LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021219\
Data File : BG039469.D
Acq On : 12 Feb 2019 18:32
Operator : JU/SJ
Sample : K1462-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-1-D

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	3.222	17	23	32	rBV	81383	160001	3.92%	0.678%
2	3.299	32	36	45	rVB	53553	80100	1.96%	0.339%
3	5.249	363	368	375	rBV	63330	98890	2.42%	0.419%
4	5.713	439	447	457	rBV	1055363	1703484	41.76%	7.216%
5	7.311	711	719	732	rBV	1133257	2101955	51.53%	8.905%
6	7.699	776	785	796	rBV	1043328	1778534	43.61%	7.534%
7	8.168	858	865	876	rVB	171653	305270	7.48%	1.293%
8	8.497	913	921	928	rBV	708162	1244905	30.52%	5.274%
9	9.349	1057	1066	1074	rBV	647523	1160488	28.45%	4.916%
10	10.994	1338	1346	1354	rVB	256887	460545	11.29%	1.951%
11	13.420	1751	1759	1766	rBV	1735961	2675333	65.59%	11.334%
12	14.237	1891	1898	1904	rBV	155311	230570	5.65%	0.977%
13	14.795	1986	1993	2001	rBV2	444832	724560	17.76%	3.069%
14	16.281	2239	2246	2262	rBV	1531200	2447119	60.00%	10.367%
15	17.538	2453	2460	2467	rBV	634518	963258	23.62%	4.081%
16	18.396	2600	2606	2614	rBV2	99699	178516	4.38%	0.756%
17	19.653	2815	2820	2828	rBV3	36369	64014	1.57%	0.271%
18	20.135	2895	2902	2908	rBV	3005805	4078738	100.00%	17.279%
19	21.421	3114	3121	3130	rBV	177994	277134	6.79%	1.174%
20	21.826	3183	3190	3199	rVB2	648357	1112863	27.28%	4.714%
21	21.985	3213	3217	3225	rVB	45766	64866	1.59%	0.275%
22	22.620	3320	3325	3335	rBV	54814	93373	2.29%	0.396%
23	23.342	3442	3448	3457	rVB	63872	123111	3.02%	0.522%
24	23.548	3476	3483	3491	rBV3	45807	95738	2.35%	0.406%
25	24.188	3585	3592	3601	rBV2	55200	124080	3.04%	0.526%
26	25.210	3754	3766	3778	rBV	375667	1168609	28.65%	4.951%
27	26.385	3956	3966	3977	rVB4	29309	89424	2.19%	0.379%

Sum of corrected areas: 23605478

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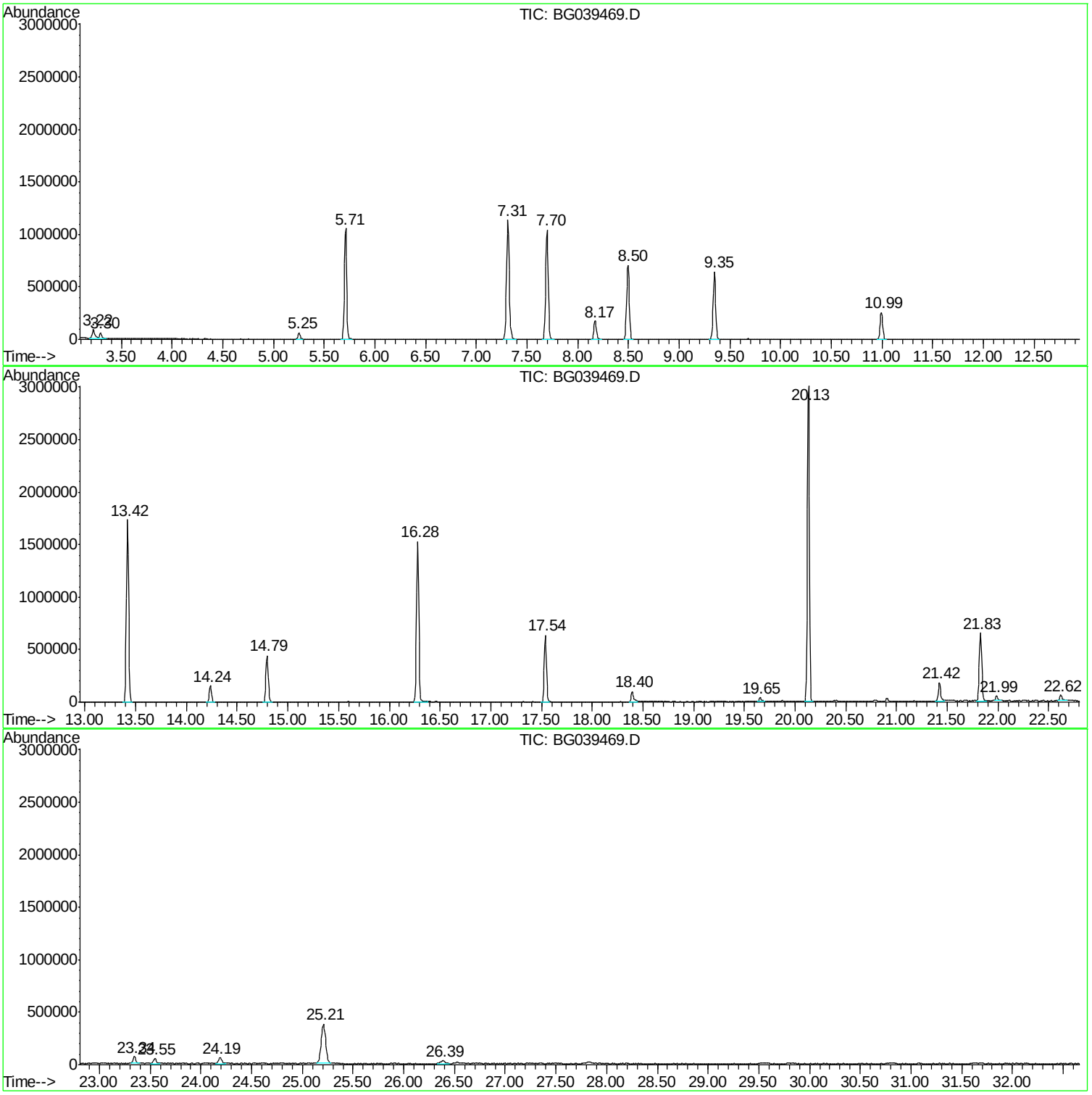
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-1-D

