LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062719\
Data File : BG041488.D
Acq On : 27 Jun 2019 13:06
Operator : HP/JU
Sample : K3539-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MH-J-A-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	4.557	246	250	256	rVB	70040	104311	3.52%	0.799%
2	5.567	416	422	433	rBV	216615	366796	12.37%	2.810%
3	7.077	675	679	684	rVB	46706	65463	2.21%	0.502%
4	7.189	692	698	710	rVB	128150	257080	8.67%	1.970%
5	7.424	733	738	747	rVB	37761	67411	2.27%	0.516%
6	7.559	754	761	778	rVB	485843	875572	29.53%	6.708%
7	8.029	835	841	850	rBV	119435	205970	6.95%	1.578%
8	8.352	889	896	906	rVB	504462	848911	28.63%	6.504%
9	9.134	1023	1029	1035	rBV	170466	286478	9.66%	2.195%
10	9.210	1035	1042	1055	rVB	405842	752217	25.37%	5.763%
11	9.527	1091	1096	1101	rVB3	26123	38595	1.30%	0.296%
12	10.855	1315	1322	1331	rVB	142825	257221	8.67%	1.971%
13	13.294	1730	1737	1746	rBV	1194570	1829036	61.68%	14.014%
14	14.122	1873	1878	1887	rBV2	21934	36339	1.23%	0.278%
15	14.439	1927	1932	1942	rBV2	18959	36605	1.23%	0.280%
16	14.674	1965	1972	1979	rBV2	248308	402924	13.59%	3.087%
17	16.167	2219	2226	2242	rBV	984681	1530667	51.62%	11.727%
18	17.424	2434	2440	2455	rBV	344283	520974	17.57%	3.992%
19	18.282	2581	2586	2596	rBV4	41891	79997	2.70%	0.613%
20	19.551	2798	2802	2807	rBV7	22664	38998	1.32%	0.299%
21	20.027	2876	2883	2892	rBV	2288624	2965395	100.00%	22.720%
22	20.291	2924	2928	2931	rBV4	23998	29700	1.00%	0.228%
23	21.696	3161	3167	3180	rVB2	339584	604512	20.39%	4.632%
24	21.837	3187	3191	3197	rVB2	24004	33376	1.13%	0.256%
25	22.448	3291	3295	3300	rVB3	27674	41754	1.41%	0.320%
26	23.141	3408	3413	3419	rVB4	32062	58434	1.97%	0.448%
27	23.946	3545	3550	3557	rVB3	30703	57695	1.95%	0.442%
28	24.904	3707	3713	3717	rBV4	20566	43625	1.47%	0.334%
29	24.980	3717	3726	3739	rVB	194293	578035	19.49%	4.429%
30	26.049	3902	3908	3915	rVB7	15747	37859	1.28%	0.290%

