LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043553.D
Acq On : 8 Nov 2019 00:01
Operator : JU
Sample : K5702-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : H-1

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	3.170	9	14	24	rVB	76923	129972	8.25%	1.384%
2	5.109	337	344	358	rBV	71311	113397	7.20%	1.208%
3	5.603	422	428	444	rBV	321933	581897	36.94%	6.198%
4	7.213	695	702	718	rBV	336065	664140	42.16%	7.074%
5	7.554	752	760	772	rBV	365011	661335	41.99%	7.044%
6	8.006	831	837	844	rBV	99596	172821	10.97%	1.841%
7	8.335	884	893	902	rBV	283556	519507	32.98%	5.533%
8	9.175	1027	1036	1052	rBV	177432	385149	24.45%	4.102%
9	10.814	1308	1315	1327	rBV	105033	218572	13.88%	2.328%
10	13.259	1724	1731	1743	rBV	511708	870419	55.26%	9.271%
11	14.087	1865	1872	1886	rBV	70973	126984	8.06%	1.352%
12	14.639	1960	1966	1979	rBV	209404	352931	22.41%	3.759%
13	16.132	2214	2220	2233	rBV	517705	894526	56.79%	9.527%
14	17.383	2427	2433	2446	rBV	261607	470505	29.87%	5.011%
15	17.501	2449	2453	2459	rVB7	16229	29074	1.85%	0.310%
16	18.276	2581	2585	2603	rBV2	77420	134557	8.54%	1.433%
17	19.992	2872	2877	2890	rBV	1078328	1575154	100.00%	16.777%
18	21.296	3095	3099	3108	rVB4	61242	125109	7.94%	1.332%
19	21.649	3154	3159	3173	rVB	305202	615591	39.08%	6.556%
20	23.306	3437	3441	3452	rVB2	65047	124104	7.88%	1.322%
21	24.851	3695	3704	3714	rVB	217009	623304	39.57%	6.639%

