LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062719\
Data File : BG041489.D
Acq On : 27 Jun 2019 13:44
Operator : HP/JU
Sample : K3539-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MH-J-B-UNTREATED

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-BG062619.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	4.562	246	251	258	rVB	60611	88934	3.18%	0.735%
2	5.567	416	422	433	rBV	232540	400791	14.35%	3.312%
3	7.077	675	679	684	rVB2	35395	53371	1.91%	0.441%
4	7.189	692	698	713	rVB	136713	271928	9.73%	2.247%
5	7.424	734	738	744	rBV2	28712	51517	1.84%	0.426%
6	7.559	754	761	771	rBV	474218	826845	29.59%	6.833%
7	8.029	835	841	849	rBV	112384	191253	6.85%	1.580%
8	8.352	889	896	904	rBV	472309	795044	28.46%	6.570%
9	9.133	1024	1029	1035	rBV	128161	214558	7.68%	1.773%
10	9.210	1035	1042	1057	rVB	364979	708052	25.34%	5.851%
11	9.527	1092	1096	1102	rVB3	21460	32163	1.15%	0.266%
12	10.855	1315	1322	1333	rBV	136543	247672	8.86%	2.047%
13	13.293	1731	1737	1753	rBV	1116282	1715031	61.39%	14.172%
14	14.674	1966	1972	1984	rVB3	227208	377386	13.51%	3.119%
15	16.166	2219	2226	2239	rBV	929933	1434864	51.36%	11.857%
16	17.424	2434	2440	2452	rBV2	317415	488838	17.50%	4.039%
17	18.282	2582	2586	2594	rBV3	30501	52827	1.89%	0.437%
18	19.551	2799	2802	2808	rBV4	20931	33281	1.19%	0.275%
19	20.027	2877	2883	2893	rBV	2213872	2793892	100.00%	23.087%
20	21.695	3160	3167	3179	rVB	344084	580806	20.79%	4.799%
21	21.836	3187	3191	3198	rVB	20639	30536	1.09%	0.252%
22	22.441	3290	3294	3302	rVB	25668	43988	1.57%	0.363%
23	23.141	3407	3413	3421	rBV5	29152	62384	2.23%	0.516%
24	23.951	3545	3551	3558	rVB4	24424	50407	1.80%	0.417%
25	24.980	3717	3726	3738	rVB	190948	555145	19.87%	4.587%

