LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021119\
Data File : BG039432.D
Acq On : 11 Feb 2019 13:37
Operator : JU/SJ
Sample : K1404-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A0C12-SS1-7.5-8.0

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-BG012919.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	3.223	18	23	31	rBV	81298	156947	3.14%	0.556%
2	3.293	31	35	44	rVB	58651	90128	1.81%	0.319%
3	5.255	362	369	376	rVB	75630	123241	2.47%	0.437%
4	5.713	439	447	457	rBV	1243709	2032438	40.70%	7.199%
5	7.311	710	719	734	rBV	1348070	2471362	49.49%	8.754%
6	7.699	776	785	793	rBV	1226922	2140175	42.86%	7.581%
7	8.169	858	865	877	rBV	203111	365723	7.32%	1.295%
8	8.498	912	921	930	rBV	819270	1434442	28.73%	5.081%
9	9.350	1056	1066	1075	rBV	763060	1359116	27.22%	4.814%
10	10.994	1337	1346	1354	rBV	304402	534804	10.71%	1.894%
11	13.420	1751	1759	1766	rBV	1902265	2920086	58.48%	10.343%
12	14.237	1891	1898	1905	rBV	181876	260435	5.22%	0.922%
13	14.795	1983	1993	2001	rBV2	518843	823876	16.50%	2.918%
14	16.281	2239	2246	2257	rBV	1825123	2850924	57.10%	10.098%
15	17.538	2453	2460	2467	rBV2	740712	1128945	22.61%	3.999%
16	18.396	2600	2606	2618	rBV	118931	207024	4.15%	0.733%
17	20.135	2895	2902	2909	rBV	3673511	4993240	100.00%	17.686%
18	20.904	3029	3033	3038	rVB	54541	66857	1.34%	0.237%
19	21.427	3115	3122	3132	rBV	244002	382613	7.66%	1.355%
20	21.827	3183	3190	3204	rVB2	779785	1355773	27.15%	4.802%
21	21.991	3212	3218	3224	rBV	130509	183979	3.68%	0.652%
22	22.626	3319	3326	3333	rBV	144232	244299	4.89%	0.865%
23	23.348	3443	3449	3460	rVB	137862	261849	5.24%	0.927%
24	24.194	3585	3593	3601	rVB2	105015	232366	4.65%	0.823%
25	25.210	3754	3766	3778	rBV3	466279	1444832	28.94%	5.118%
26	26.385	3958	3966	3977	rBV3	39268	113277	2.27%	0.401%
27	27.836	4204	4213	4219	rBV6	16734	53255	1.07%	0.189%