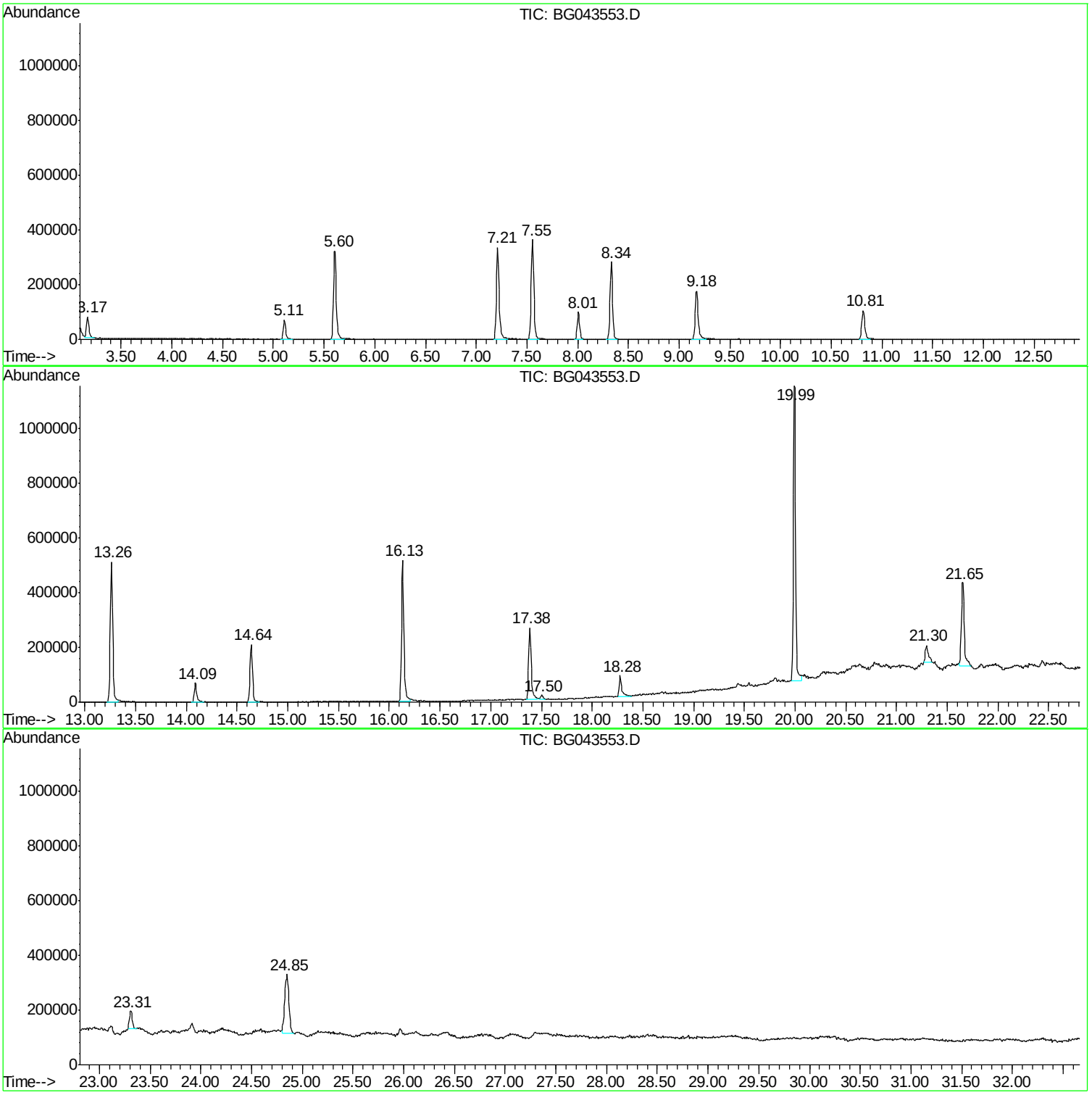
Sum of corrected areas: 9389048

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043553.D
Acq On : 8 Nov 2019 00:01
Operator : JU
Sample : K5702-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : H-1

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\BG110719\
Data File : BG043553.D
Acq On : 8 Nov 2019 00:01
Operator : JU
Sample : K5702-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : H-1

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

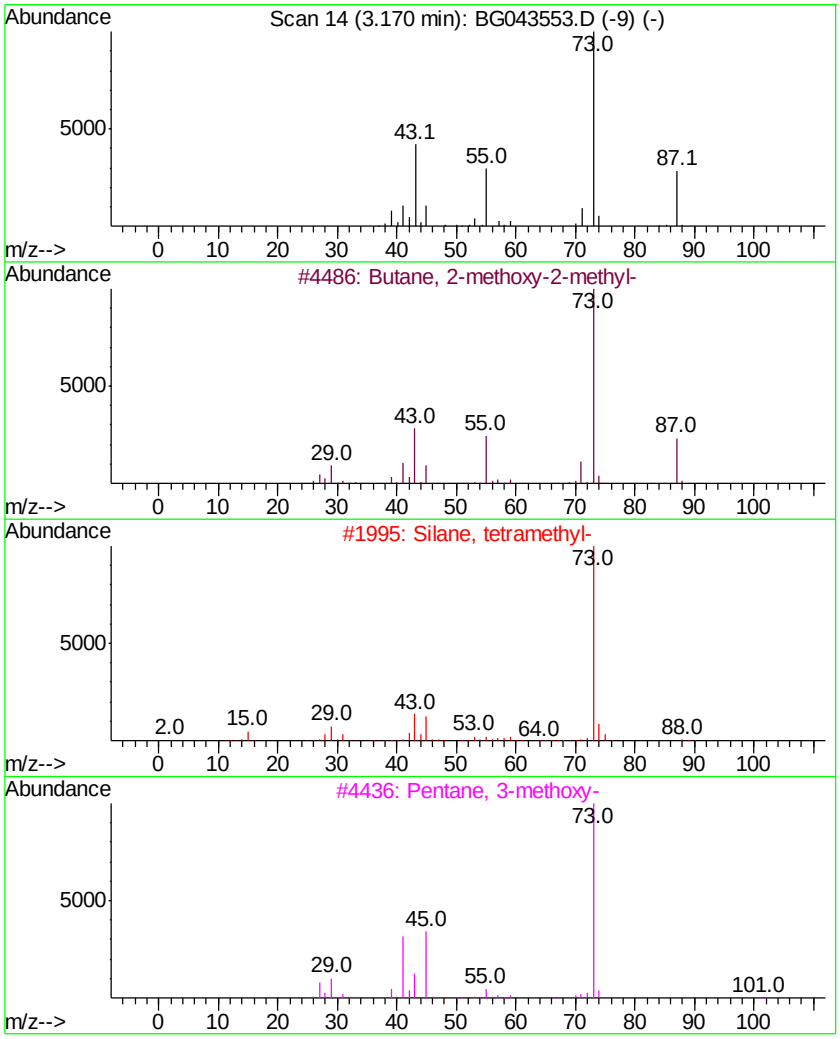
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

