LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044081.D
Acq On : 17 Jan 2020 19:18
Operator : JU
Sample : PB126154BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126154BL

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-BG123019.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	5.038	324	332	344	rBV	96393	161099	2.82%	0.573%
2	5.508	405	412	435	rVB	698791	1186405	20.79%	4.221%
3	7.101	672	683	697	rBV	470844	820715	14.38%	2.920%
4	7.465	737	745	758	rBV	1290134	2292813	40.18%	8.157%
5	7.929	818	824	832	rBV	233078	403670	7.07%	1.436%
6	8.258	870	880	893	rBV	991353	1796961	31.49%	6.393%
7	9.087	1013	1021	1035	rBV	854308	1543734	27.05%	5.492%
8	10.738	1292	1302	1314	rBV	314678	594844	10.42%	2.116%
9	13.194	1712	1720	1742	rBV	2286295	3766776	66.01%	13.400%
10	14.568	1945	1954	1969	rBV2	592272	967776	16.96%	3.443%
11	16.055	2200	2207	2227	rBV	2103251	3378678	59.21%	12.020%
12	17.312	2414	2421	2435	rBV	740982	1158457	20.30%	4.121%
13	19.927	2860	2866	2881	rBV	4274725	5706235	100.00%	20.300%
14	21.560	3137	3144	3152	rBV	716380	1188091	20.82%	4.227%
15	22.365	3276	3281	3288	rVB3	86285	146883	2.57%	0.523%
16	23.035	3390	3395	3401	rVB	60107	104821	1.84%	0.373%
17	23.229	3422	3428	3440	rVB4	87953	215492	3.78%	0.767%
18	23.816	3522	3528	3535	rVB2	54301	107497	1.88%	0.382%
19	24.263	3597	3604	3618	rVB3	118135	356675	6.25%	1.269%
20	24.668	3663	3673	3681	rBV2	435106	1196637	20.97%	4.257%
21	25.538	3811	3821	3843	rBV3	119617	555293	9.73%	1.975%
22	27.142	4084	4094	4114	rVB7	82333	460110	8.06%	1.637%

Sum of corrected areas: 28109662

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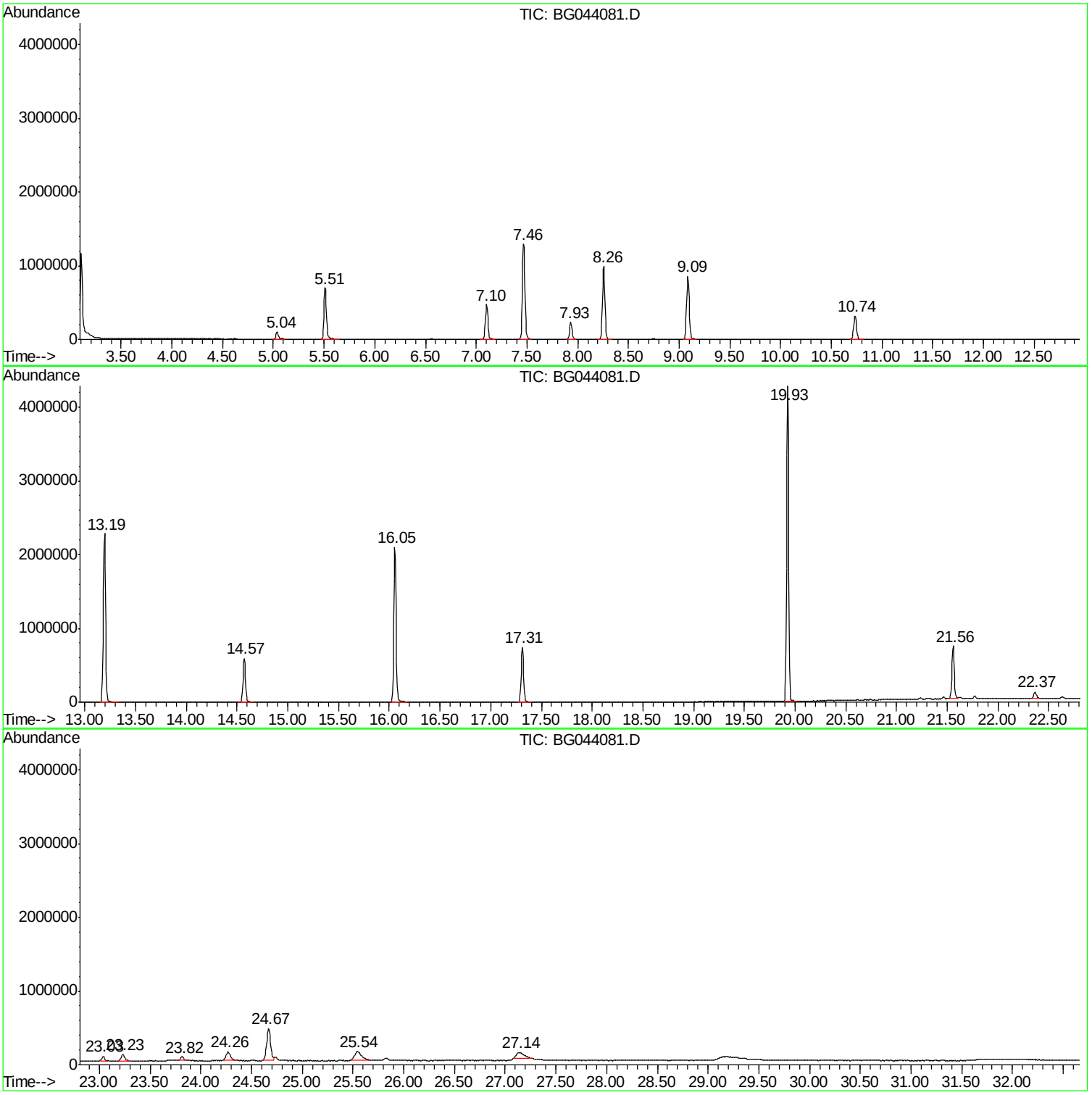
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB126154BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