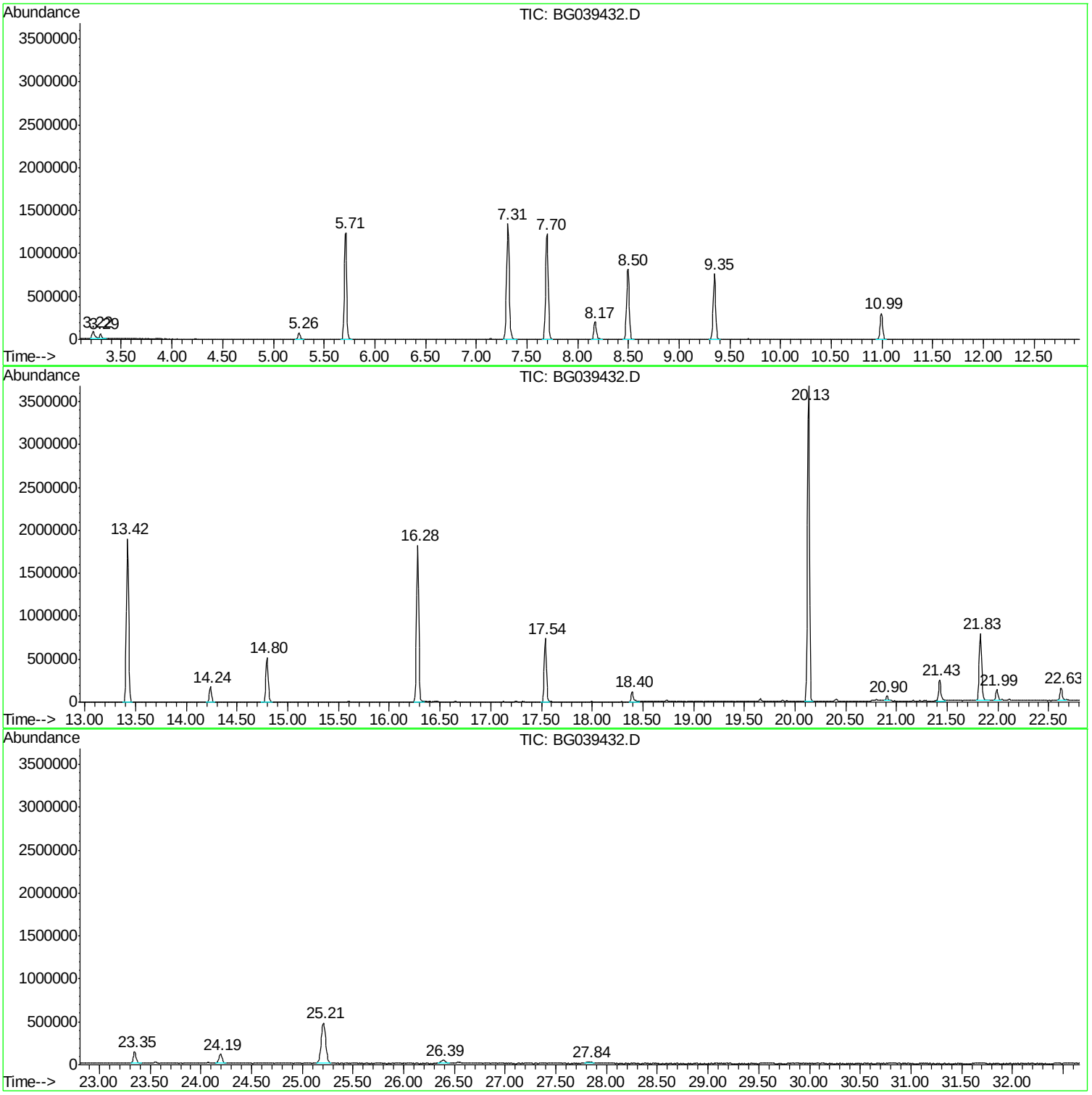
Sum of corrected areas: 28232006

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021119\
Data File : BG039432.D
Acq On : 11 Feb 2019 13:37
Operator : JU/SJ
Sample : K1404-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A0C12-SS1-7.5-8.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021119\
Data File : BG039432.D
Acq On : 11 Feb 2019 13:37
Operator : JU/SJ
Sample : K1404-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A0C12-SS1-7.5-8.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

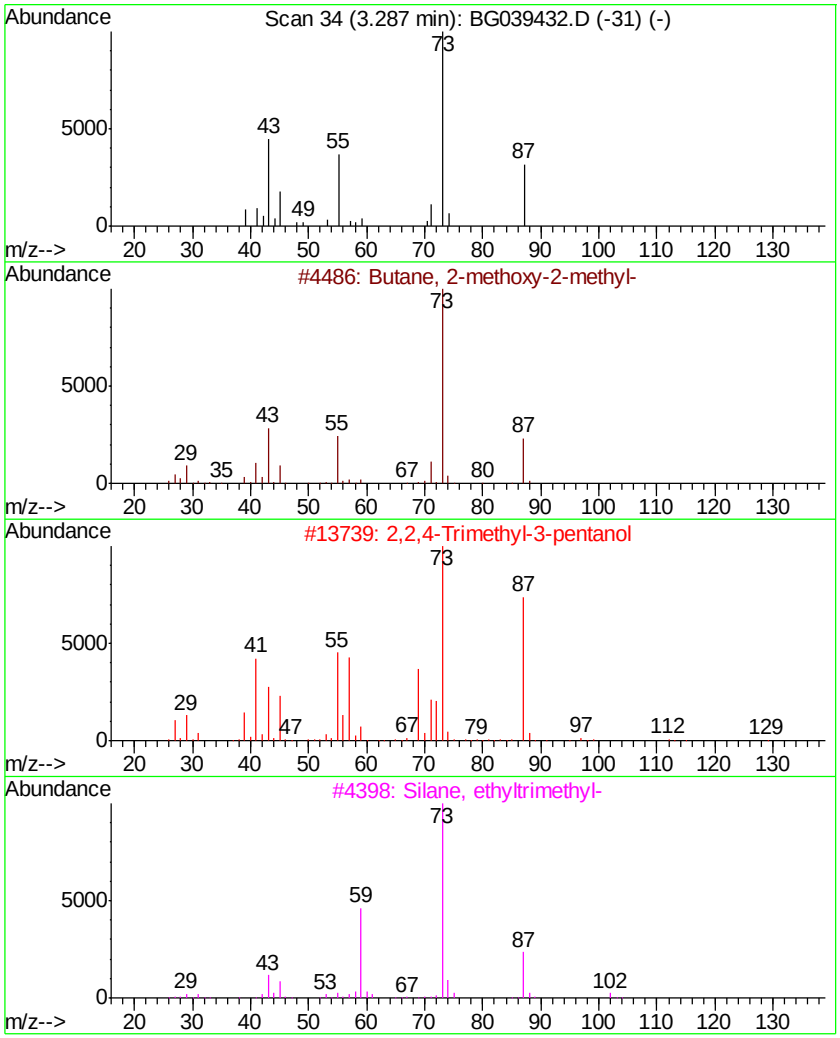
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

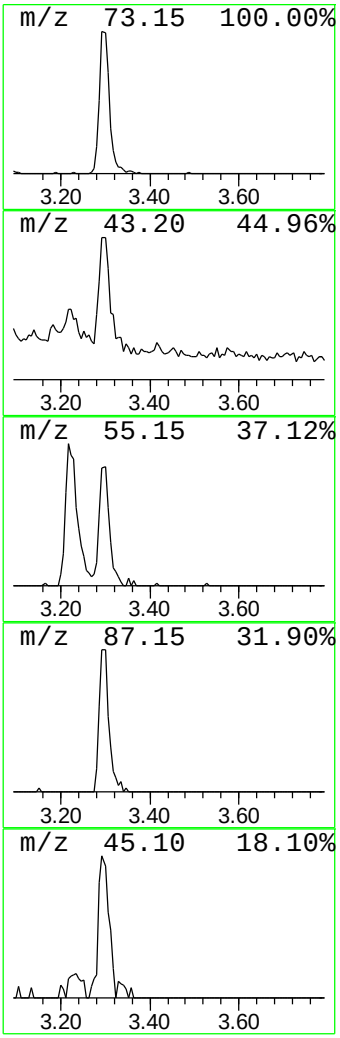
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.29	4.93 ng	90128	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	38
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021119\
Data File : BG039432.D
Acq On : 11 Feb 2019 13:37
Operator : JU/SJ
Sample : K1404-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A0C12-SS1-7.5-8.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