Sum of corrected areas: 12101513

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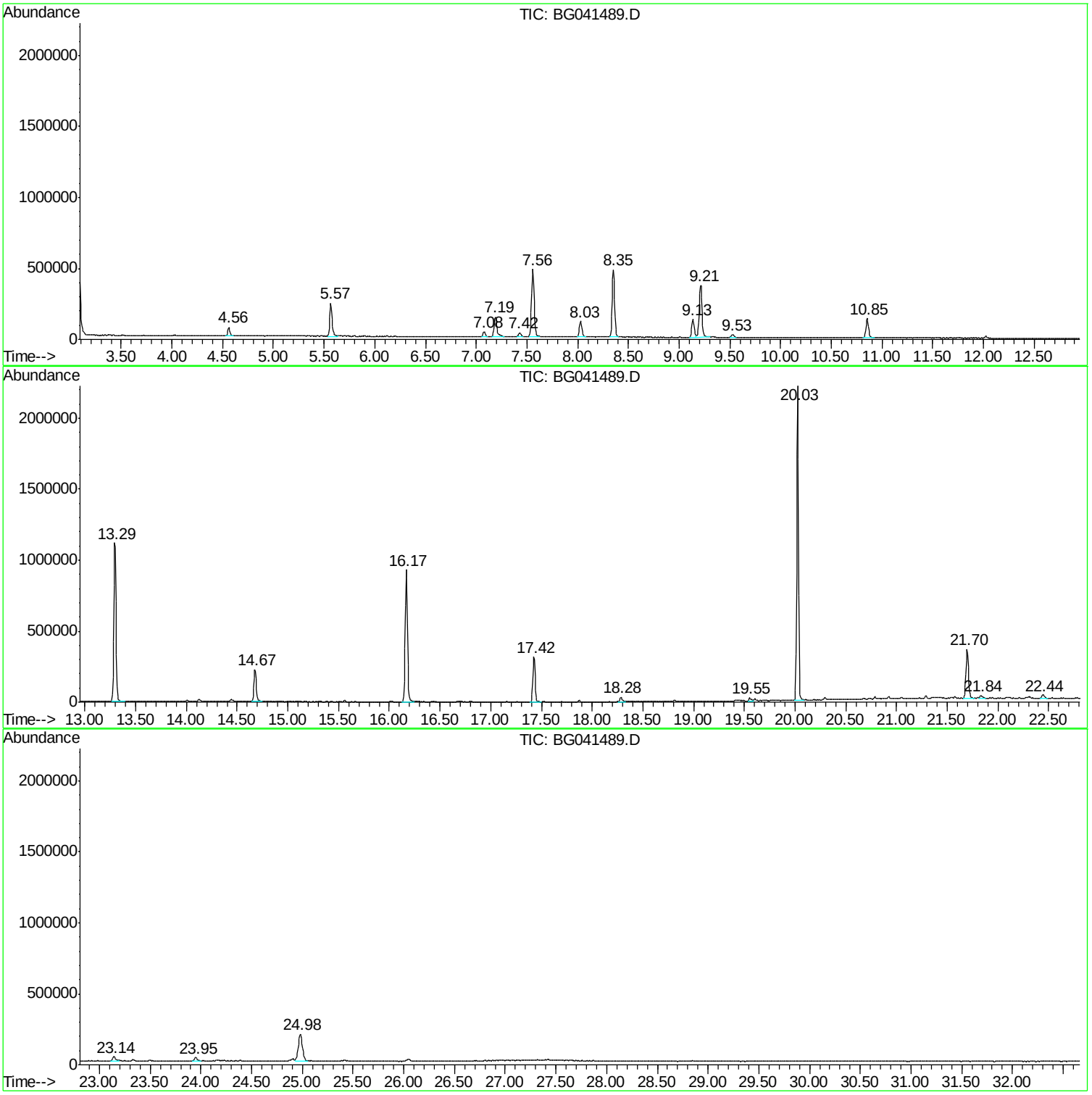
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-J-B-UNTREATED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062719\
Data File : BG041489.D
Acq On : 27 Jun 2019 13:44
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Sample : K3539-02
Misc :
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Instrument : BNA_G
ClientSampleId : MH-J-B-UNTREATED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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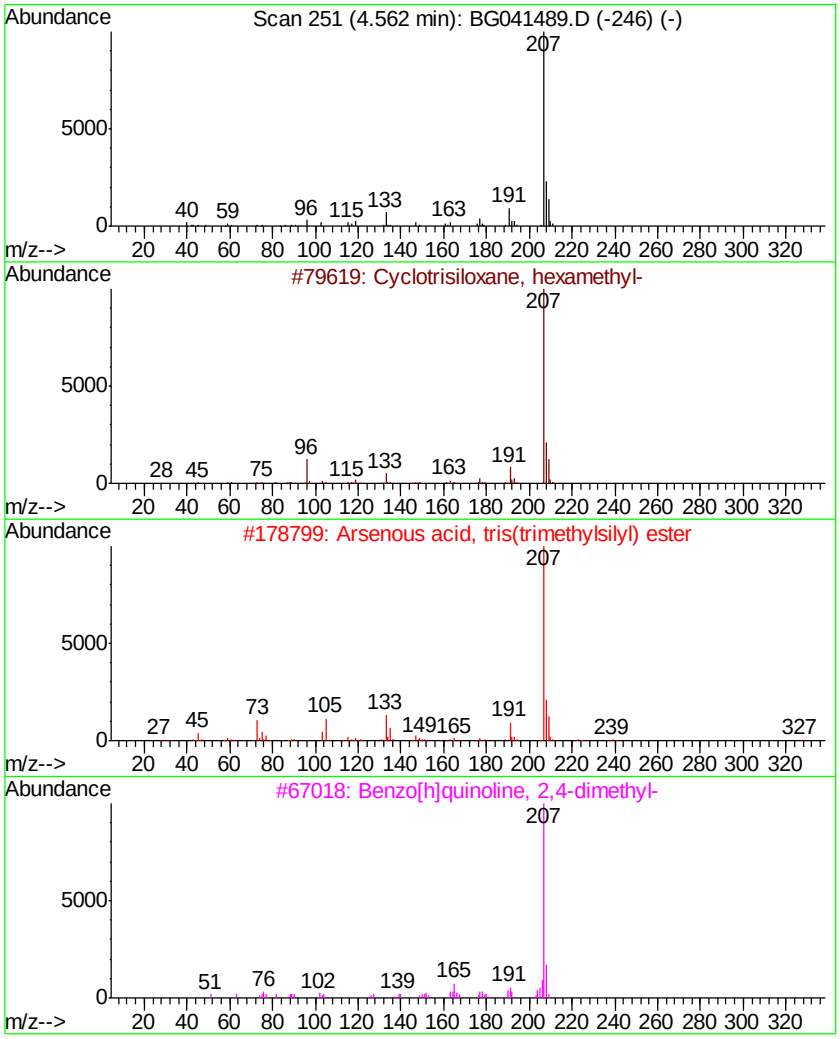
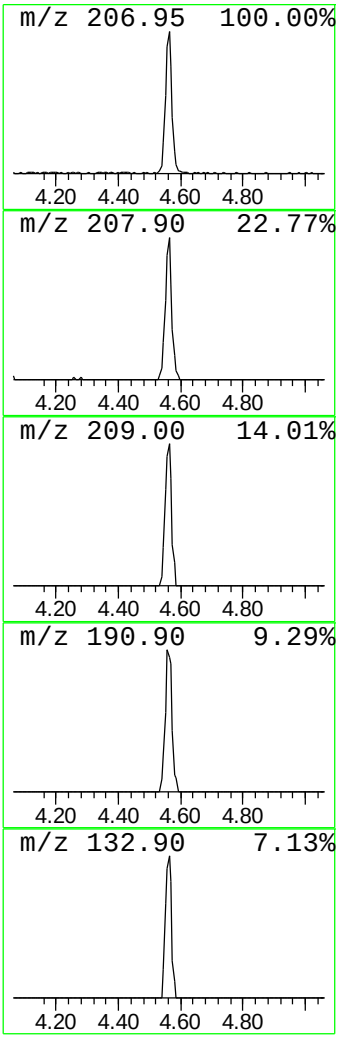
****

Peak Number 1 Cyclotrisiloxane, hexamethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	9.30 ng	88934	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	90
2	Arsenous acid, tris(trimethylsil...	342	C9H27AsO3Si3	055429-29-3	64
3	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	59
4	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	39
5	1H-Indole, 5-methyl-2-phenyl-	207	C15H13N	013228-36-9	9