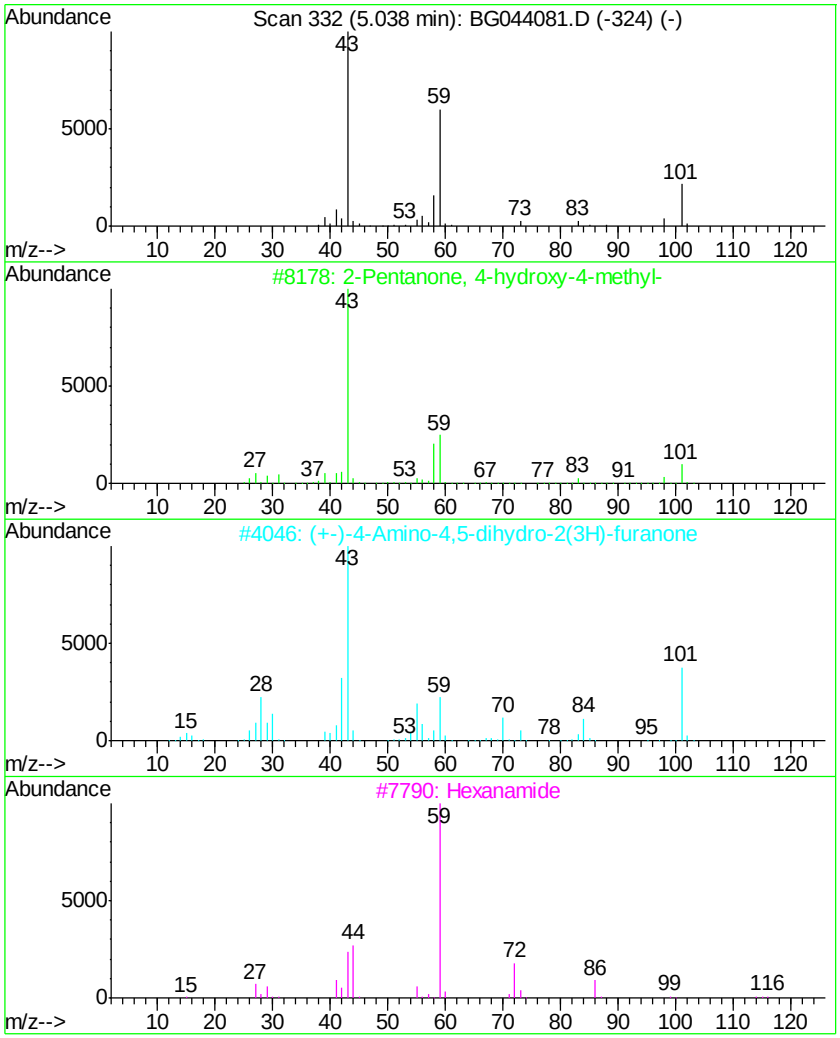
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

