LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022719\
Data File : BG039637.D
Acq On : 27 Feb 2019 16:38
Operator : JU/SJ
Sample : K1631-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : Z31W

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	17	23	31	rBV	218403	433213	10.63%	2.282%
2	3.294	31	35	49	rVB	146709	229702	5.63%	1.210%
3	5.708	440	446	458	rBV	387766	627694	15.40%	3.306%
4	7.312	710	719	729	rBV2	245168	473072	11.61%	2.492%
5	7.694	776	784	792	rBV	739169	1268491	31.12%	6.681%
6	8.164	858	864	876	rVB	161544	291305	7.15%	1.534%
7	8.493	909	920	930	rBV	652779	1169382	28.69%	6.159%
8	9.344	1056	1065	1076	rBV	568558	1038392	25.47%	5.469%
9	10.989	1337	1345	1352	rBV	220859	404466	9.92%	2.130%
10	13.415	1750	1758	1767	rBV	1554986	2450207	60.11%	12.906%
11	14.232	1891	1897	1904	rBV	118065	178628	4.38%	0.941%
12	14.790	1984	1992	2002	rBV2	367500	608805	14.93%	3.207%
13	16.276	2237	2245	2259	rBV	1330961	2033946	49.90%	10.713%
14	17.533	2452	2459	2470	rBV	542146	826086	20.27%	4.351%
15	18.385	2597	2604	2611	rBV2	54909	93508	2.29%	0.493%
16	20.124	2894	2900	2910	rBV	3030806	4076382	100.00%	21.471%
17	21.416	3115	3120	3134	rBV4	47946	133146	3.27%	0.701%
18	21.822	3182	3189	3200	rVB	585646	973797	23.89%	5.129%
19	21.968	3210	3214	3220	rVB	26758	43121	1.06%	0.227%
20	22.597	3316	3321	3328	rVB	47989	78265	1.92%	0.412%
21	23.320	3438	3444	3452	rVB2	67702	127658	3.13%	0.672%
22	24.154	3579	3586	3597	rVB	69459	153903	3.78%	0.811%
23	25.199	3748	3764	3776	rVB2	315619	1065180	26.13%	5.611%
24	26.339	3948	3958	3967	rBV4	39539	130643	3.20%	0.688%
25	27.755	4191	4199	4211	rVB6	20031	76409	1.87%	0.402%

Sum of corrected areas: 18985401

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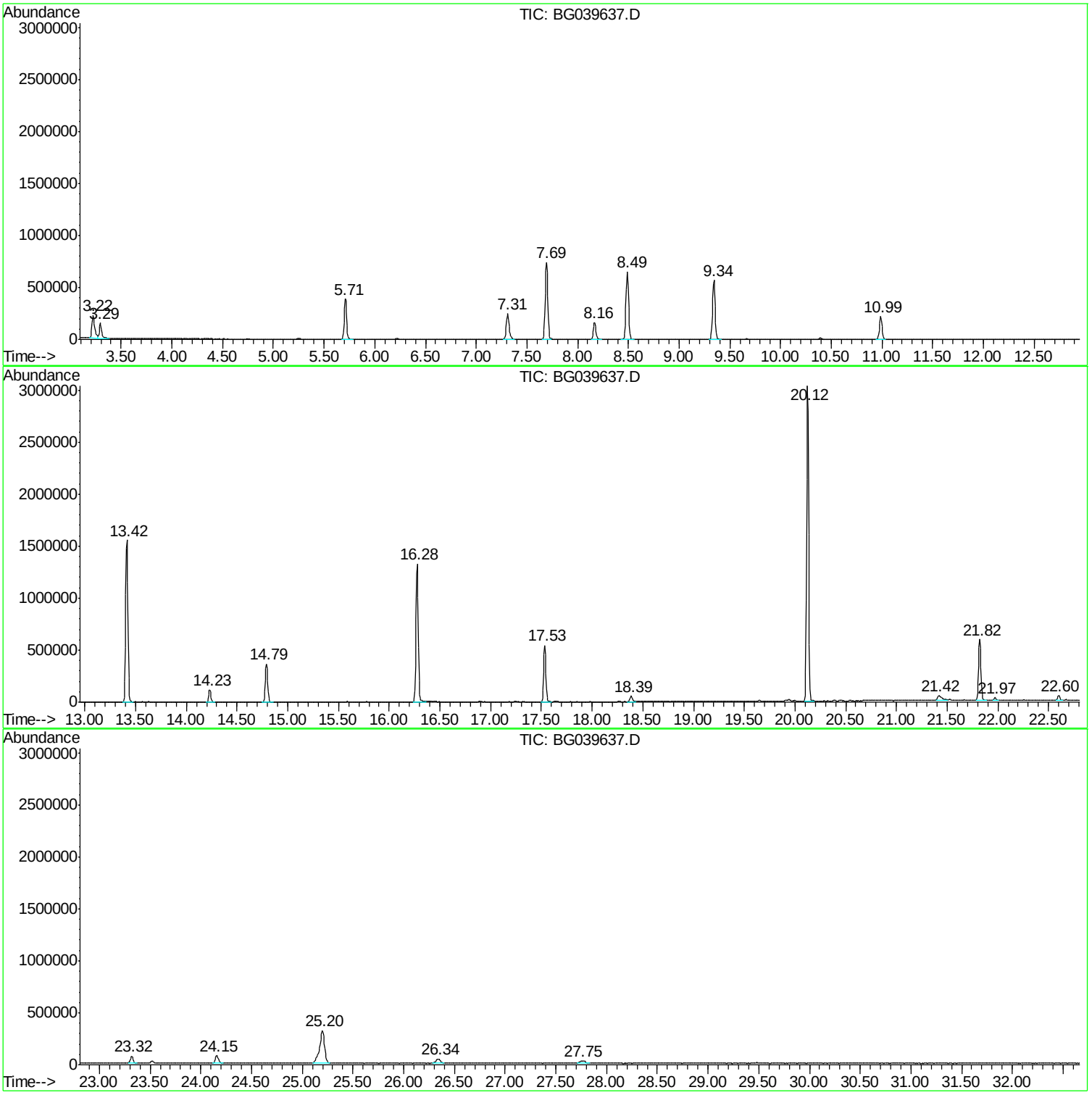
Instrument :
BNA_G
ClientSampleId :
Z31W

