LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111519\
Data File : BG043661.D
Acq On : 15 Nov 2019 21:50
Operator : JU
Sample : PB124780BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124780BL

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	3.176	9	15	29	rVB2	360826	681293	27.58%	6.490%
2	3.464	60	64	70	rBV	34778	42194	1.71%	0.402%
3	5.097	338	342	353	rVB	80657	123277	4.99%	1.174%
4	5.585	418	425	437	rBV	348729	607933	24.61%	5.791%
5	7.189	690	698	716	rBV	342285	665815	26.96%	6.342%
6	7.536	749	757	770	rBV	372502	682457	27.63%	6.501%
7	7.988	825	834	844	rBV2	66818	121409	4.92%	1.157%
8	8.317	883	890	901	rBV	274252	482936	19.55%	4.600%
9	9.157	1026	1033	1049	rBV	177765	380773	15.42%	3.627%
10	10.797	1305	1312	1324	rBV	59850	142282	5.76%	1.355%
11	13.247	1722	1729	1744	rBV	569226	1000920	40.52%	9.534%
12	14.627	1956	1964	1975	rBV	127078	242027	9.80%	2.305%
13	16.114	2211	2217	2235	rBV	462931	937178	37.94%	8.927%
14	17.371	2425	2431	2445	rBV	183132	343319	13.90%	3.270%
15	19.610	2806	2812	2826	rBV	97400	257391	10.42%	2.452%
16	19.980	2869	2875	2892	rBV	1872202	2469970	100.00%	23.528%
17	20.238	2913	2919	2931	rBV	33936	69842	2.83%	0.665%
18	20.720	2996	3001	3009	rBV2	64334	96528	3.91%	0.919%
19	21.637	3150	3157	3171	rBV	246183	491450	19.90%	4.681%
20	23.088	3399	3404	3411	rVB4	15900	31709	1.28%	0.302%
21	23.887	3534	3540	3546	rVB7	14507	30629	1.24%	0.292%
22	24.815	3686	3698	3717	rBV2	172712	562548	22.78%	5.359%
23	25.914	3878	3885	3895	rBV7	11496	34076	1.38%	0.325%

Sum of corrected areas: 10497956

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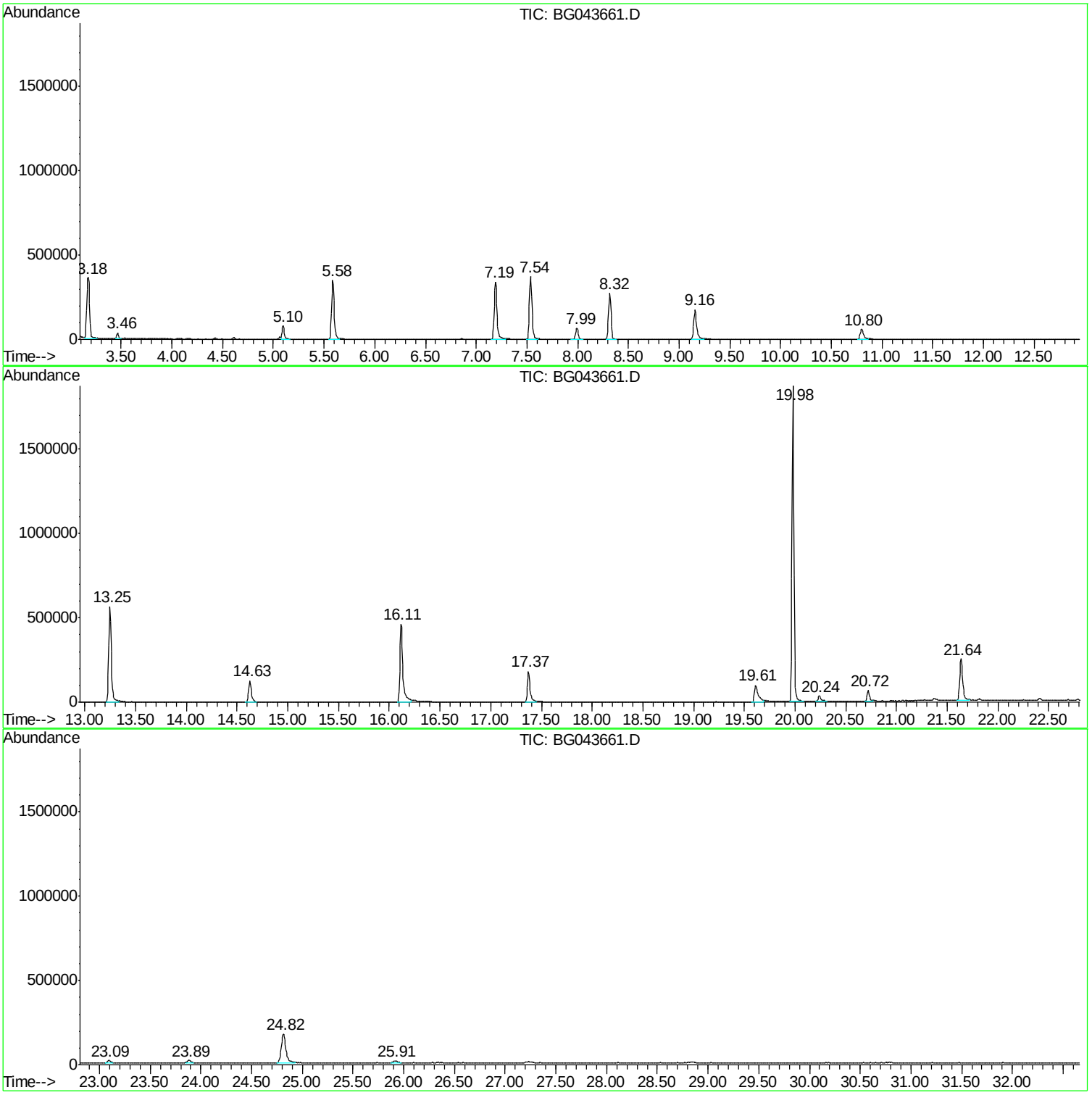
Instrument : BNA_G
ClientSampleId : PB124780BL