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Data File : BG041489.D
Acq On : 27 Jun 2019 13:44
Operator : HP/JU
Sample : K3539-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MH-J-B-UNTREATED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.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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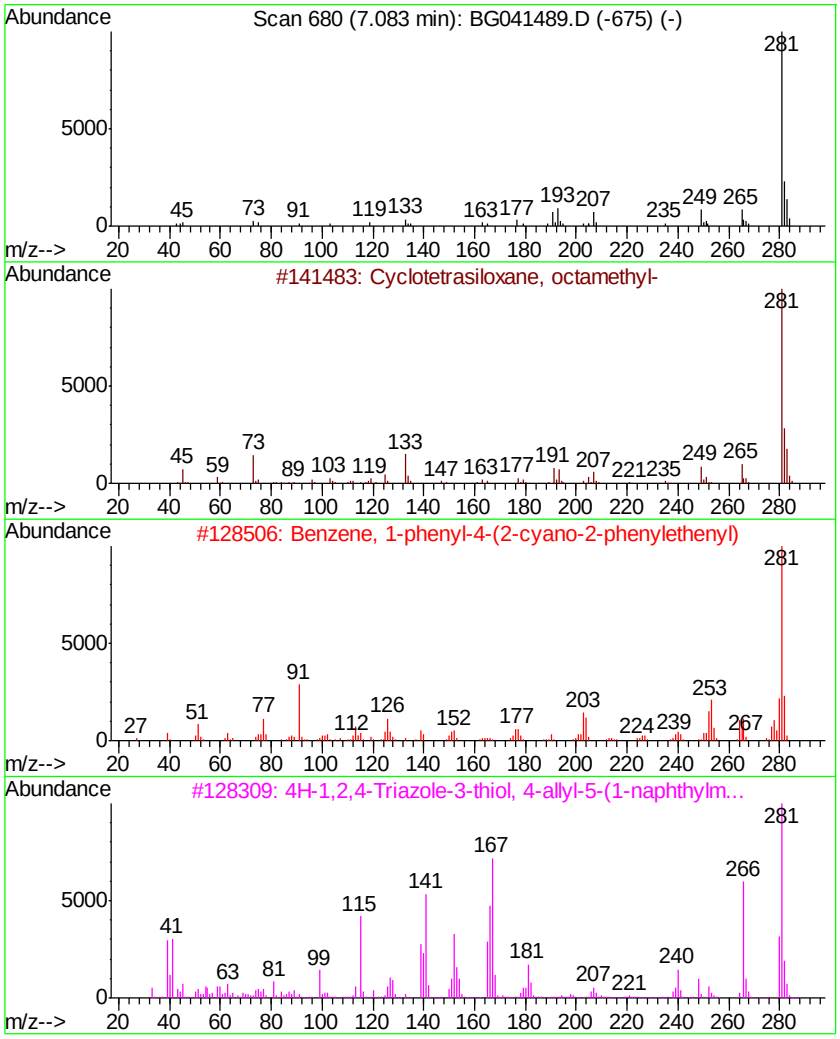
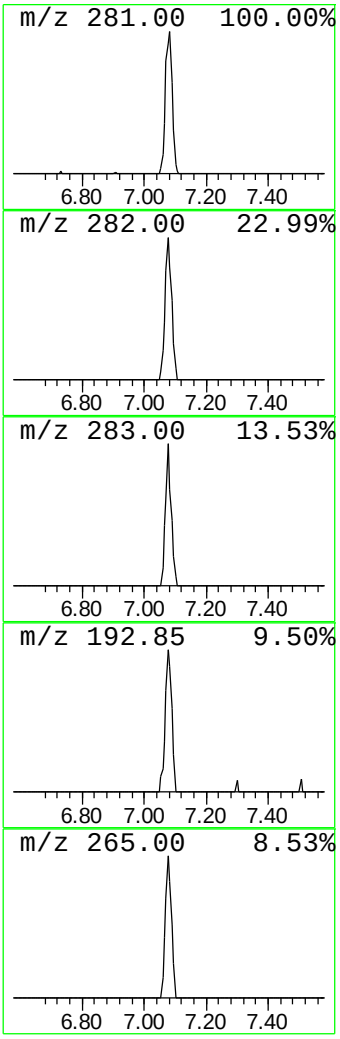
Peak Number 2 Cyclotetrasiloxane, octamet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.08	5.58 ng	53371	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetrasiloxane, octamethyl-	296	C8H24O4Si4	000556-67-2	91
2	Benzene, 1-phenyl-4-(2-cyano-2-p...	281	C21H15N	027869-56-3	50
3	4H-1,2,4-Triazole-3-thiol, 4-all...	281	C16H15N3S	031803-13-1	47
4	2-(4-Chlorophenyl)-5,7-dimethyli...	281	C16H12ClN3	1000305-50-9	42
5	Benzoic acid, 3-methyl-2-trimeth...	296	C14H24O3Si2	1000153-57-1	40





