LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043470.D
Acq On : 1 Nov 2019 17:57
Operator : JU
Sample : K5602-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190938-COMPOSITE-A

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	3.182	12	16	26	rVB	93448	153746	6.27%	1.174%
2	5.115	337	345	356	rBV	90233	152852	6.23%	1.167%
3	5.596	420	427	440	rBV	425477	775712	31.62%	5.923%
4	7.194	689	699	713	rBV	482831	908161	37.02%	6.934%
5	7.553	752	760	783	rBV	507556	909353	37.07%	6.943%
6	8.011	831	838	850	rBV	140241	249463	10.17%	1.905%
7	8.334	885	893	908	rBV	357376	646088	26.34%	4.933%
8	9.175	1028	1036	1055	rBV2	244962	519031	21.16%	3.963%
9	10.820	1306	1316	1328	rBV	152152	318797	13.00%	2.434%
10	13.264	1724	1732	1750	rBV	741060	1285132	52.39%	9.812%
11	14.092	1867	1873	1884	rBV	72450	138202	5.63%	1.055%
12	14.639	1960	1966	1981	rBV2	304393	519770	21.19%	3.969%
13	16.131	2212	2220	2236	rBV	759770	1292611	52.69%	9.869%
14	17.388	2427	2434	2445	rBV	387615	669895	27.31%	5.115%
15	17.506	2449	2454	2464	rVB3	24188	42390	1.73%	0.324%
16	18.276	2581	2585	2594	rBV4	21546	38610	1.57%	0.295%
17	19.997	2872	2878	2895	rBV	1775445	2453170	100.00%	18.731%
18	21.290	3093	3098	3107	rBV3	81562	154550	6.30%	1.180%
19	21.654	3153	3160	3172	rBV	457278	848833	34.60%	6.481%
20	22.441	3290	3294	3298	rBV7	14884	25109	1.02%	0.192%
21	23.123	3404	3410	3416	rBV5	20873	44433	1.81%	0.339%
22	23.916	3541	3545	3556	rVB4	25223	50803	2.07%	0.388%
23	24.844	3693	3703	3714	rBV2	295575	900457	36.71%	6.875%

