LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043432.D
Acq On : 31 Oct 2019 12:46
Operator : JU
Sample : K5599-03
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : Z3-20B

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	3.188	13	17	29	rVB	103126	168960	7.43%	1.405%
2	5.127	342	347	354	rBV	78620	125426	5.51%	1.043%
3	5.609	422	429	448	rBV	371906	678287	29.82%	5.639%
4	7.207	692	701	717	rBV	386252	774476	34.05%	6.438%
5	7.560	754	761	775	rBV	407790	766189	33.68%	6.369%
6	8.018	830	839	850	rBV	128207	235121	10.34%	1.955%
7	8.347	887	895	907	rBV	319104	582097	25.59%	4.839%
8	9.181	1029	1037	1055	rBV	192054	439133	19.31%	3.651%
9	10.827	1310	1317	1329	rBV	136617	297854	13.09%	2.476%
10	13.271	1725	1733	1748	rBV	674520	1200983	52.80%	9.984%
11	14.105	1867	1875	1889	rBV	43283	100892	4.44%	0.839%
12	14.652	1961	1968	1982	rBV2	290869	516546	22.71%	4.294%
13	16.138	2214	2221	2238	rBV	582379	1075587	47.29%	8.941%
14	17.395	2428	2435	2447	rBV	382140	671374	29.52%	5.581%
15	17.513	2450	2455	2462	rVB3	22839	41985	1.85%	0.349%
16	18.288	2581	2587	2592	rBV3	17482	36239	1.59%	0.301%
17	20.004	2873	2879	2896	rBV	1655329	2274608	100.00%	18.909%
18	21.314	3096	3102	3111	rBV8	30118	94078	4.14%	0.782%
19	21.661	3154	3161	3179	rBV2	434950	855756	37.62%	7.114%
20	23.136	3405	3412	3416	rBV3	23910	44252	1.95%	0.368%
21	23.935	3540	3548	3555	rBV4	25317	55969	2.46%	0.465%
22	24.857	3694	3705	3720	rBV	310493	942354	41.43%	7.834%
23	25.985	3888	3897	3905	rBV7	15878	51193	2.25%	0.426%