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

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Misc :
ALS Vial : 9 Sample Multiplier: 1

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

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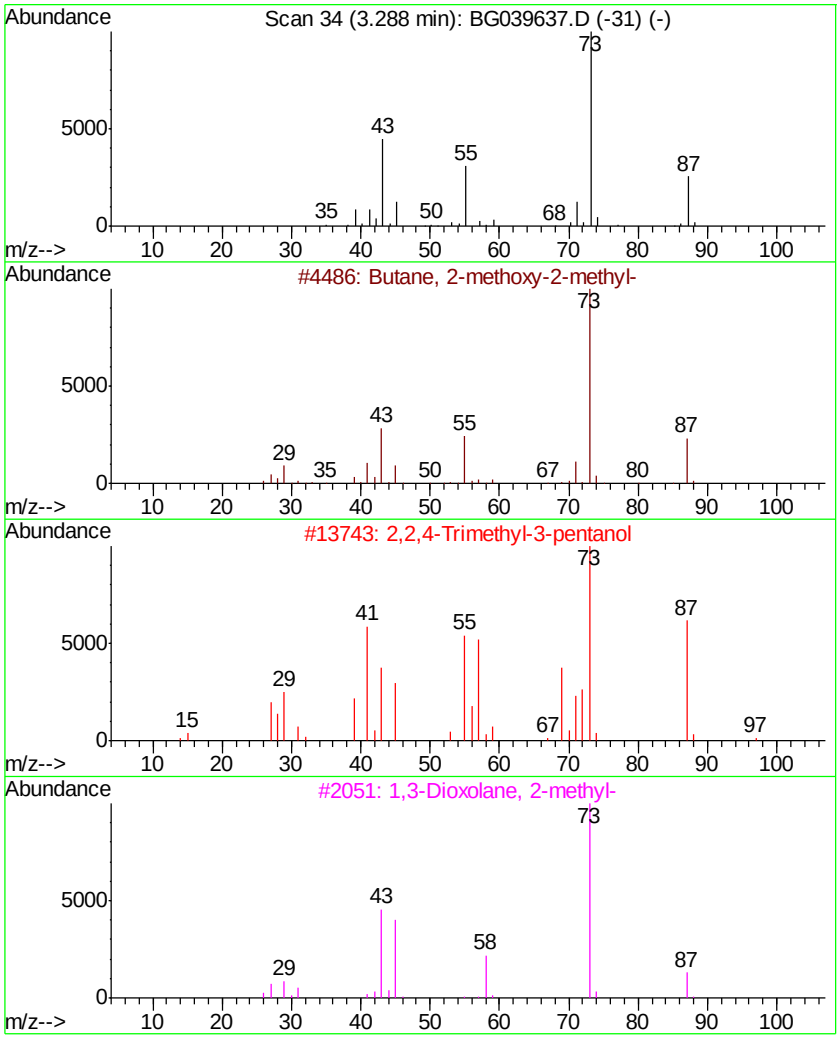
TIC Integration Parameters: LSCINT.P

