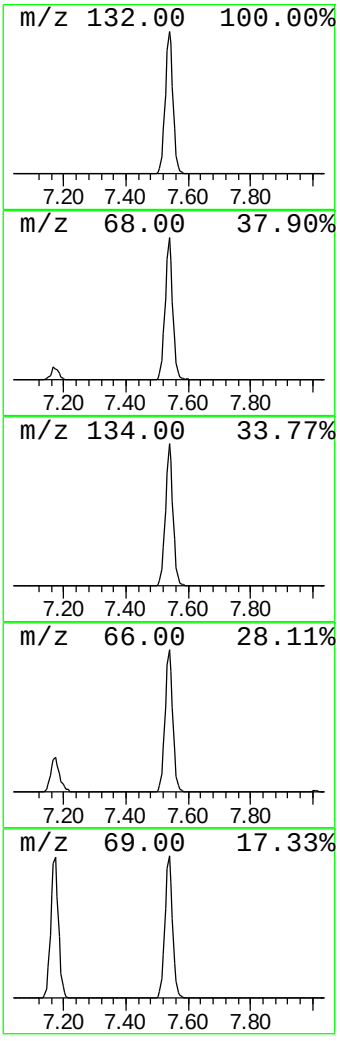
****

Peak Number 3 unknown7.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	117.43 ng	460564	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Aminoindole	132	C8H8N2	005192-03-0	27
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	12
5	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012119\
Data File : BG039232.D
Acq On : 21 Jan 2019 14:03
Operator : JU/SJ
Sample : K1205-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

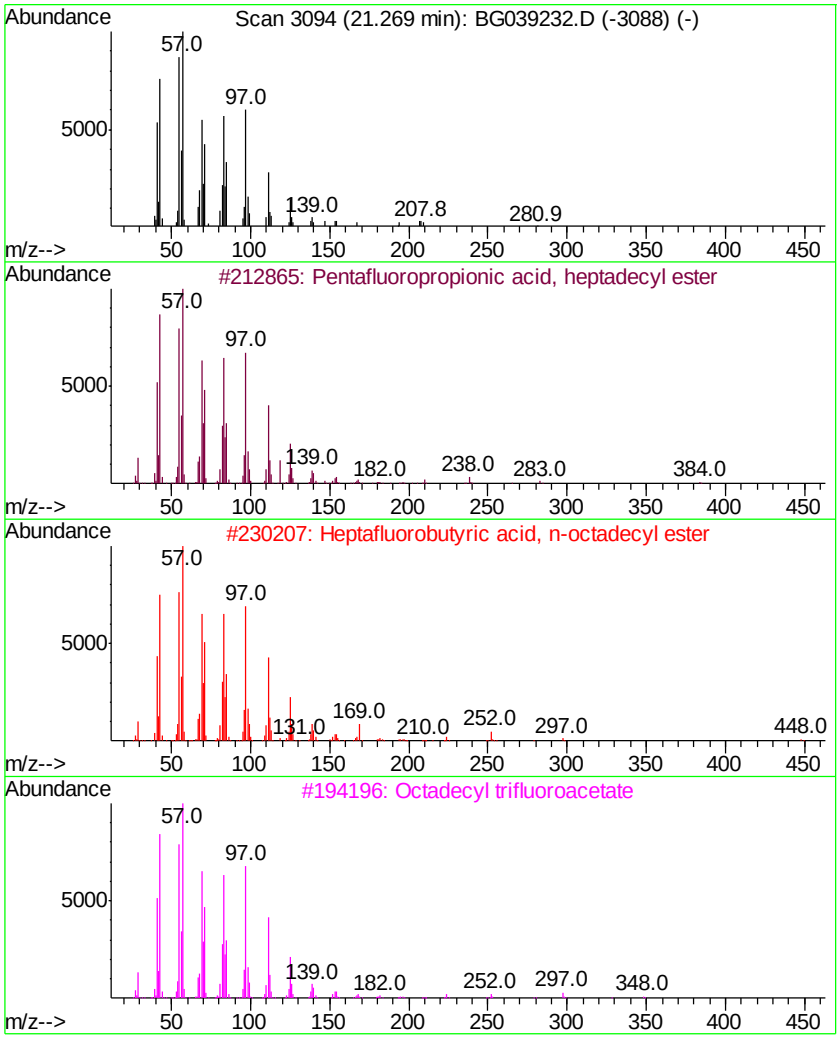
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