Sum of corrected areas: 12029359

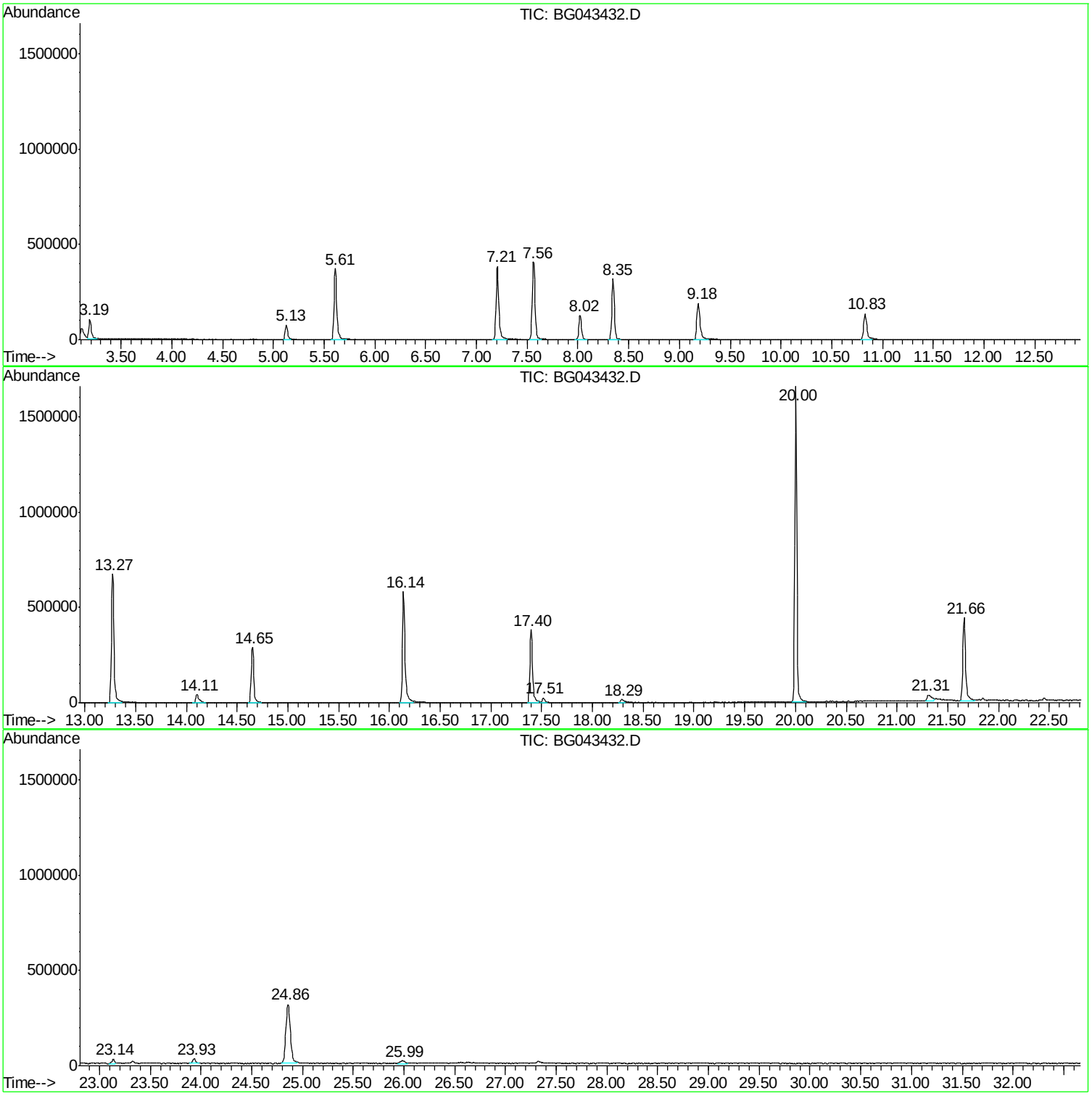
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043432.D
Acq On : 31 Oct 2019 12:46
Operator : JU
Sample : K5599-03
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : Z3-20B

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043432.D
Acq On : 31 Oct 2019 12:46
Operator : JU
Sample : K5599-03
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : Z3-20B

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

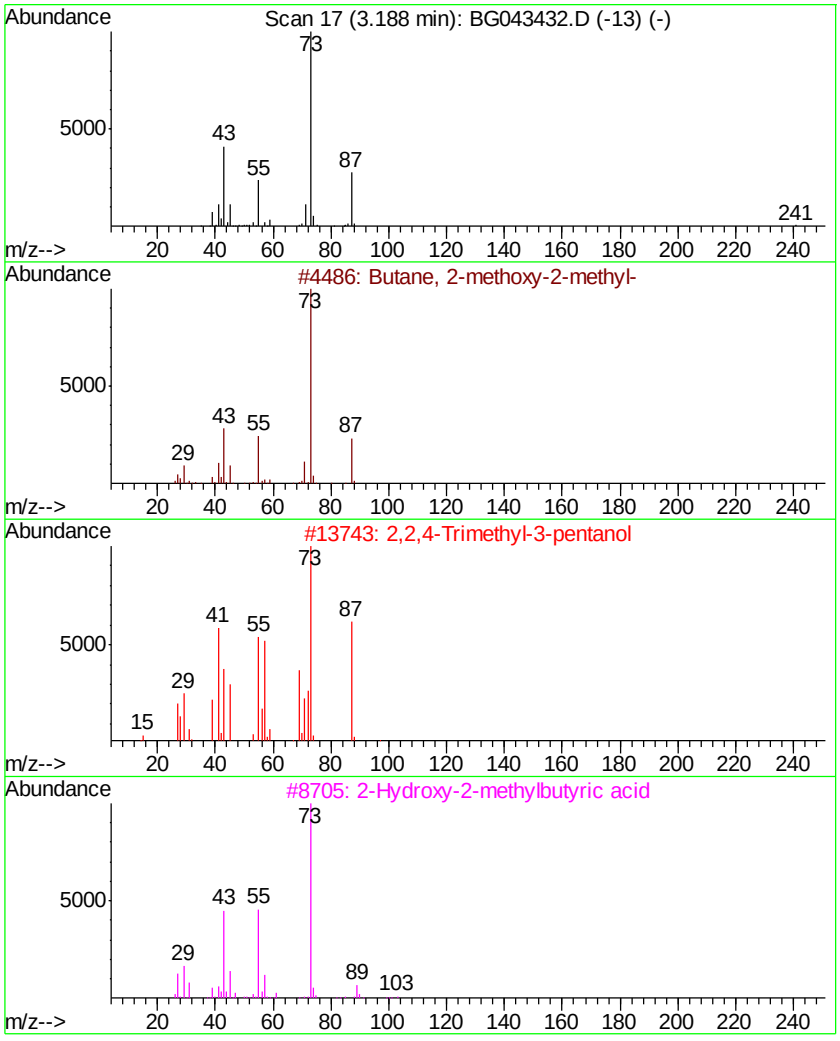
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

