LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050919\
Data File : BG040833.D
Acq On : 10 May 2019 2:05
Operator : HP/JU
Sample : K2764-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS001-0612-01

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-BG042319.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	3.153	6	11	20	rBV	116306	211877	4.27%	0.741%
2	3.229	20	24	36	rVB	265092	350127	7.05%	1.225%
3	5.673	432	440	450	rBV	1221259	1915274	38.57%	6.702%
4	7.283	704	714	727	rBV	1302458	2299718	46.31%	8.048%
5	7.665	771	779	791	rBV	1246096	2107374	42.44%	7.375%
6	8.141	852	860	867	rBV	216776	364086	7.33%	1.274%
7	8.464	907	915	923	rBV	868165	1436182	28.92%	5.026%
8	9.322	1052	1061	1068	rBV	773330	1416364	28.52%	4.956%
9	10.961	1333	1340	1347	rBV	278593	511659	10.30%	1.791%
10	13.394	1744	1754	1762	rBV	2085556	3068789	61.79%	10.739%
11	14.210	1888	1893	1898	rBV	149900	200987	4.05%	0.703%
12	14.768	1981	1988	1999	rBV2	521218	827096	16.65%	2.894%
13	16.255	2234	2241	2258	rBV	1982136	2989883	60.21%	10.463%
14	17.512	2446	2455	2460	rBV	735131	1119563	22.54%	3.918%
15	18.370	2593	2601	2611	rBV	353200	593235	11.95%	2.076%
16	19.557	2798	2803	2808	rVB	45884	70375	1.42%	0.246%
17	19.627	2808	2815	2825	rBV2	117682	196819	3.96%	0.689%
18	19.915	2857	2864	2871	rBV	89161	132955	2.68%	0.465%
19	20.109	2891	2897	2912	rBV	3774535	4966119	100.00%	17.379%
20	20.379	2937	2943	2951	rVB10	23206	58995	1.19%	0.206%
21	21.396	3112	3116	3132	rBV4	182448	568377	11.45%	1.989%
22	21.795	3175	3184	3190	rBV2	706414	1244101	25.05%	4.354%
23	22.630	3324	3326	3338	rVB2	31790	69467	1.40%	0.243%
24	23.294	3431	3439	3450	rBV2	184576	410567	8.27%	1.437%
25	23.493	3467	3473	3479	rVB3	49738	94997	1.91%	0.332%
26	24.122	3574	3580	3590	rVB7	46110	115911	2.33%	0.406%
27	25.144	3741	3754	3768	rBV2	336121	1170840	23.58%	4.097%
28	26.296	3942	3950	3957	rVB3	22519	64173	1.29%	0.225%