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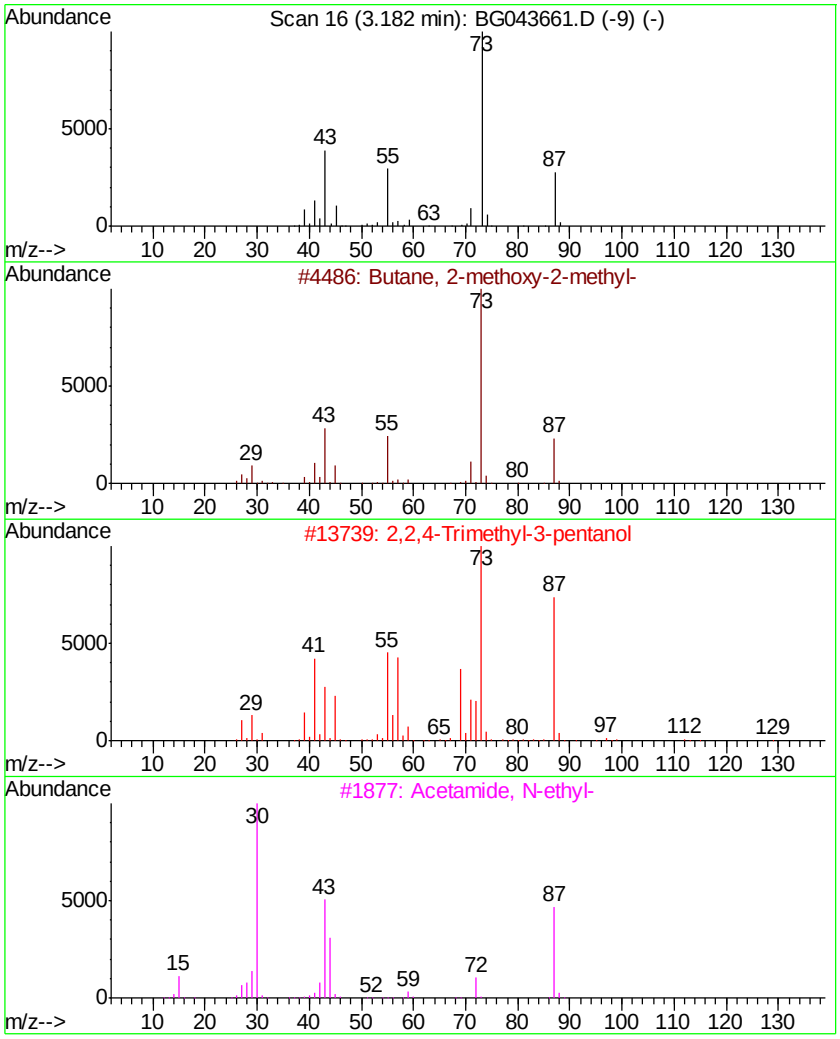
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