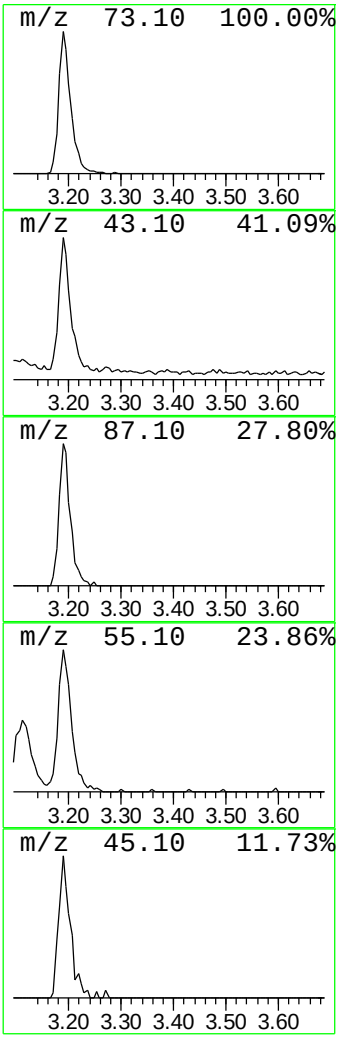
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	14.37 ng	168960	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	50
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	17
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043432.D
Acq On : 31 Oct 2019 12:46
Operator : JU
Sample : K5599-03
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : Z3-20B

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

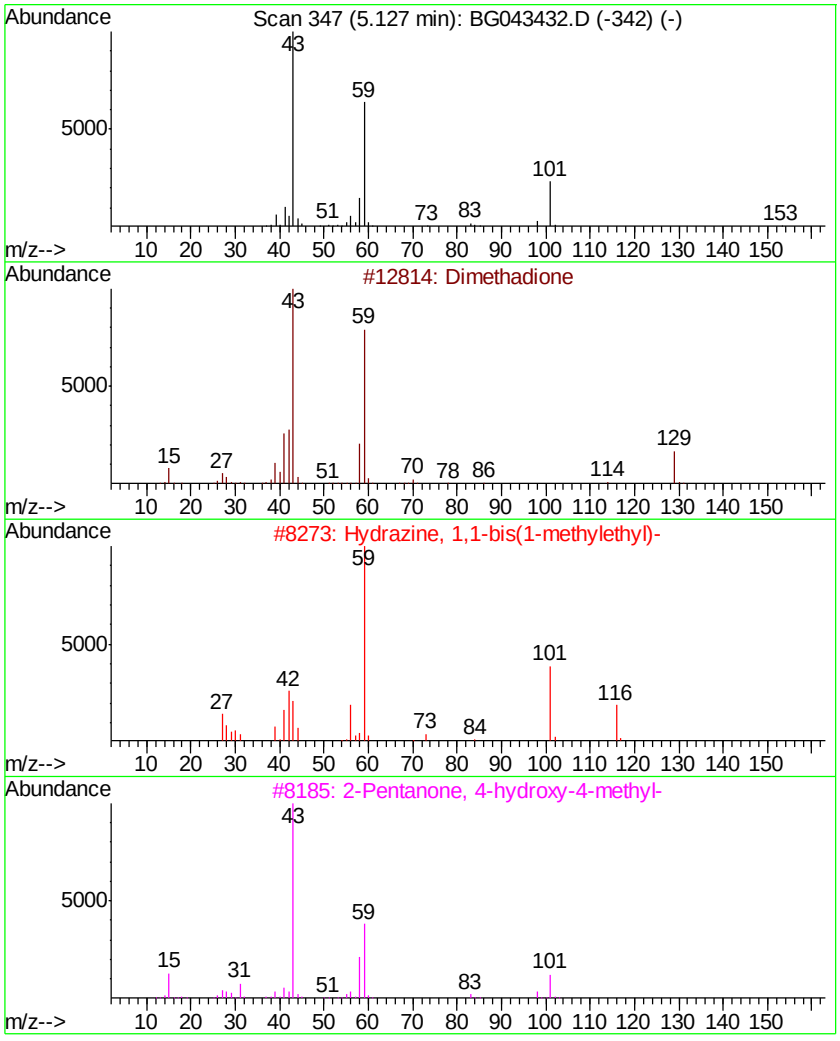
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