Sum of corrected areas: 28575910

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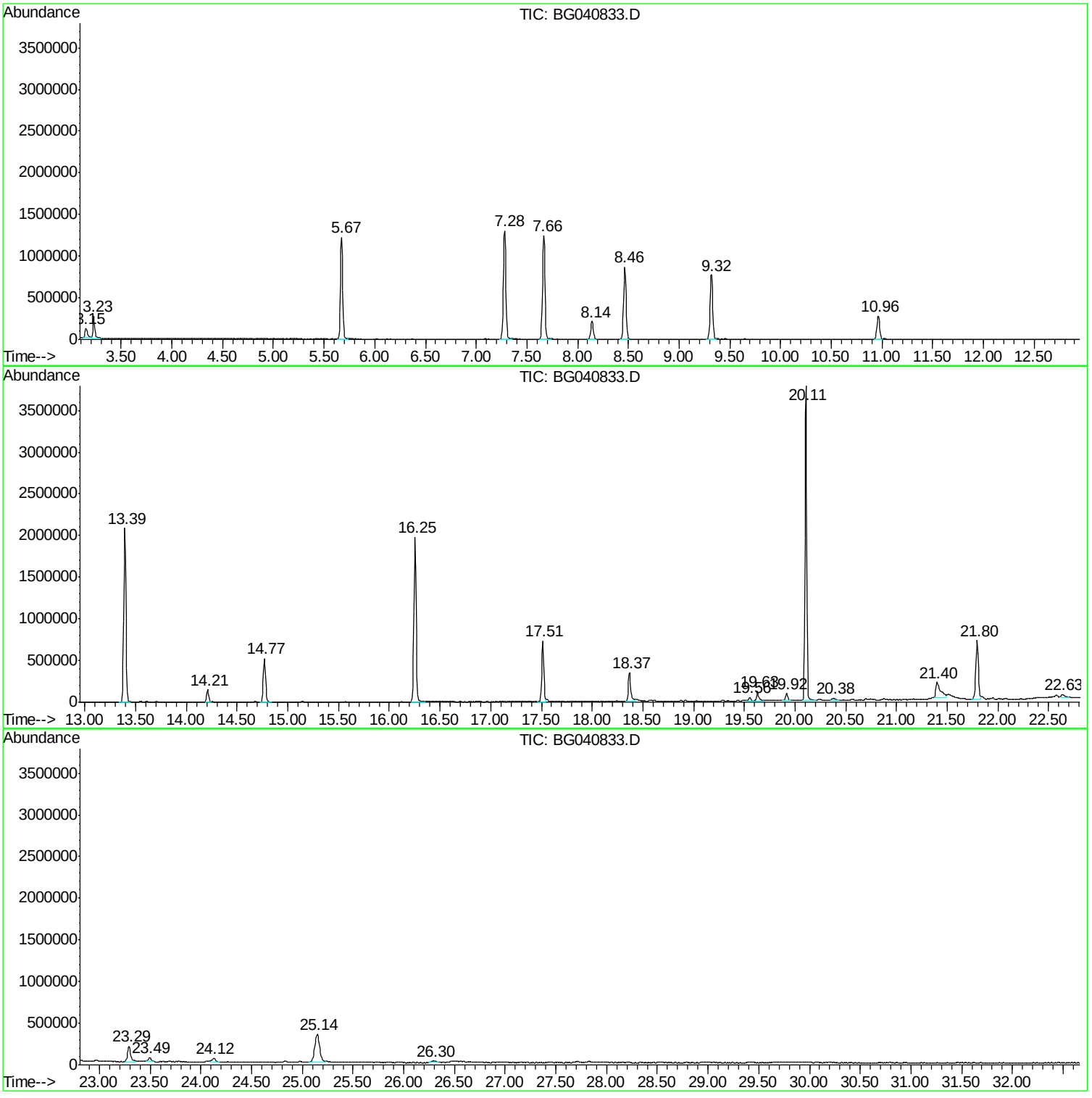
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P026-SS001-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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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Data File : BG040833.D
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Misc :
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Instrument : BNA_G
ClientSampleId : P026-SS001-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

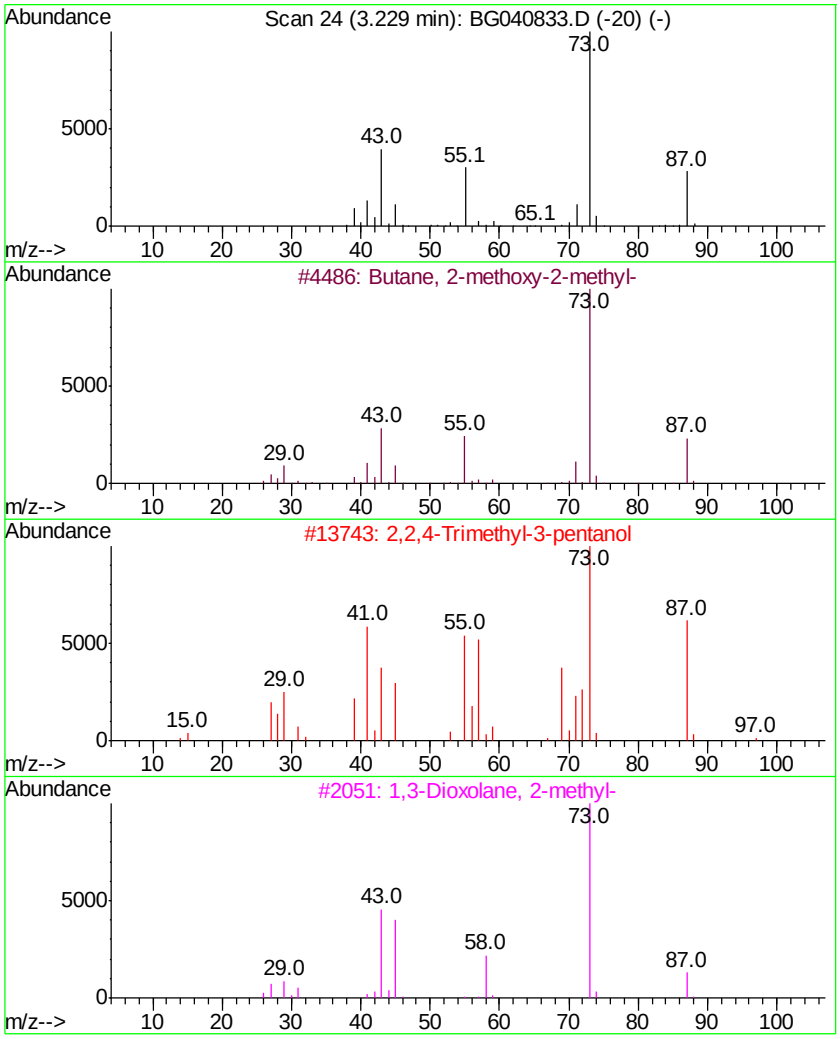
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