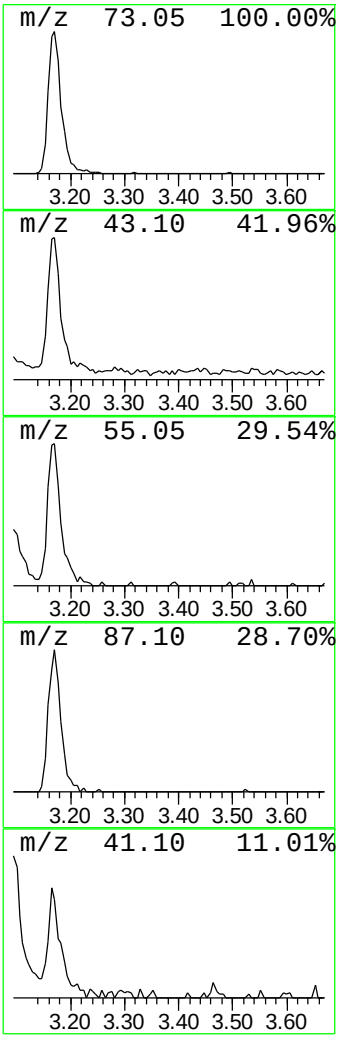
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	15.04 ng	129972	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	72
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043553.D
Acq On : 8 Nov 2019 00:01
Operator : JU
Sample : K5702-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : H-1

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

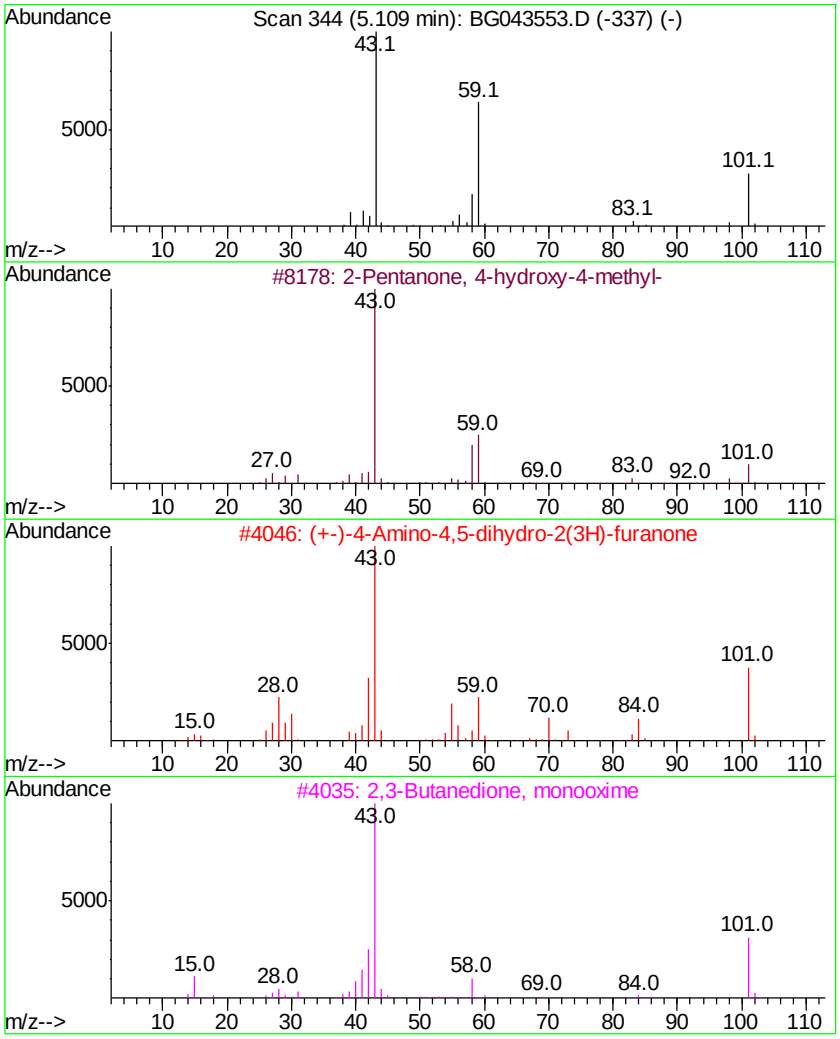
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