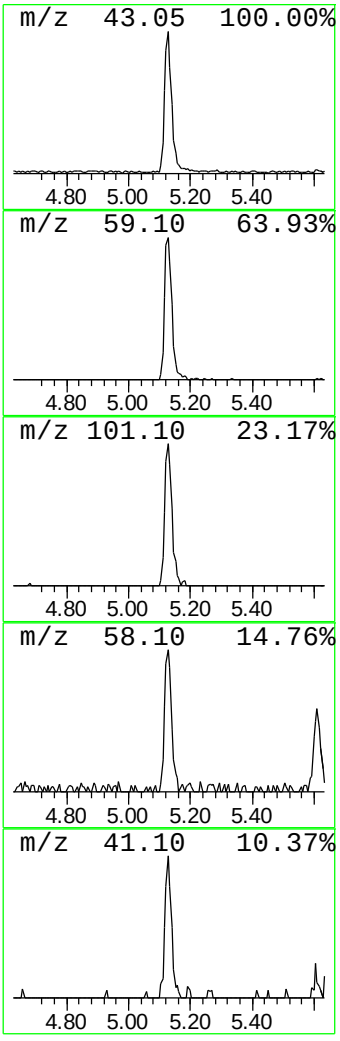
****

Peak Number 2 unknown5.13 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	10.67 ng	125426	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethadione	129	C5H7NO3	000695-53-4	42
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	40
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043432.D
Acq On : 31 Oct 2019 12:46
Operator : JU
Sample : K5599-03
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : Z3-20B

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

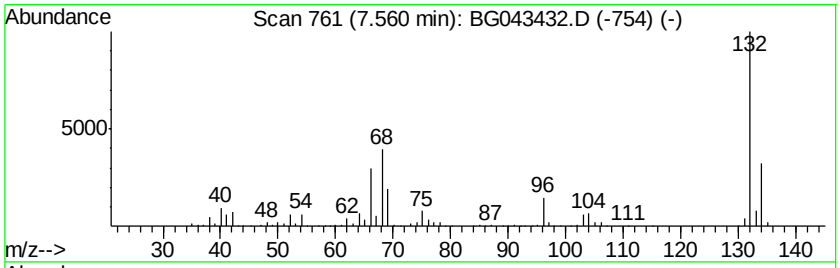
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

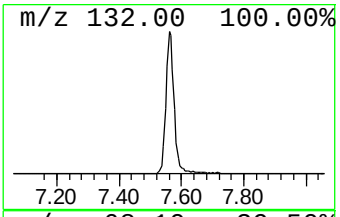
****

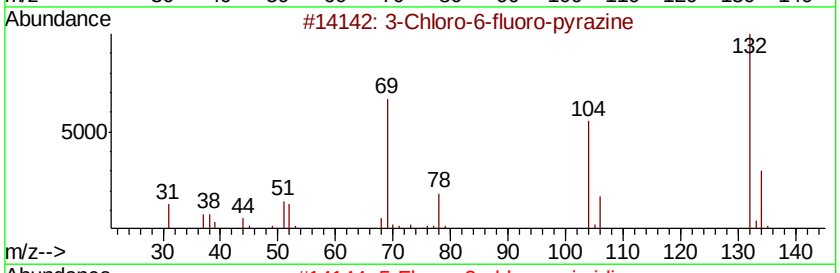
Peak Number 3 unknown7.56 Concentration Rank 1

