LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110819\
Data File : BG043571.D
Acq On : 8 Nov 2019 16:06
Operator : JU
Sample : PB124640BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124640BL

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-BG102119.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	3.166	8	13	22	rVB	85825	127000	4.08%	0.931%
2	5.105	338	343	352	rBV	102390	165285	5.30%	1.212%
3	5.604	421	428	440	rBV	476613	856428	27.48%	6.281%
4	7.208	693	701	718	rBV	522302	976120	31.32%	7.159%
5	7.549	751	759	775	rBV	538787	976946	31.35%	7.165%
6	8.001	829	836	845	rBV	89598	158110	5.07%	1.160%
7	8.330	883	892	902	rBV	424555	763276	24.49%	5.598%
8	9.171	1027	1035	1048	rBV	283509	572738	18.38%	4.200%
9	10.810	1306	1314	1324	rBV	90772	194345	6.24%	1.425%
10	13.260	1723	1731	1744	rBV	913170	1519898	48.77%	11.146%
11	14.635	1957	1965	1977	rBV	190176	324421	10.41%	2.379%
12	16.127	2212	2219	2235	rBV	868639	1493132	47.91%	10.950%
13	17.384	2425	2433	2444	rBV	260721	450002	14.44%	3.300%
14	18.278	2578	2585	2591	rBV2	34918	60182	1.93%	0.441%
15	19.993	2871	2877	2895	rBV	2328229	3116366	100.00%	22.854%
16	21.292	3094	3098	3107	rBV7	31866	87746	2.82%	0.644%
17	21.650	3152	3159	3167	rBV2	303163	553335	17.76%	4.058%
18	21.832	3185	3190	3196	rVB2	25980	38069	1.22%	0.279%
19	22.431	3287	3292	3297	rBV2	28262	47157	1.51%	0.346%
20	23.113	3404	3408	3414	rVB2	29847	50749	1.63%	0.372%
21	23.307	3433	3441	3448	rVB	196670	374650	12.02%	2.748%
22	23.912	3538	3544	3553	rVB4	32092	74231	2.38%	0.544%
23	24.840	3692	3702	3717	rBV2	204362	616009	19.77%	4.518%
24	25.951	3888	3891	3901	rVB5	18263	39486	1.27%	0.290%