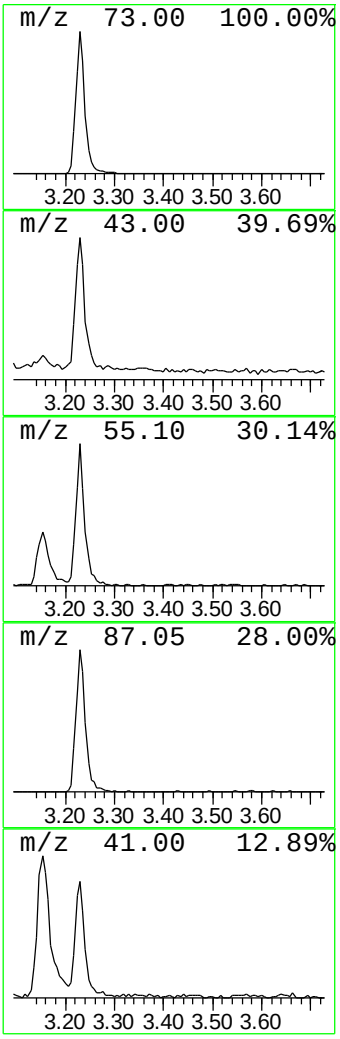
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	19.23 ng	350127	1,4-Dichlorobenzene-d4	8.14