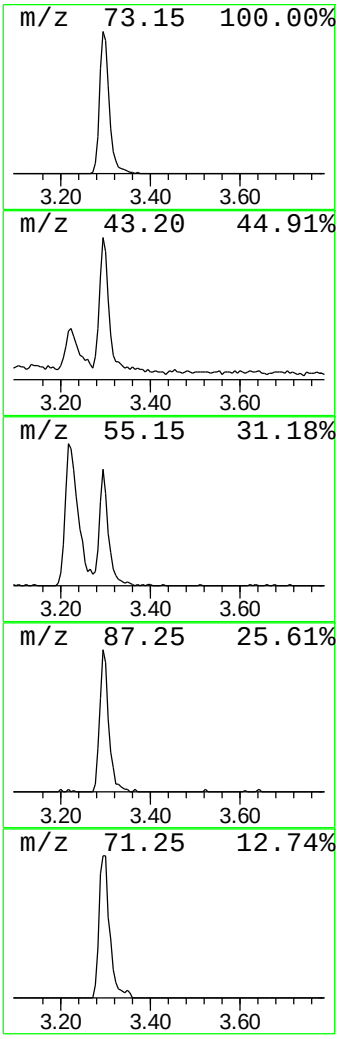
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.29	15.77 ng	229702	1,4-Dichlorobenzene-d4	8.16

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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Library Search Compound Report

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Operator : JU/SJ
Sample : K1631-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : Z31W

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

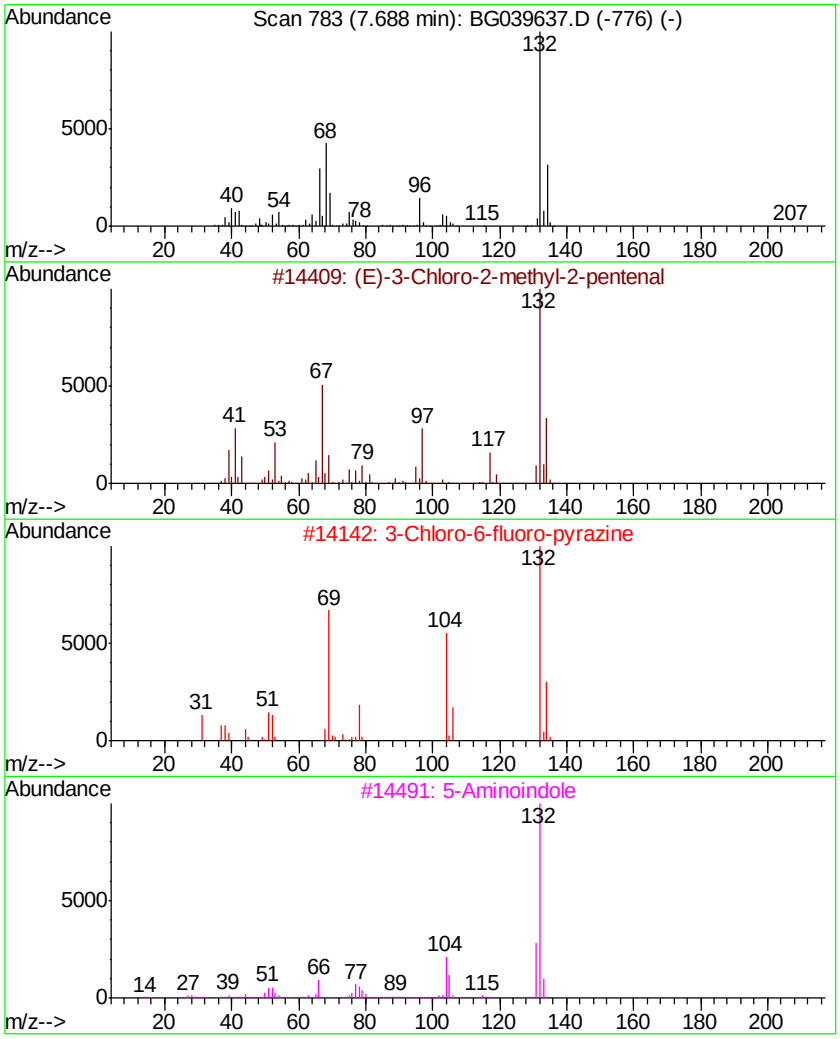
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