Sum of corrected areas: 13635681

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110819\
Data File : BG043571.D
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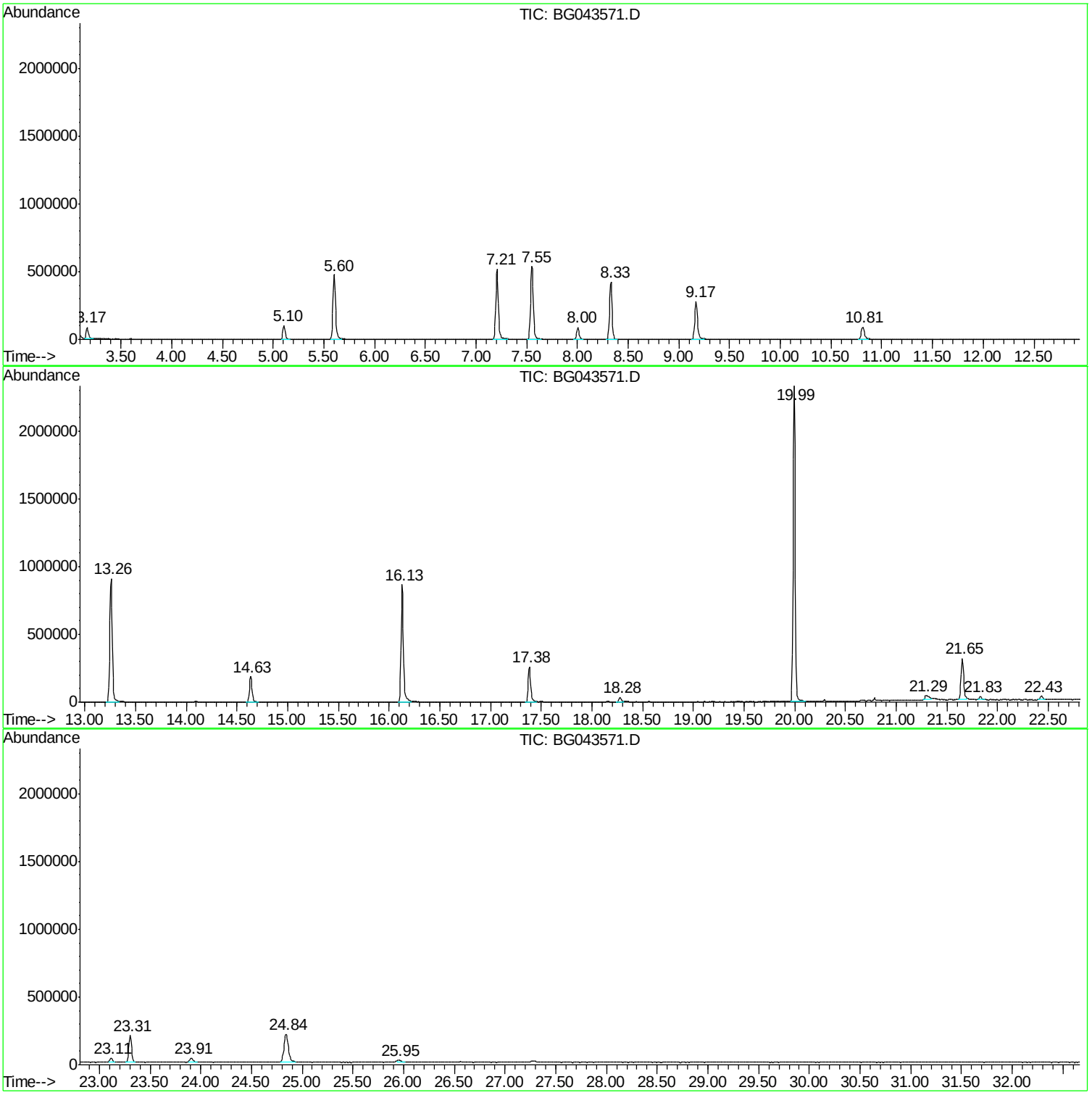
Sample : PB124640BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124640BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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\BG110819\
Data File : BG043571.D
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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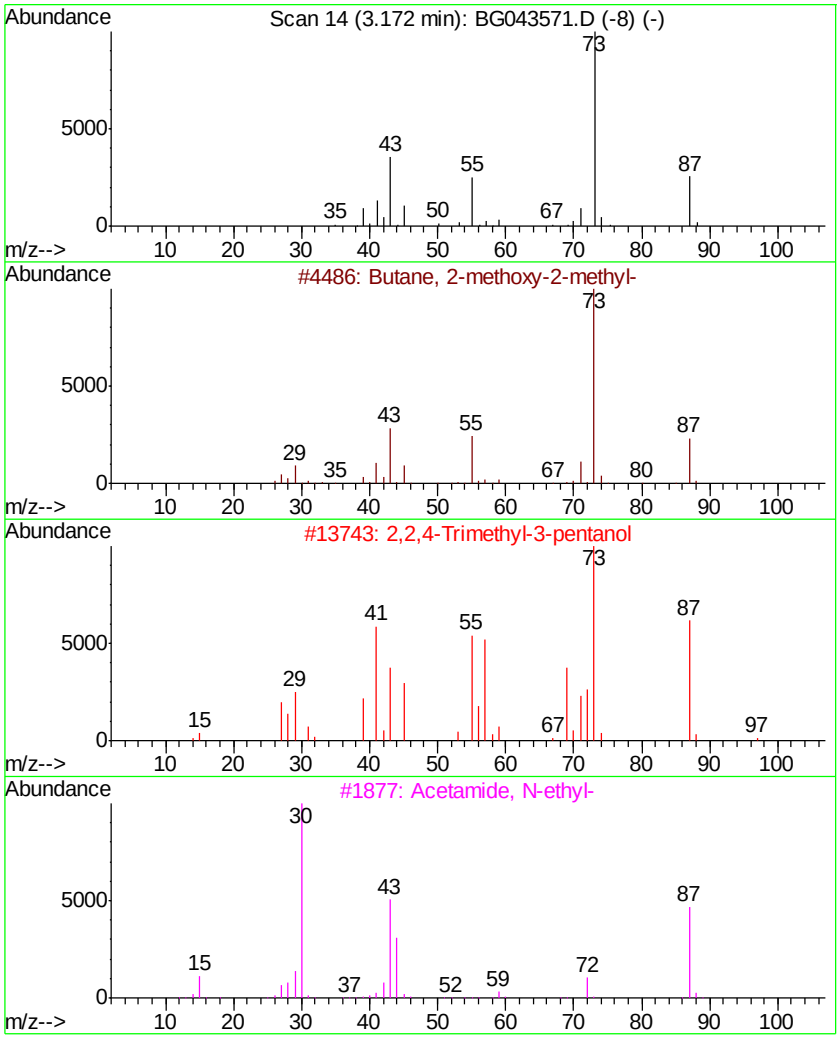
TIC Integration Parameters: LSCINT.P