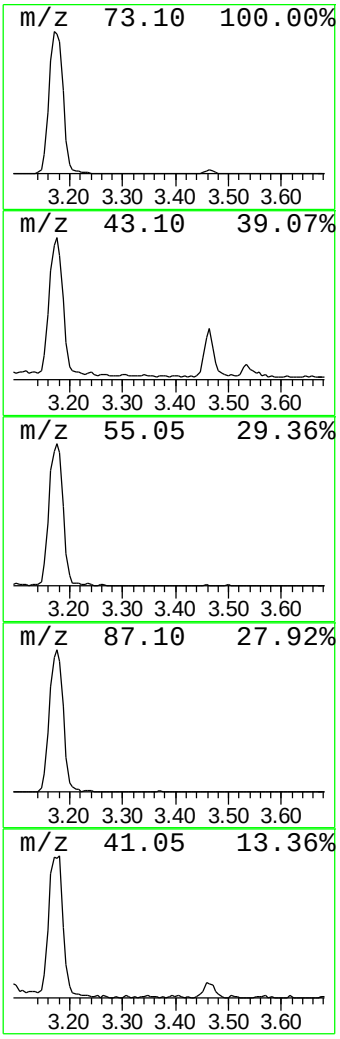
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	112.23 ng	681293	1,4-Dichlorobenzene-d4	7.99

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	38
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	1,4-Butanediamine	88	C4H12N2	000110-60-1	9





Library Search Compound Report

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Data File : BG043661.D
Acq On : 15 Nov 2019 21:50
Operator : JU
Sample : PB124780BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124780BL

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

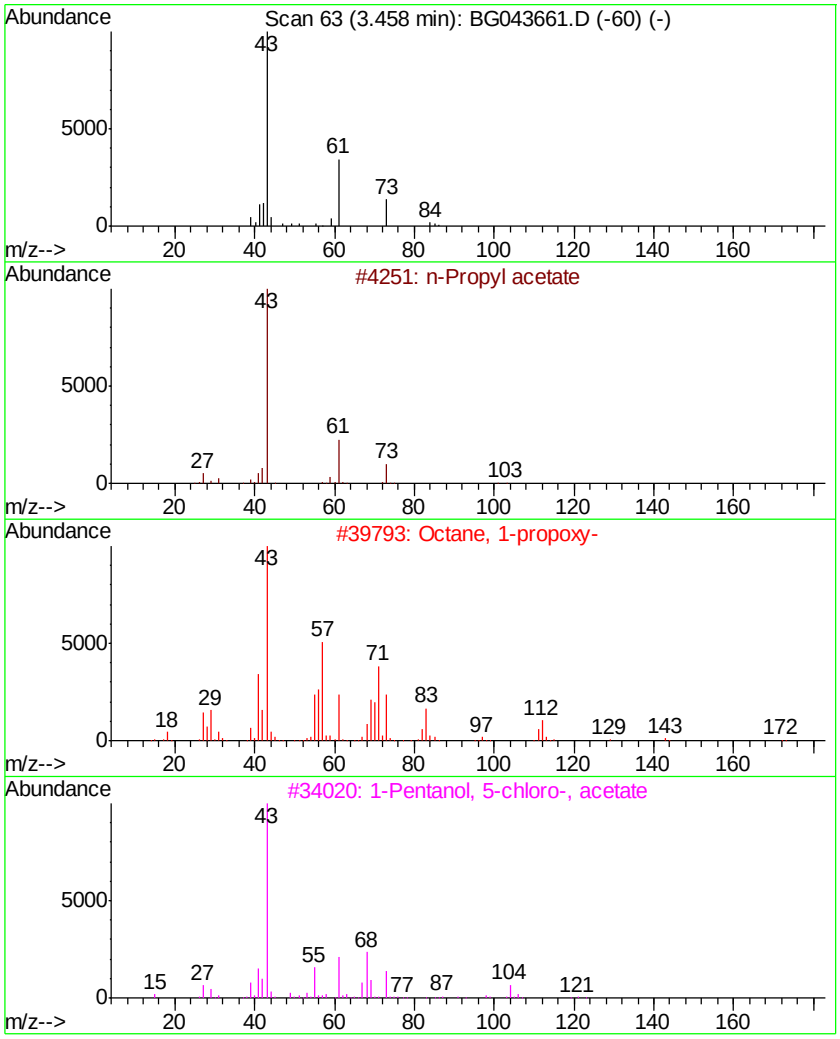
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