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062719\
Data File : BG041489.D
Acq On : 27 Jun 2019 13:44
Operator : HP/JU
Sample : K3539-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MH-J-B-UNTREATED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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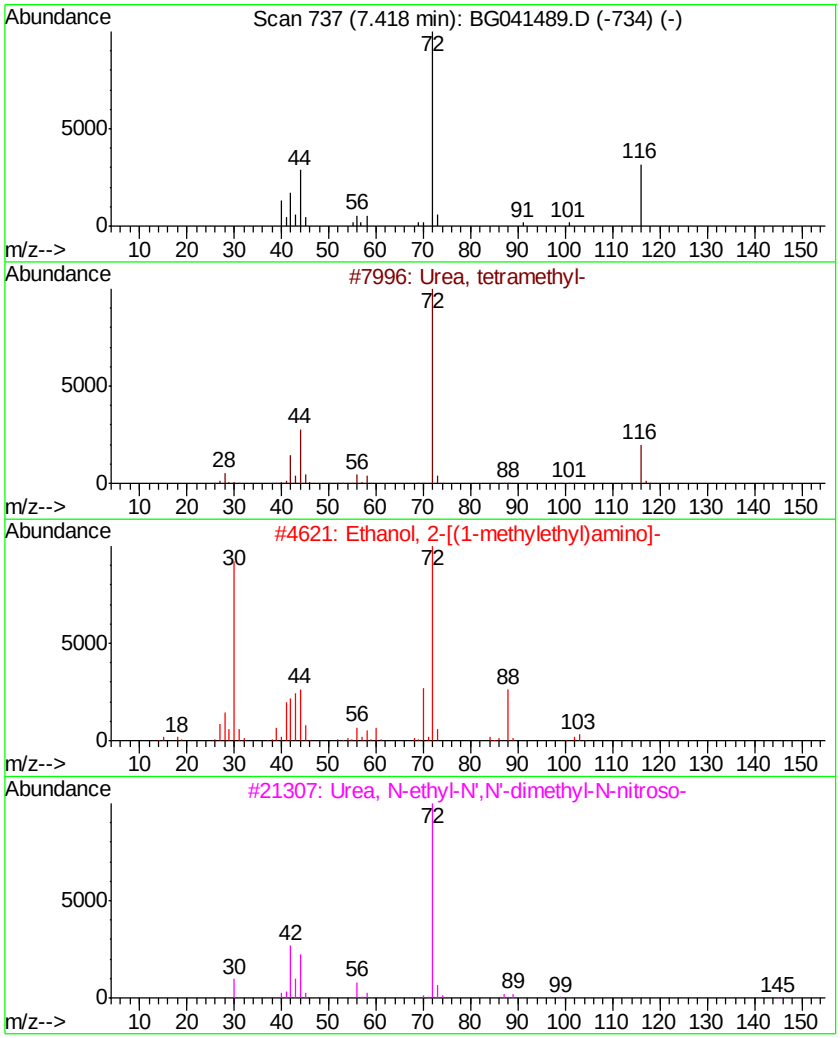
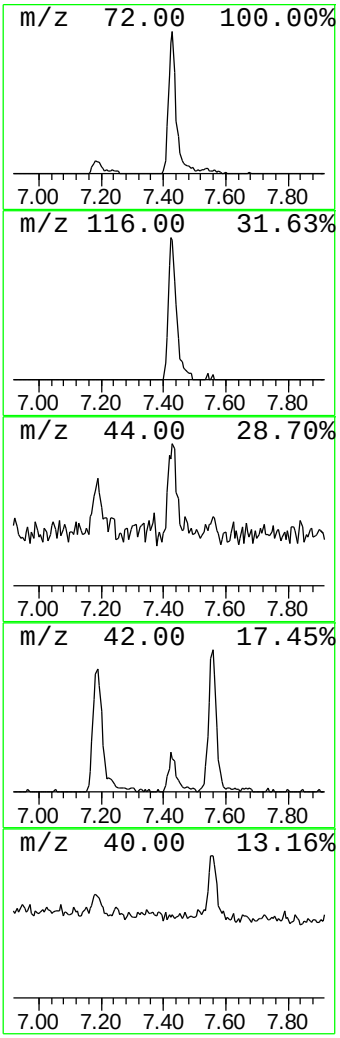
****

Peak Number 3 Urea, tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	5.39 ng	51517	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Urea, tetramethyl-	116	C5H12N2O	000632-22-4	80
2	Ethanol, 2-[(1-methylethyl)amino]-	103	C5H13NO	000109-56-8	50
3	Urea, N-ethyl-N',N'-dimethyl-N-n...	145	C5H11N3O2	050285-71-7	50
4	Urea, trimethylnitroso-	131	C4H9N3O2	003475-63-6	42
5	N(1)-[1-[4-Chlorophenyl]-1H-tetr...	280	C12H17ClN6	1000213-45-7	40





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062719\
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Acq On : 27 Jun 2019 13:44
Operator : HP/JU
Sample : K3539-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MH-J-B-UNTREATED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