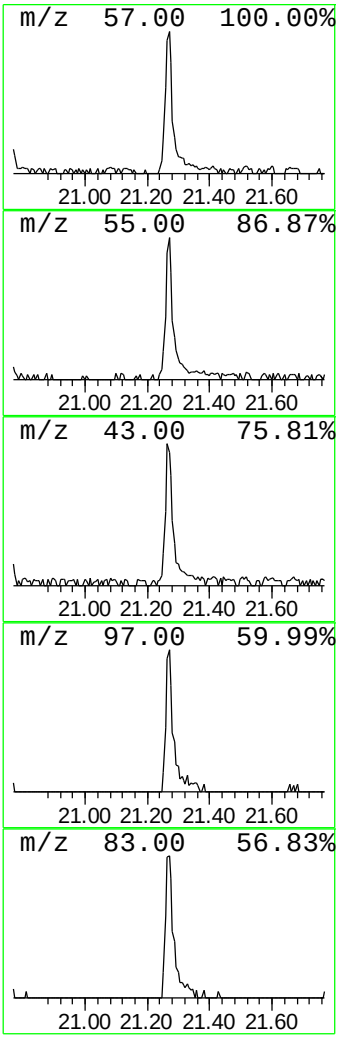
****

Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.27	6.05 ng	88199	Chrysene-d12	21.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4	Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	91
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012119\
Data File : BG039232.D
Acq On : 21 Jan 2019 14:03
Operator : JU/SJ
Sample : K1205-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

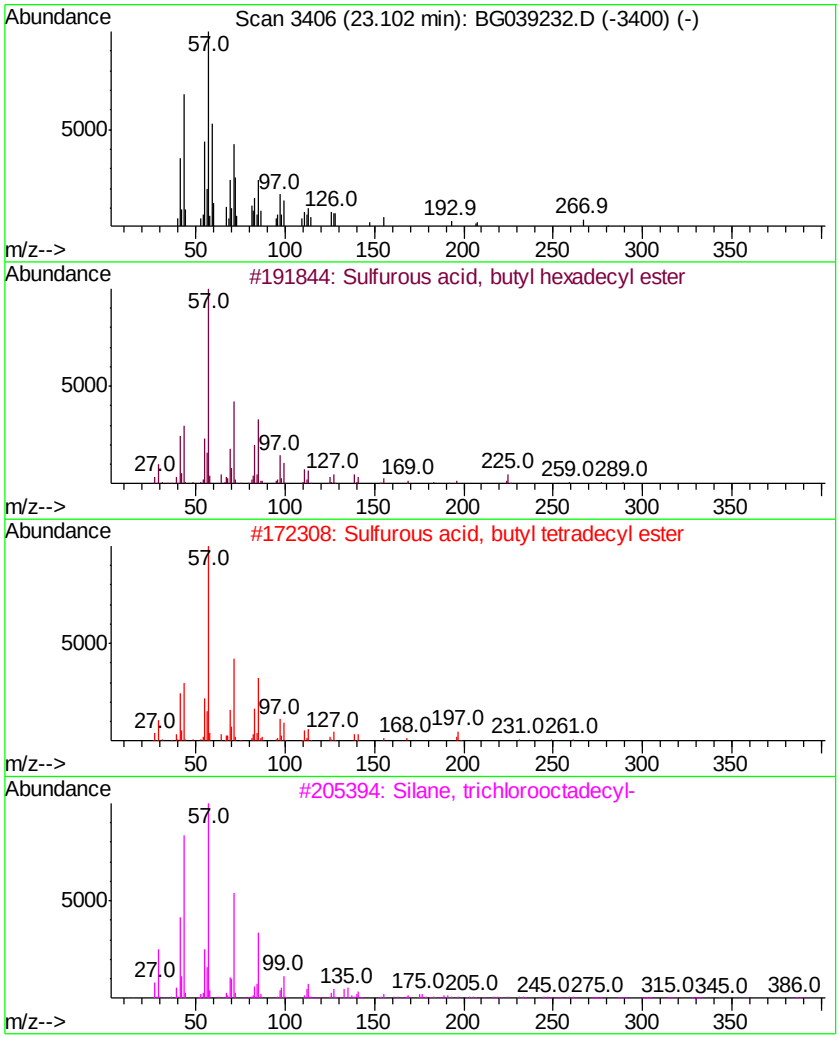
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