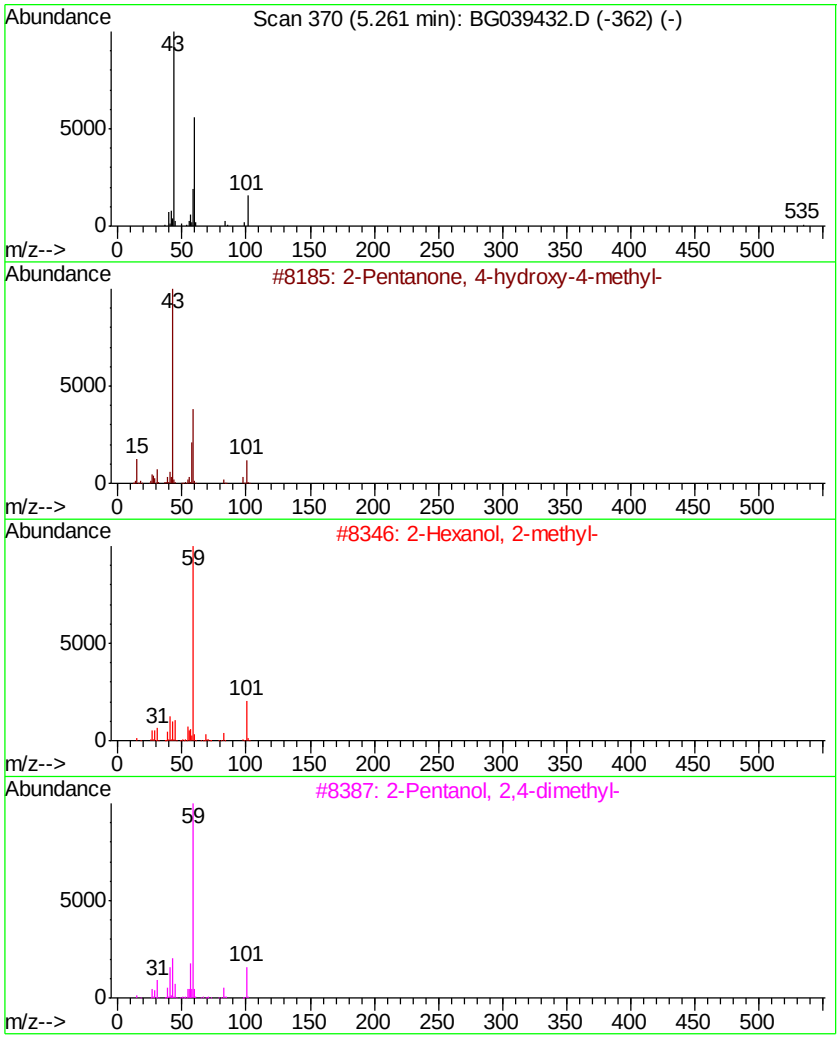
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

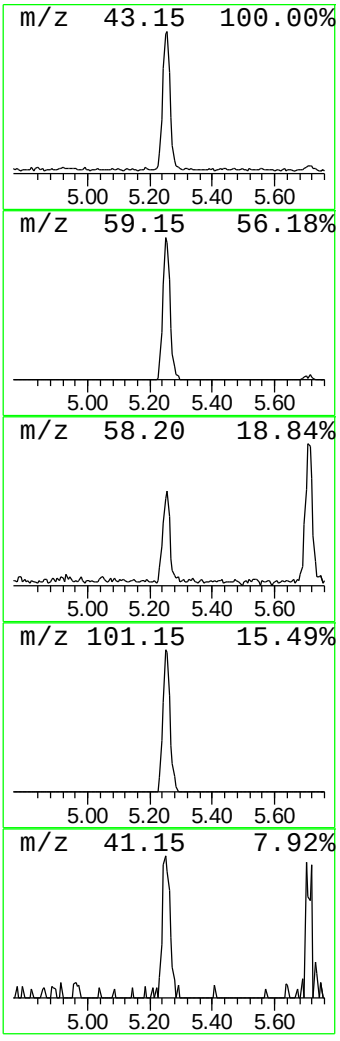
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	6.74 ng	123241	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021119\
Data File : BG039432.D
Acq On : 11 Feb 2019 13:37
Operator : JU/SJ
Sample : K1404-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A0C12-SS1-7.5-8.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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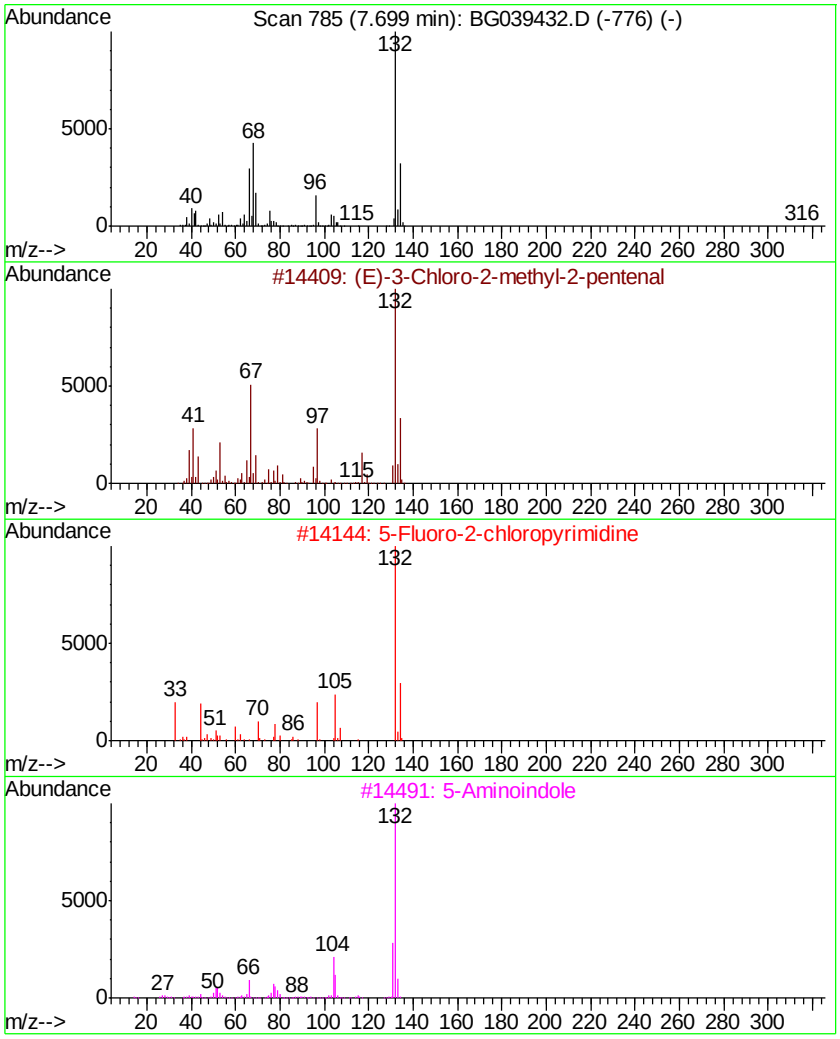
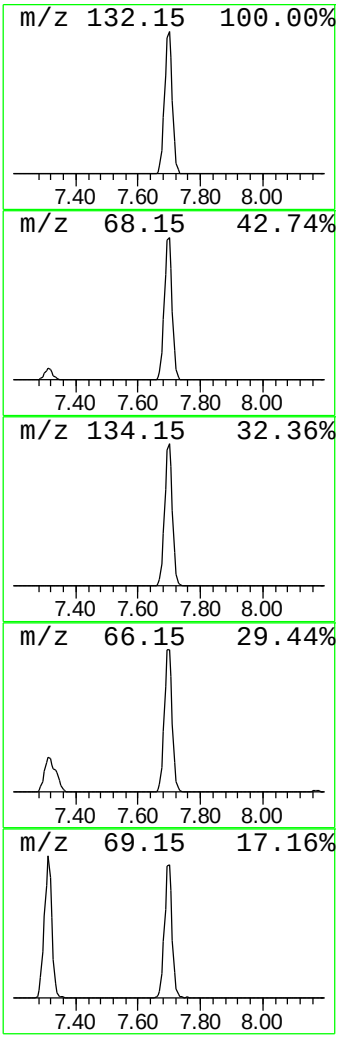
****