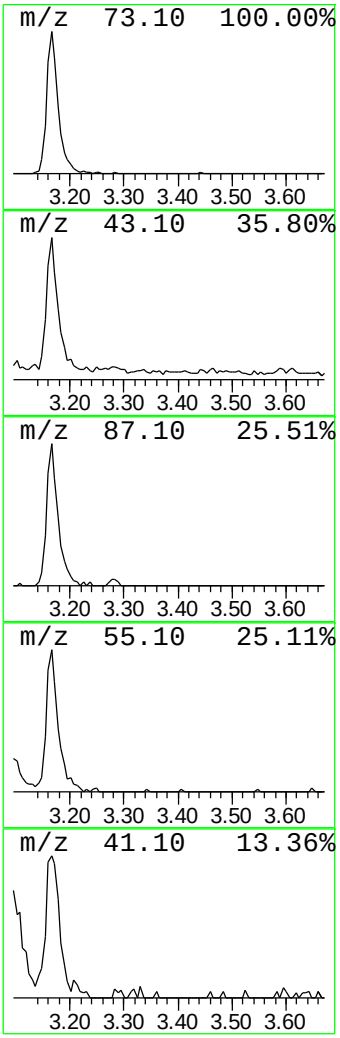
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	16.06 ng	127000	1,4-Dichlorobenzene-d4	8.00

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	38
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9





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Data File : BG043571.D
Acq On : 8 Nov 2019 16:06
Operator : JU
Sample : PB124640BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124640BL

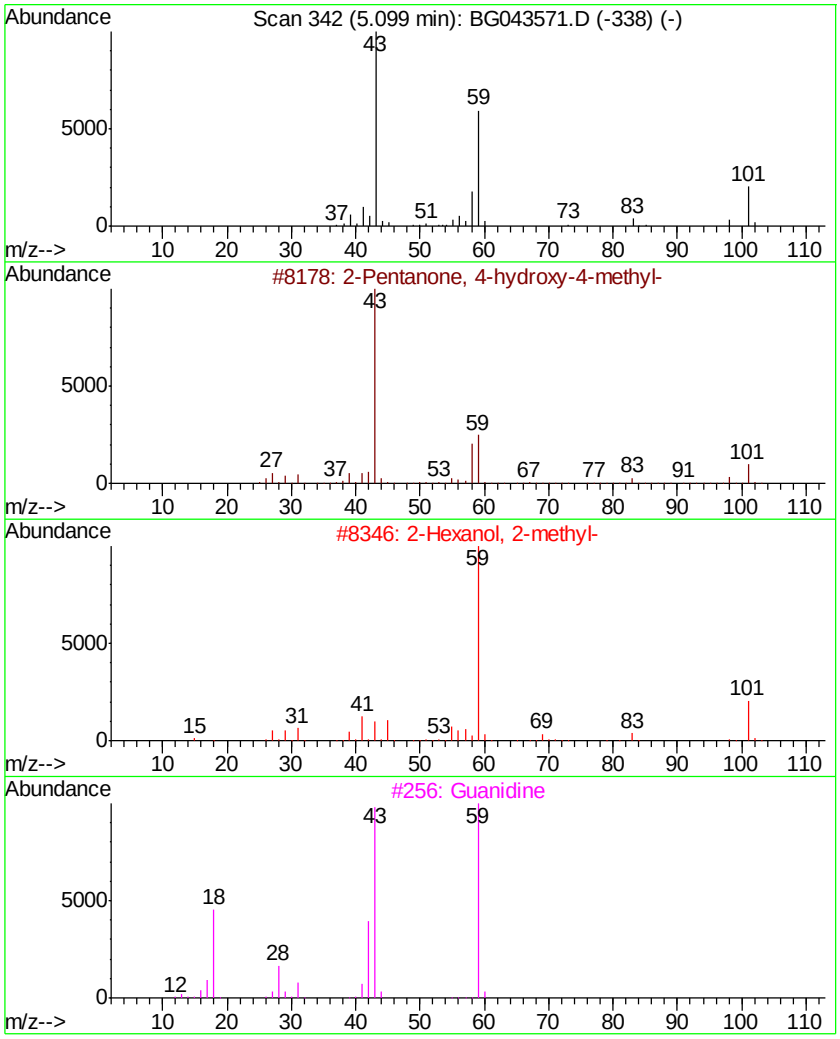
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