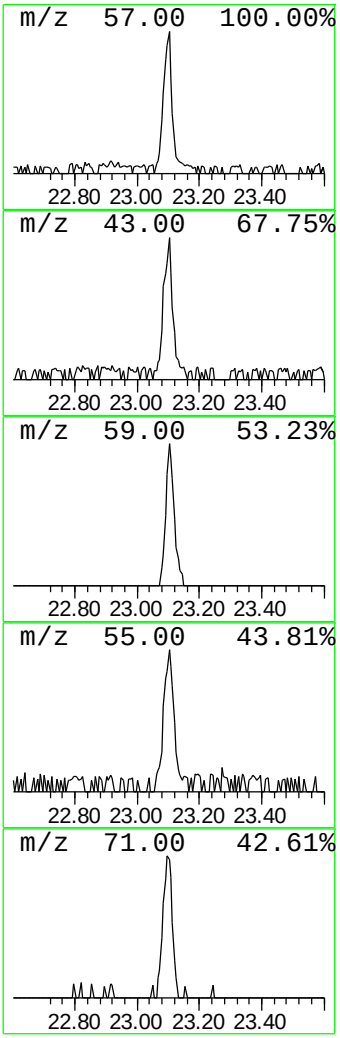
****

Peak Number 6 unknown23.10 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.10	3.07 ng	44789	Chrysene-d12	21.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	47
2	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	47
3	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	46
4	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	43
5	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	43





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012119\
Data File : BG039232.D
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Operator : JU/SJ
Sample : K1205-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

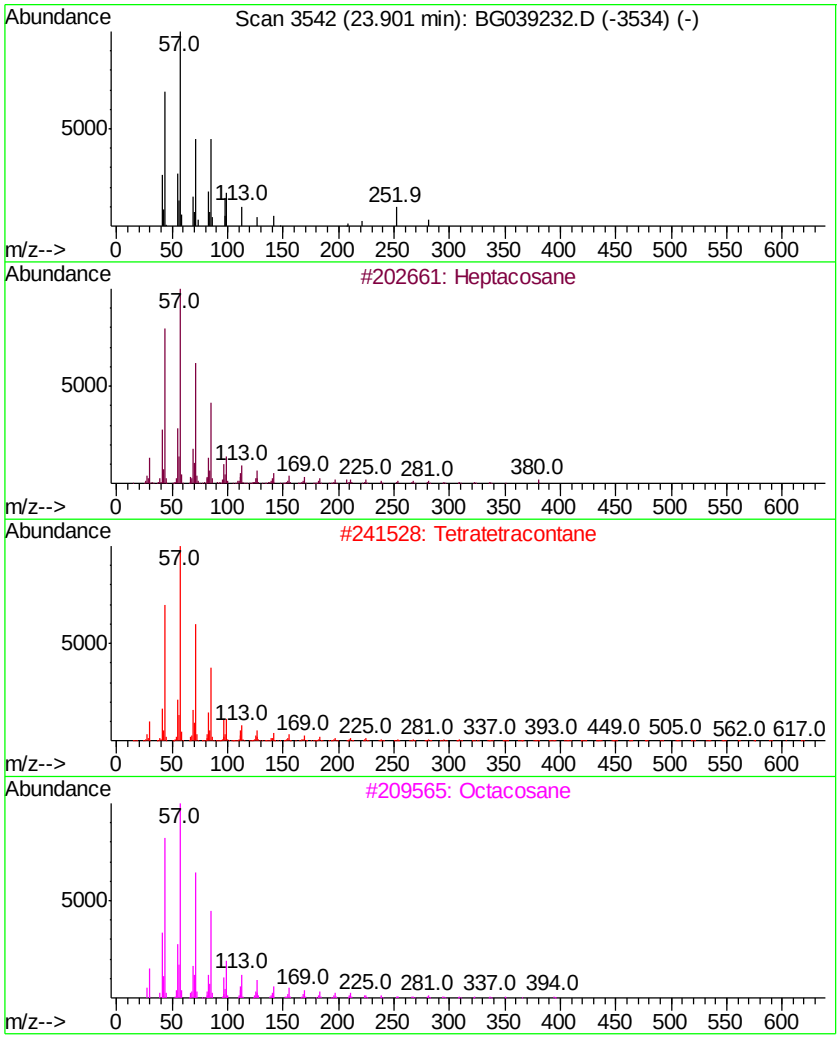
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