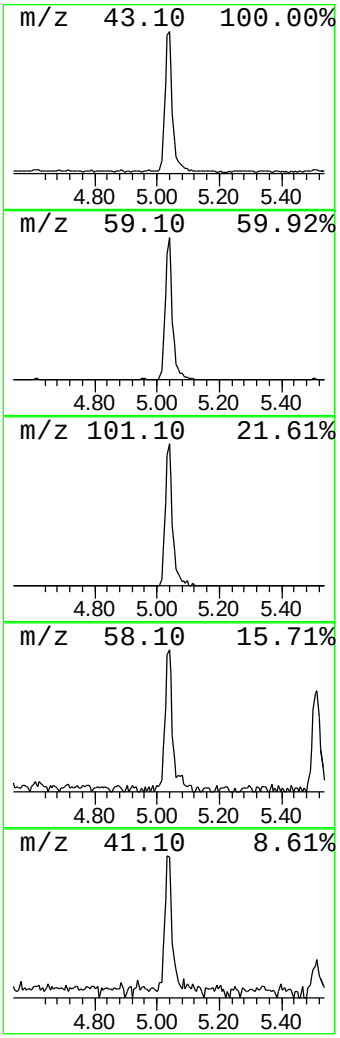
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	7.98 ng	161099	1,4-Dichlorobenzene-d4	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	35
3	Hexanamide	115	C6H13NO	000628-02-4	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044081.D
Acq On : 17 Jan 2020 19:18
Operator : JU
Sample : PB126154BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126154BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

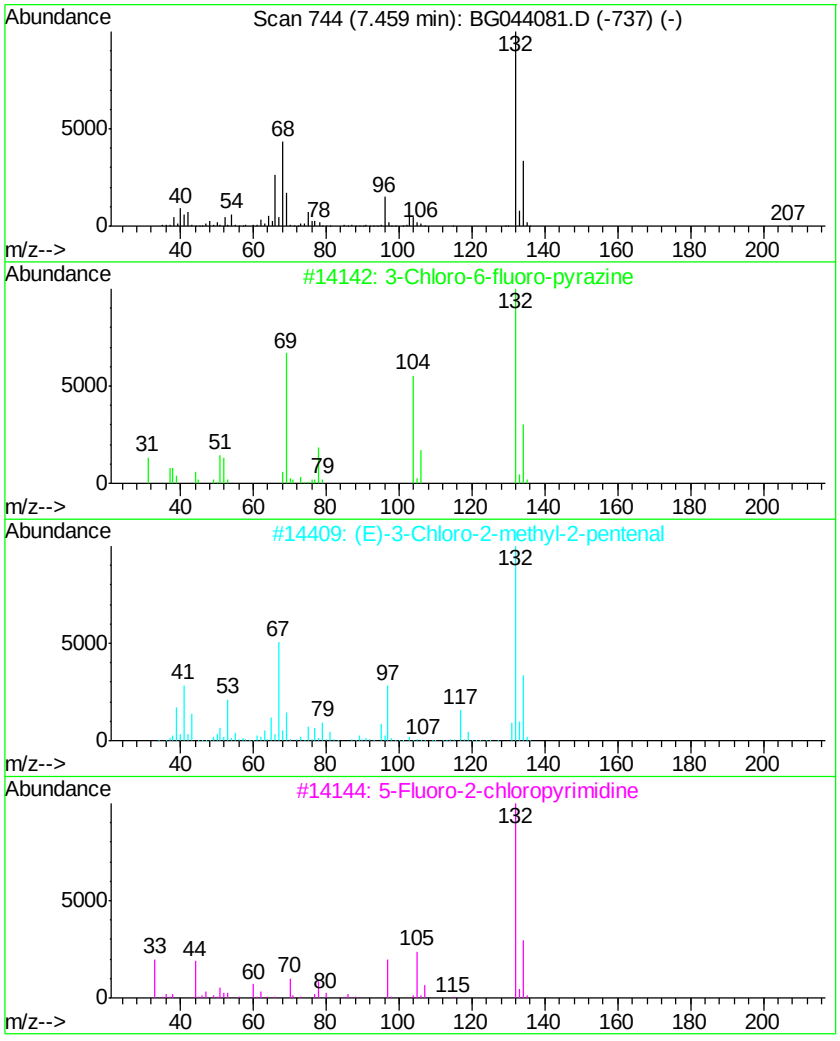
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