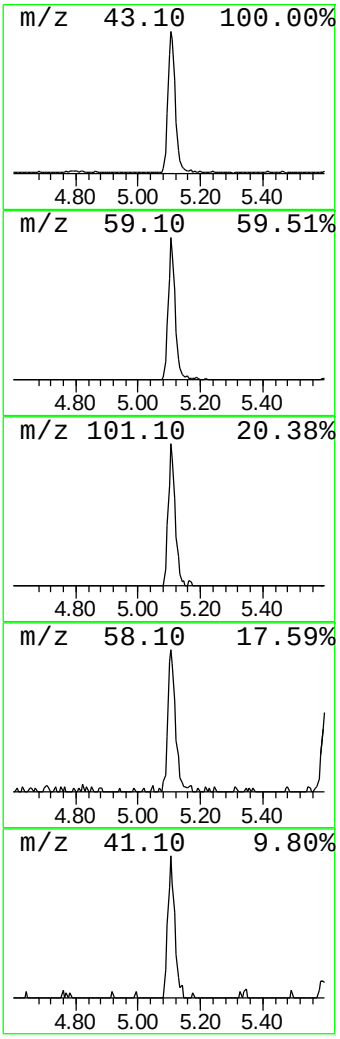
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	20.91 ng	165285	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	53
3	Guanidine	59	CH5N3	000113-00-8	43
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





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Data File : BG043571.D
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Sample : PB124640BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124640BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

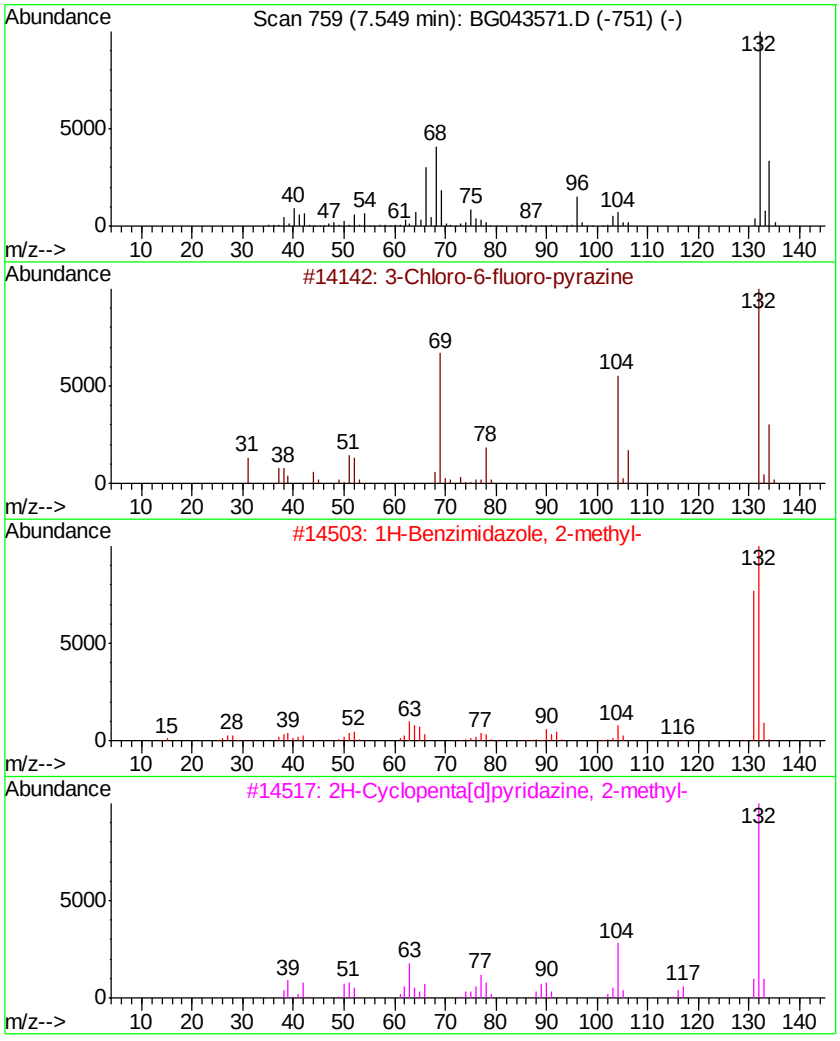
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