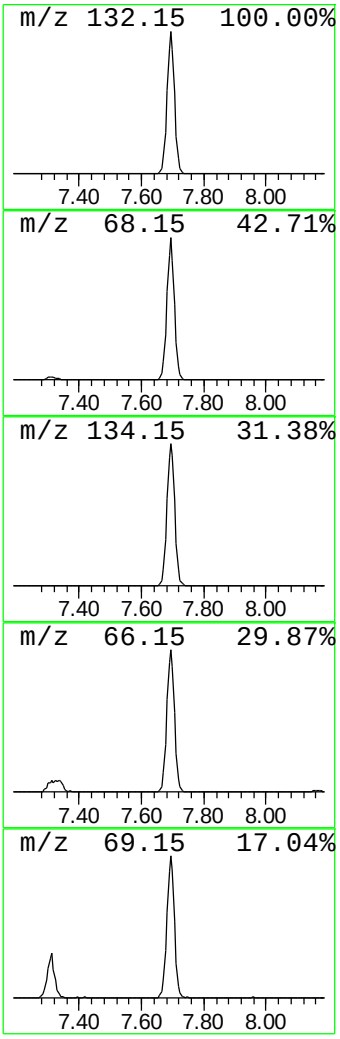
****

Peak Number 3 unknown7.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	87.09 ng	1268490	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9





Library Search Compound Report

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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : Z31W

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

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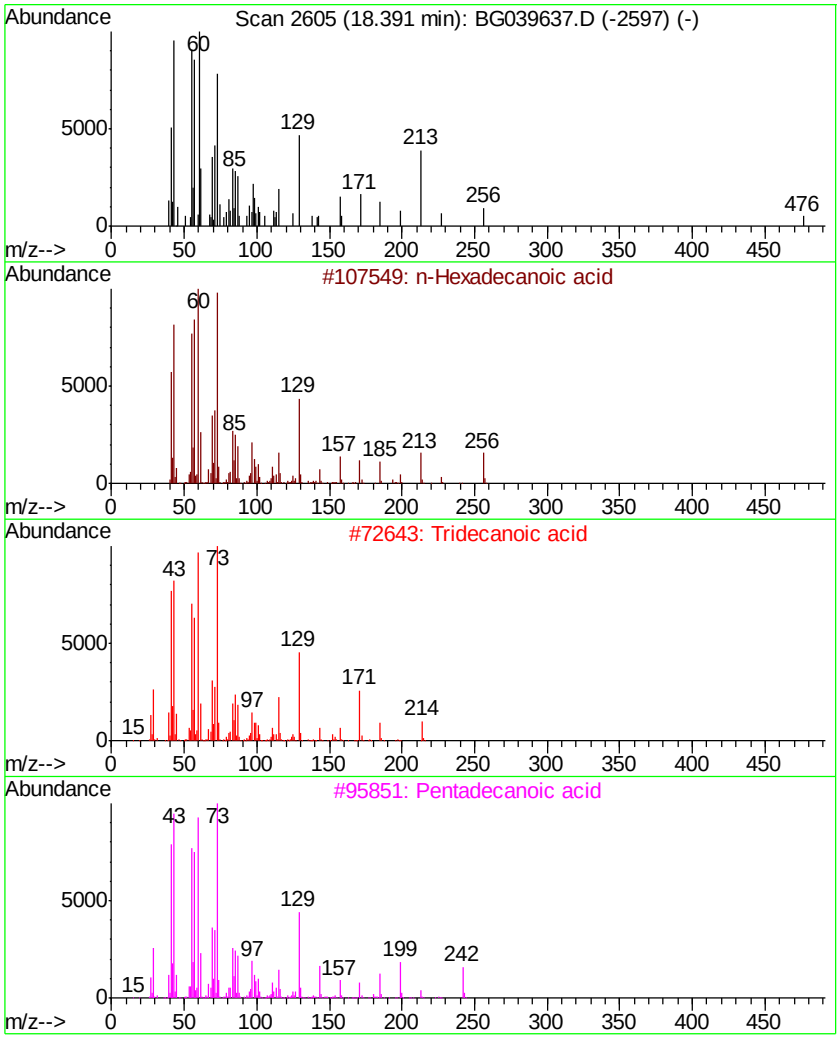
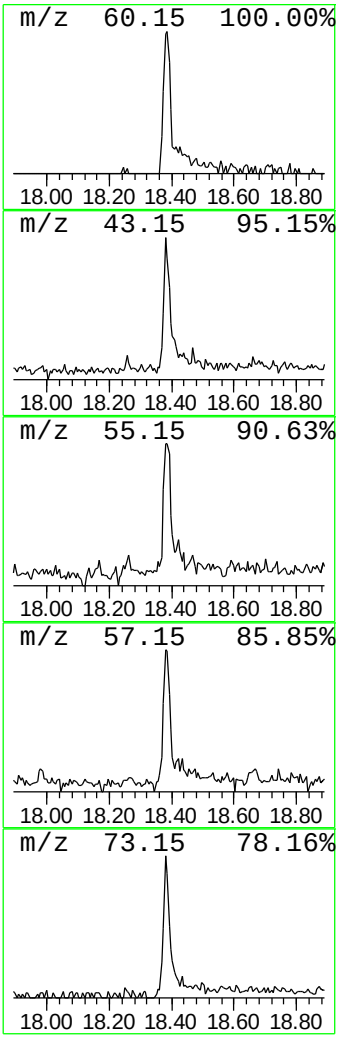
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	2.26 ng	93508	Phenanthrene-d10	17.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5	Trehalose	342	C12H22O11	000099-20-7	43