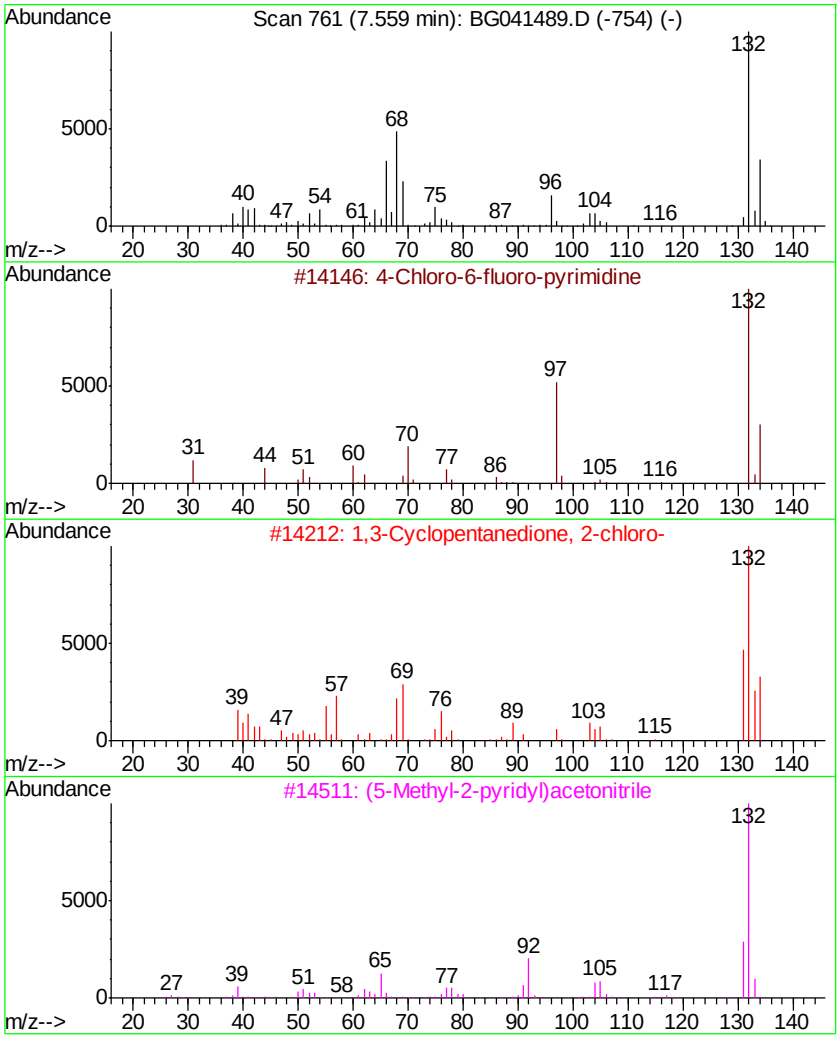
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

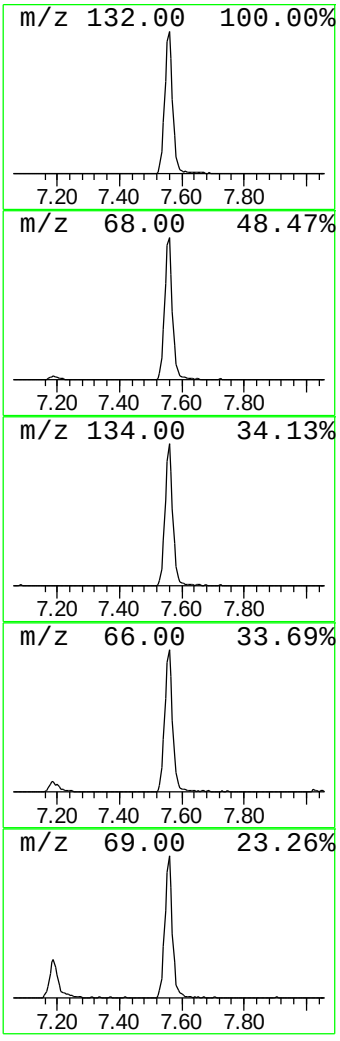
****

Peak Number 4 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	86.47 ng	826845	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	22
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MH-J-B-UNTREATED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

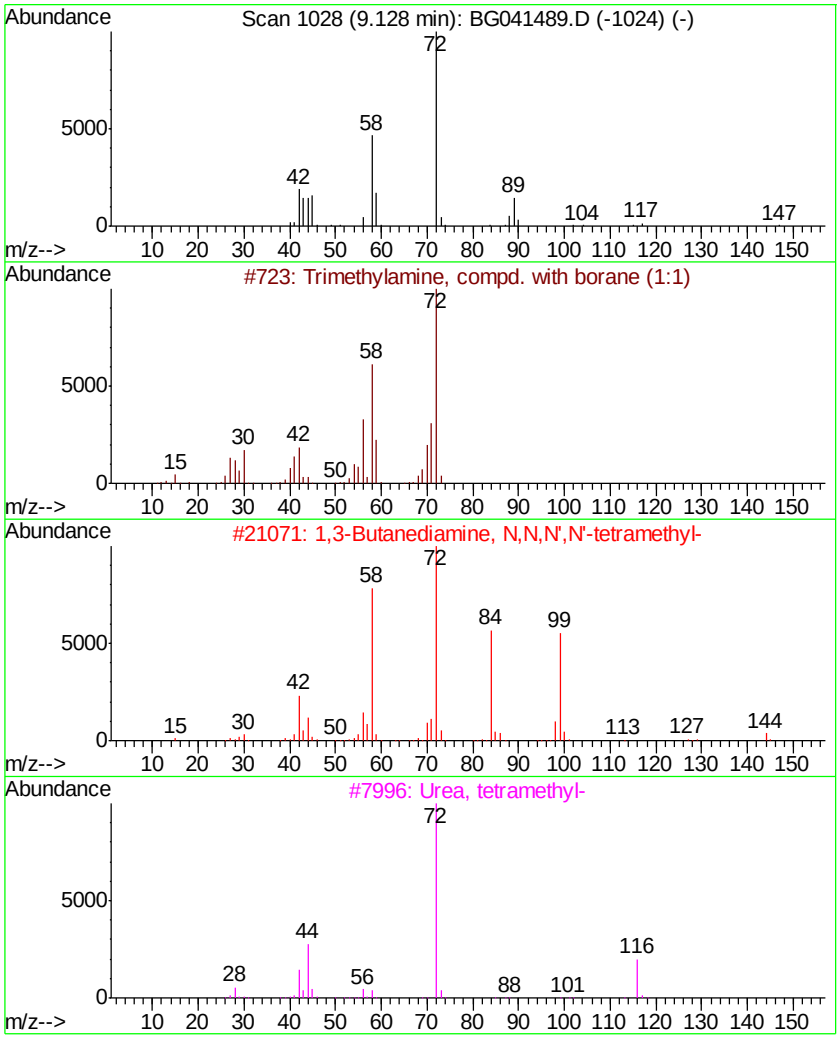
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