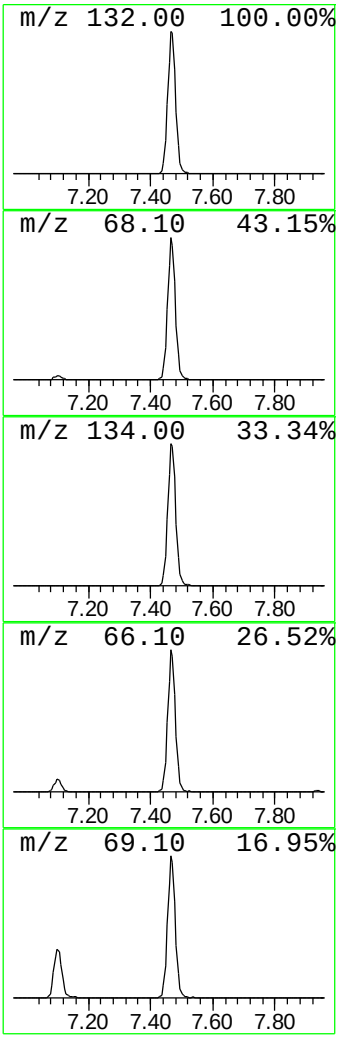
****

Peak Number 2 unknown7.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.46	113.60 ng	2292810	1,4-Dichlorobenzene-d4	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	Amphetaminil	250	C17H18N2	017590-01-1	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044081.D
Acq On : 17 Jan 2020 19:18
Operator : JU
Sample : PB126154BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126154BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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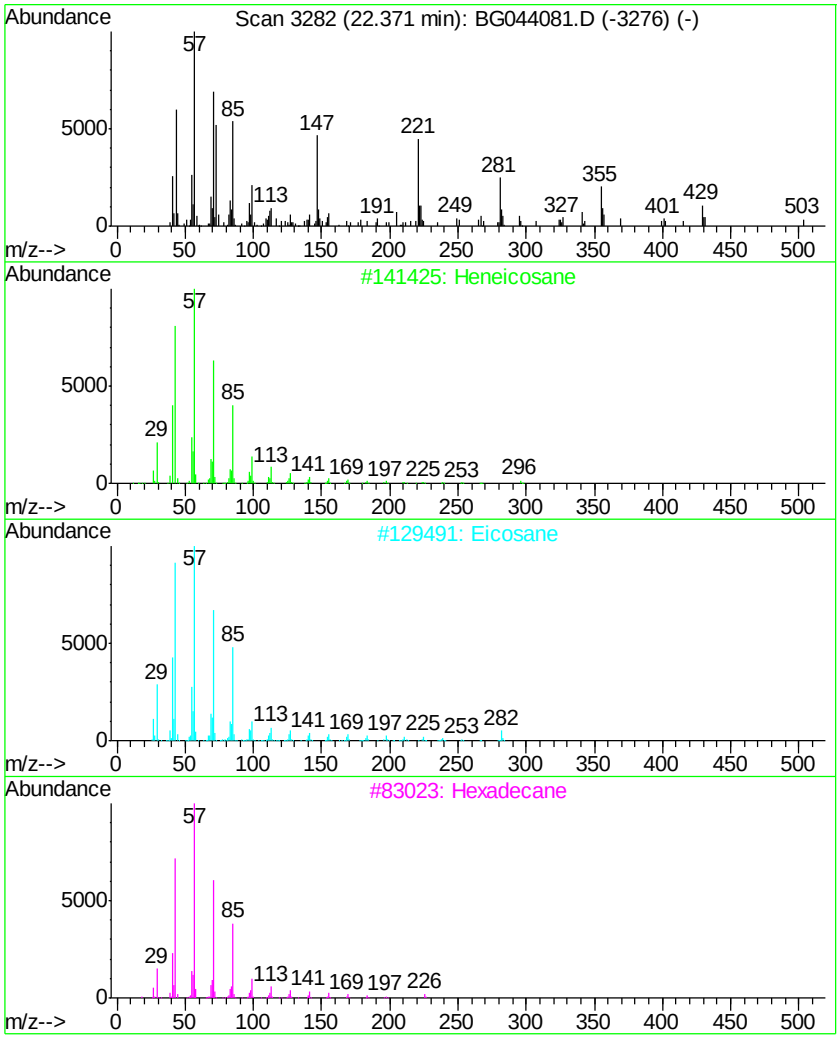
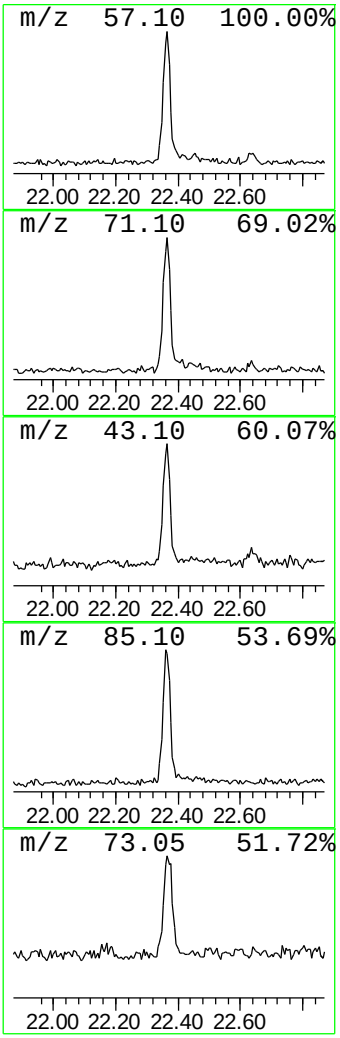
Peak Number 4 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.37	2.47 ng	146883	Chrysene-d12	21.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	64
2	Eicosane	282	C20H42	000112-95-8	64
3	Hexadecane	226	C16H34	000544-76-3	50
4	Tetracosane	338	C24H50	000646-31-1	50
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	50