Sum of corrected areas: 13051950

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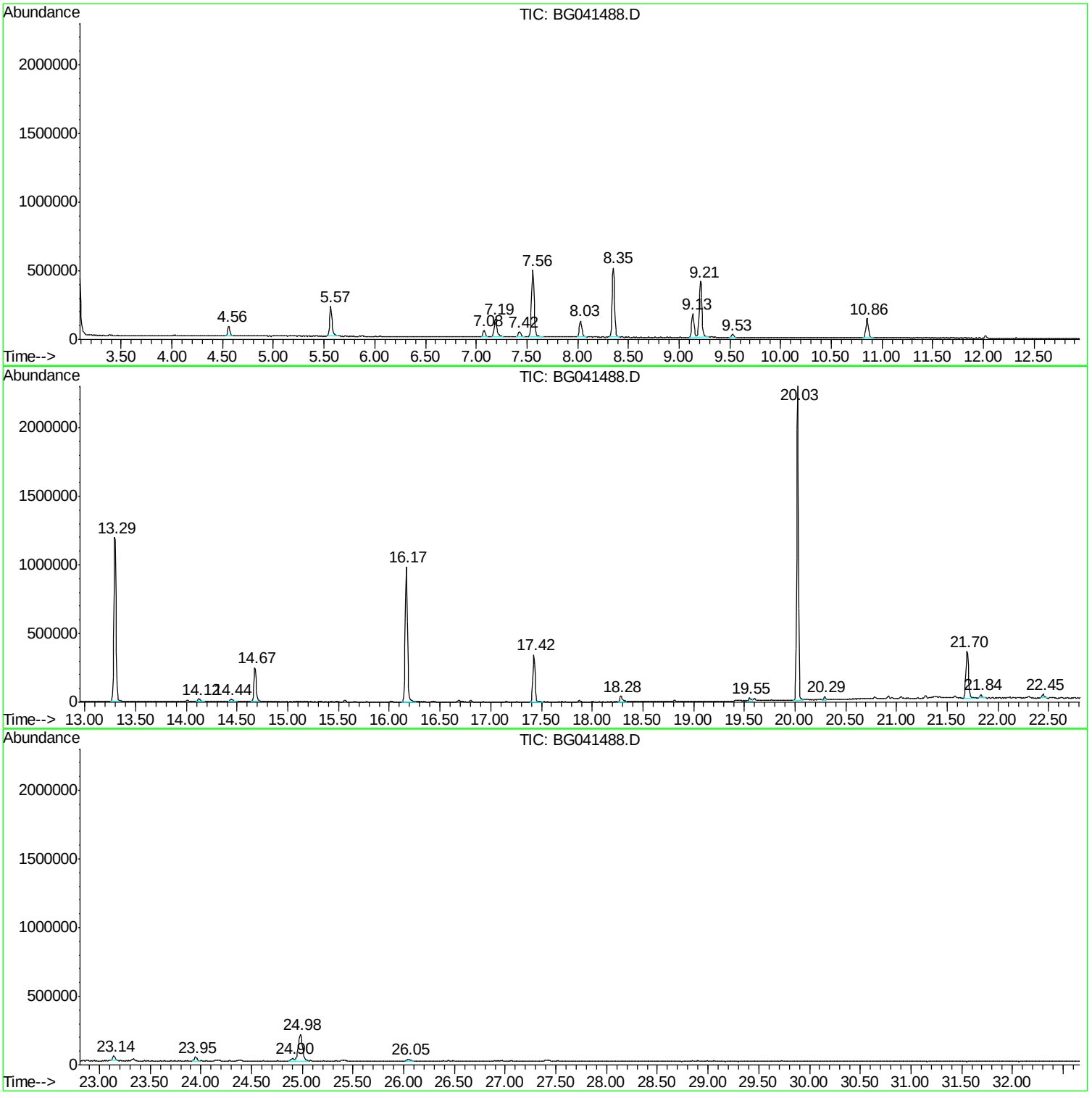
Misc :
ALS Vial : 10 Sample Multiplier: 1

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

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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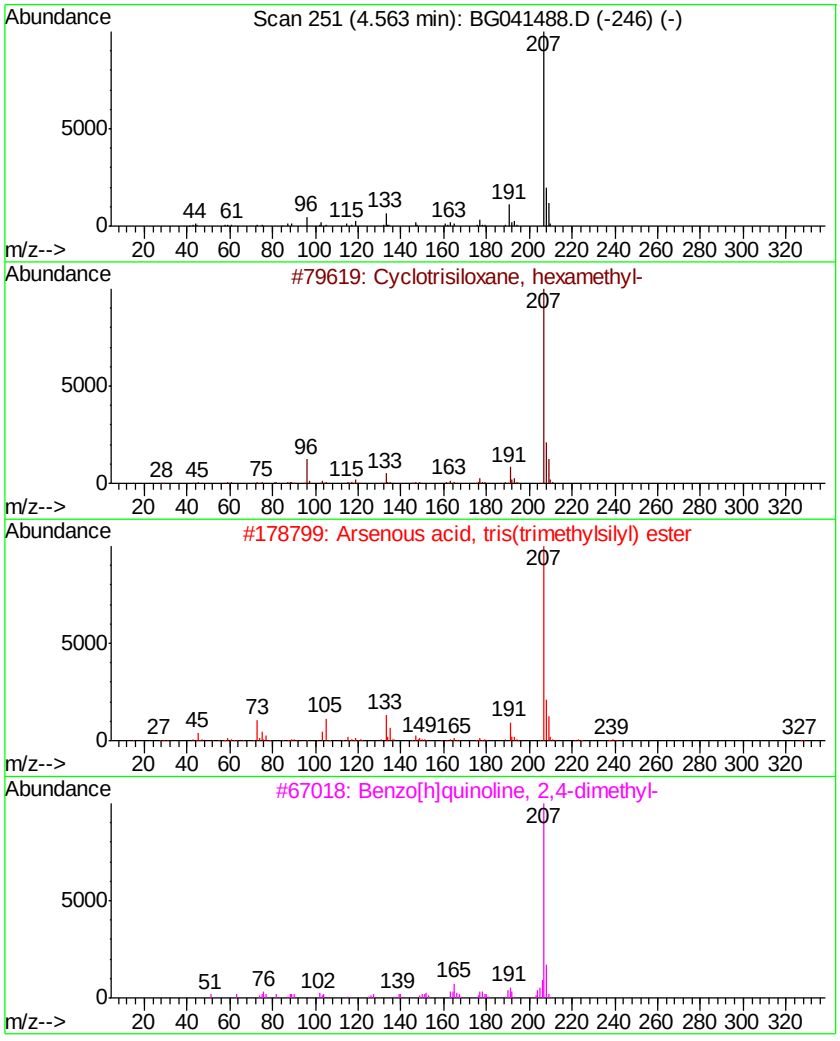
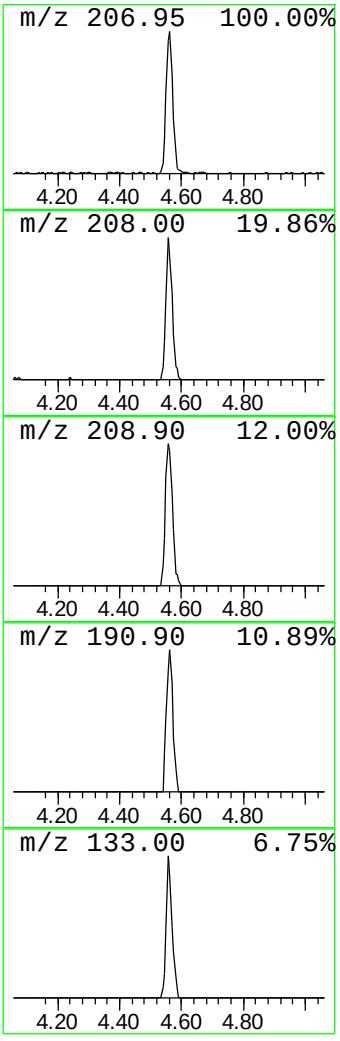
****