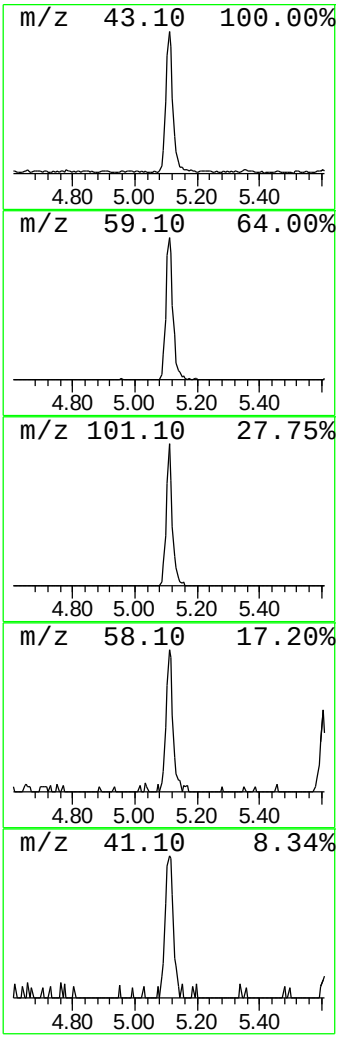
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	13.12 ng	113397	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	59
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043553.D
Acq On : 8 Nov 2019 00:01
Operator : JU
Sample : K5702-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : H-1

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

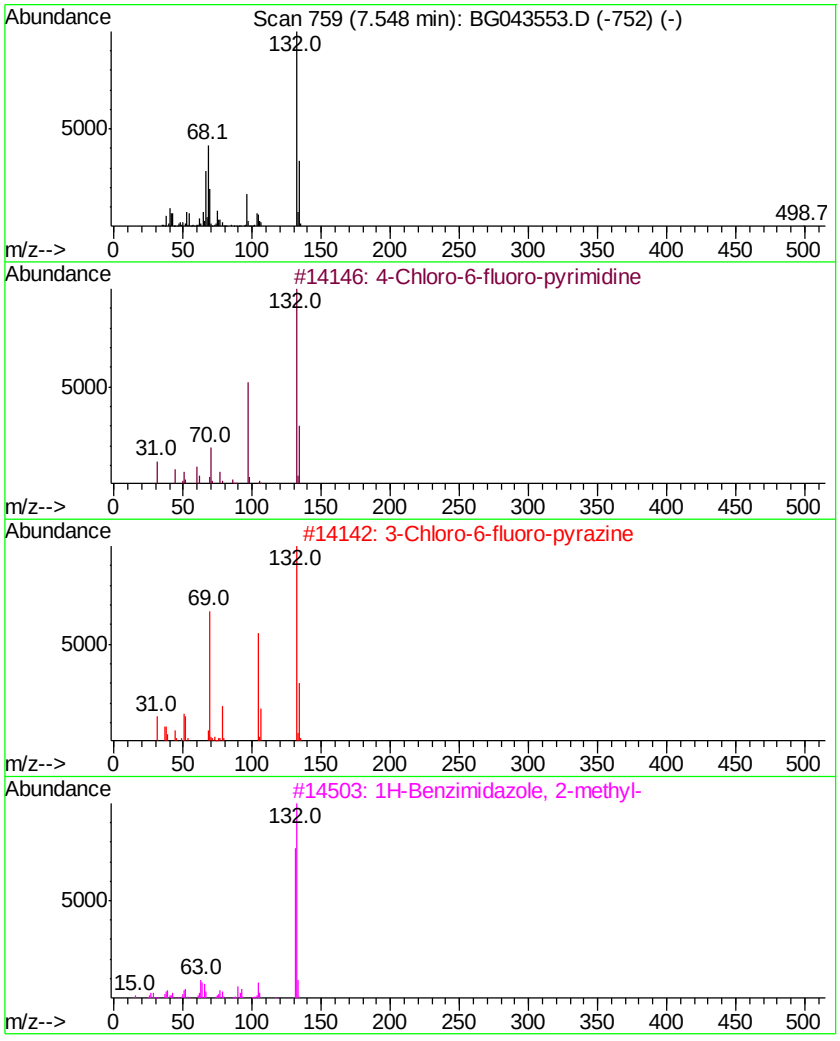
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