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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS001-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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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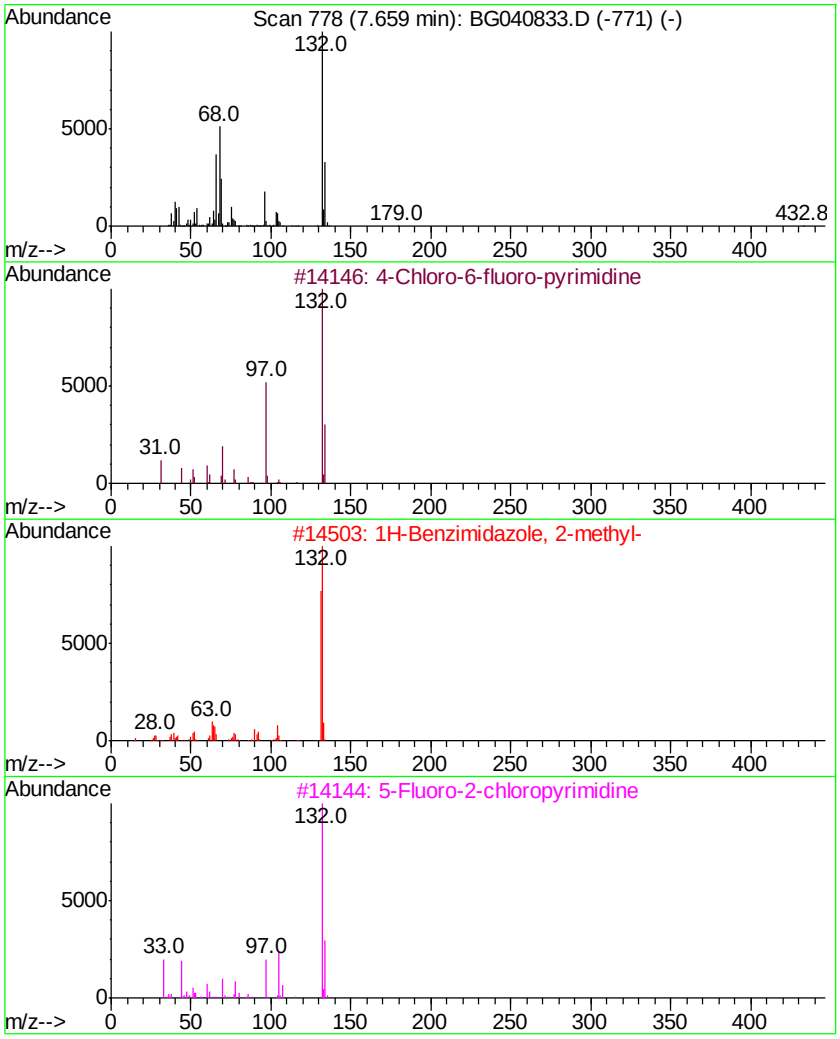
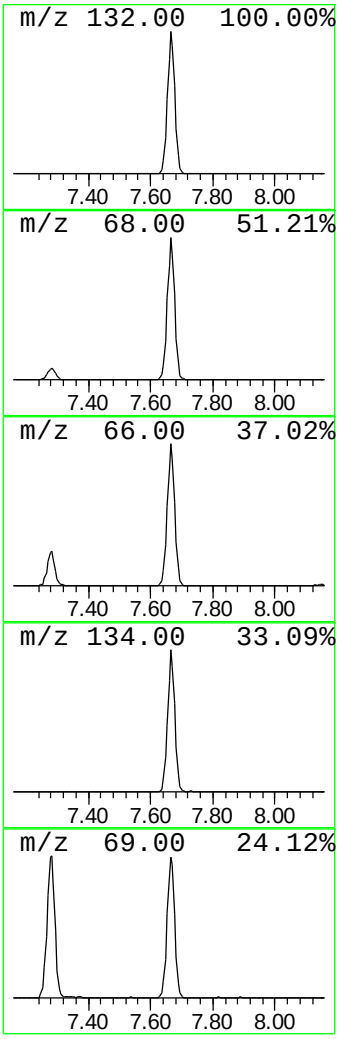
Peak Number 3 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	115.76 ng	2107370	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	14