Peak Number 4 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	117.04 ng	2140180	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021119\
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Operator : JU/SJ
Sample : K1404-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A0C12-SS1-7.5-8.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

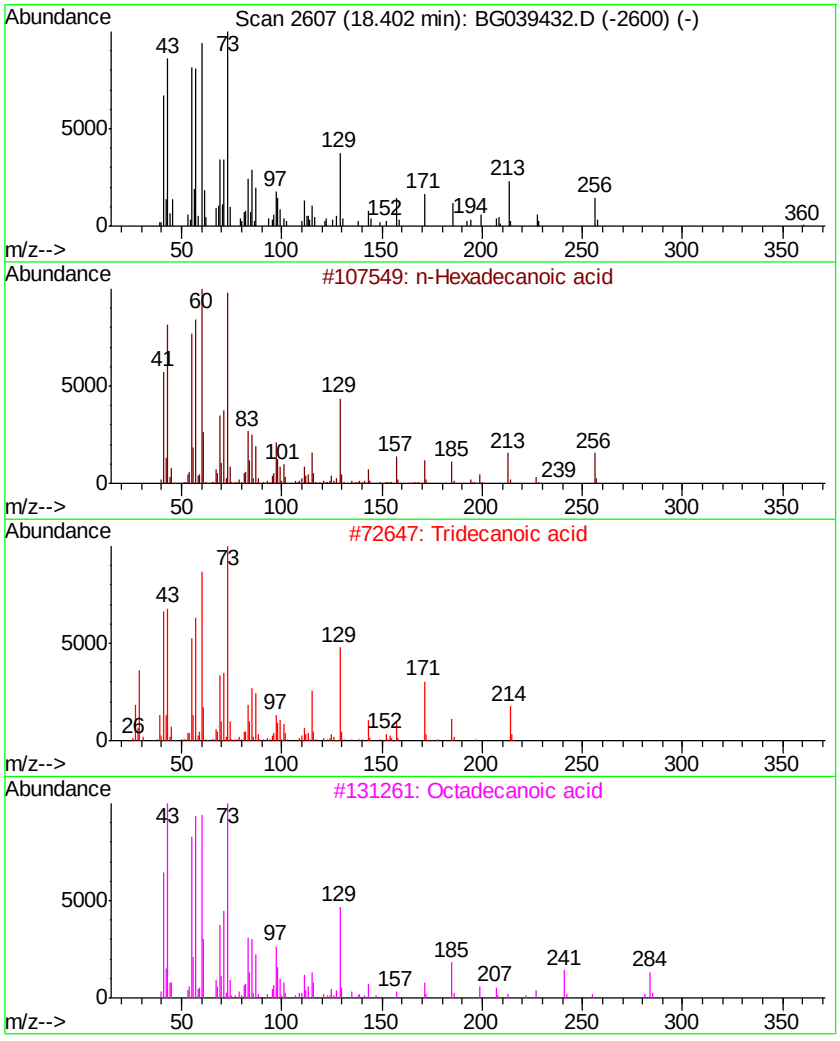
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

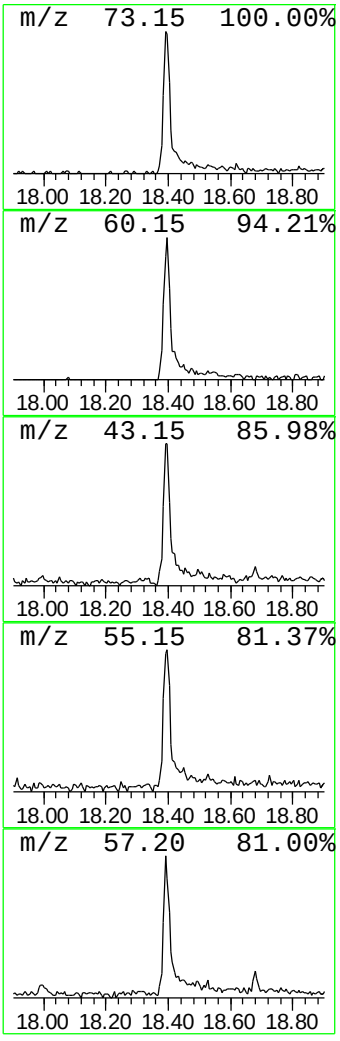
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.40	3.67 ng	207024	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021119\
Data File : BG039432.D
Acq On : 11 Feb 2019 13:37
Operator : JU/SJ
Sample : K1404-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A0C12-SS1-7.5-8.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