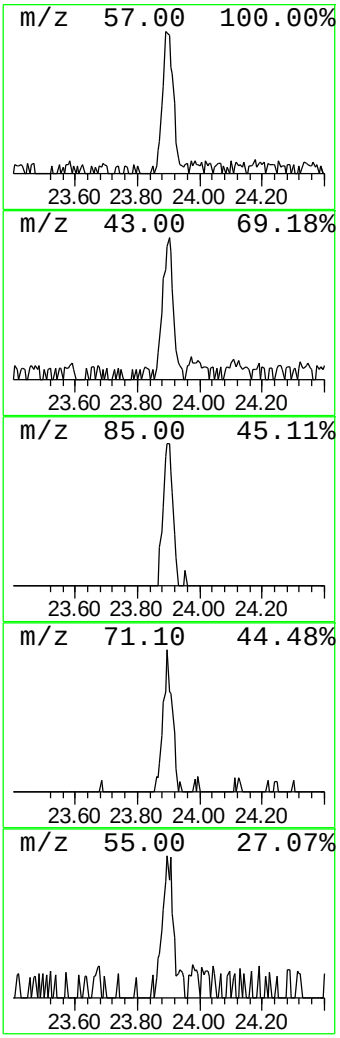
****

Peak Number 7 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.90	2.45 ng	34301	Perylene-d12	24.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	87
2	Tetratetracontane	619	C44H90	007098-22-8	86
3	Octacosane	394	C28H58	000630-02-4	86
4	Hentriacontane	437	C31H64	000630-04-6	86
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86





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Acq On : 21 Jan 2019 14:03
Operator : JU/SJ
Sample : K1205-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

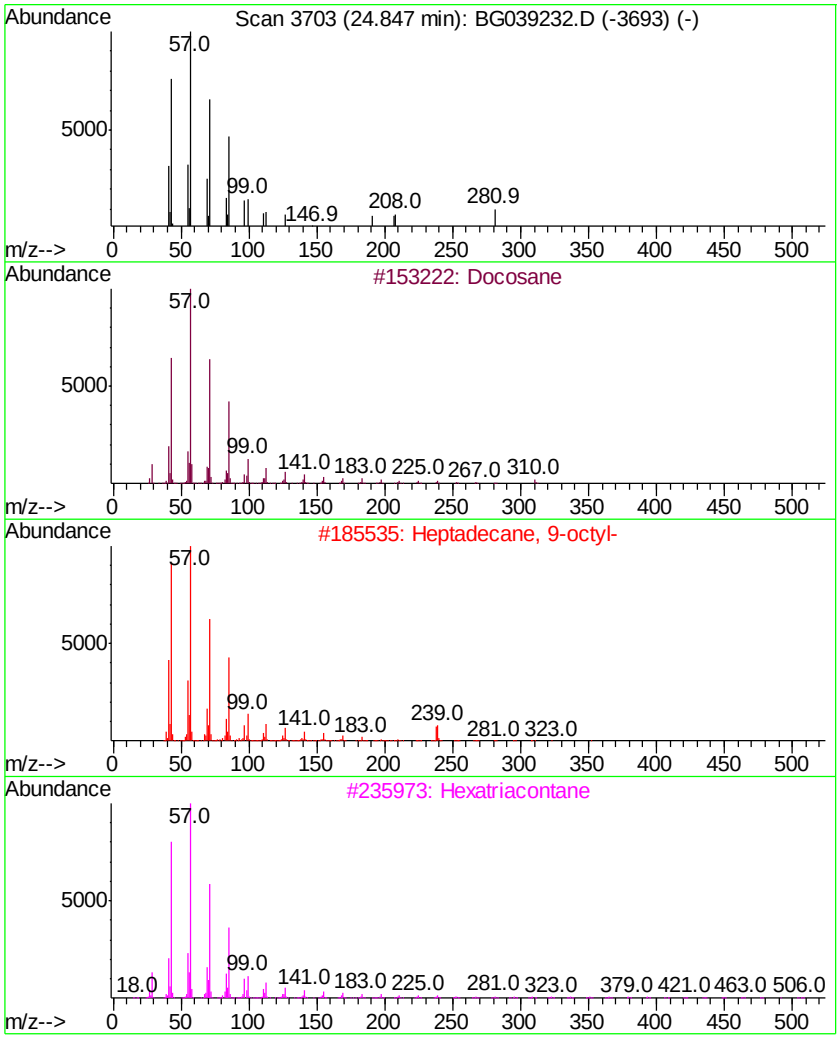
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