Library Search Compound Report

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Sample : K2764-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS001-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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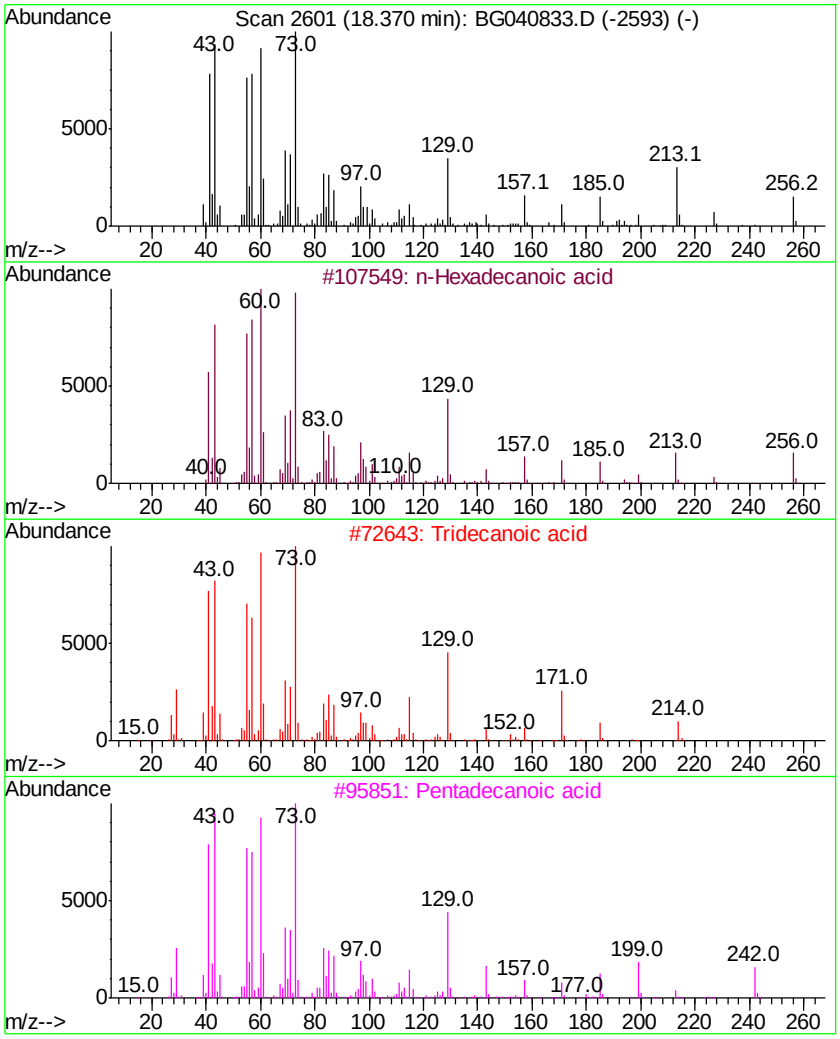
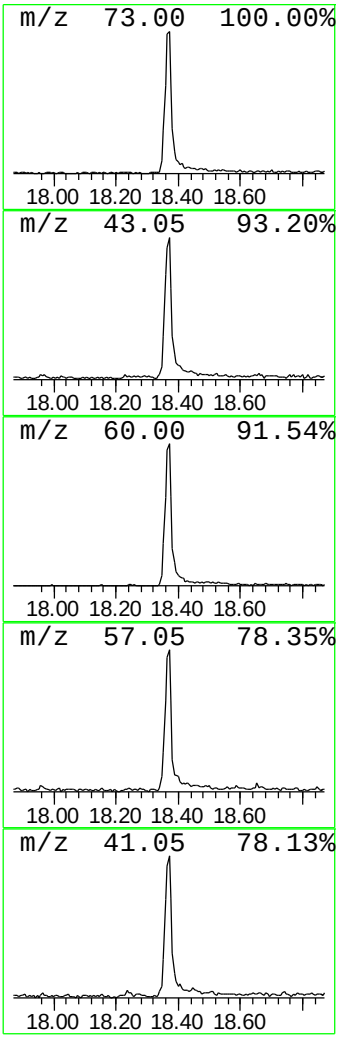
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	10.60 ng	593235	Phenanthrene-d10	17.51

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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	53