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Data File : BG044081.D
Acq On : 17 Jan 2020 19:18
Operator : JU
Sample : PB126154BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126154BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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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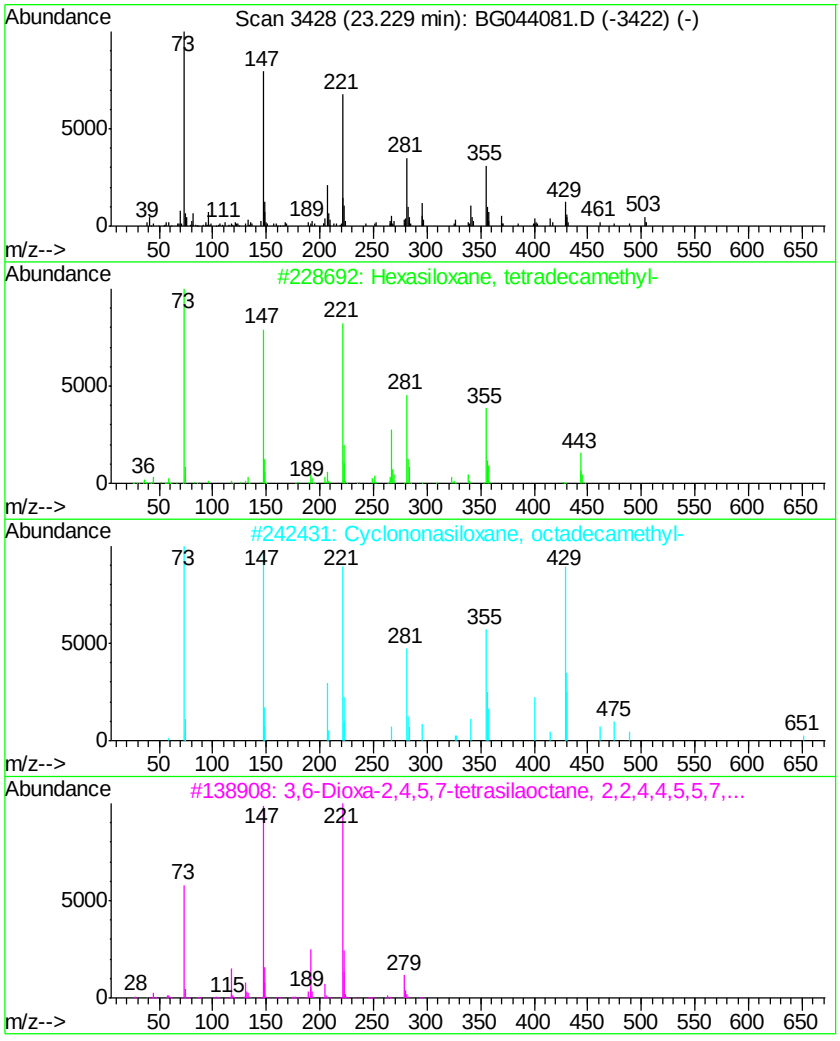
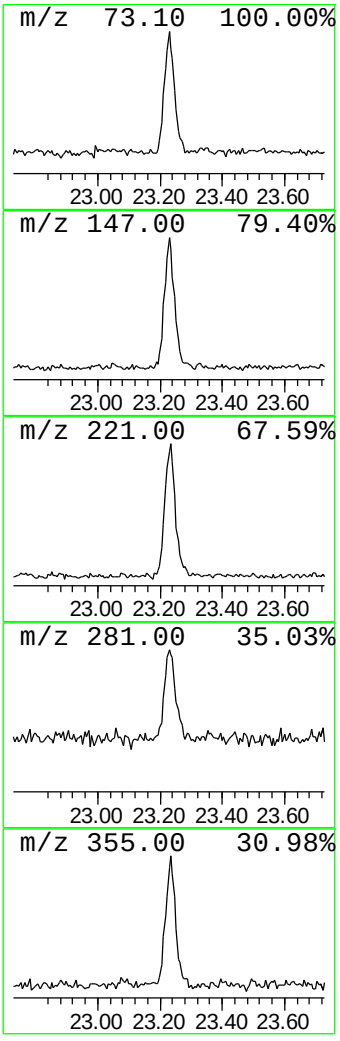
Peak Number 5 Hexasiloxane, tetradecamethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.23	3.60 ng	215492	Perylene-d12	24.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	87
2	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	78
3	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	50
4	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	43
5	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044081.D
Acq On : 17 Jan 2020 19:18
Operator : JU
Sample : PB126154BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126154BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