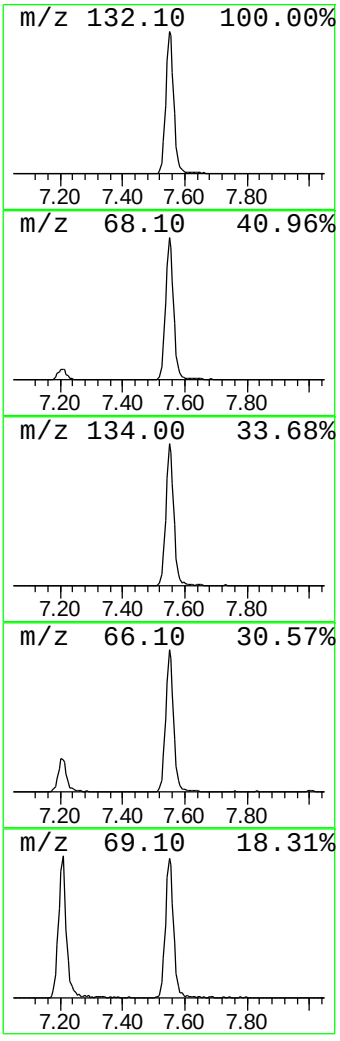
****

Peak Number 3 unknown7.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	123.58 ng	976946	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12
4	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110819\
Data File : BG043571.D
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Operator : JU
Sample : PB124640BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124640BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

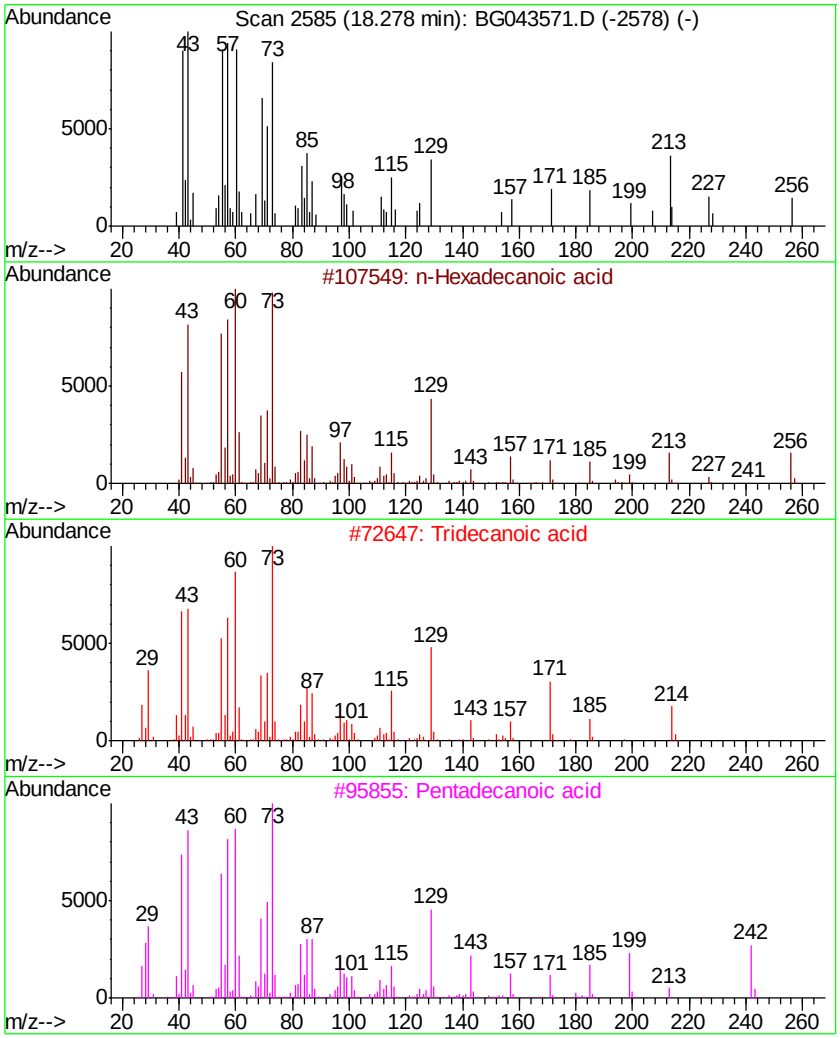
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