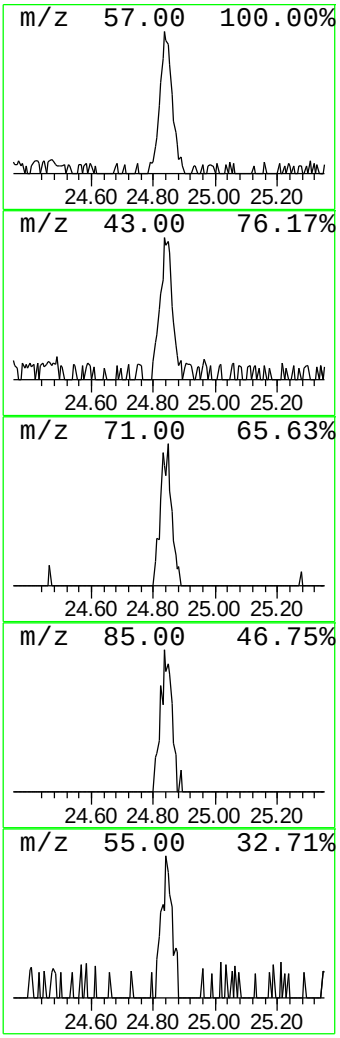
****

Peak Number 8 Docosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.85	2.08 ng	29158	Perylene-d12	24.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	64
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	64
3	Hexatriacontane	507	C36H74	000630-06-8	64
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	64
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	64