Library Search Compound Report

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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS001-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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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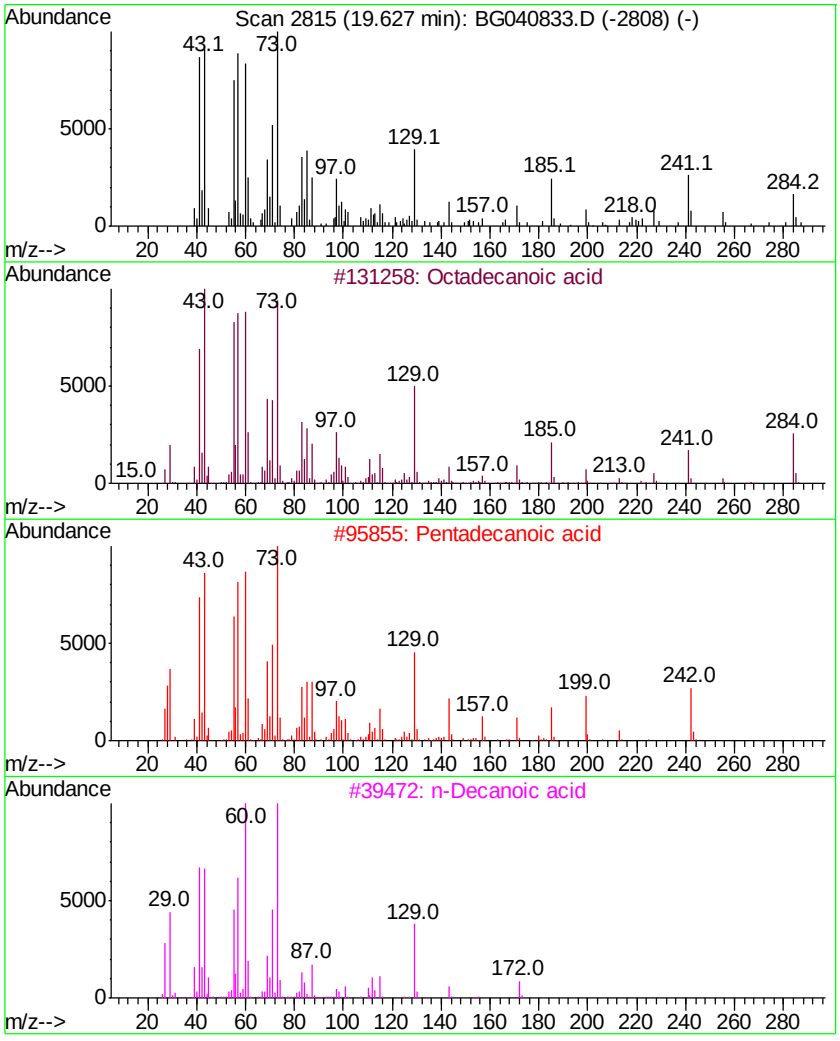
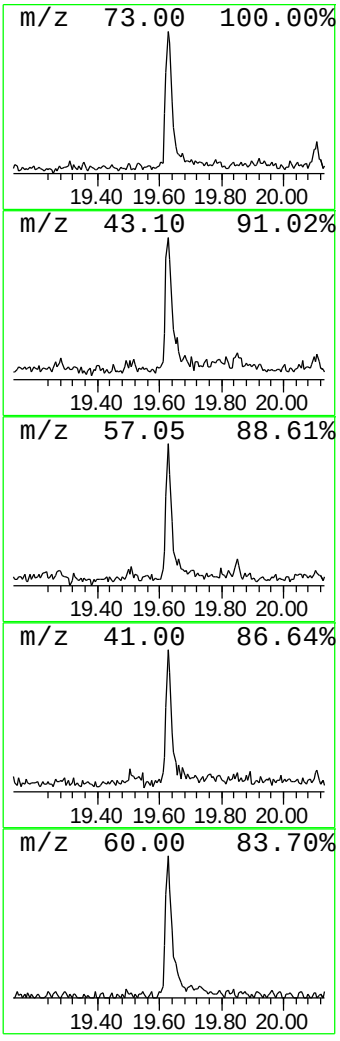
Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.63	3.52 ng	196819	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Decanoic acid	172	C10H20O2	000334-48-5	58
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	52





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050919\
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Sample : K2764-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS001-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