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021219\
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ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

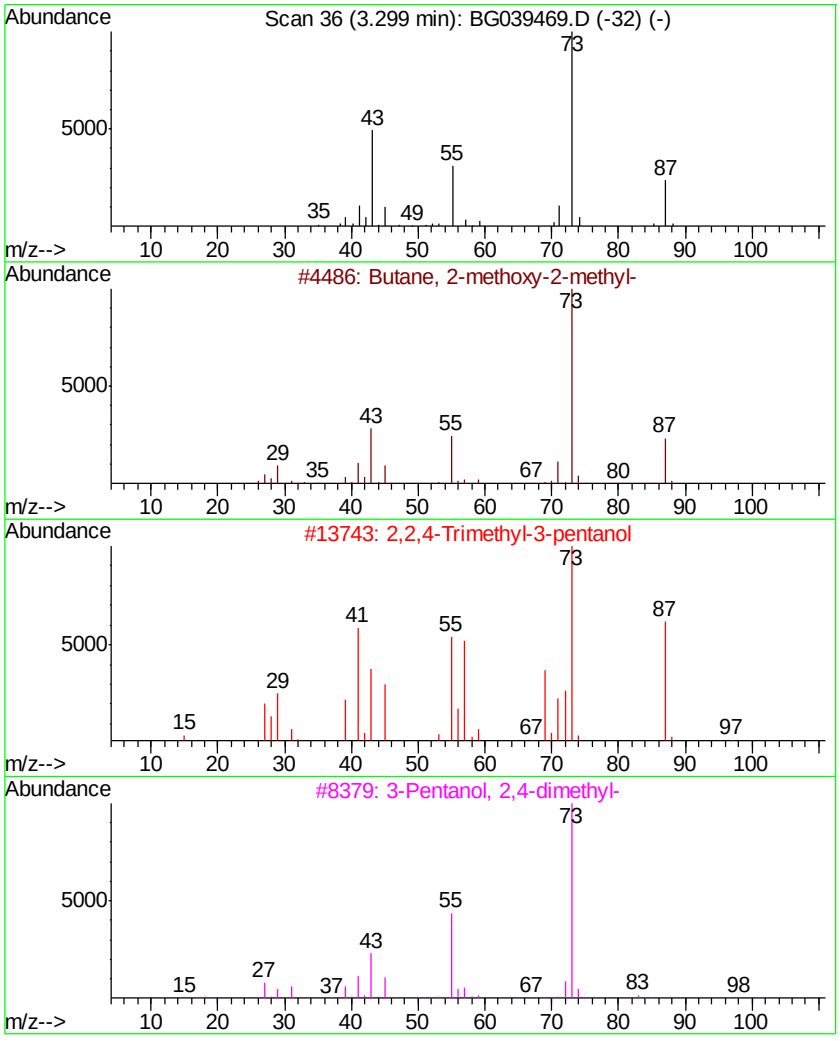
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