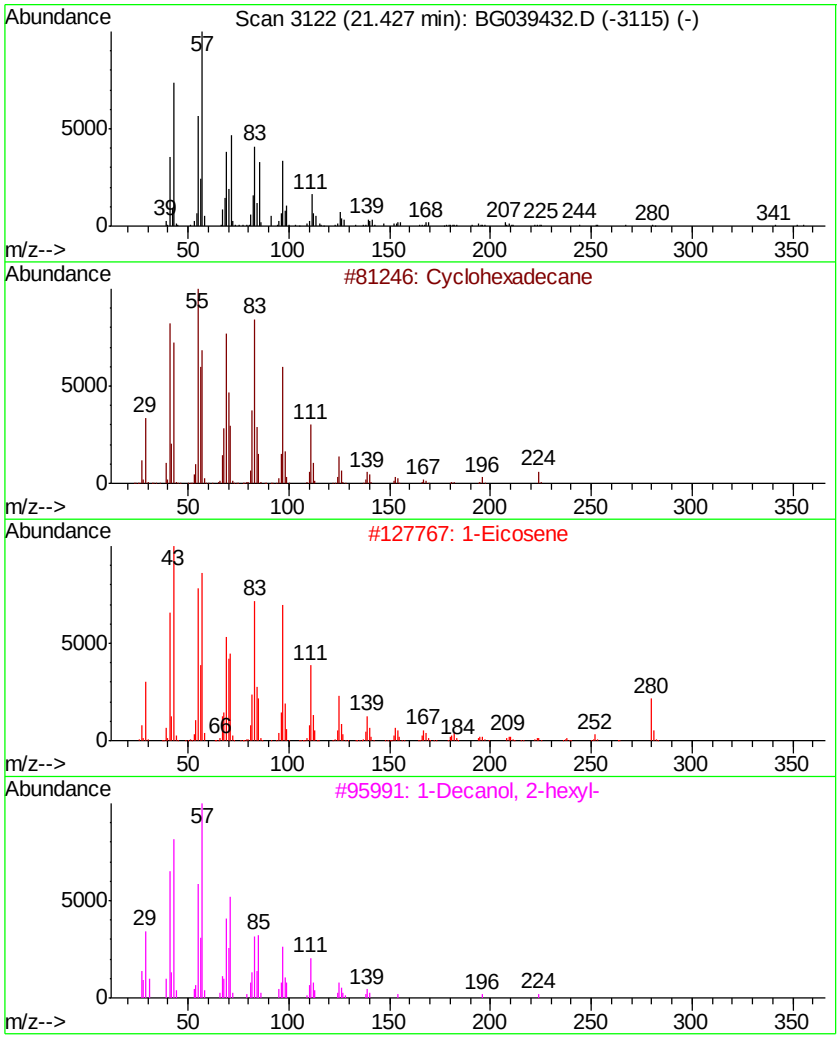
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

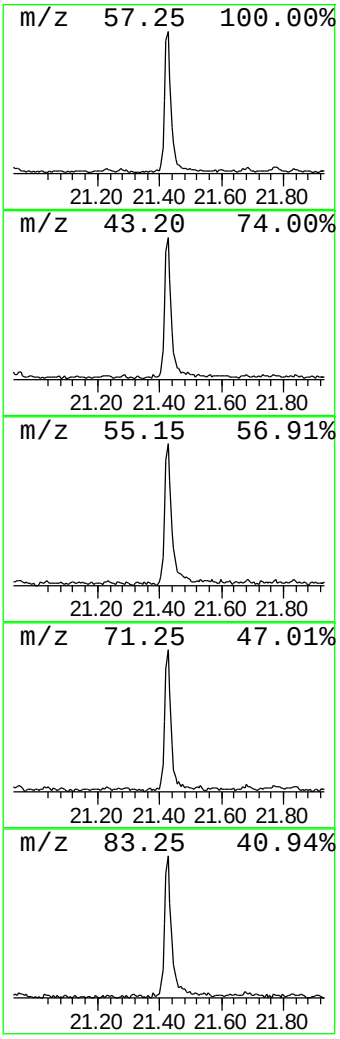
****

Peak Number 7 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.43	5.64 ng	382613	Chrysene-d12	21.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	96
2	1-Eicosene	280	C20H40	003452-07-1	93
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	87
4	1-Pentadecanethiol	244	C15H32S	025276-70-4	83
5	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021119\
Data File : BG039432.D
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Operator : JU/SJ
Sample : K1404-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A0C12-SS1-7.5-8.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