Sum of corrected areas: 13097168

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Misc :
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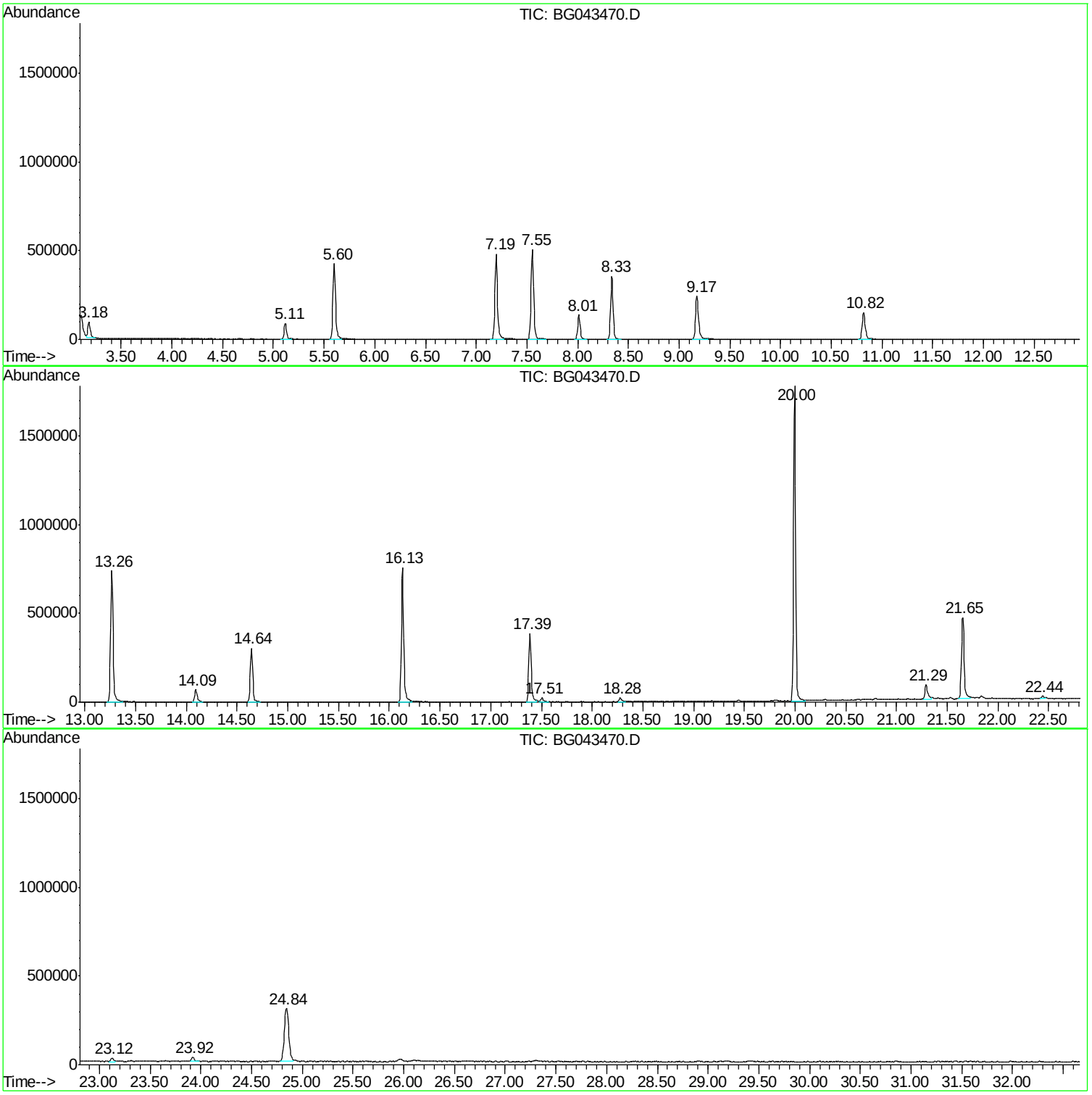
Instrument :
BNA_G
ClientSampleId :
20190938-COMPOSITE-A

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



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Data File : BG043470.D
Acq On : 1 Nov 2019 17:57
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Misc :
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Instrument : BNA_G
ClientSampleId : 20190938-COMPOSITE-A

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

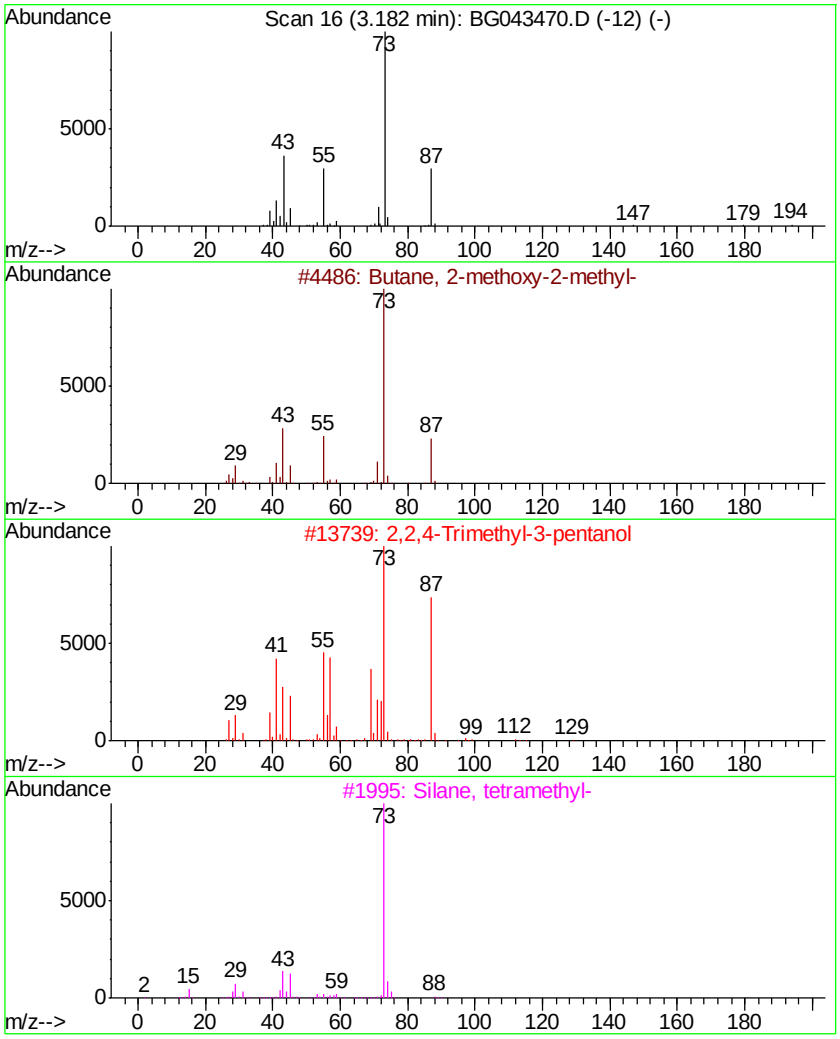
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