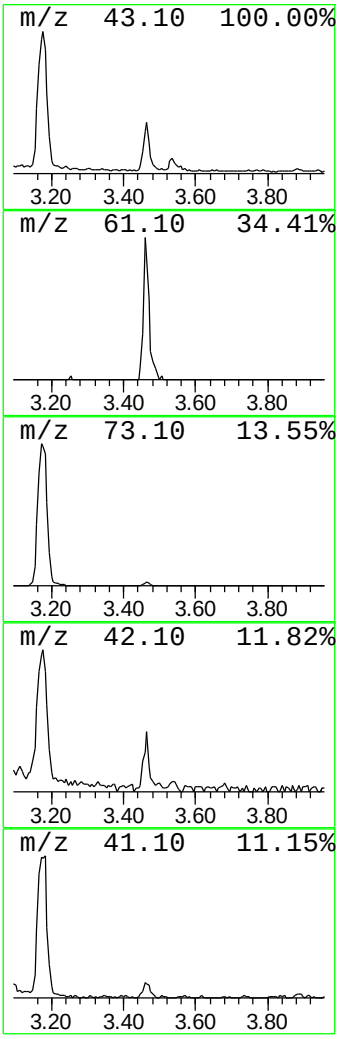
****

Peak Number 2 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.46	6.95 ng	42194	1,4-Dichlorobenzene-d4	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	56
2	Octane, 1-propoxy-	172	C11H24O	029379-41-7	9
3	1-Pentanol, 5-chloro-, acetate	164	C7H13ClO2	020395-28-2	9
4	Pentanoic acid, 3-hydroxy-4-meth...	146	C7H14O3	065596-31-8	9
5	Ethanamine, N-ethyl-	73	C4H11N	000109-89-7	7





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Data File : BG043661.D
Acq On : 15 Nov 2019 21:50
Operator : JU
Sample : PB124780BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124780BL