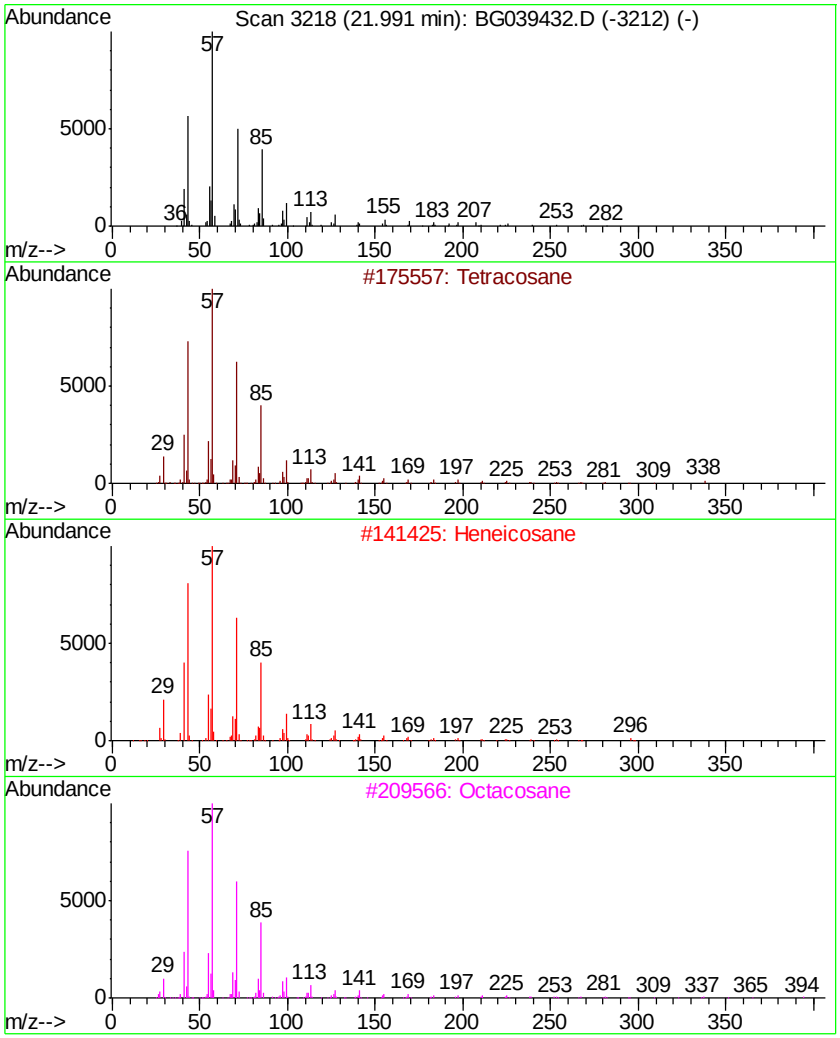
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

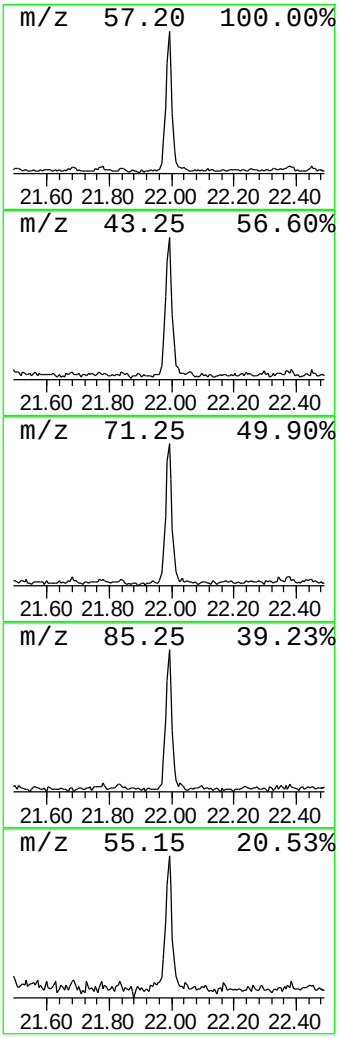
****

Peak Number 8 Tetracosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.99	2.71 ng	183979	Chrysene-d12	21.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86





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Acq On : 11 Feb 2019 13:37
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Sample : K1404-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A0C12-SS1-7.5-8.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

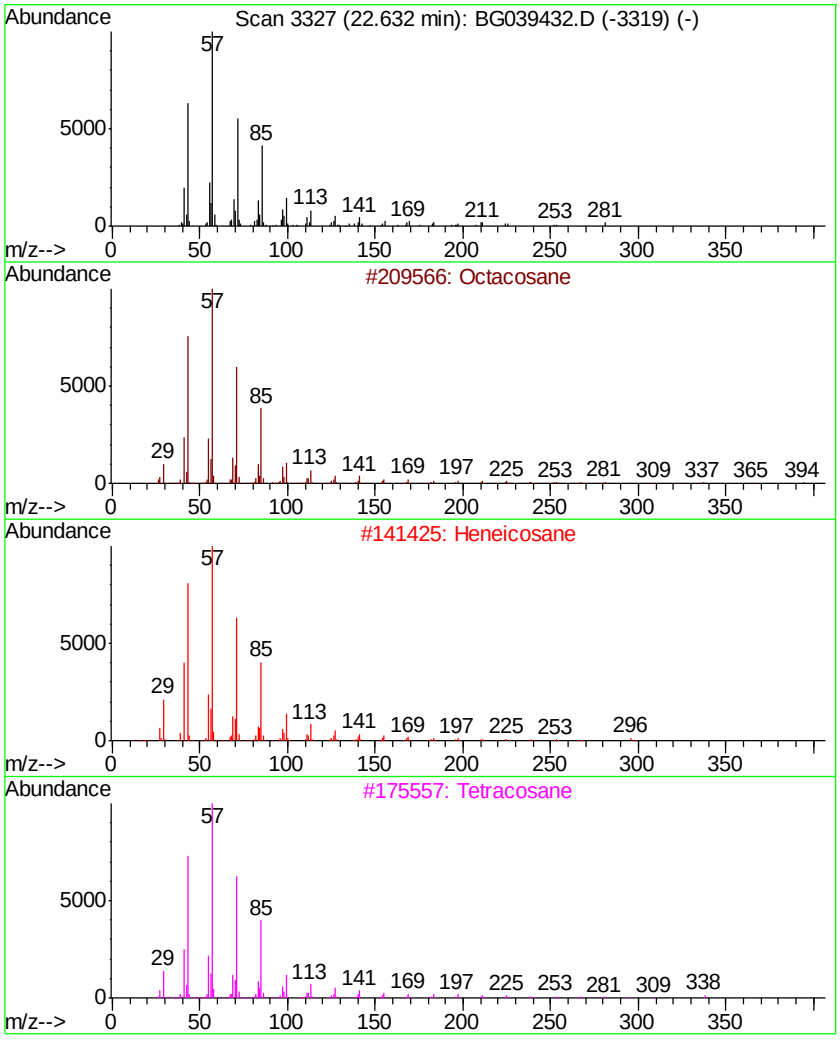
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