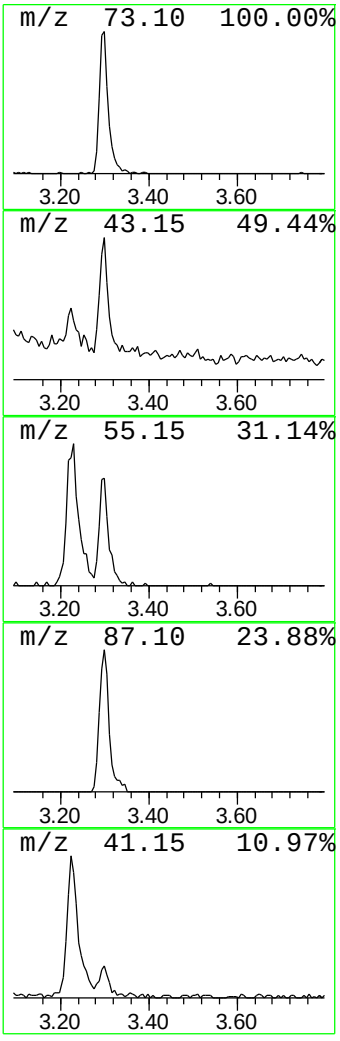
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.30	5.25 ng	80100	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	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
4	1,3-Dioxolane, 2-(1-methylpropyl)-	130	C7H14O2	014447-25-7	23
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BG039469.D
Acq On : 12 Feb 2019 18:32
Operator : JU/SJ
Sample : K1462-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-1-D

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

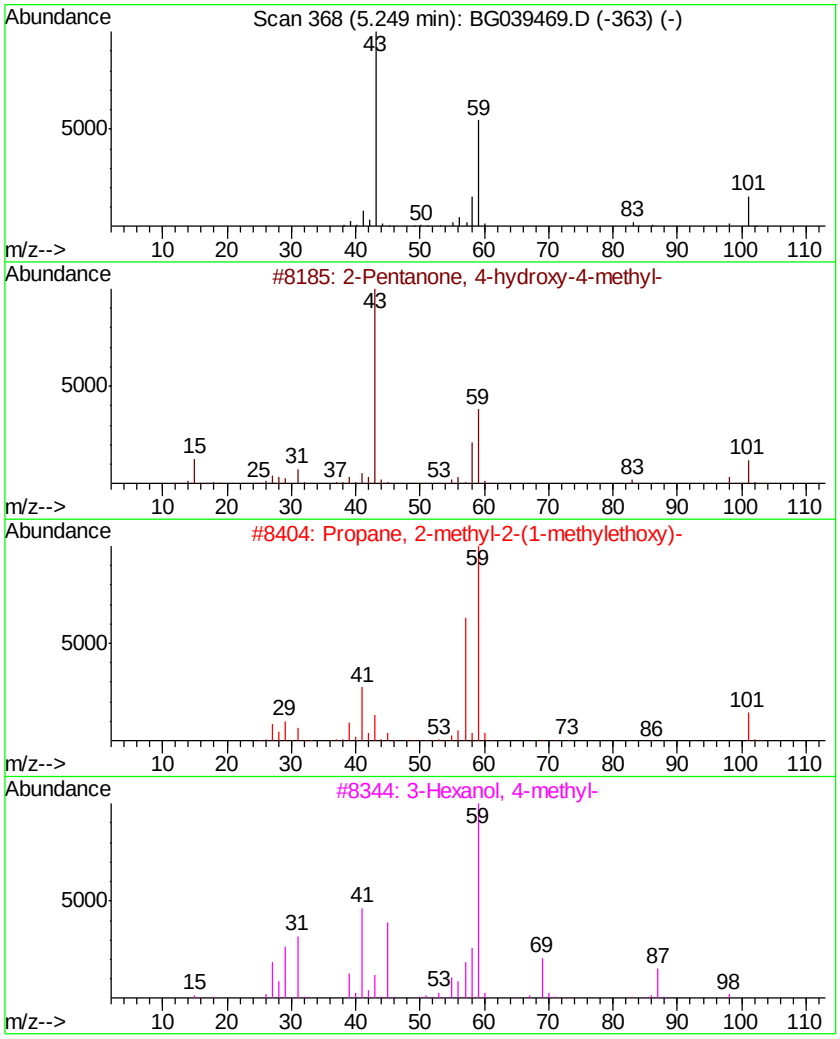
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