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

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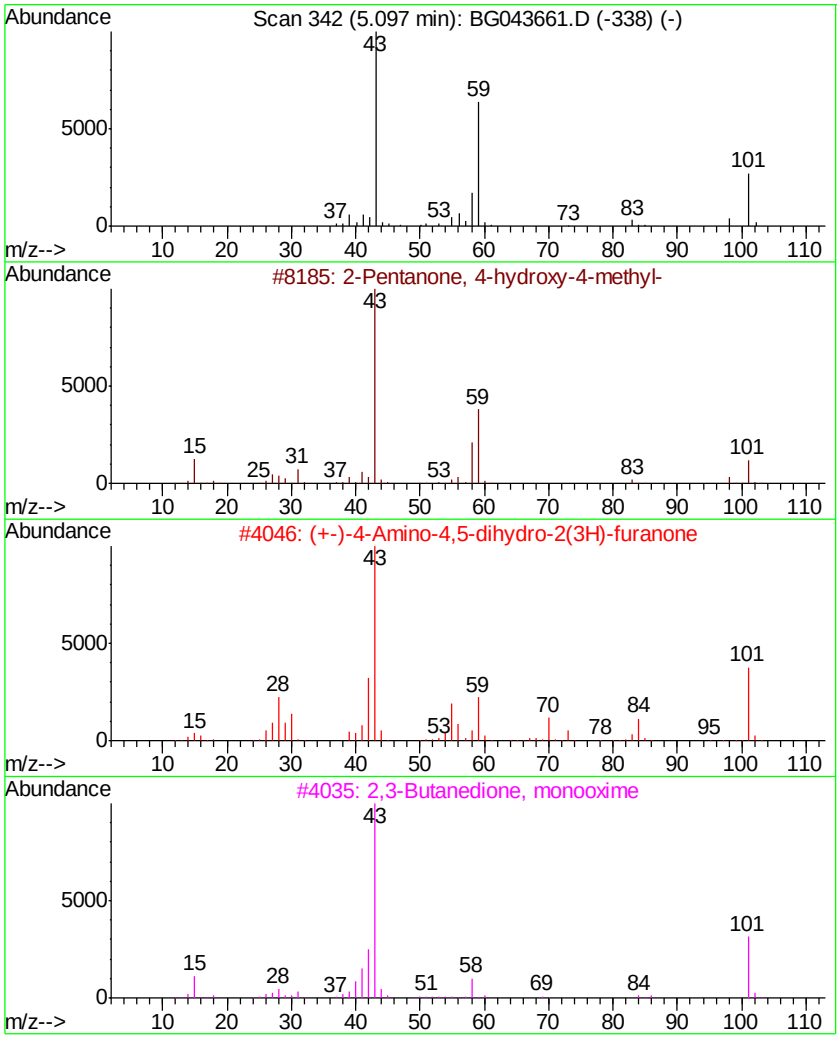
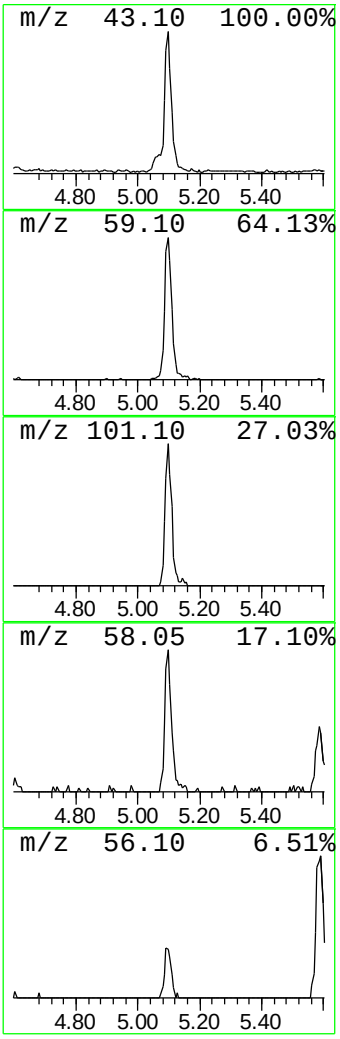
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	20.31 ng	123277	1,4-Dichlorobenzene-d4	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	37
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	17
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16





Library Search Compound Report

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Operator : JU
Sample : PB124780BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124780BL