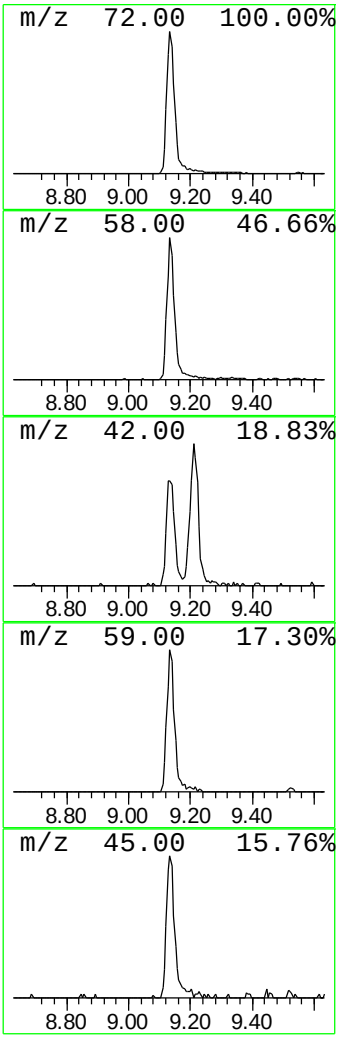
****

Peak Number 6 Trimethylamine, compd. with... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.13	22.44 ng	214558	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trimethylamine, compd. with bora...	73	C3H12BN	000075-22-9	50
2	1,3-Butanediamine, N,N,N',N'-tet...	144	C8H20N2	000097-84-7	38
3	Urea, tetramethyl-	116	C5H12N2O	000632-22-4	25
4	Acetaldehyde, methylhydrazone	72	C3H8N2	017167-73-6	23
5	Methylamine, N,N-dimethyl-	59	C3H9N	000075-50-3	22





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ClientSampleId : MH-J-B-UNTREATED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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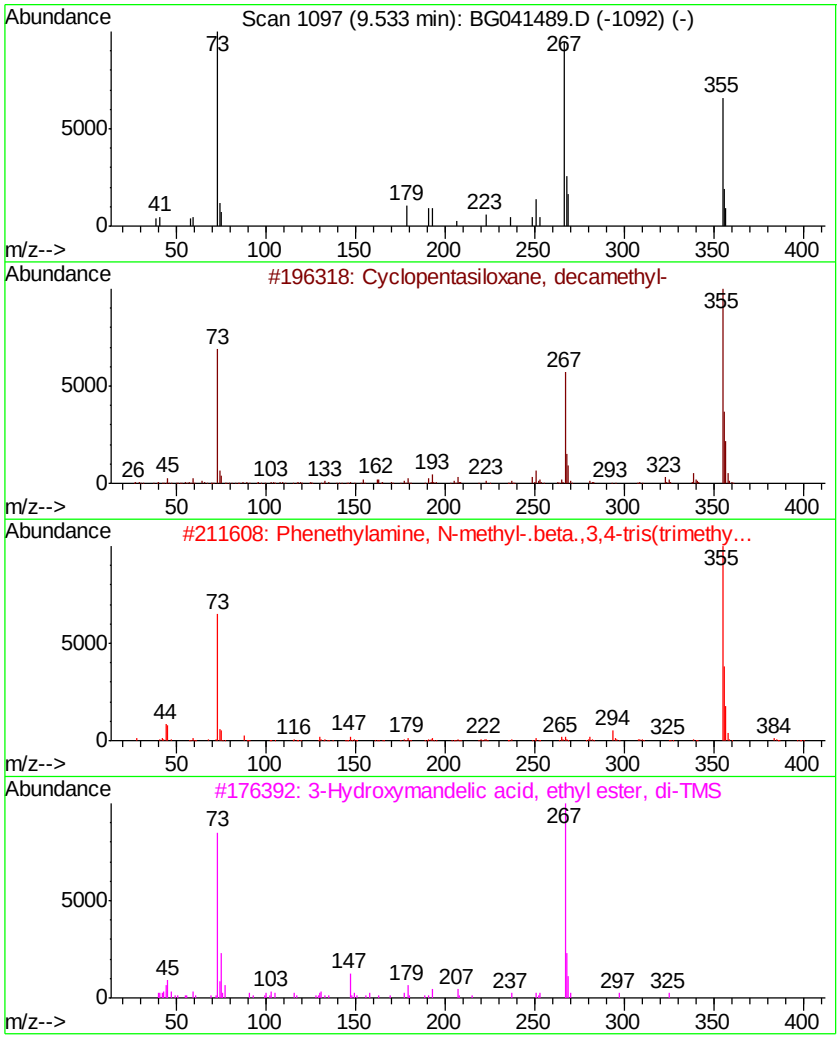
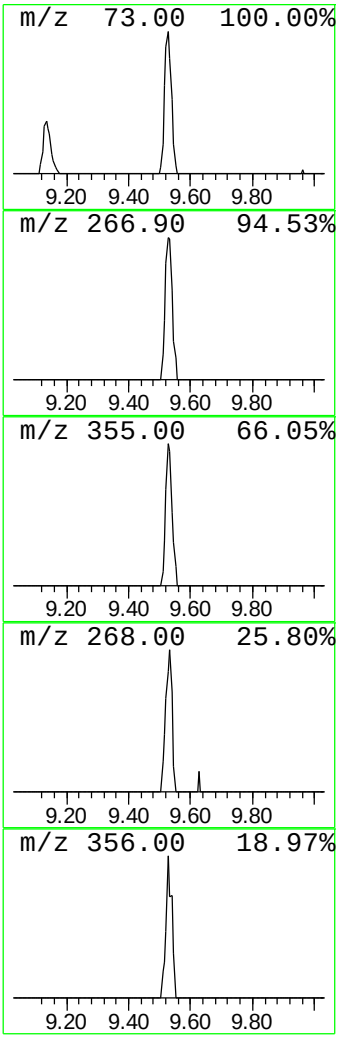
****