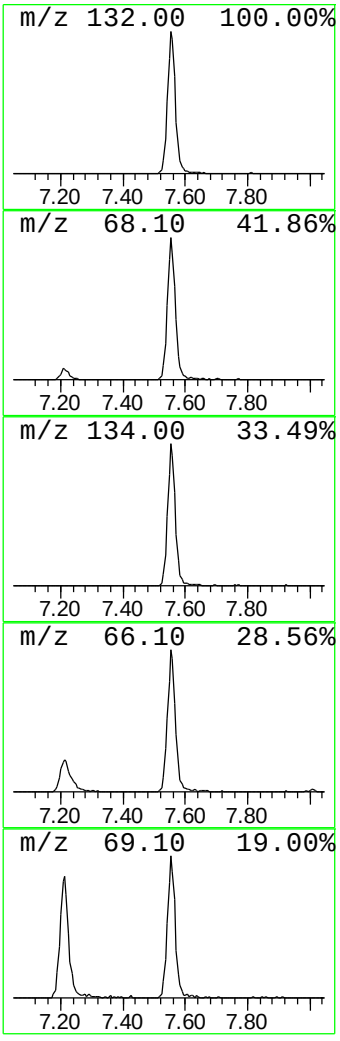
****

Peak Number 3 unknown7.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	76.53 ng	661335	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043553.D
Acq On : 8 Nov 2019 00:01
Operator : JU
Sample : K5702-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : H-1

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

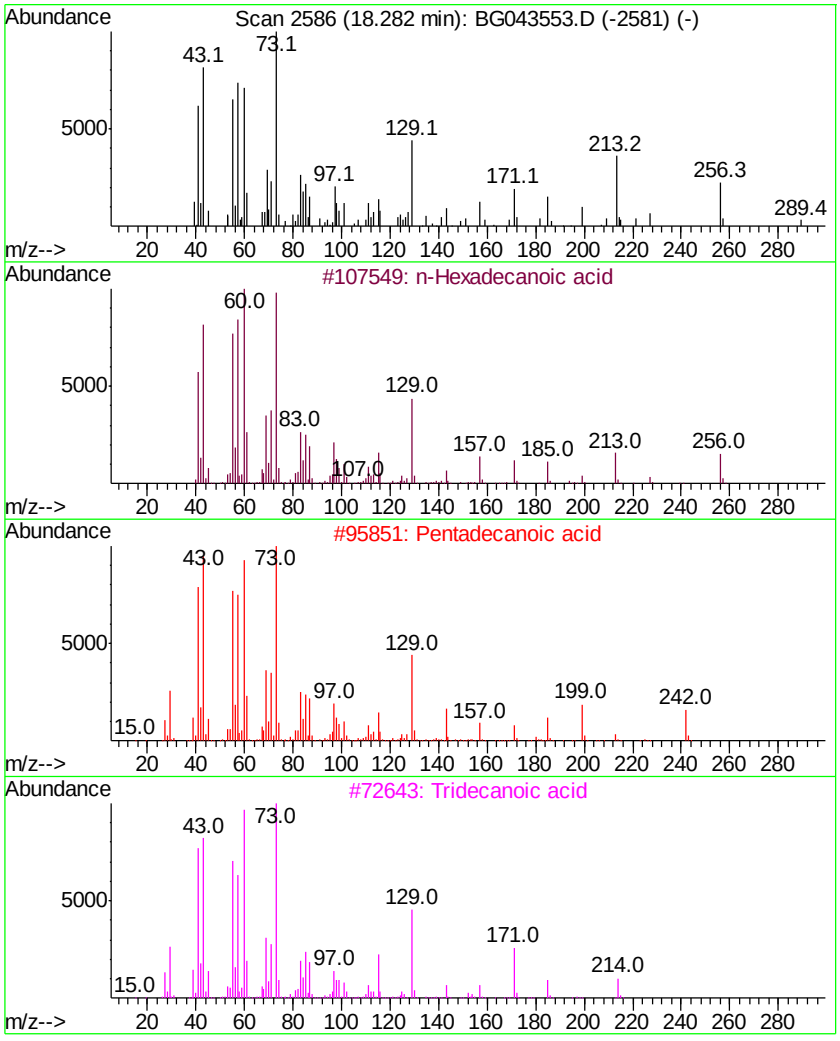
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