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
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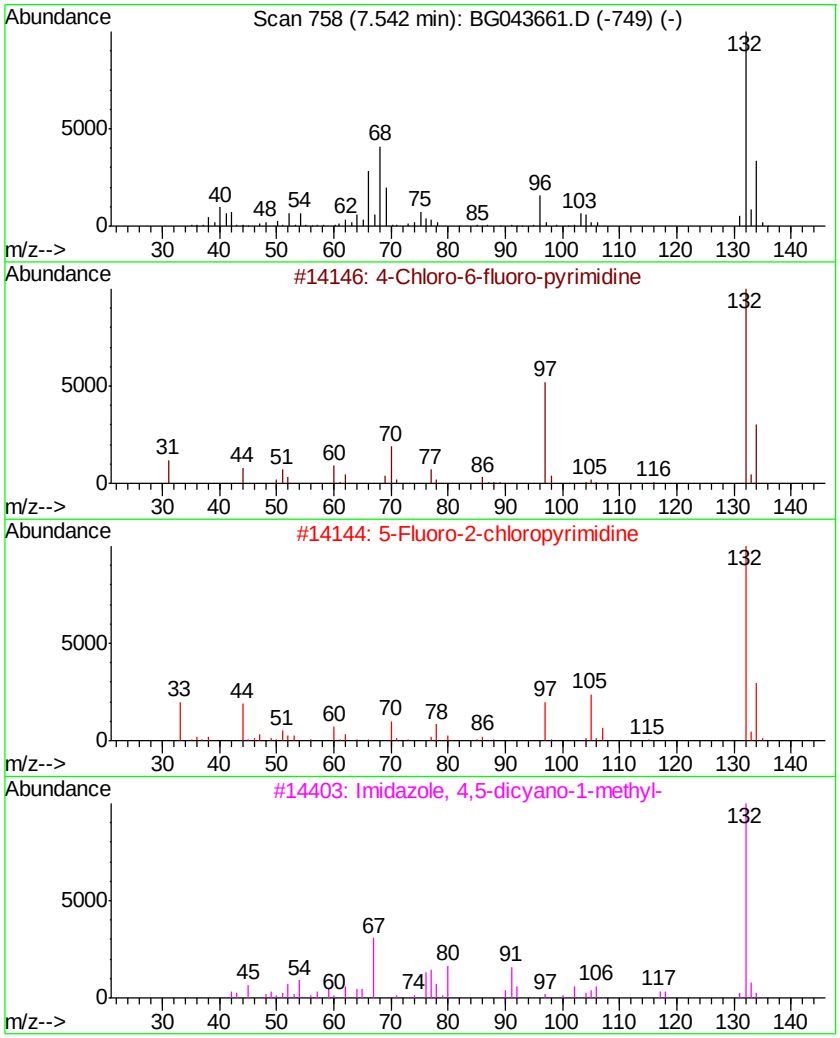
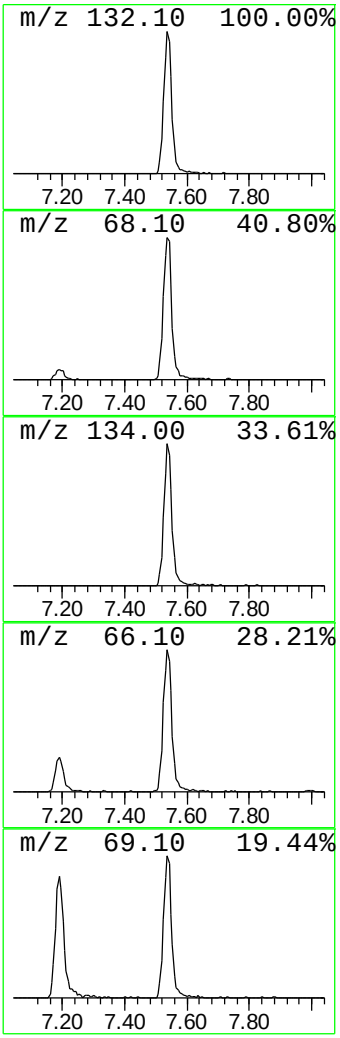
****

Peak Number 4 unknown7.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	112.42 ng	682457	1,4-Dichlorobenzene-d4	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12





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Acq On : 15 Nov 2019 21:50
Operator : JU
Sample : PB124780BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124780BL

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

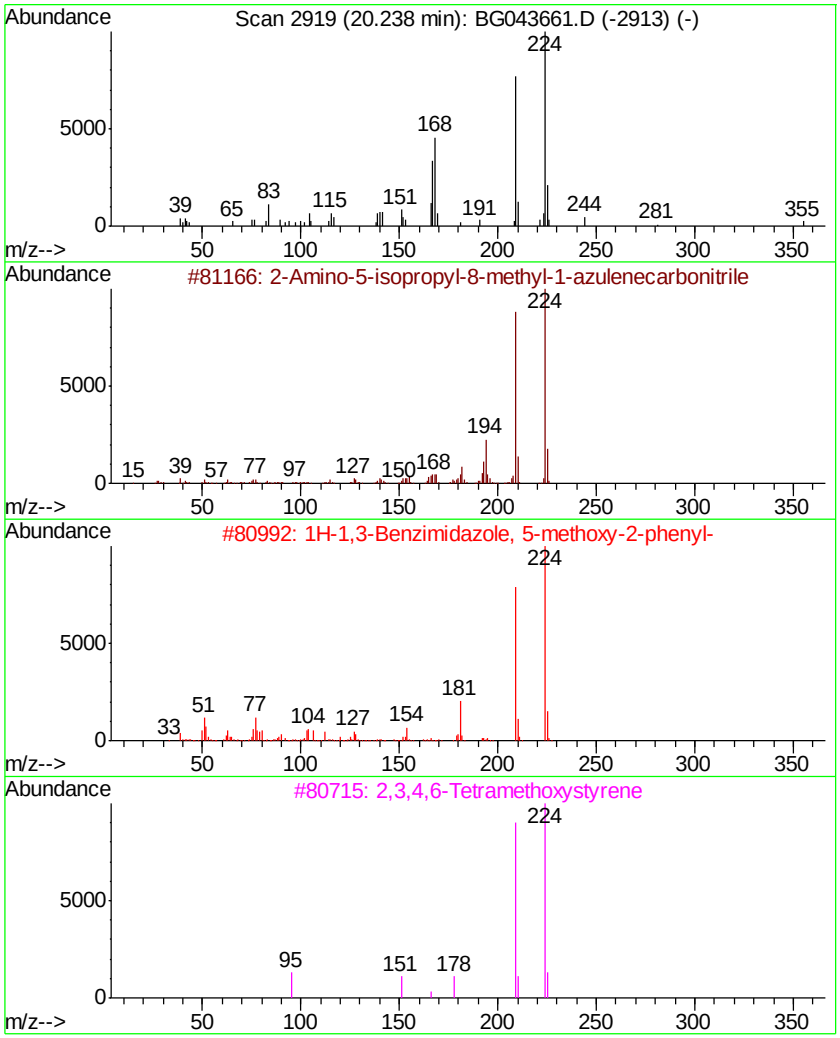
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