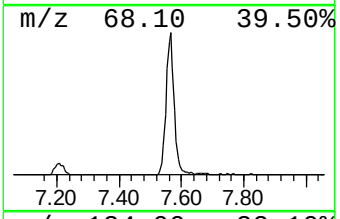
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	65.17 ng	766189	1,4-Dichlorobenzene-d4	8.02

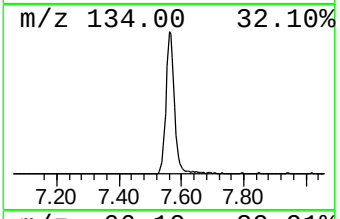
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
5	5-Aminoindole	132	C8H8N2	005192-03-0	12

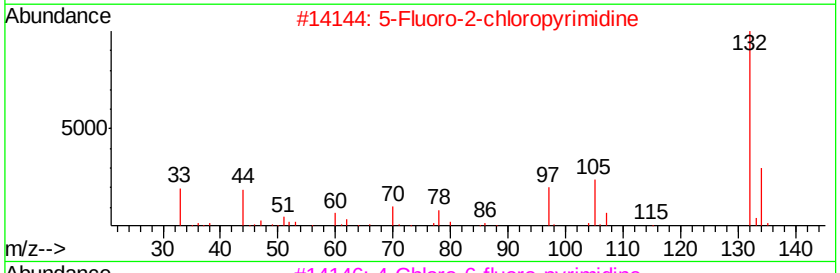


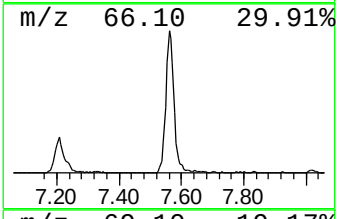


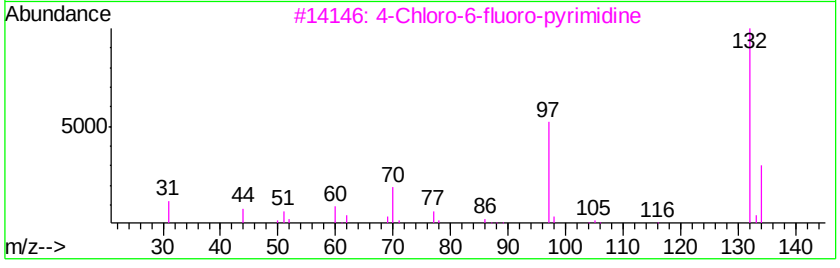


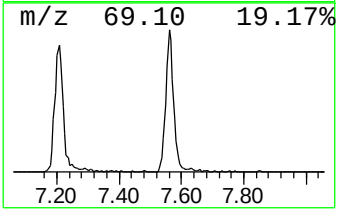












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

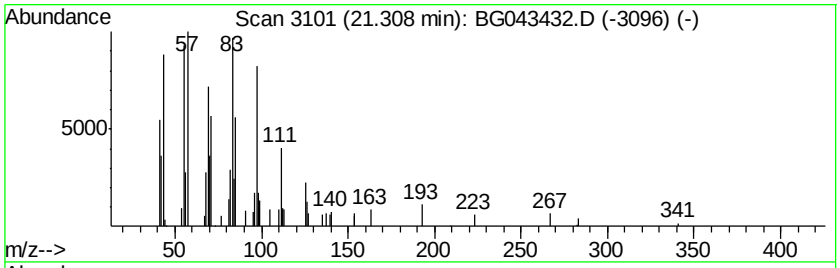
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