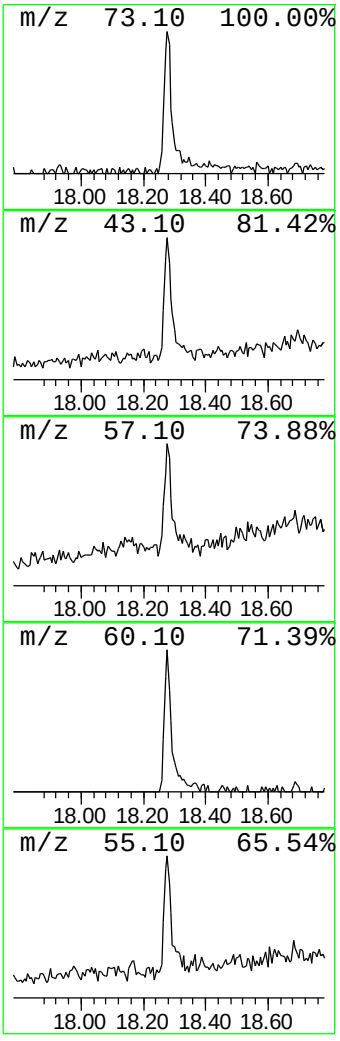
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	5.72 ng	134557	Phenanthrene-d10	17.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	Tridecanoic acid	214	C13H26O2	000638-53-9	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	47





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043553.D
Acq On : 8 Nov 2019 00:01
Operator : JU
Sample : K5702-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : H-1