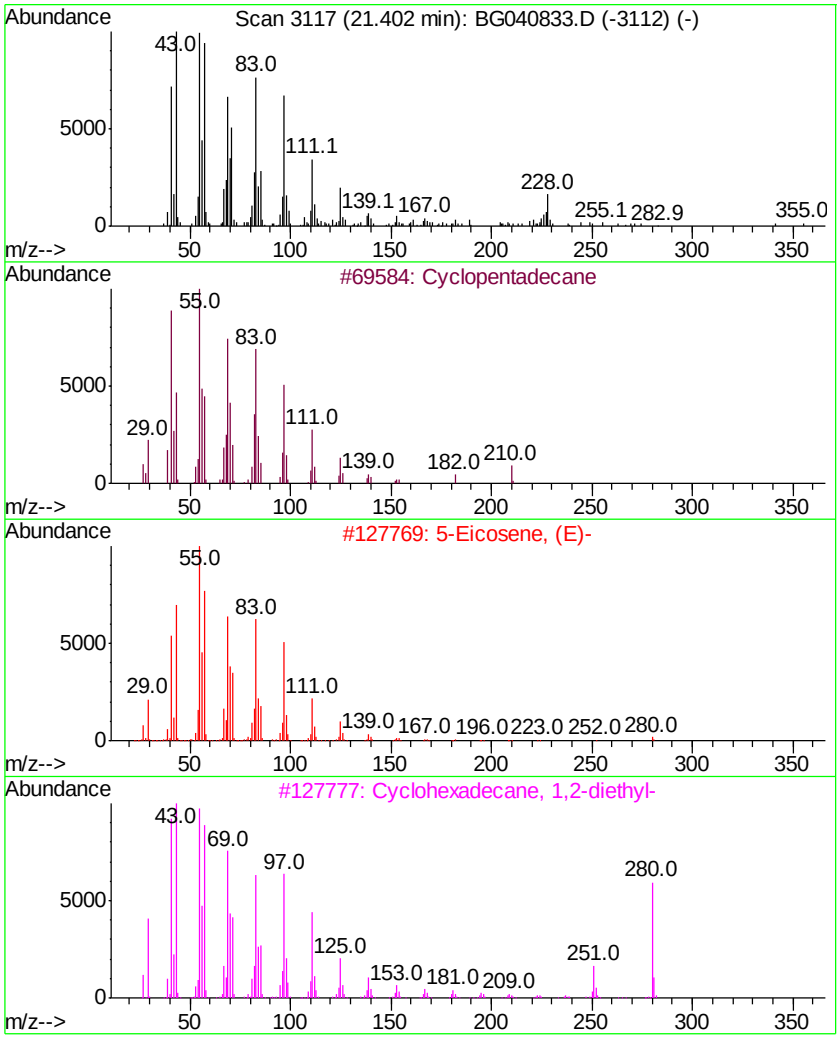
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

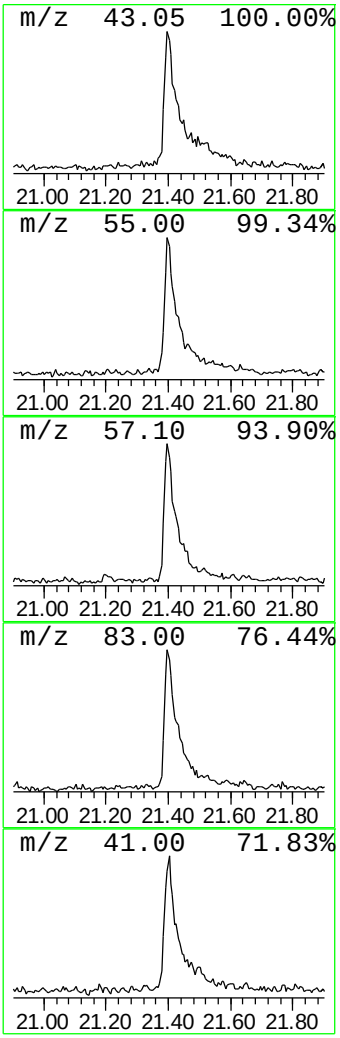
****

Peak Number 7 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	9.14 ng	568377	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	97
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	93
3	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	93
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
5	1-Docosene	308	C22H44	001599-67-3	92





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Misc :
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Instrument : BNA_G
ClientSampleId : P026-SS001-0612-01

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

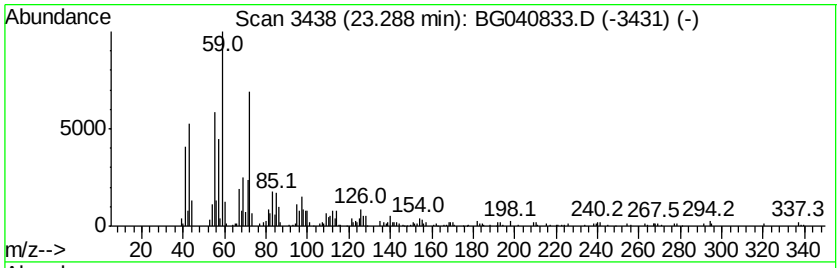
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