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Operator : JU/SJ
Sample : K1631-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : Z31W

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

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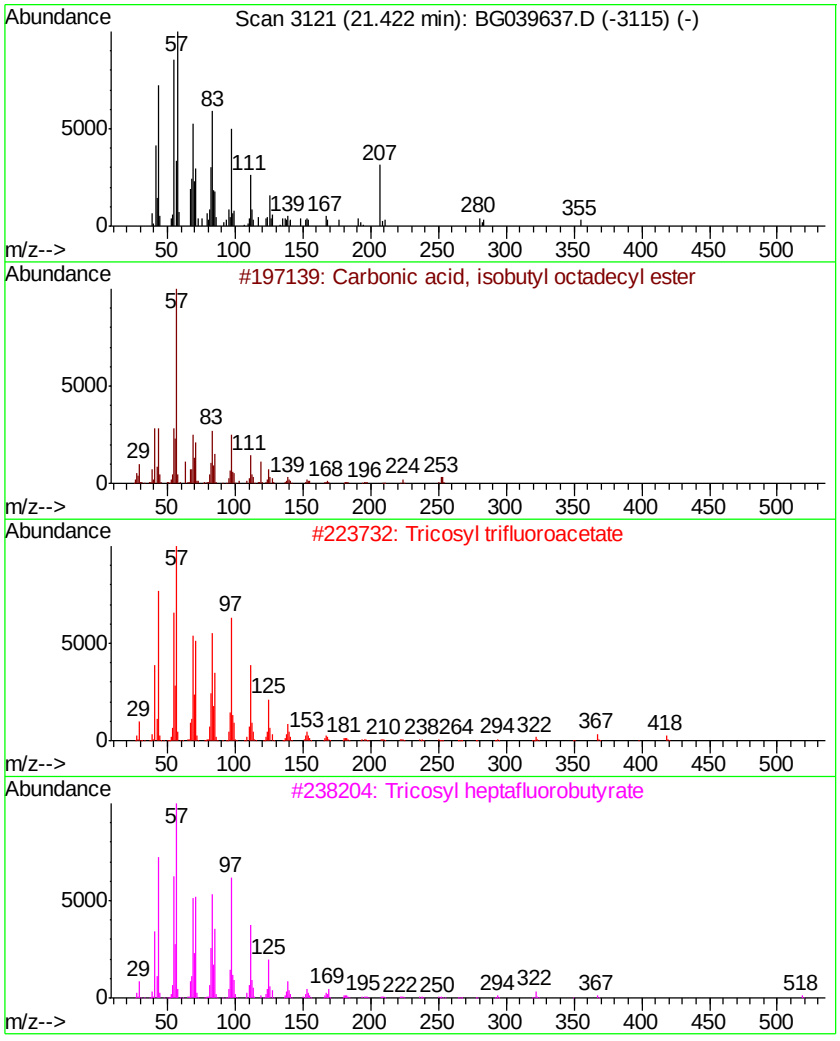
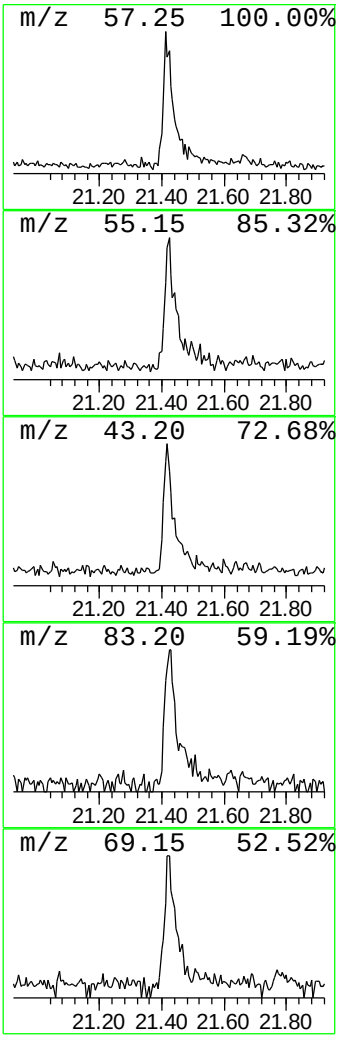
Peak Number 6 Carbonic acid, isobutyl oct... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.42	2.73 ng	133146	Chrysene-d12	21.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	91
2	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	87
3	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	86
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	83
5	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	83