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

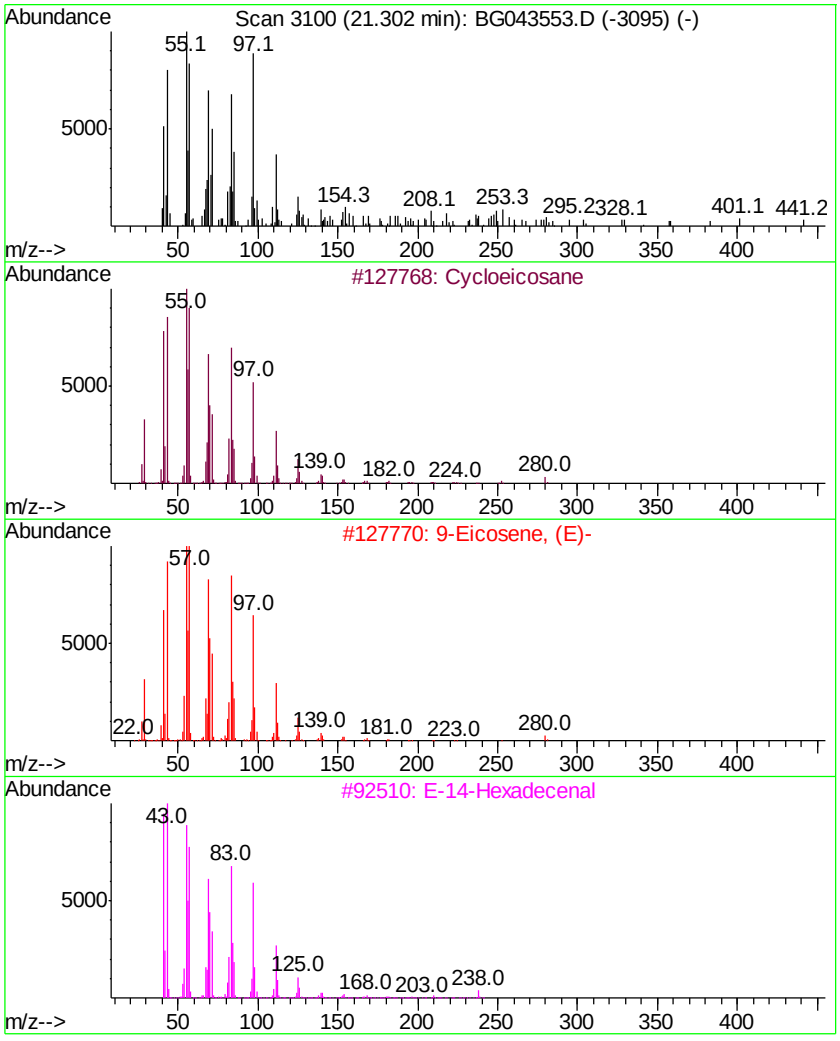
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

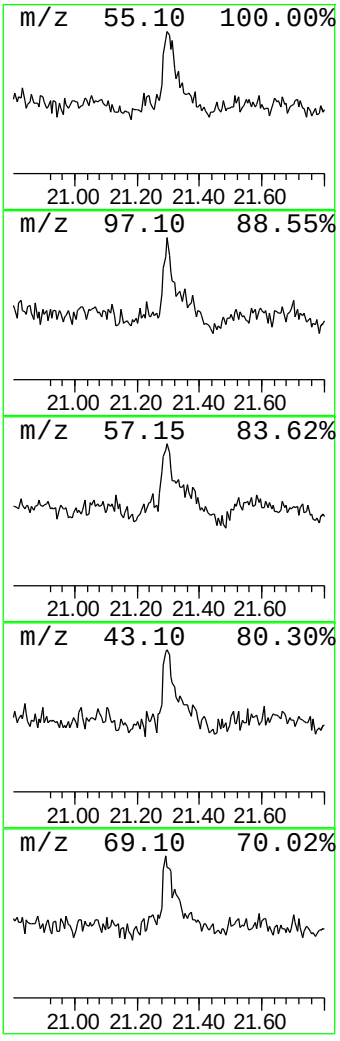
****

Peak Number 6 Cycloeicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	4.06 ng	125109	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	90
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	87
3	E-14-Hexadecenal	238	C16H30O	330207-53-9	83
4	1-Octadecene	252	C18H36	000112-88-9	70
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043553.D
Acq On : 8 Nov 2019 00:01
Operator : JU
Sample : K5702-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : H-1