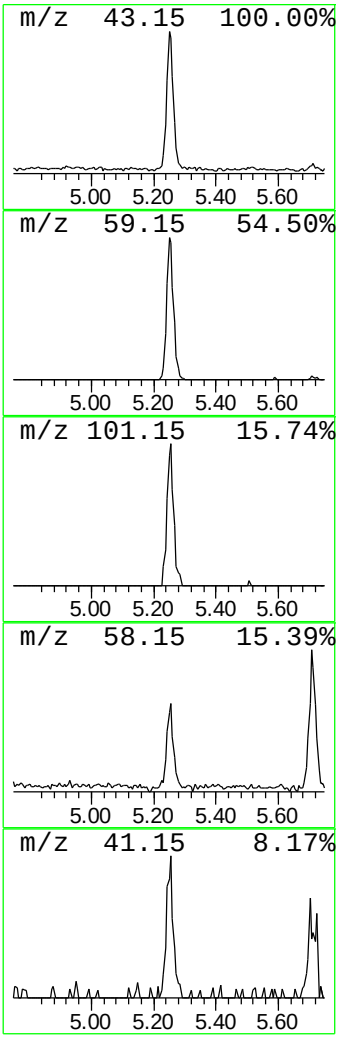
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	6.48 ng	98890	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	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021219\
Data File : BG039469.D
Acq On : 12 Feb 2019 18:32
Operator : JU/SJ
Sample : K1462-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-1-D

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

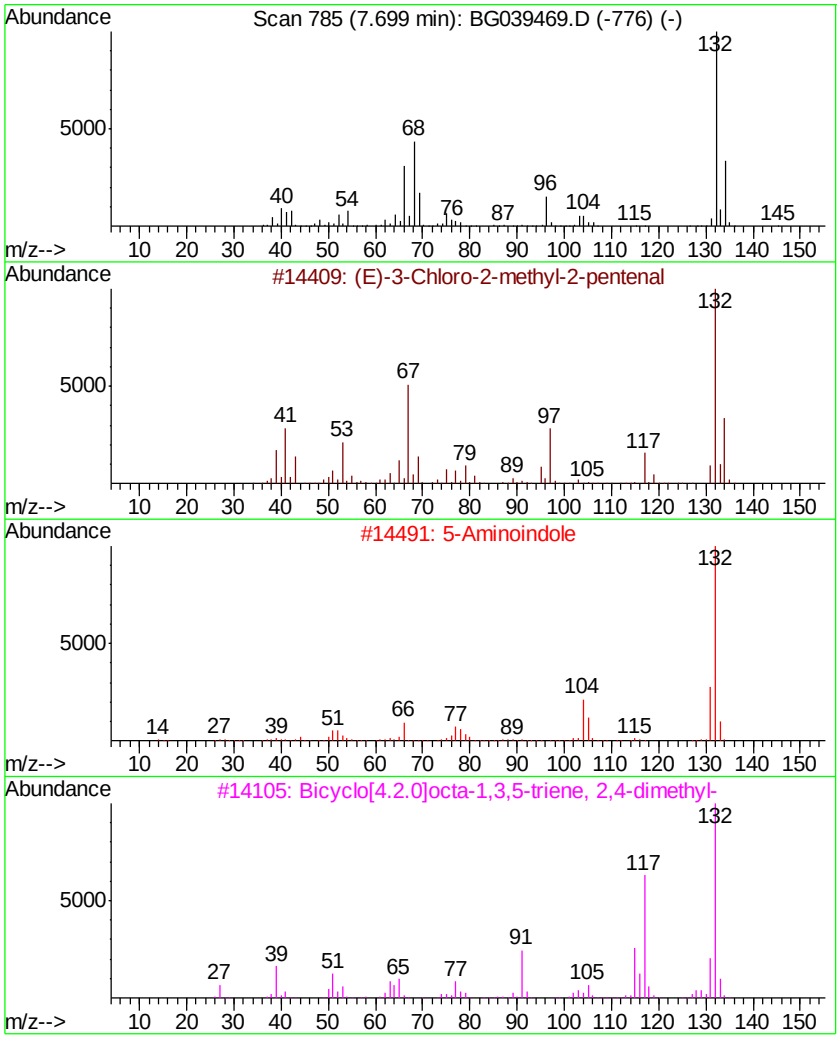
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

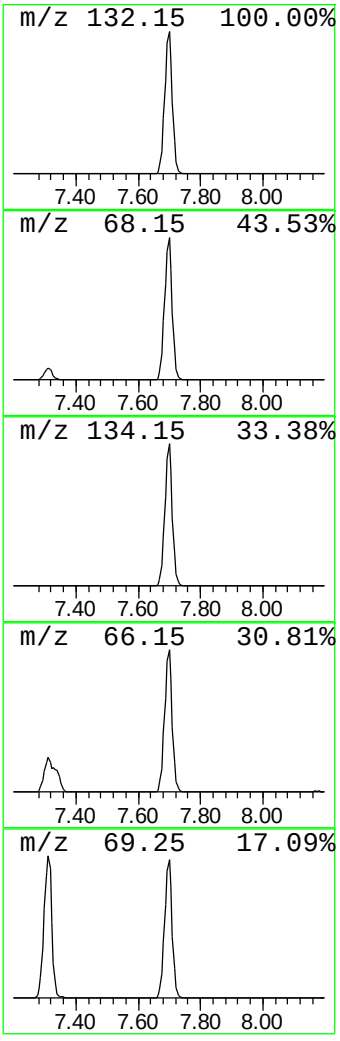
****

Peak Number 4 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	116.52 ng	1778530	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	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021219\
Data File : BG039469.D
Acq On : 12 Feb 2019 18:32
Operator : JU/SJ
Sample : K1462-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-1-D