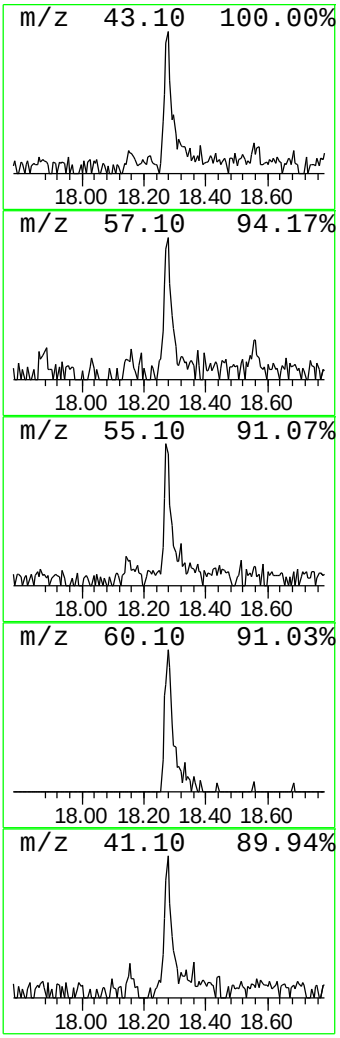
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	2.67 ng	60182	Phenanthrene-d10	17.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Tridecanoic acid	214	C13H26O2	000638-53-9	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110819\
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Acq On : 8 Nov 2019 16:06
Operator : JU
Sample : PB124640BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124640BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

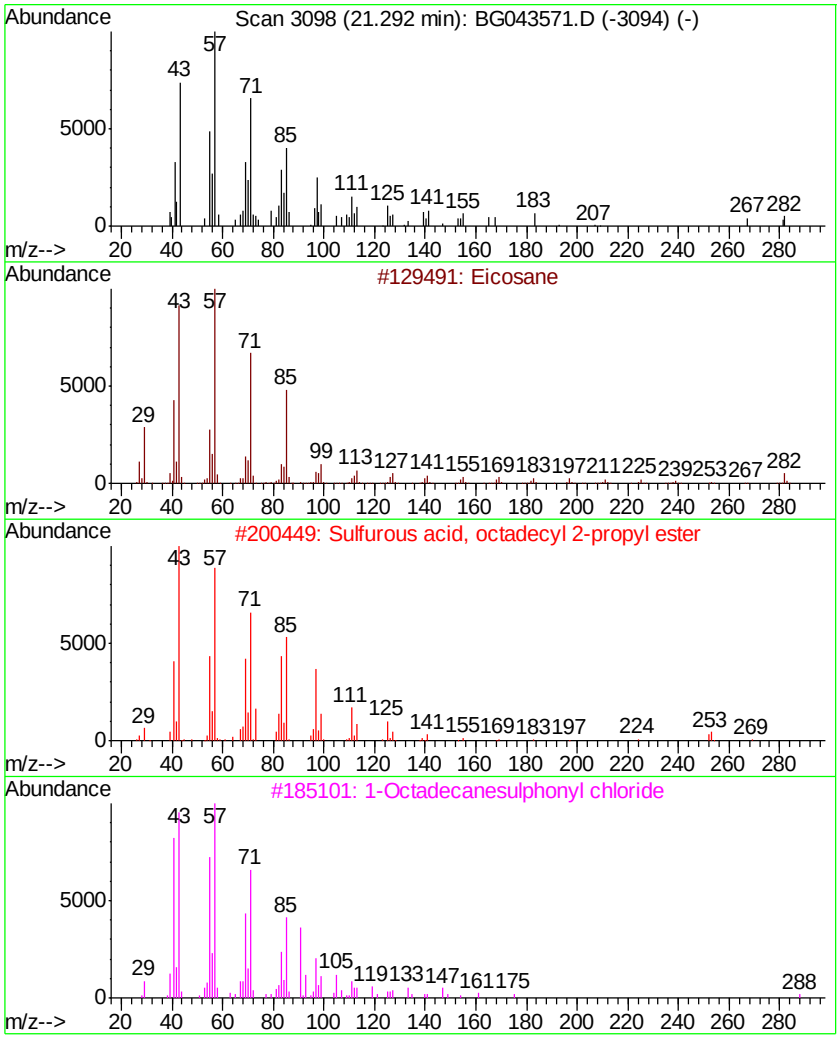
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