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

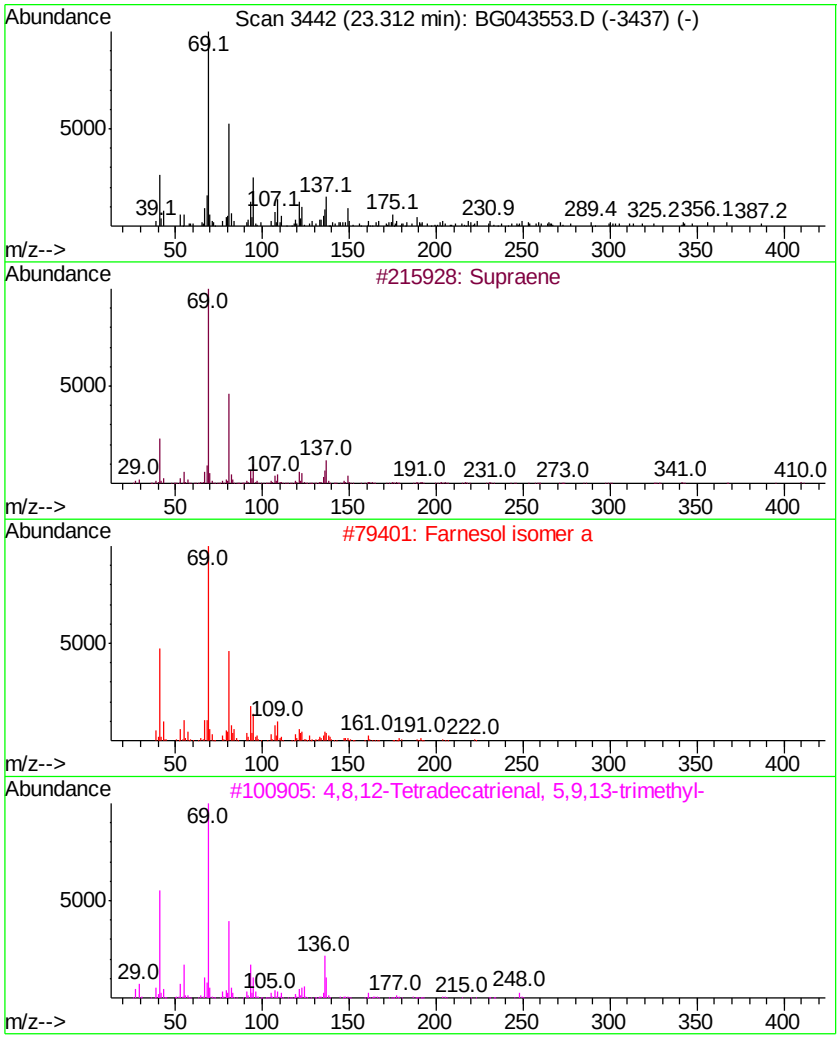
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

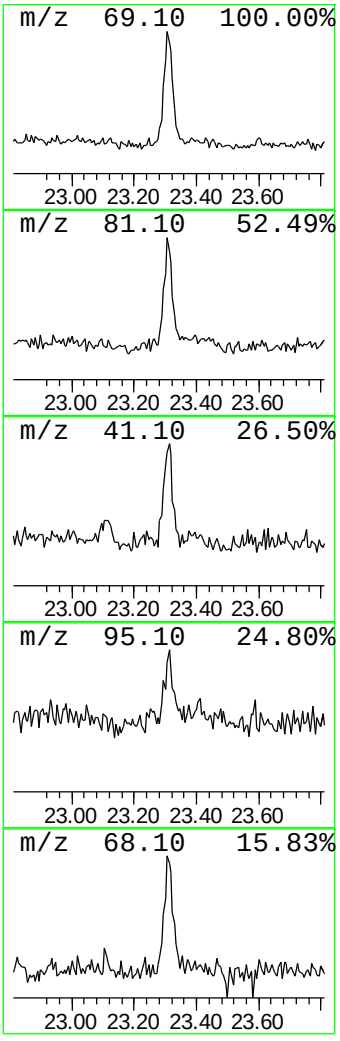
****

Peak Number 7 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.31	3.98 ng	124104	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	72
2	Farnesol isomer a	222	C15H26O	1000108-92-4	64
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	56
5	Squalene	410	C30H50	000111-02-4	56





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110719\
Data File : BG043553.D
Acq On : 8 Nov 2019 00:01
Operator : JU
Sample : K5702-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : H-1

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...	3.17	15.0	ng	129972	1	8.01	172821	20.0
2-Pentanone, 4-hy...	5.11	13.1	ng	113397	1	8.01	172821	20.0
unknown7.55	7.55	76.5	ng	661335	1	8.01	172821	20.0
n-Hexadecanoic acid	18.28	5.7	ng	134557	4	17.38	470505	20.0
Cycloeicosane	21.30	4.1	ng	125109	5	21.65	615591	20.0
Supraene	23.31	4.0	ng	124104	6	24.85	623304	20.0