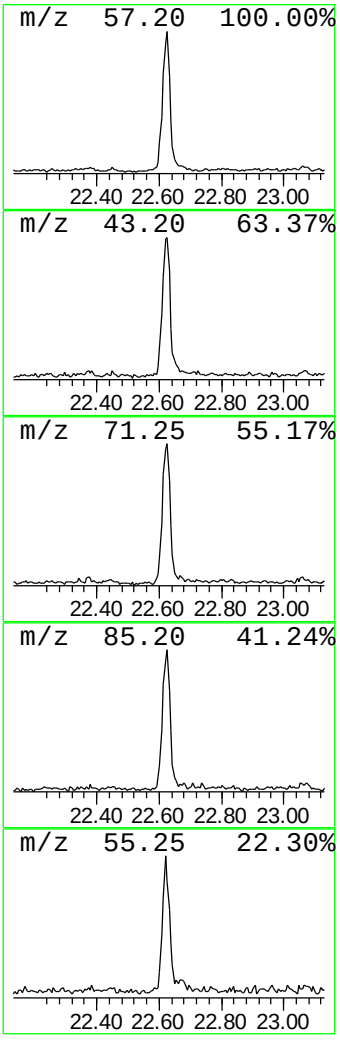
****

Peak Number 9 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.63	3.60 ng	244299	Chrysene-d12	21.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Octadecane	254	C18H38	000593-45-3	90





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Operator : JU/SJ
Sample : K1404-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A0C12-SS1-7.5-8.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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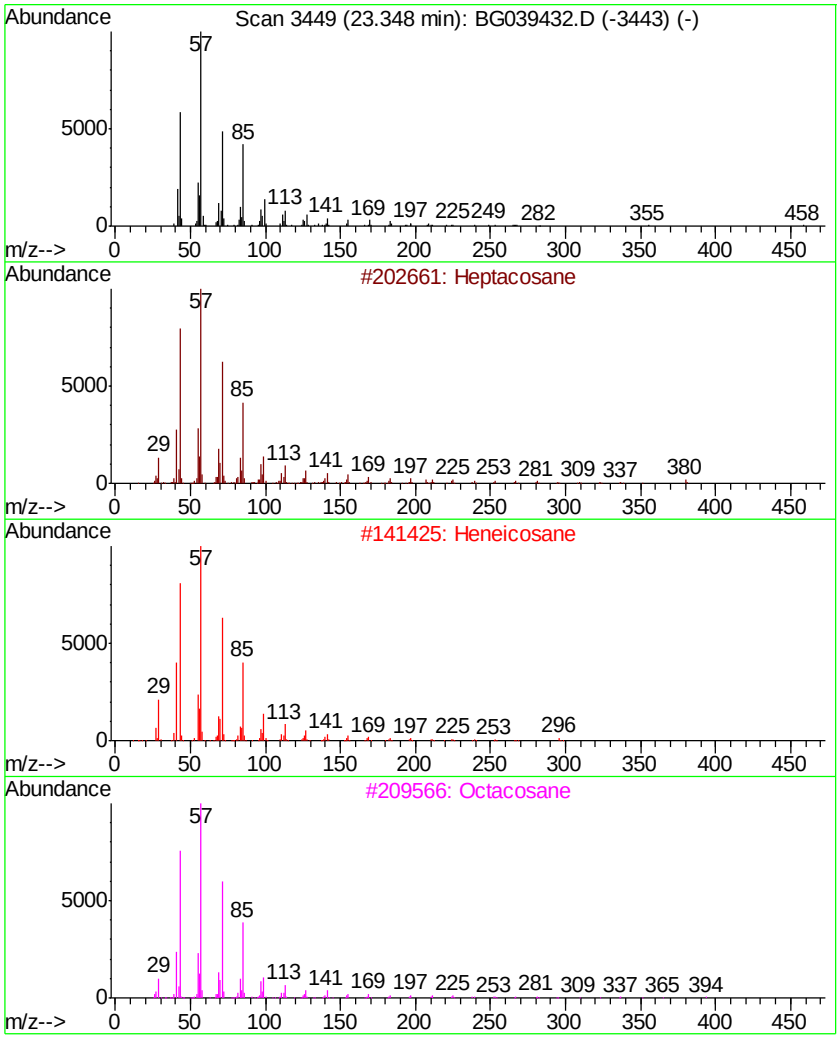
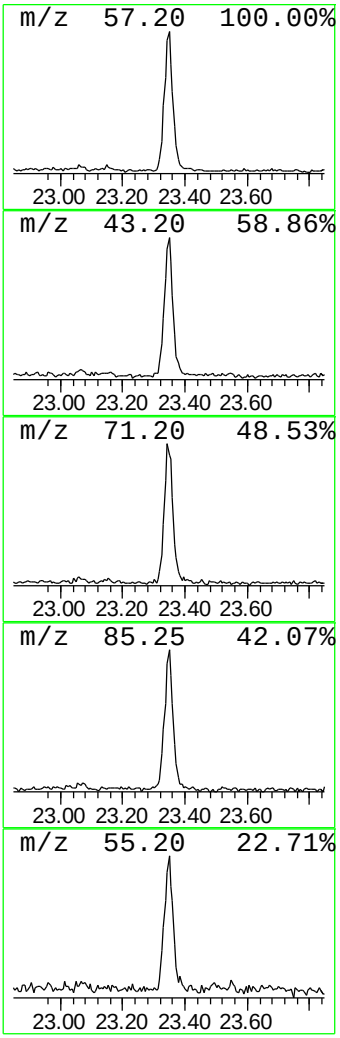
Peak Number 10 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.35	3.86 ng	261849	Chrysene-d12	21.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Octadecane	254	C18H38	000593-45-3	91