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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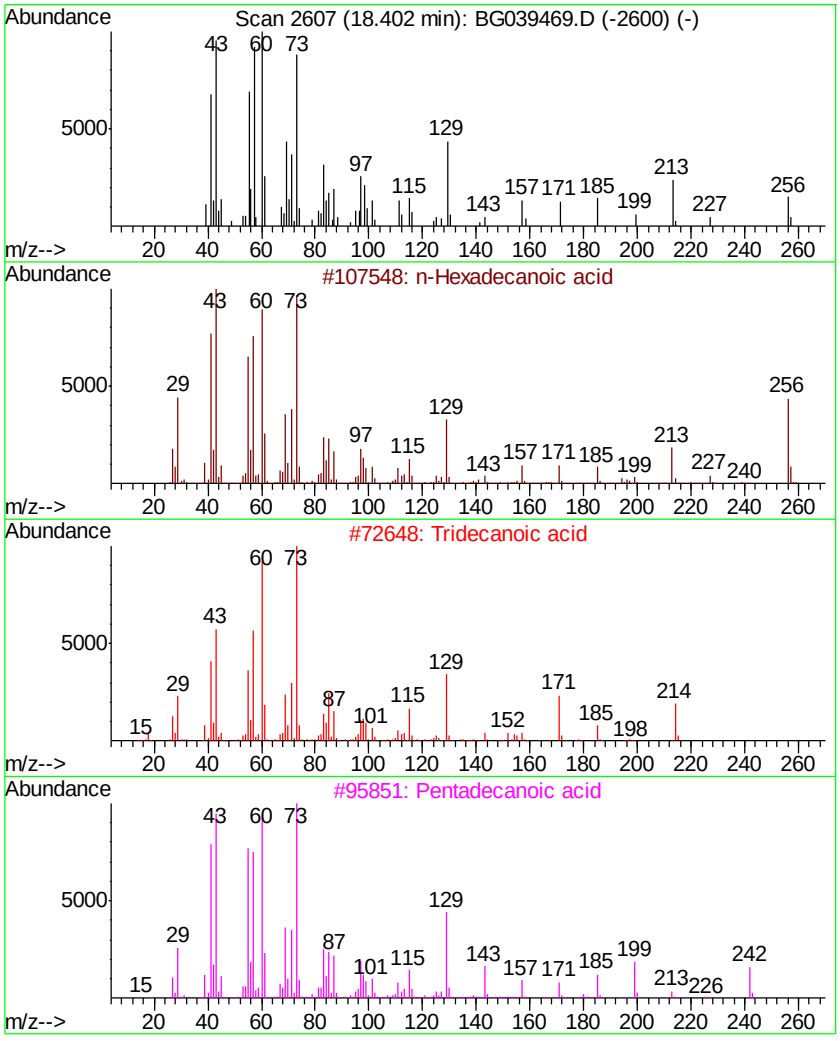
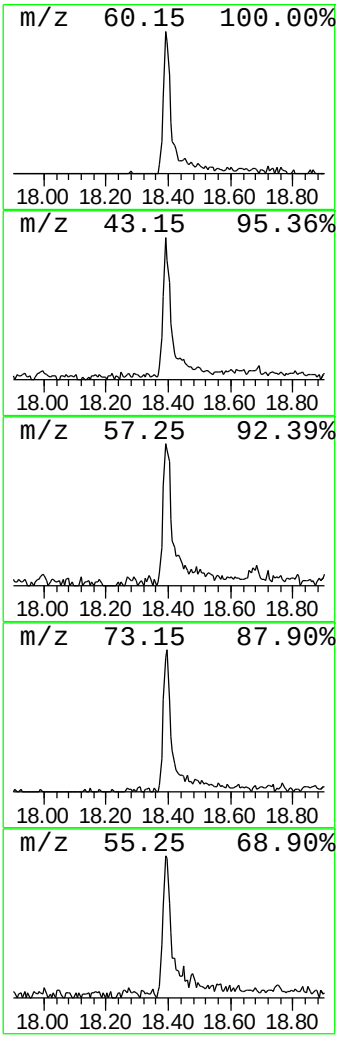
Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.40	3.71 ng	178516	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	78
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021219\
Data File : BG039469.D
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Misc :
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Instrument : BNA_G
ClientSampleId : TP-1-D