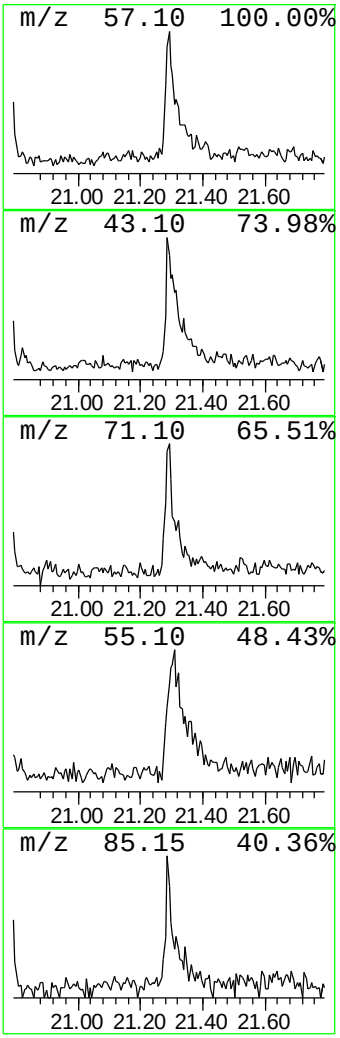
****

Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	3.17 ng	87746	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
3	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	83
4	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	80
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	52





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Sample : PB124640BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124640BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

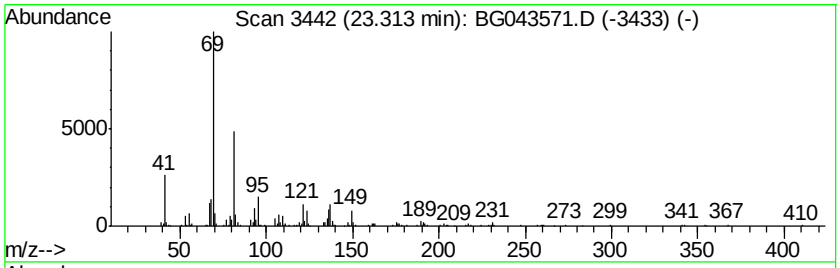
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

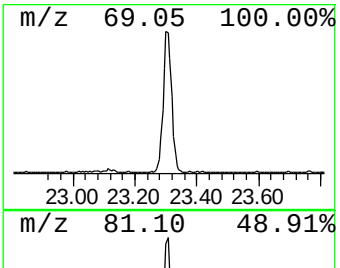
****

Peak Number 7 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.31	12.16 ng	374650	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
4	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72
5	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64





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Instrument : BNA_G
ClientSampleId : PB124640BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

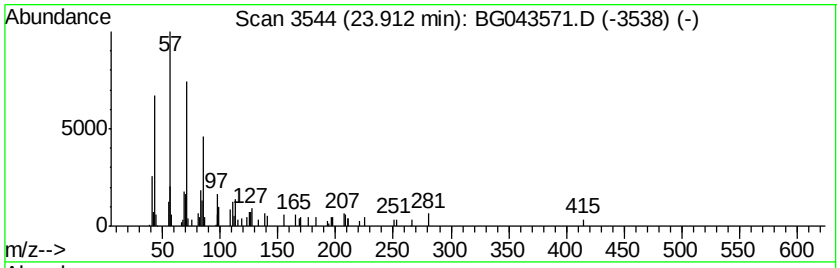
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