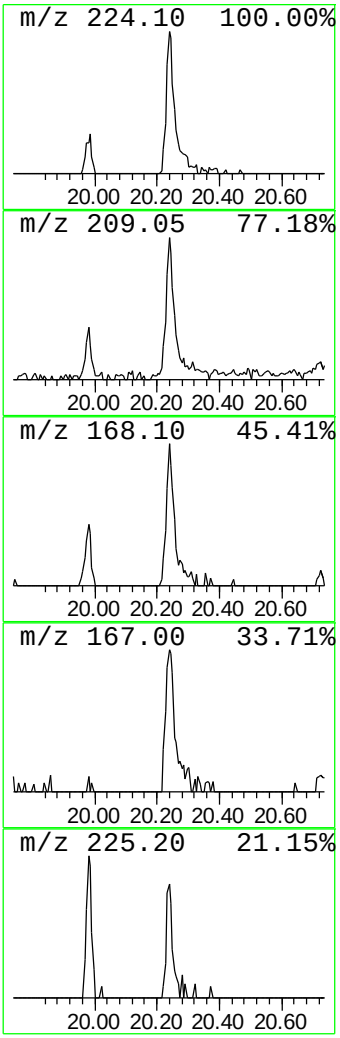
****

Peak Number 6 2-Amino-5-isopropyl-8-methy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.24	2.84 ng	69842	Chrysene-d12	21.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-5-isopropyl-8-methyl-1-a...	224	C15H16N2	093946-48-6	59
2	1H-1,3-Benzimidazole, 5-methoxy-...	224	C14H12N2O	1000350-62-4	53
3	2,3,4,6-Tetramethoxystyrene	224	C12H16O4	048153-74-8	50
4	3,5(2H)-Dihydroindazol-5-one, 2-...	266	C16H14N2O2	059341-21-8	42
5	8-Methyl-3a,4,5,6-tetrahydro-1H-...	224	C15H16N2	1000300-23-2	38





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Instrument : BNA_G
ClientSampleId : PB124780BL