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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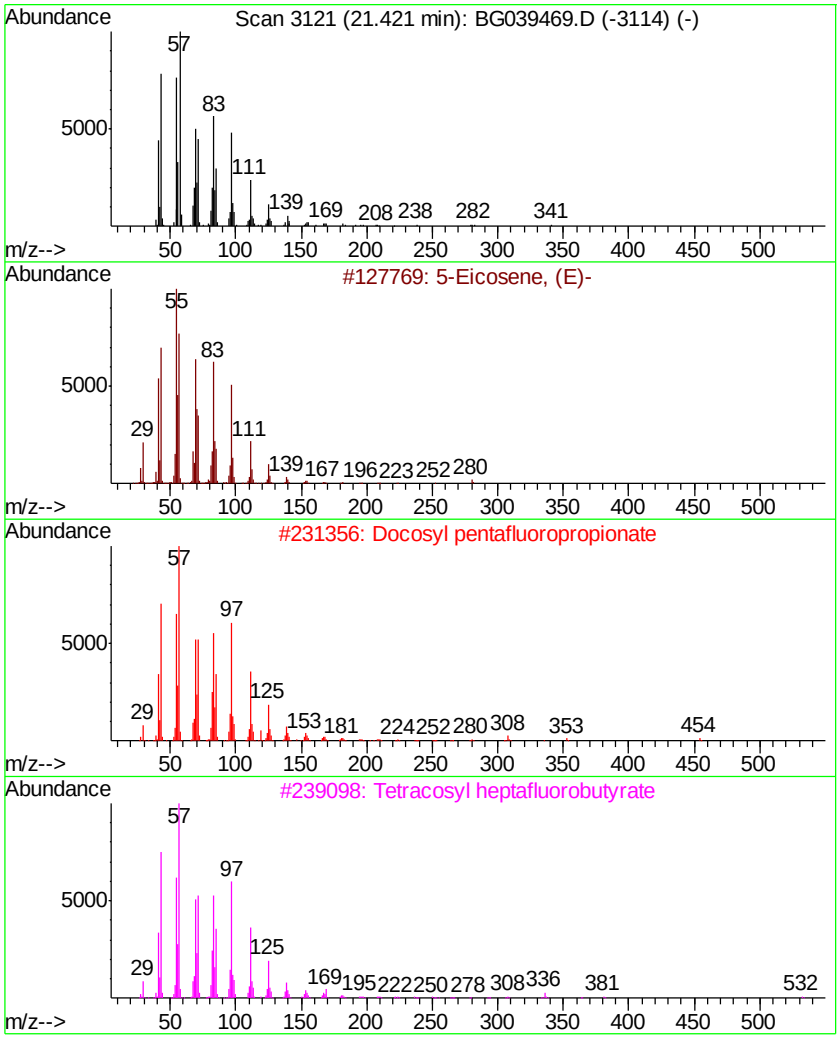
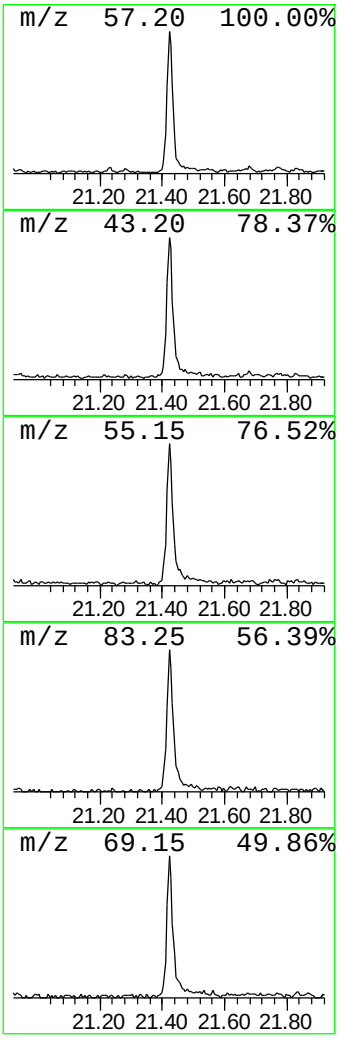
****

Peak Number 7 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.42	4.98 ng	277134	Chrysene-d12	21.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
3	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
4	Tetracosyl pentafluoropropionate	500	C27H49F5O2	1000351-81-3	91
5	Docosyl heptafluorobutyrate	522	C26H45F7O2	1000351-83-1	91