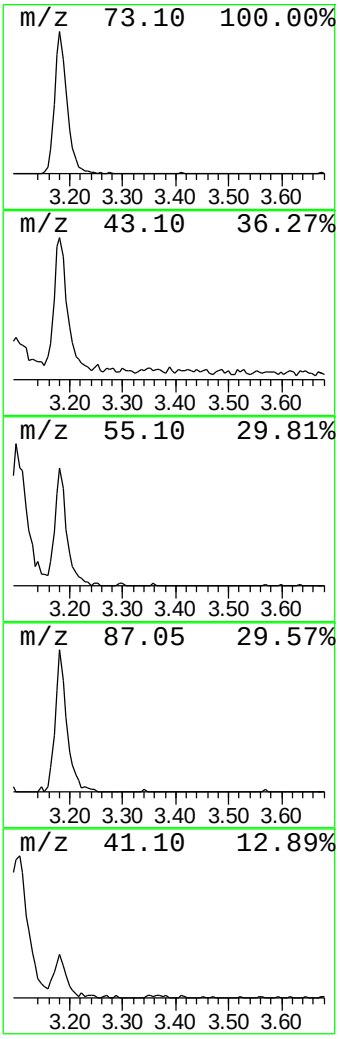
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	12.33 ng	153746	1,4-Dichlorobenzene-d4	8.01

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	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Acq On : 1 Nov 2019 17:57
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Sample : K5602-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190938-COMPOSITE-A