Peak Number 7 Cyclopentasiloxane, decamet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.53	2.60 ng	32163	Naphthalene-d8	10.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	90
2	Phenethylamine, N-methyl-.beta.,...	399	C18H37NO3Si3	010538-85-9	38
3	3-Hydroxymandelic acid, ethyl es...	340	C16H28O4Si2	1000071-88-9	37
4	4-Hydroxymandelic acid, ethyl es...	340	C16H28O4Si2	1000071-53-3	37
5	Auramine	267	C17H21N3	000492-80-8	35





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Misc :
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Instrument : BNA_G
ClientSampleId : MH-J-B-UNTREATED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

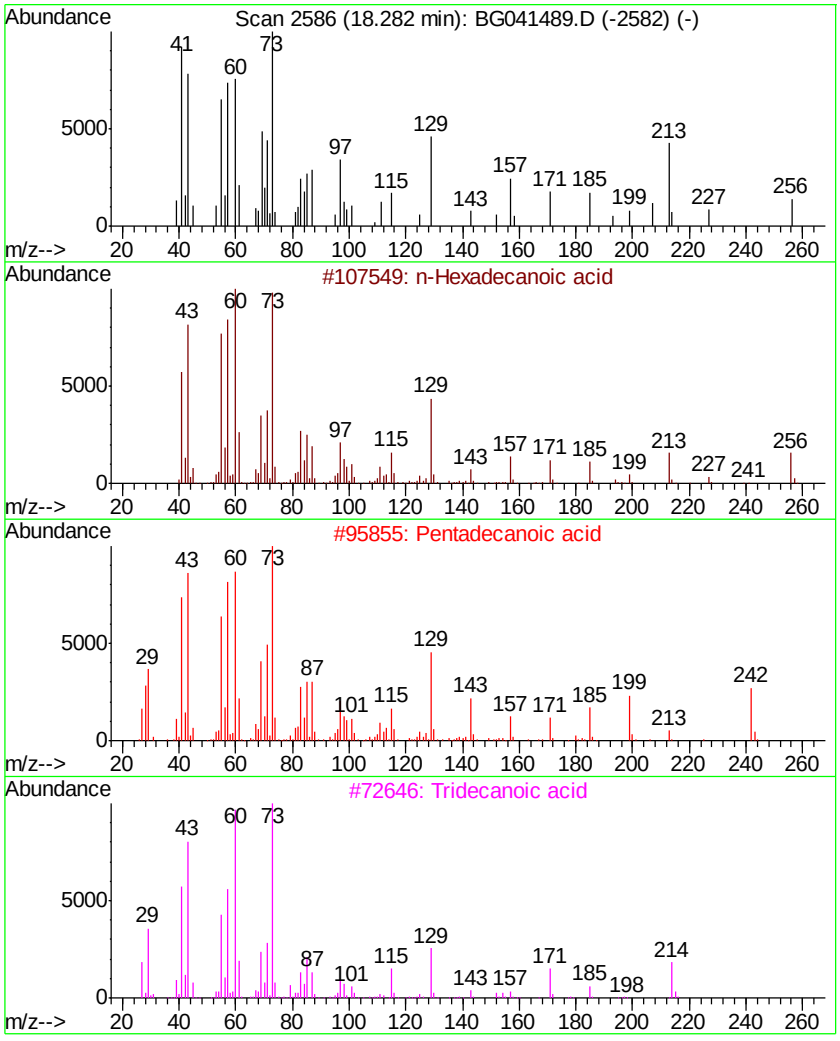
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