Library Search Compound Report

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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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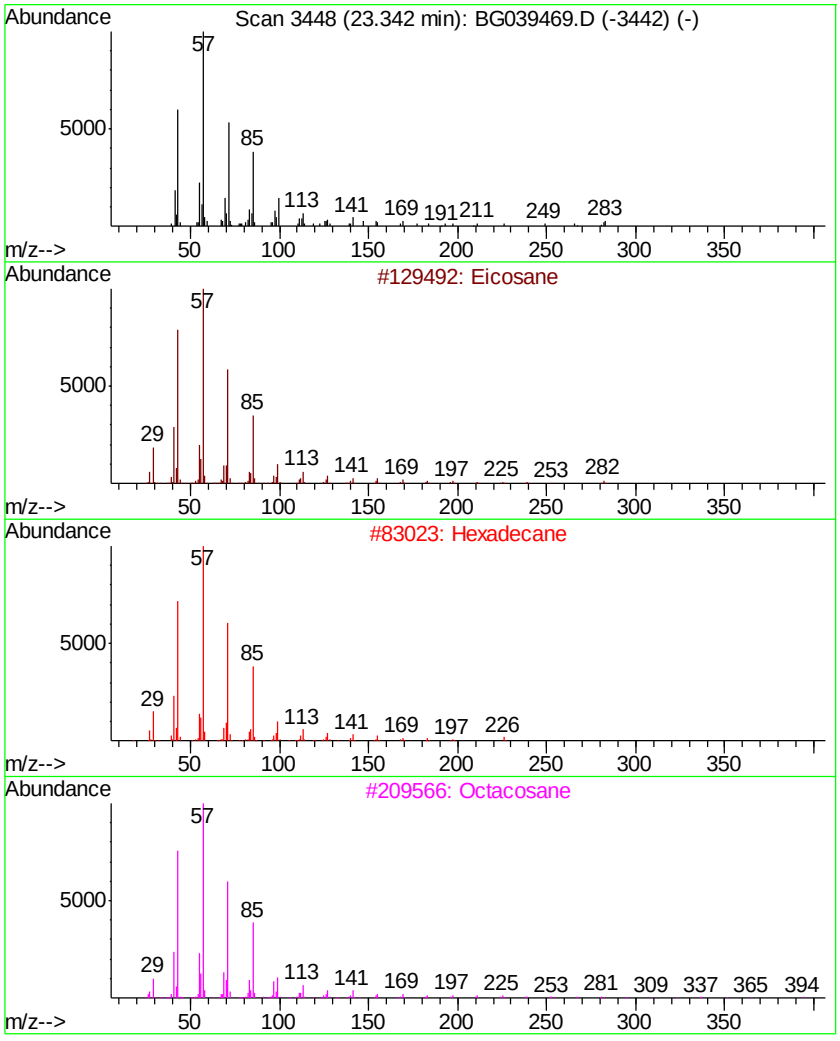
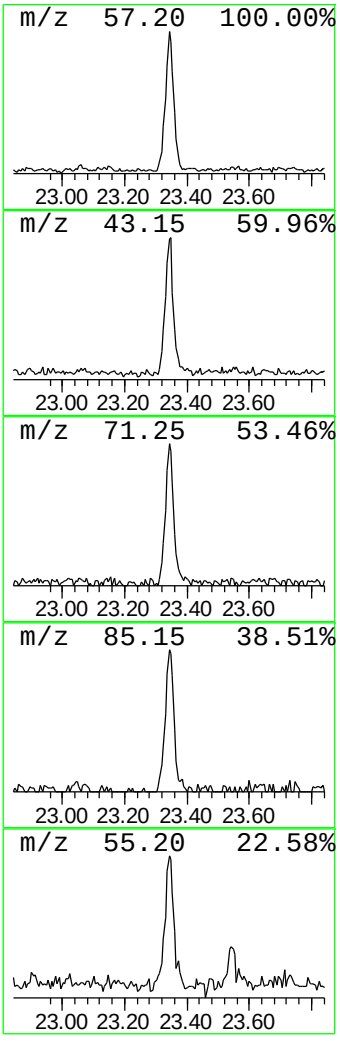
****

Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.34	2.21 ng	123111	Chrysene-d12	21.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Hexadecane	226	C16H34	000544-76-3	96
3	Octacosane	394	C28H58	000630-02-4	90
4	Heptacosane	380	C27H56	000593-49-7	87
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	80