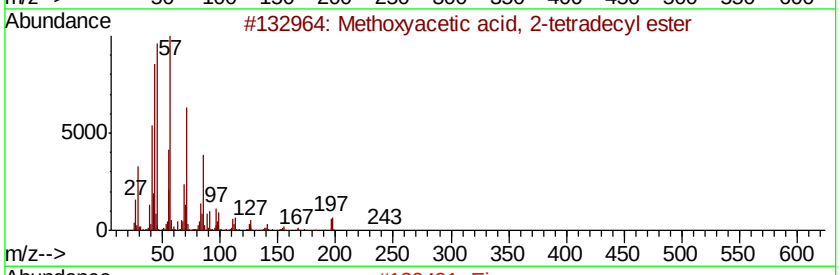
****

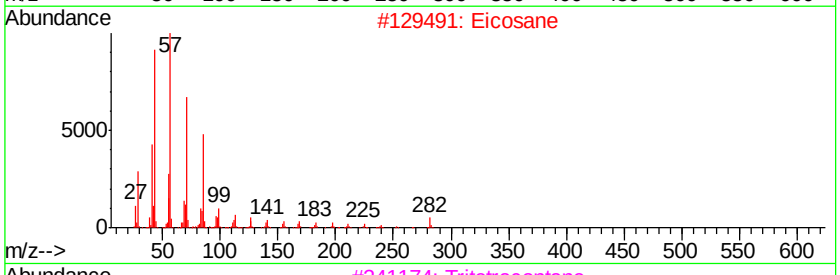
Peak Number 8 Methoxyacetic acid, 2-tetra... Concentration Rank 8

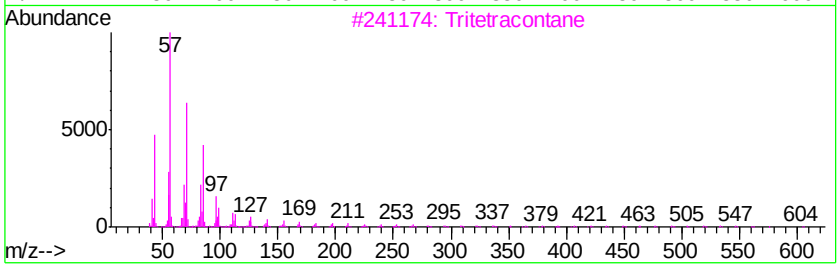
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.91	2.41 ng	74231	Perylene-d12	24.84

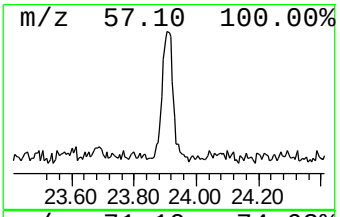
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	86
2	Eicosane	282	C20H42	000112-95-8	83
3	Tritetracontane	605	C43H88	007098-21-7	80
4	Hentriacontane	437	C31H64	000630-04-6	80
5	Tetracosane	338	C24H50	000646-31-1	80

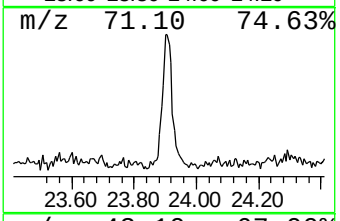


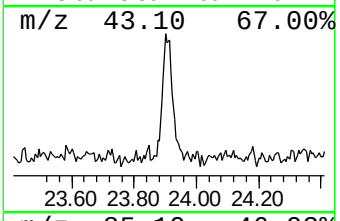


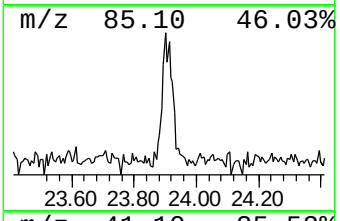


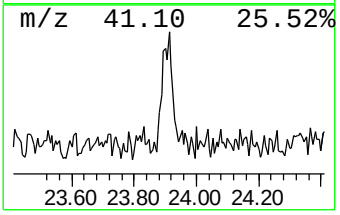












Tentatively Identified Compound (LSC) summary

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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...	3.17	16.1	ng	127000	1	8.00	158110	20.0
2-Pentanone, 4-hy...	5.10	20.9	ng	165285	1	8.00	158110	20.0
unknown7.55	7.55	123.6	ng	976946	1	8.00	158110	20.0
n-Hexadecanoic acid	18.28	2.7	ng	60182	4	17.38	450002	20.0
Eicosane	21.29	3.2	ng	87746	5	21.65	553335	20.0
Squalene	23.31	12.2	ng	374650	6	24.84	616009	20.0
Methoxyacetic aci...	23.91	2.4	ng	74231	6	24.84	616009	20.0