Library Search Compound Report

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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.M
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TIC Library : C:\Database\NIST11.L
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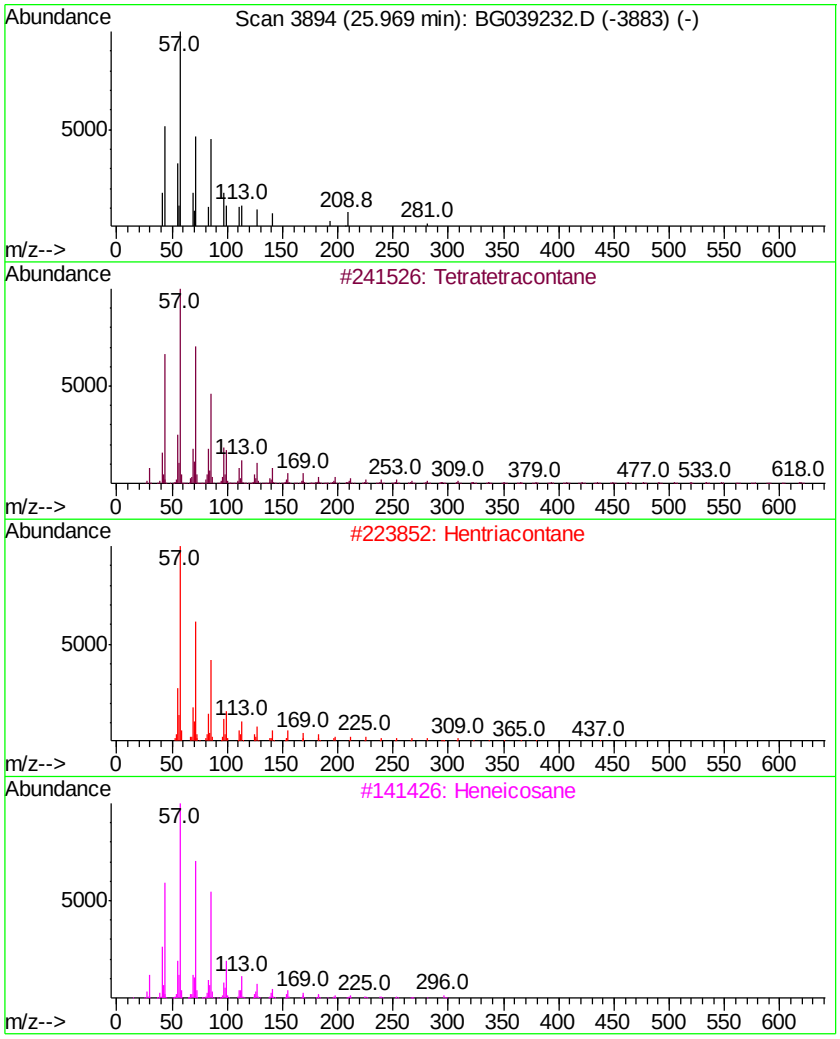
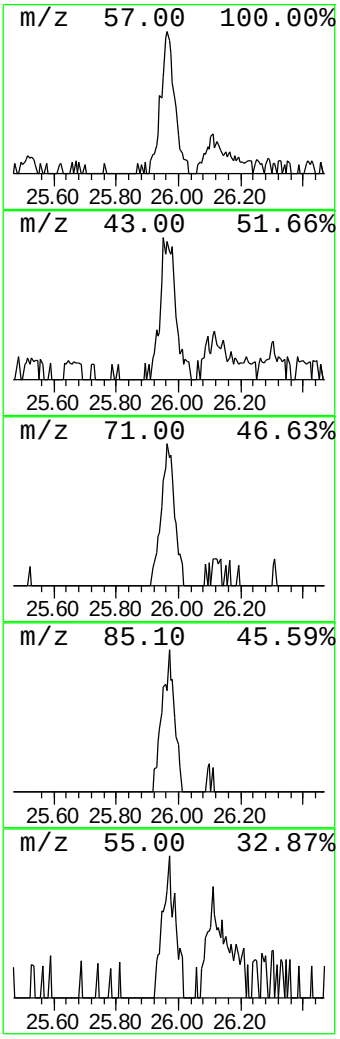
****

Peak Number 9 Tetratetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.97	2.10 ng	29444	Perylene-d12	24.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	72
2	Hentriacontane	437	C31H64	000630-04-6	72
3	Heneicosane	296	C21H44	000629-94-7	72
4	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	64
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG012119\
Data File : BG039232.D
Acq On : 21 Jan 2019 14:03
Operator : JU/SJ
Sample : K1205-01
Misc :
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Instrument : BNA_G
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.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
Butane, 2-methoxy...	3.13	3.4	ng	13431	1	8.01	78442	20.0
2-Pentanone, 4-hy...	5.09	6.0	ng	23644	1	8.01	78442	20.0
unknown7.54	7.54	117.4	ng	460564	1	8.01	78442	20.0
Pentafluoropropio...	21.27	6.0	ng	88199	5	21.67	291777	20.0
unknown23.10	23.10	3.1	ng	44789	5	21.67	291777	20.0
Heptacosane	23.90	2.5	ng	34301	6	24.93	279762	20.0
Docosane	24.85	2.1	ng	29158	6	24.93	279762	20.0
Tetratetracontane	25.97	2.1	ng	29444	6	24.93	279762	20.0