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : TP-1-D

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

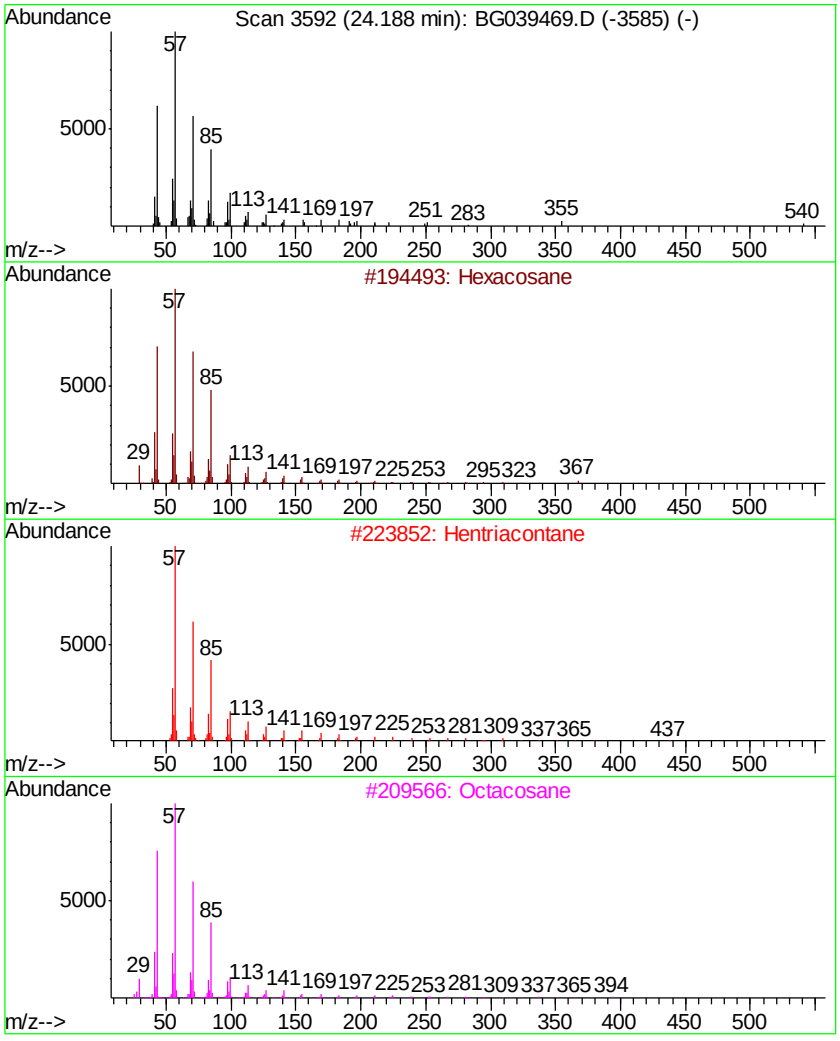
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

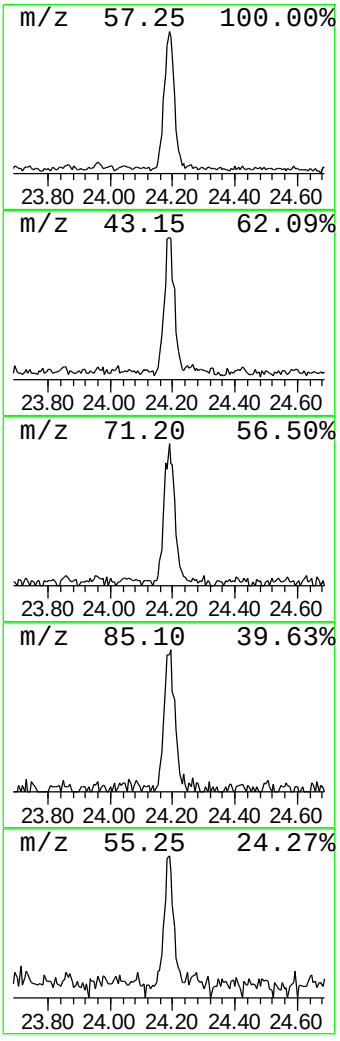
****

Peak Number 9 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.19	2.12 ng	124080	Perylene-d12	25.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Hentriacontane	437	C31H64	000630-04-6	90
3	Octacosane	394	C28H58	000630-02-4	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Tetratetracontane	619	C44H90	007098-22-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG021219\
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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...	3.30	5.3	ng	80100	1	8.17	305270	20.0
2-Pentanone, 4-hy...	5.25	6.5	ng	98890	1	8.17	305270	20.0
unknown7.70	7.70	116.5	ng	1778530	1	8.17	305270	20.0
n-Hexadecanoic acid	18.40	3.7	ng	178516	4	17.54	963258	20.0
5-Eicosene, (E)-	21.42	5.0	ng	277134	5	21.83	1112860	20.0
Eicosane	23.34	2.2	ng	123111	5	21.83	1112860	20.0
Hexacosane	24.19	2.1	ng	124080	6	25.21	1168610	20.0