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

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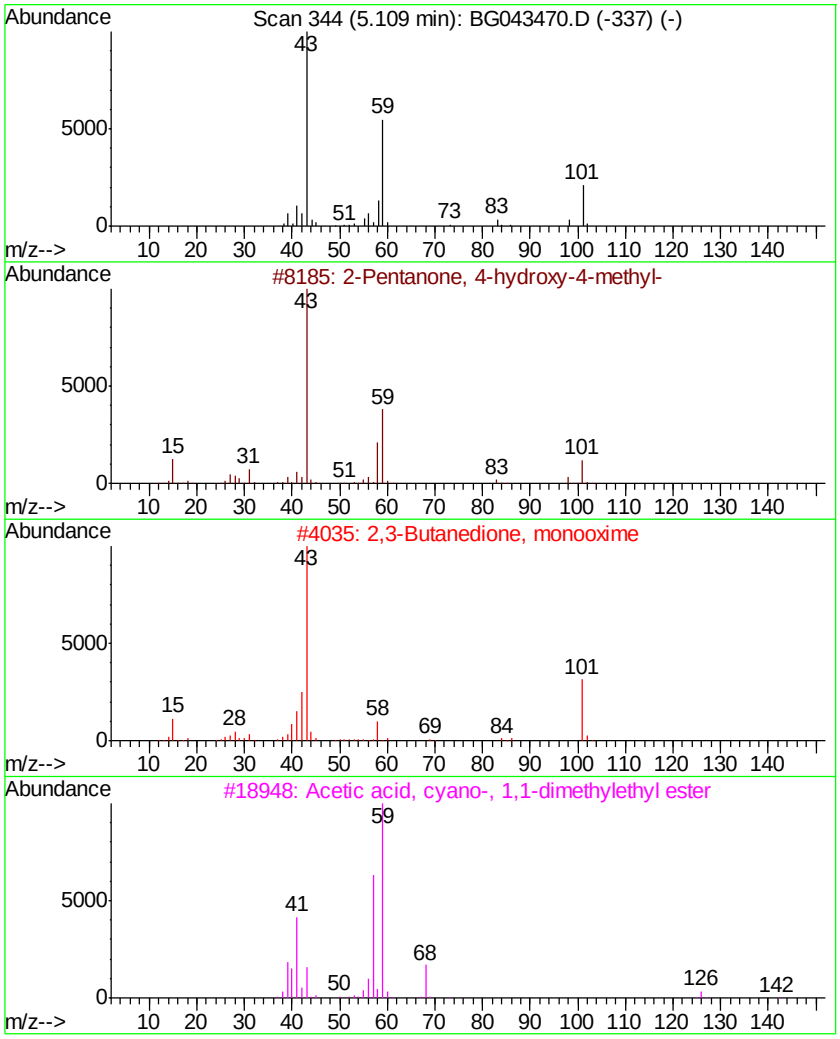
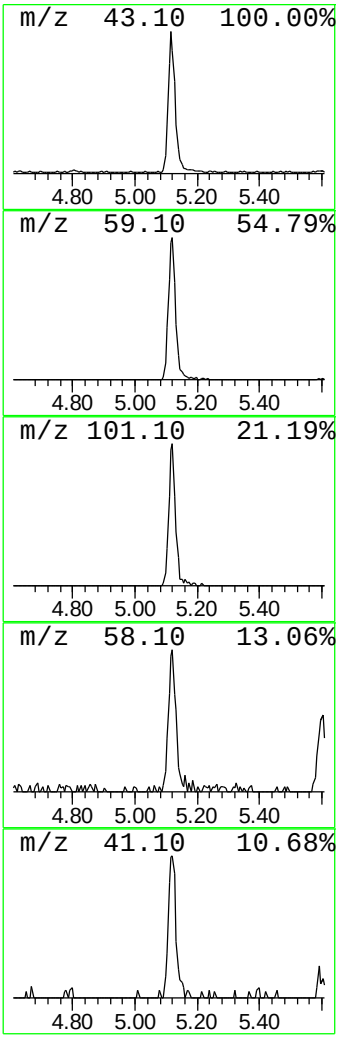
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	12.25 ng	152852	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

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Data File : BG043470.D
Acq On : 1 Nov 2019 17:57
Operator : JU
Sample : K5602-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190938-COMPOSITE-A