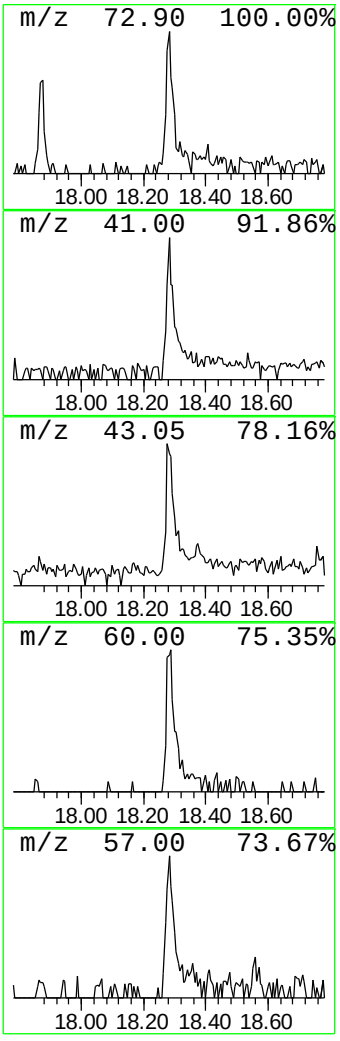
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	2.16 ng	52827	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	50
5	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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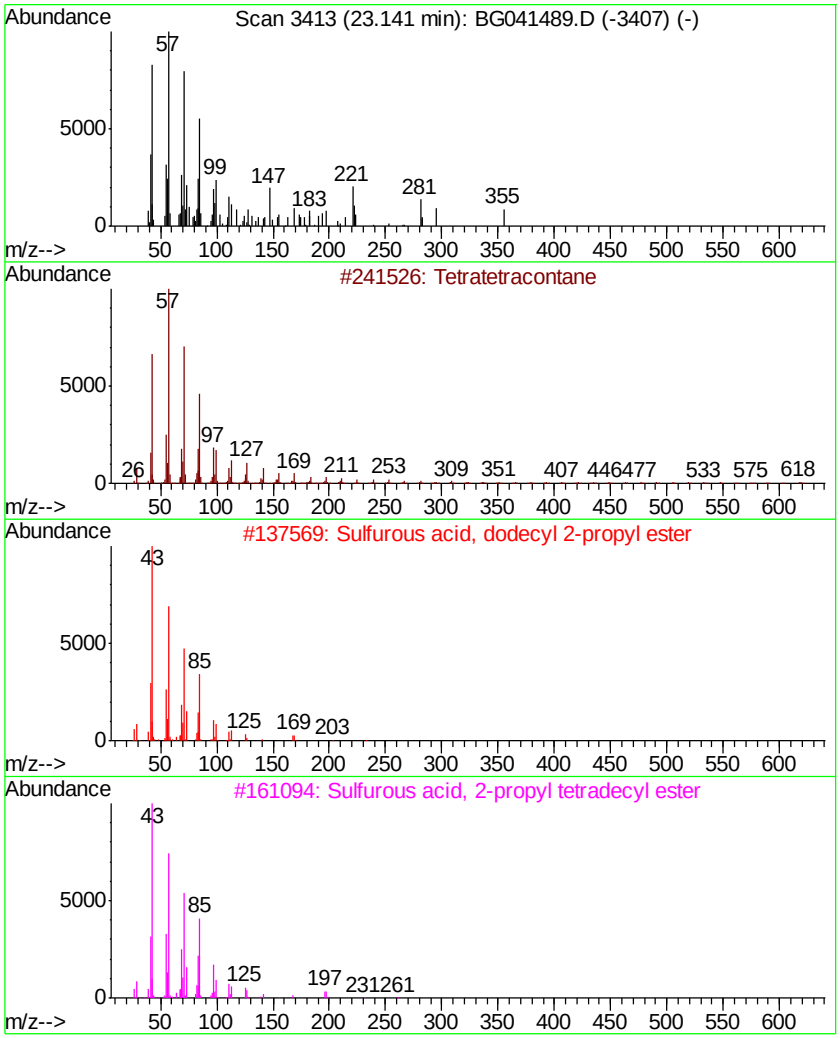
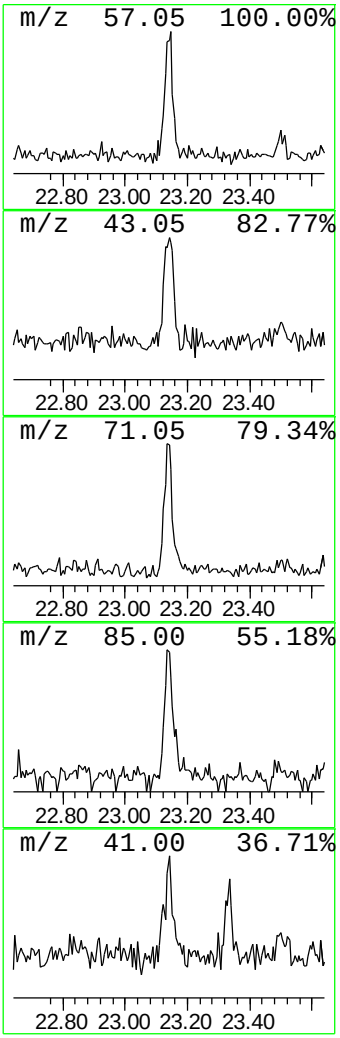
****

Peak Number 9 Tetratetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.14	2.15 ng	62384	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	52
2	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	52
3	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	52
4	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	52
5	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG062719\
Data File : BG041489.D
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.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
Cyclotrisiloxane,...	4.56	9.3	ng	88934	1	8.03	191253	20.0
Cyclotetrasiloxan...	7.08	5.6	ng	53371	1	8.03	191253	20.0
Urea, tetramethyl-	7.42	5.4	ng	51517	1	8.03	191253	20.0
unknown7.56	7.56	86.5	ng	826845	1	8.03	191253	20.0
Trimethylamine, c...	9.13	22.4	ng	214558	1	8.03	191253	20.0
Cyclopentasiloxan...	9.53	2.6	ng	32163	2	10.85	247672	20.0
n-Hexadecanoic acid	18.28	2.2	ng	52827	4	17.42	488838	20.0
Tetratetracontane	23.14	2.1	ng	62384	5	21.70	580806	20.0