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : Z31W

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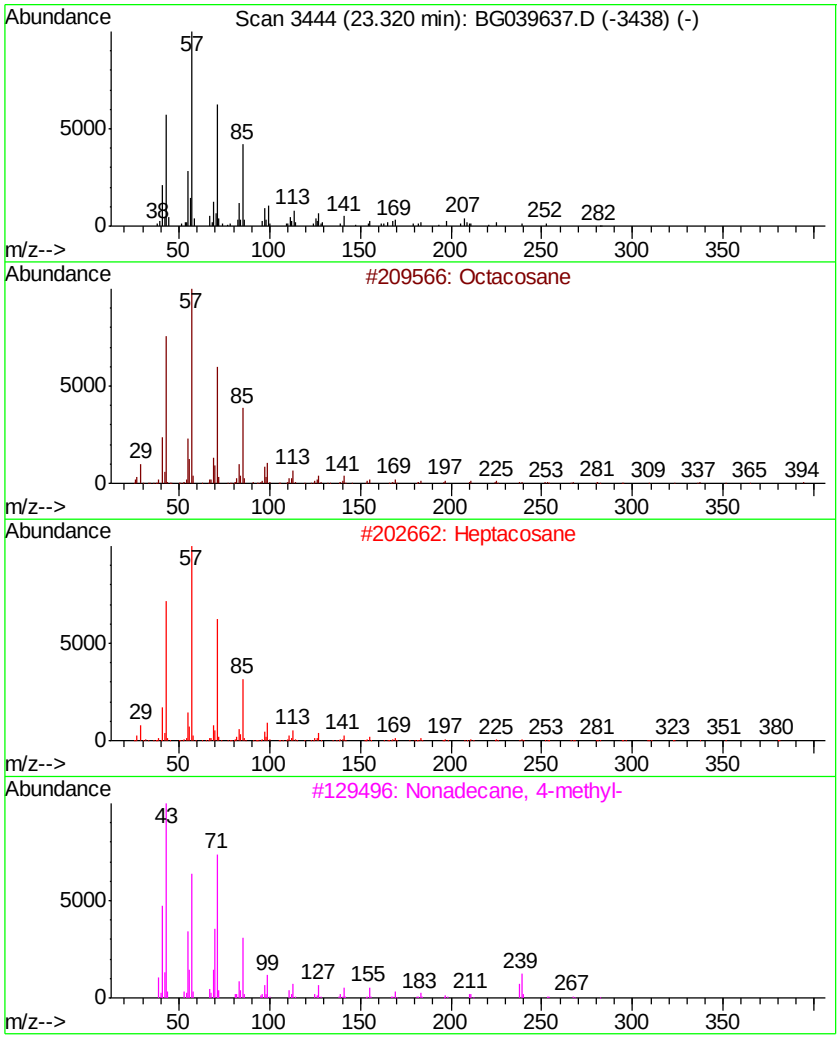
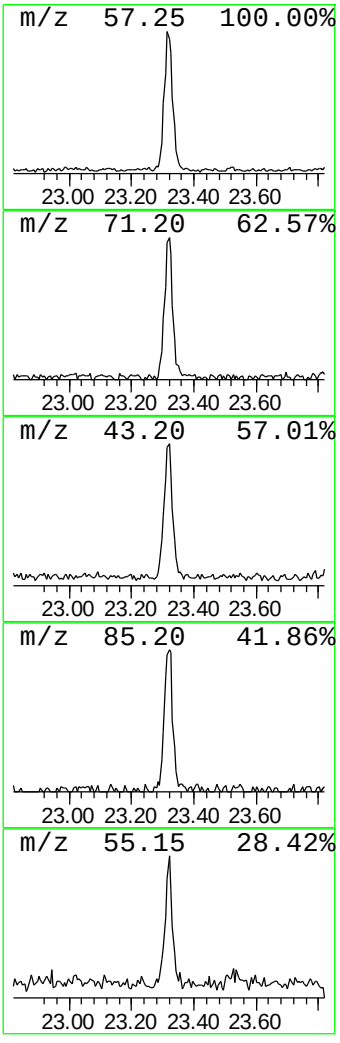
****

Peak Number 7 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.32	2.62 ng	127658	Chrysene-d12	21.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Heptacosane	380	C27H56	000593-49-7	90
3	Nonadecane, 4-methyl-	282	C20H42	025117-27-5	86
4	Docosane	310	C22H46	000629-97-0	86
5	Eicosane	282	C20H42	000112-95-8	86





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Misc :
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Instrument : BNA_G
ClientSampleId : Z31W