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

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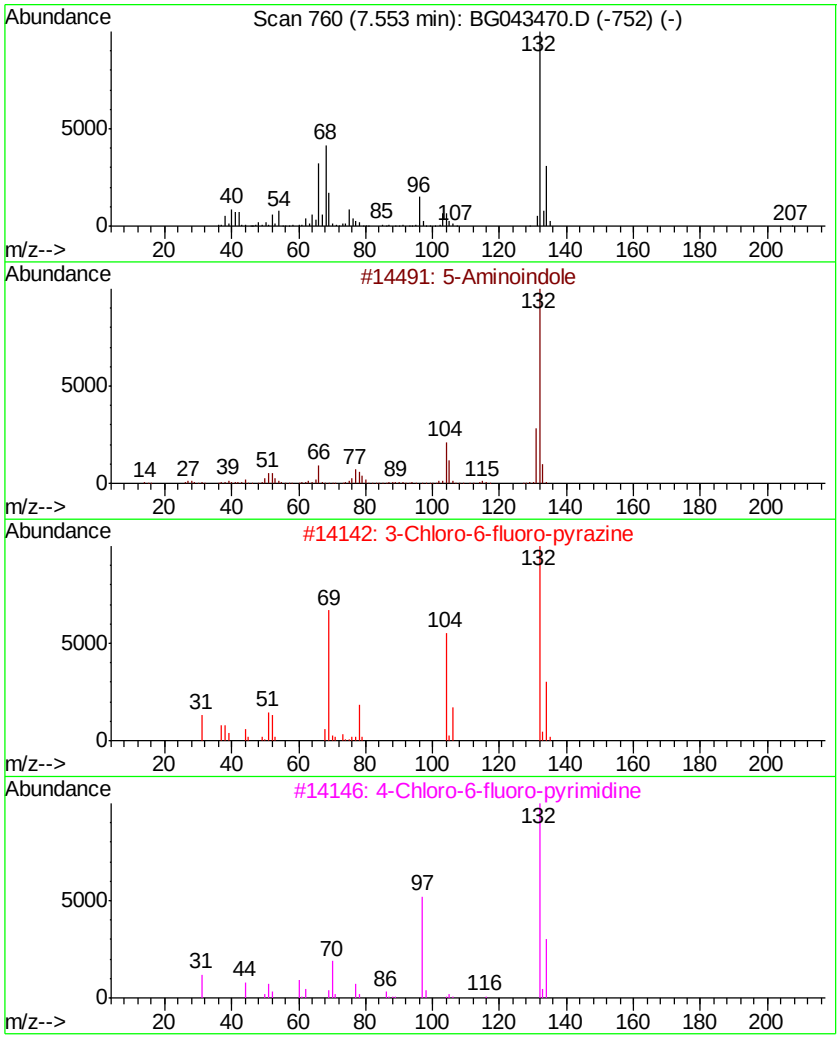
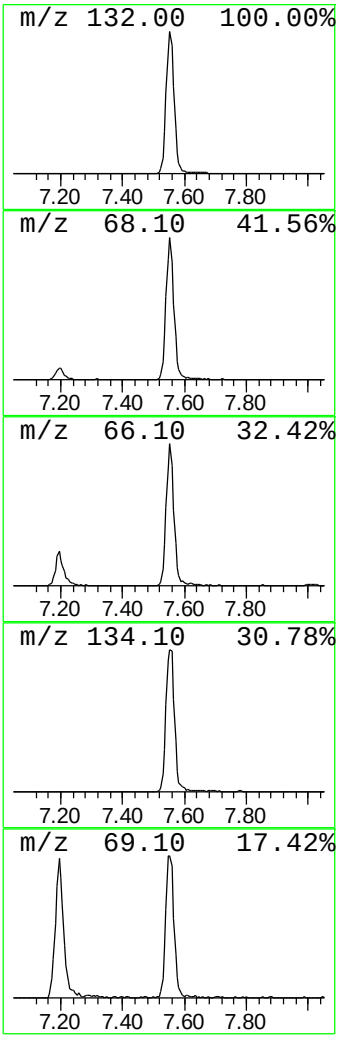
Peak Number 3 unknown7.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	72.90 ng	909353	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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Operator : JU
Sample : K5602-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190938-COMPOSITE-A