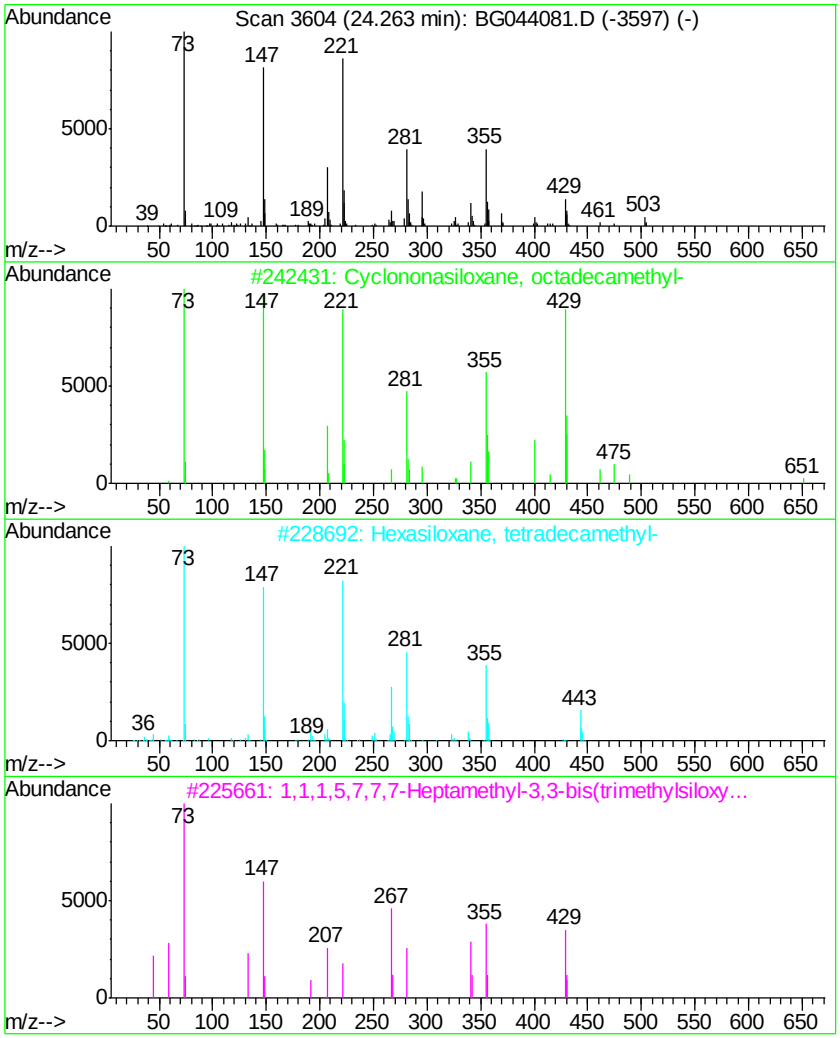
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

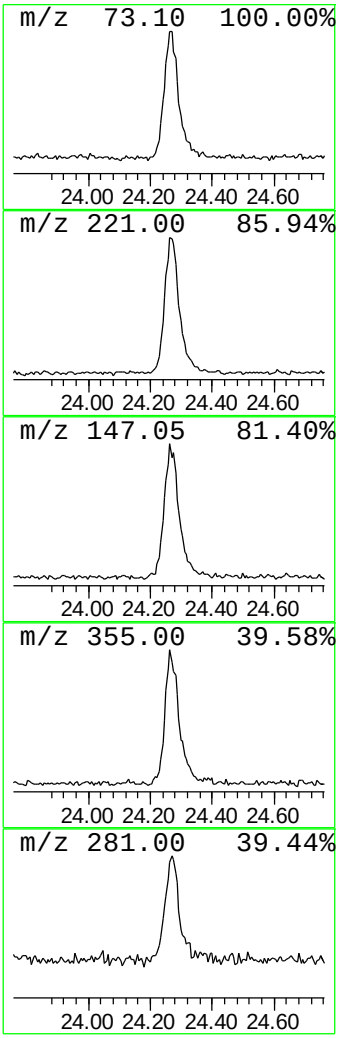
****

Peak Number 6 Cyclononasiloxane, octadeca... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.26	5.96 ng	356675	Perylene-d12	24.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	80
2	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	72
3	1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	59
4	Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	47
5	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	47





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Acq On : 17 Jan 2020 19:18
Operator : JU
Sample : PB126154BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126154BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