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

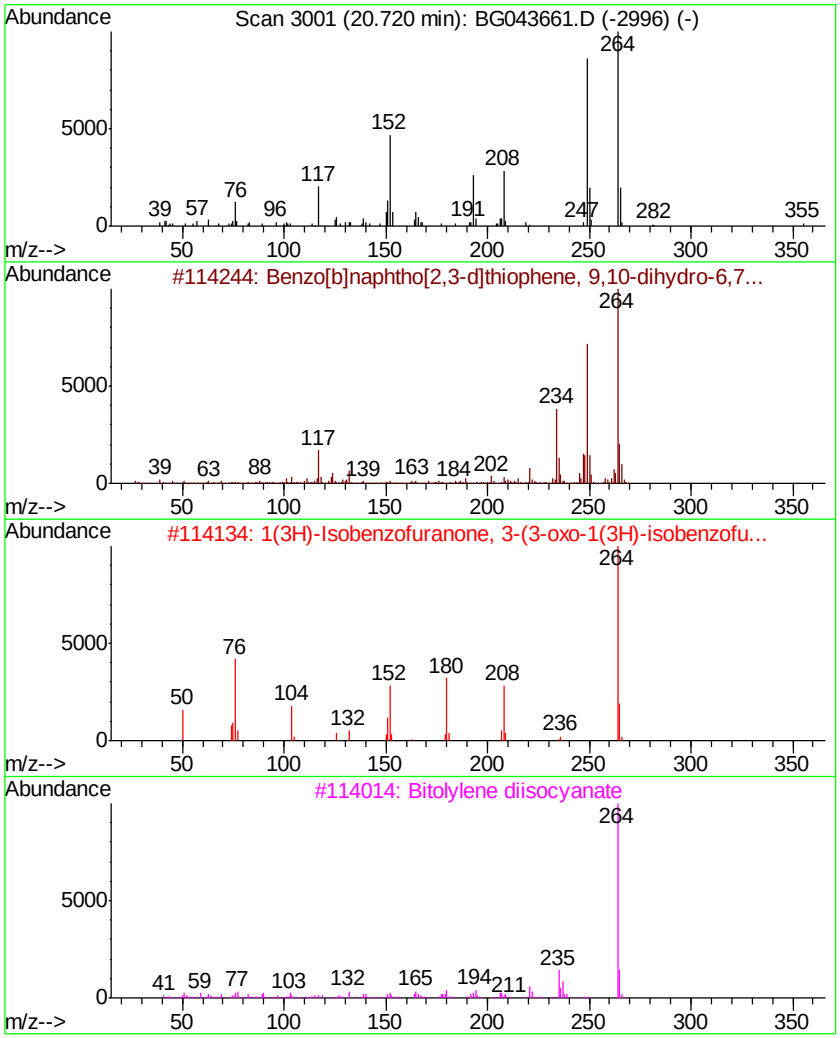
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

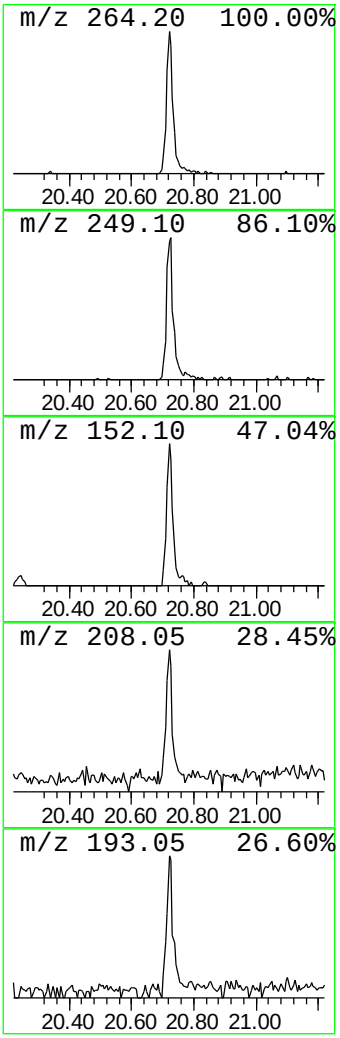
****

Peak Number 7 Benzo[b]naphtho[2,3-d]thiop... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.72	3.93 ng	96528	Chrysene-d12	21.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]naphtho[2,3-d]thiophene,...	264	C18H16S	024964-02-1	53
2	1(3H)-Isobenzofuranone, 3-(3-oxo...	264	C16H8O4	000482-23-5	38
3	Bitolylene diisocyanate	264	C16H12N2O2	000091-97-4	30
4	Iron, (.eta.-5-cyclopentadienyl)...	264	C16H16Fe	1000155-06-6	30
5	1,8-Dichlorophenazine 5-oxide	264	C12H6Cl2N2O	006479-80-7	27





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...	3.18	112.2	ng	681293	1	7.99	121409	20.0
n-Propyl acetate	3.46	7.0	ng	42194	1	7.99	121409	20.0
2-Pentanone, 4-hy...	5.10	20.3	ng	123277	1	7.99	121409	20.0
unknown7.54	7.54	112.4	ng	682457	1	7.99	121409	20.0
2-Amino-5-isoprop...	20.24	2.8	ng	69842	5	21.64	491450	20.0
Benzo[b]naphtho[2...	20.72	3.9	ng	96528	5	21.64	491450	20.0