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

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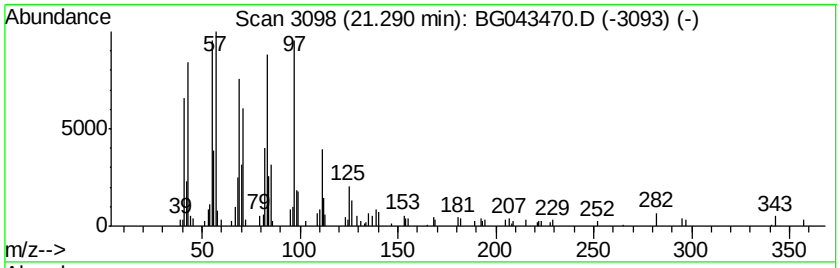
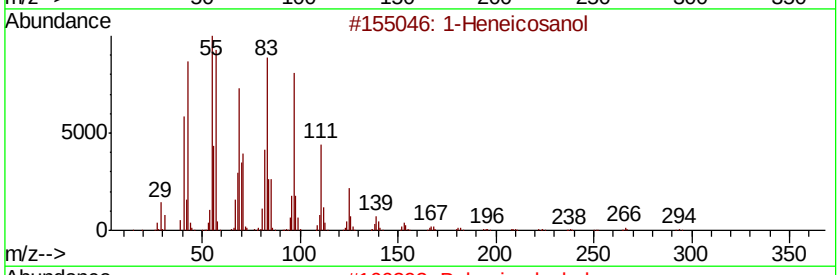
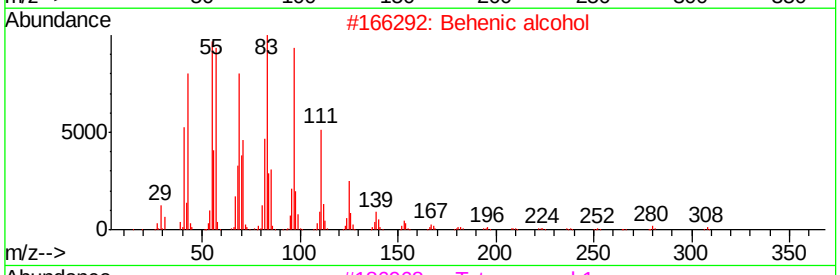
Peak Number 5 1-Heneicosanol Concentration Rank 5

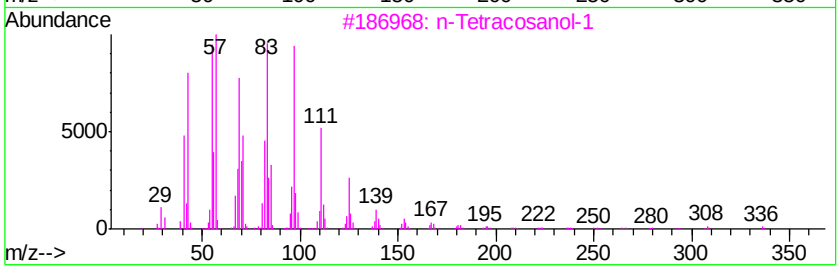
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	3.64 ng	154550	Chrysene-d12	21.65

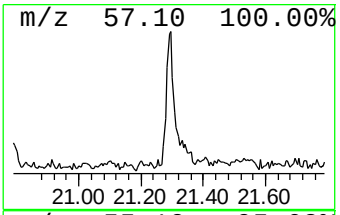
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	91
5	17-Pentatriacontene	491	C35H70	006971-40-0	91

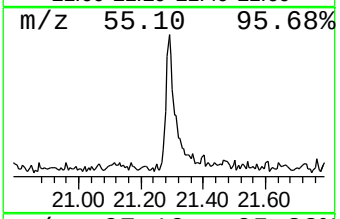


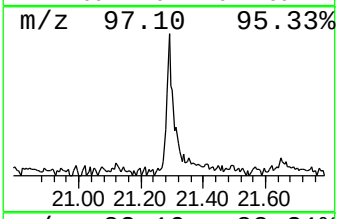


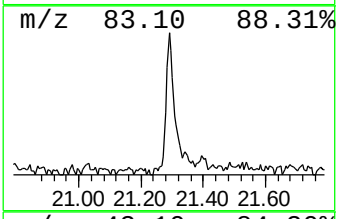


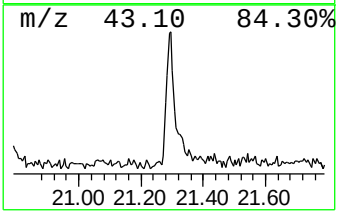












Tentatively Identified Compound (LSC) summary

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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...	3.18	12.3	ng	153746	1	8.01	249463	20.0
2-Pentanone, 4-hy...	5.11	12.3	ng	152852	1	8.01	249463	20.0
unknown7.55	7.55	72.9	ng	909353	1	8.01	249463	20.0
1-Heneicosanol	21.29	3.6	ng	154550	5	21.65	848833	20.0