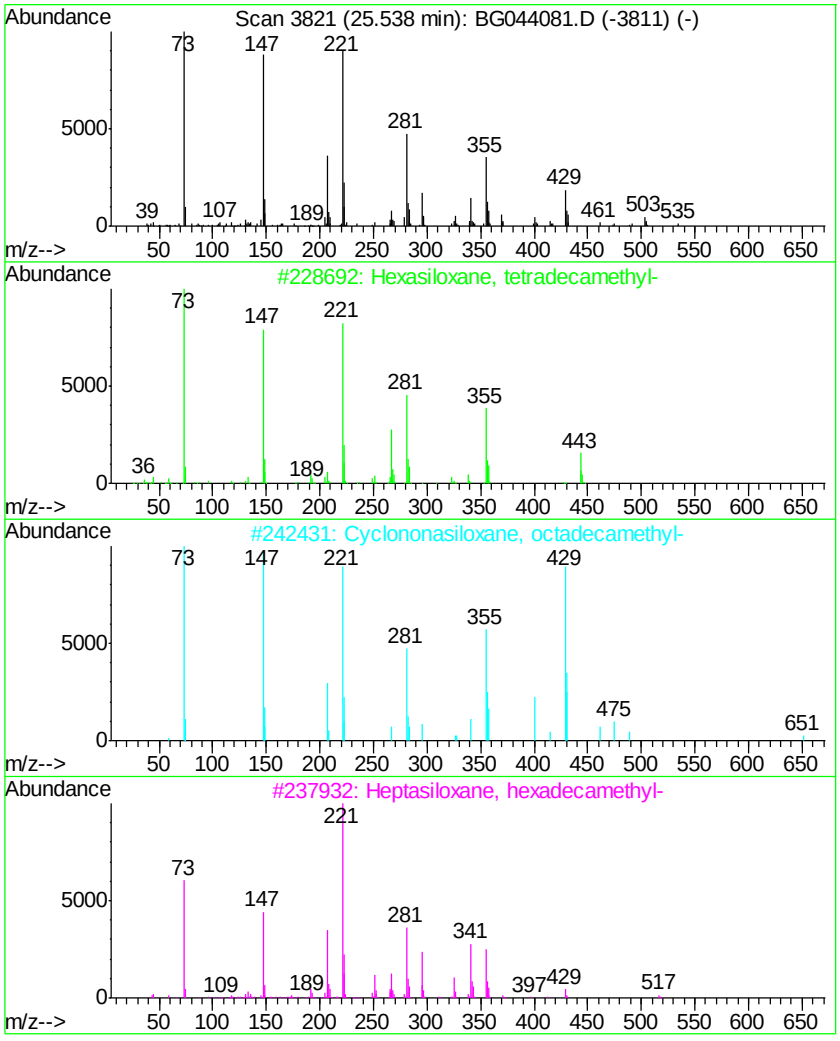
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

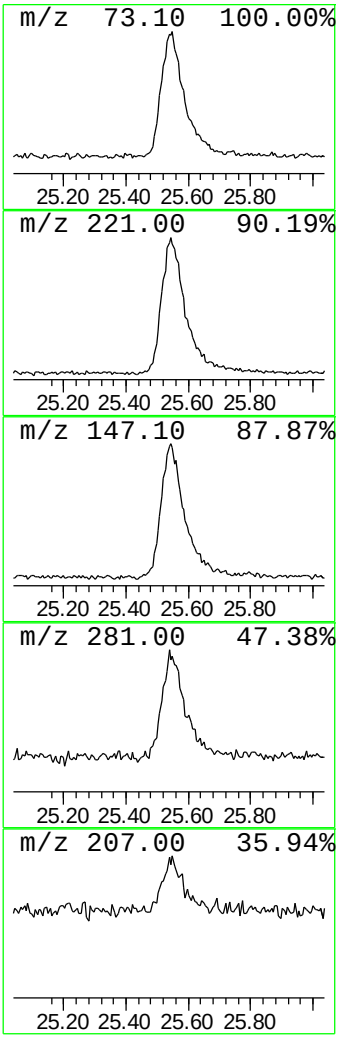
****

Peak Number 7 Heptasiloxane, hexadecamethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.54	9.28 ng	555293	Perylene-d12	24.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	90
2	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	90
3	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	80
4	Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	43
5	Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	38





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
2-Pentanone, 4-hy...	5.04	8.0	ng	161099	1	7.93	403670	20.0
unknown7.46	7.46	113.6	ng	2292810	1	7.93	403670	20.0
Heneicosane	22.37	2.5	ng	146883	5	21.56	1188090	20.0
Hexasiloxane, tet...	23.23	3.6	ng	215492	6	24.67	1196640	20.0
Cyclononasiloxane...	24.26	6.0	ng	356675	6	24.67	1196640	20.0
Heptasiloxane, he...	25.54	9.3	ng	555293	6	24.67	1196640	20.0