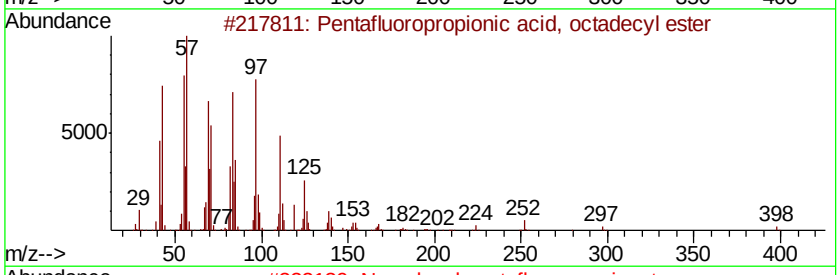
****

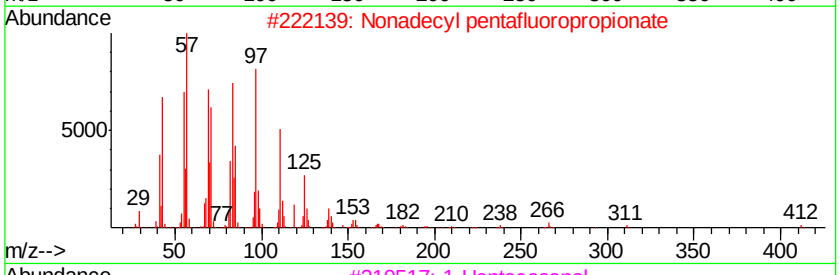
Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 5

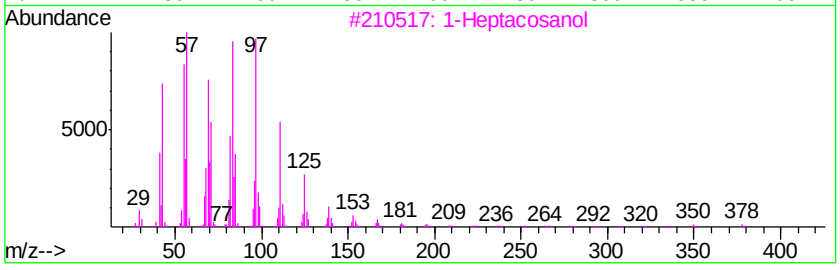
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	2.20 ng	94078	Chrysene-d12	21.66

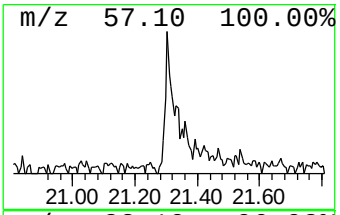
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	94
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91

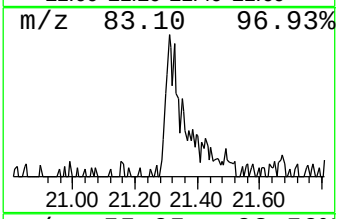


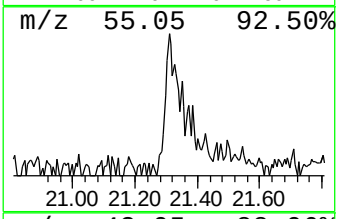


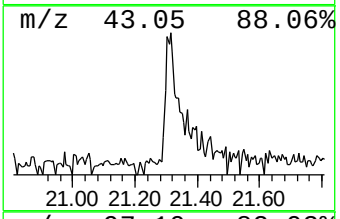


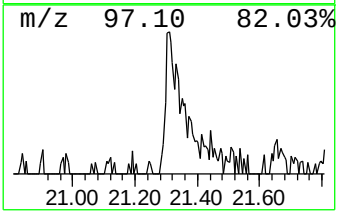












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG103019\
Data File : BG043432.D
Acq On : 31 Oct 2019 12:46
Operator : JU
Sample : K5599-03
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : Z3-20B

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.19	14.4	ng	168960	1	8.02	235121	20.0
unknown5.13	5.13	10.7	ng	125426	1	8.02	235121	20.0
unknown7.56	7.56	65.2	ng	766189	1	8.02	235121	20.0
Pentafluoropropio...	21.31	2.2	ng	94078	5	21.66	855756	20.0