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

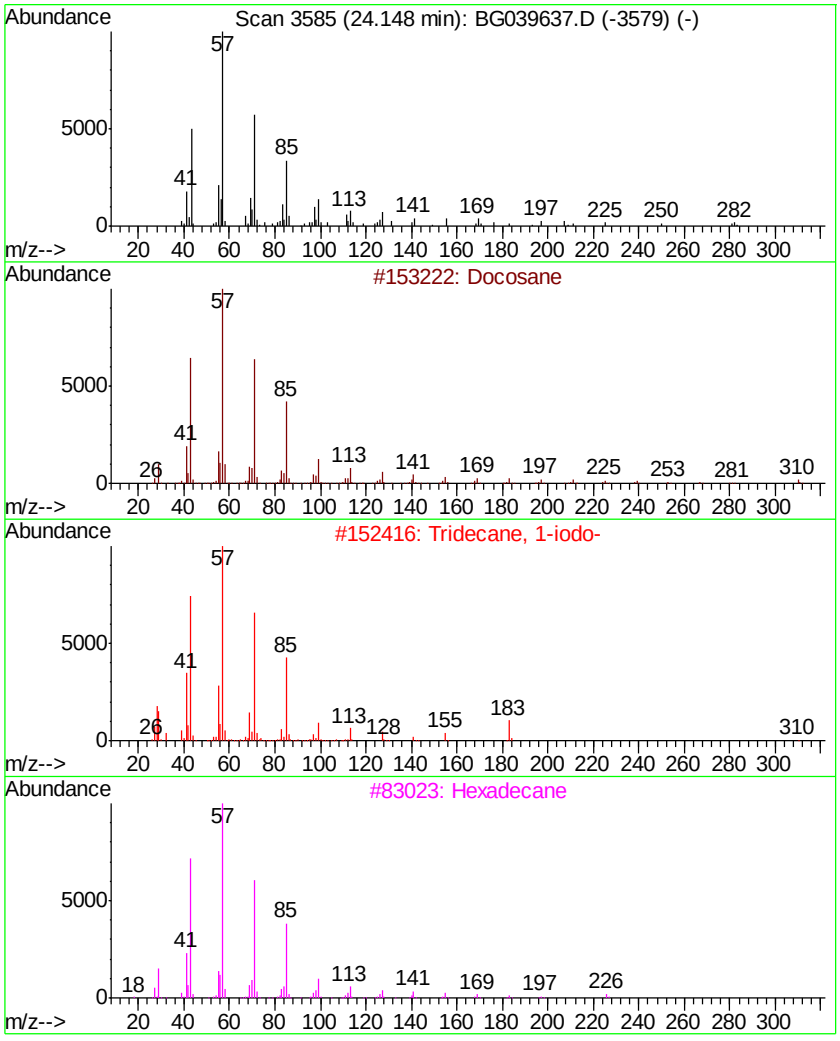
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

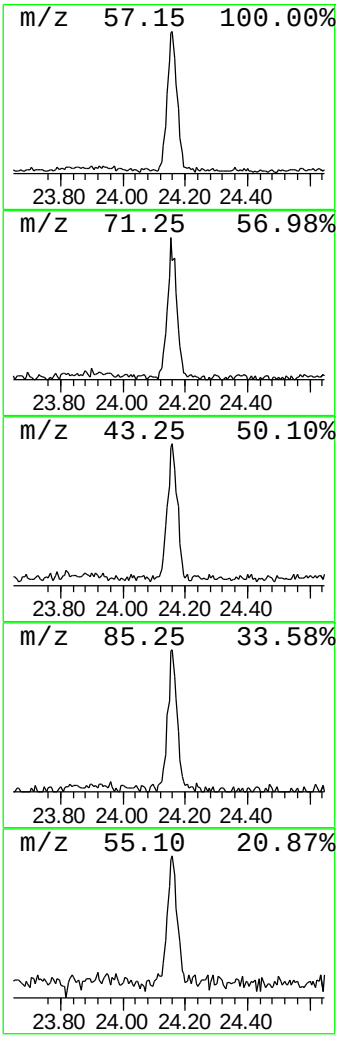
****

Peak Number 8 Docosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.15	2.89 ng	153903	Perylene-d12	25.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	87
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
3	Hexadecane	226	C16H34	000544-76-3	86
4	Heptadecane	240	C17H36	000629-78-7	86
5	Nonadecane	268	C19H40	000629-92-5	80