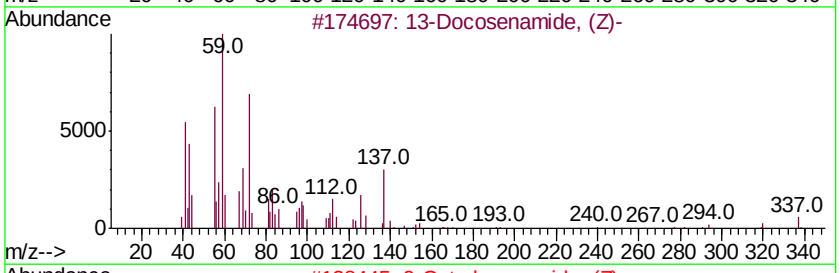
****

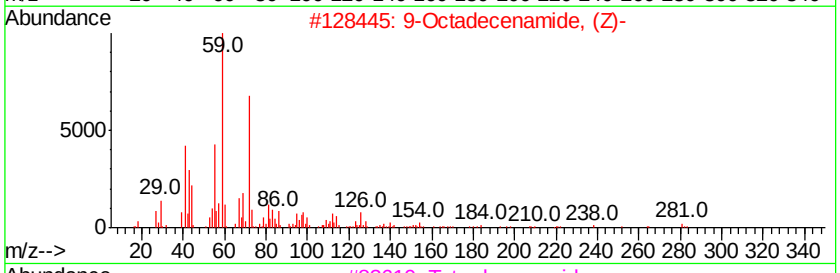
Peak Number 8 13-Docosenamide, (Z)- Concentration Rank 7

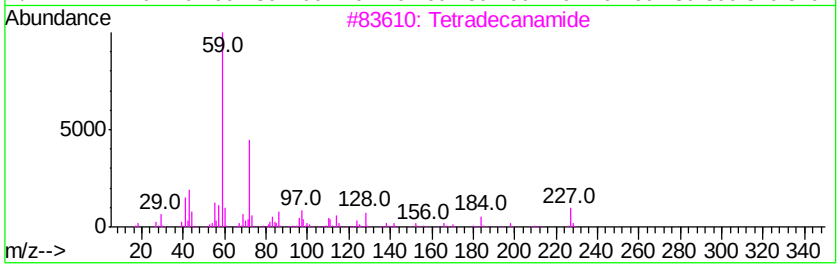
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.29	6.60 ng	410567	Chrysene-d12	21.80

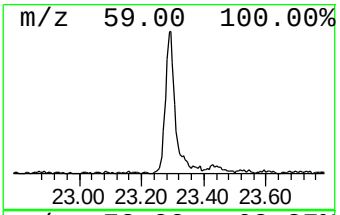
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	76
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74
3	Tetradecanamide	227	C14H29NO	000638-58-4	53
4	2-Propanone, 1-cyclohexyl-	140	C9H16O	000103-78-6	30
5	Cyclopentadecanone, 2-methyl-	238	C16H30O	052914-66-6	25

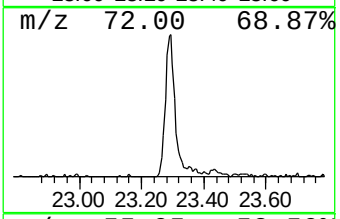


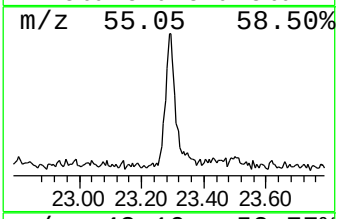


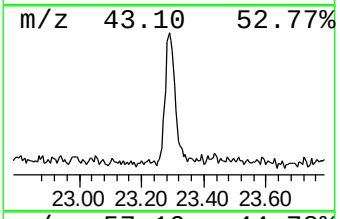


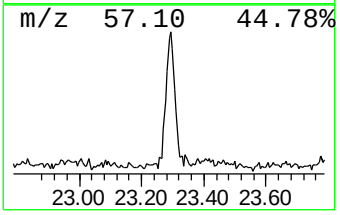












Tentatively Identified Compound (LSC) summary

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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...	3.23	19.2	ng	350127	1	8.14	364086	20.0
unknown7.66	7.66	115.8	ng	2107370	1	8.14	364086	20.0
n-Hexadecanoic acid	18.37	10.6	ng	593235	4	17.51	1119560	20.0
Octadecanoic acid	19.63	3.5	ng	196819	4	17.51	1119560	20.0
Cyclopentadecane	21.40	9.1	ng	568377	5	21.80	1244100	20.0
13-Docosenamide, ...	23.29	6.6	ng	410567	5	21.80	1244100	20.0