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Data File : BG039432.D
Acq On : 11 Feb 2019 13:37
Operator : JU/SJ
Sample : K1404-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A0C12-SS1-7.5-8.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

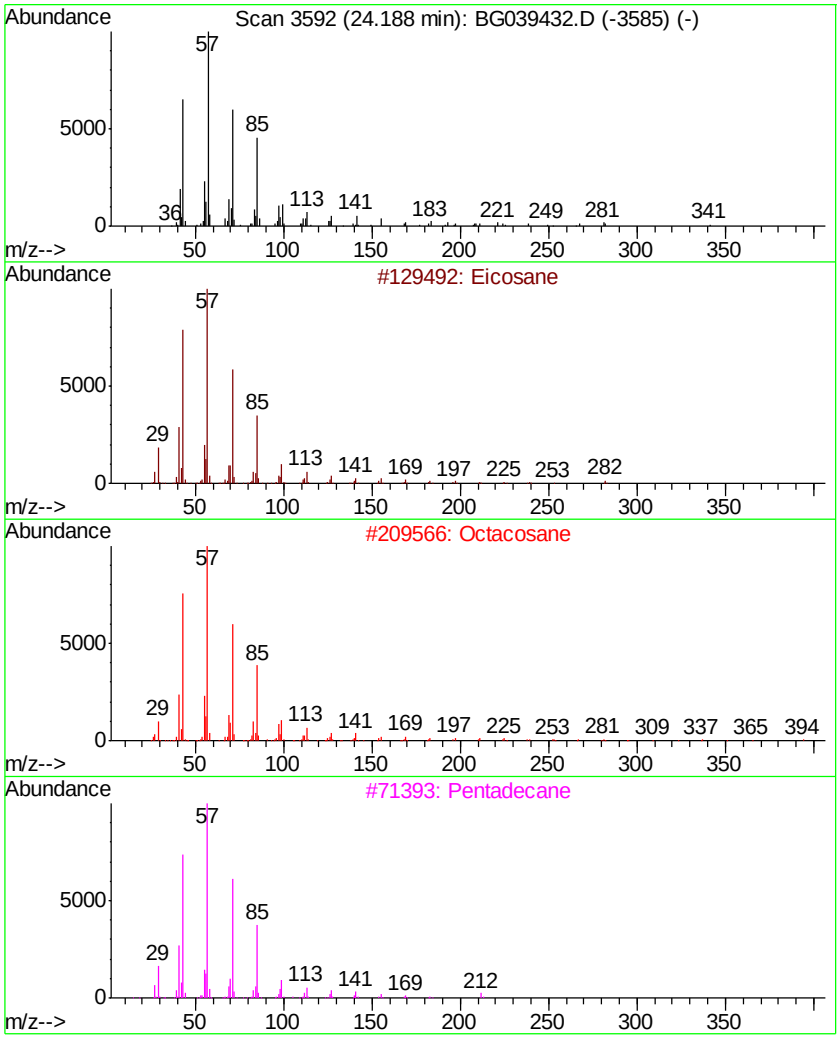
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

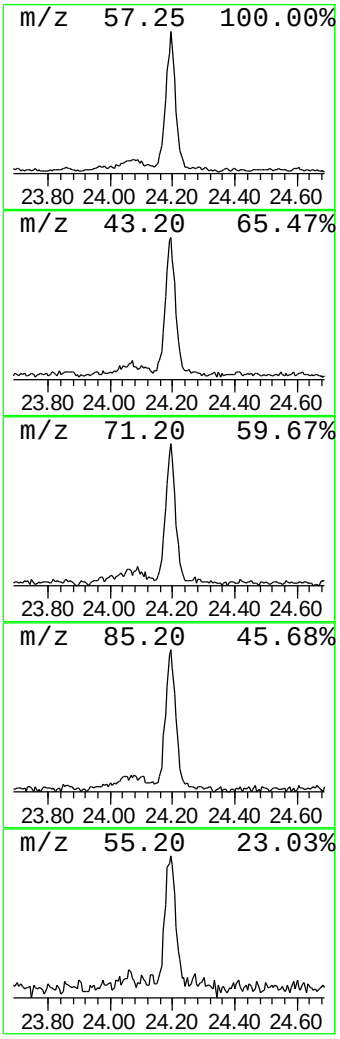
****

Peak Number 11 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.19	3.22 ng	232366	Perylene-d12	25.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Octacosane	394	C28H58	000630-02-4	90
3	Pentadecane	212	C15H32	000629-62-9	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Heneicosane	296	C21H44	000629-94-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG021119\
Data File : BG039432.D
Acq On : 11 Feb 2019 13:37
Operator : JU/SJ
Sample : K1404-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A0C12-SS1-7.5-8.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.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...	3.29	4.9	ng	90128	1	8.17	365723	20.0
2-Pentanone, 4-hy...	5.26	6.7	ng	123241	1	8.17	365723	20.0
unknown7.70	7.70	117.0	ng	2140180	1	8.17	365723	20.0
n-Hexadecanoic acid	18.40	3.7	ng	207024	4	17.54	1128950	20.0
Cyclohexadecane	21.43	5.6	ng	382613	5	21.83	1355770	20.0
Tetracosane	21.99	2.7	ng	183979	5	21.83	1355770	20.0
Octacosane	22.63	3.6	ng	244299	5	21.83	1355770	20.0
Heptacosane	23.35	3.9	ng	261849	5	21.83	1355770	20.0
Eicosane	24.19	3.2	ng	232366	6	25.21	1444830	20.0