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

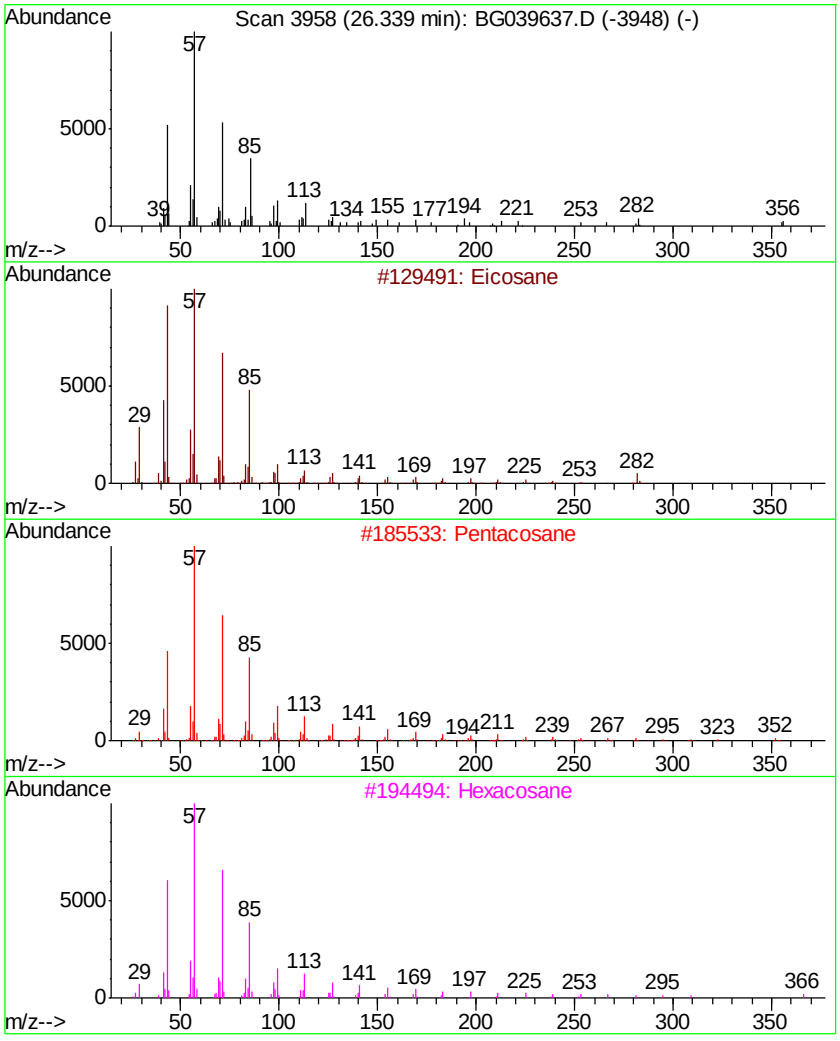
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

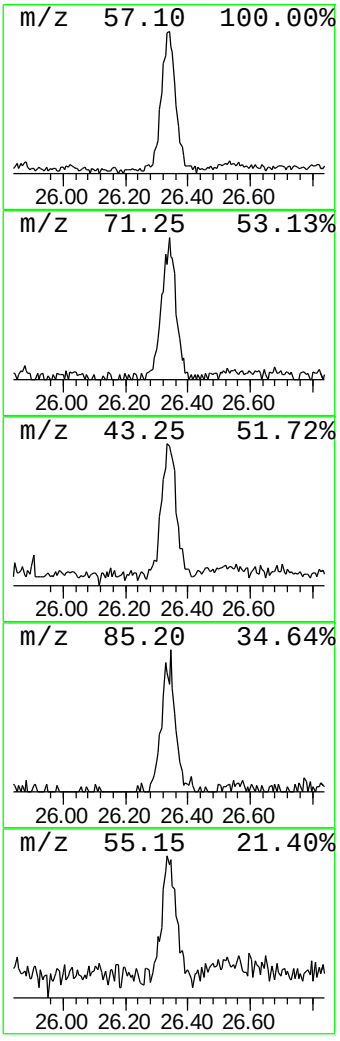
****

Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.34	2.45 ng	130643	Perylene-d12	25.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Pentacosane	352	C25H52	000629-99-2	80
3	Hexacosane	366	C26H54	000630-01-3	80
4	2-methyloctacosane	408	C29H60	1000376-72-8	74
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	74





Tentatively Identified Compound (LSC) summary

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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	15.8	ng	229702	1	8.16	291305	20.0
unknown7.69	7.69	87.1	ng	1268490	1	8.16	291305	20.0
n-Hexadecanoic acid	18.39	2.3	ng	93508	4	17.53	826086	20.0
Carbonic acid, is...	21.42	2.7	ng	133146	5	21.82	973797	20.0
Octacosane	23.32	2.6	ng	127658	5	21.82	973797	20.0
Docosane	24.15	2.9	ng	153903	6	25.20	1065180	20.0
Eicosane	26.34	2.5	ng	130643	6	25.20	1065180	20.0