Peak Number 1 Cyclotrisiloxane, hexamethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	10.13 ng	104311	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	78
3	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	40
4	1H-Indole, 5-methyl-2-phenyl-	207	C15H13N	013228-36-9	9
5	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	9





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MH-J-A-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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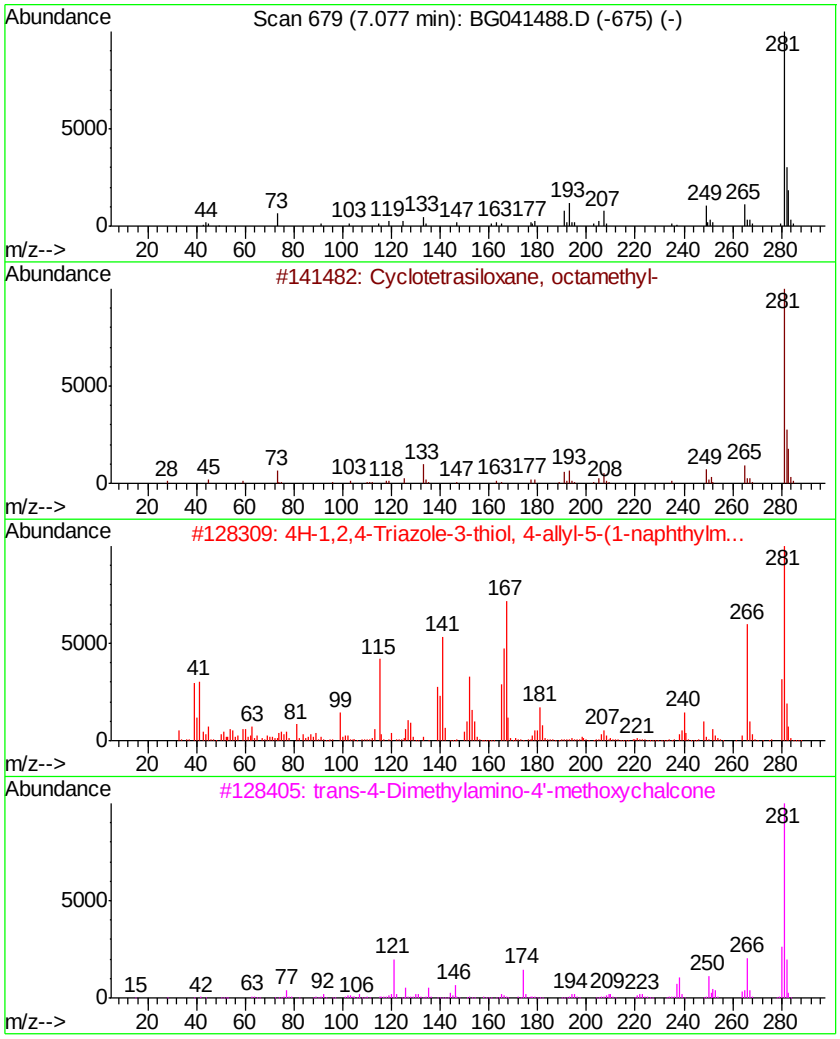
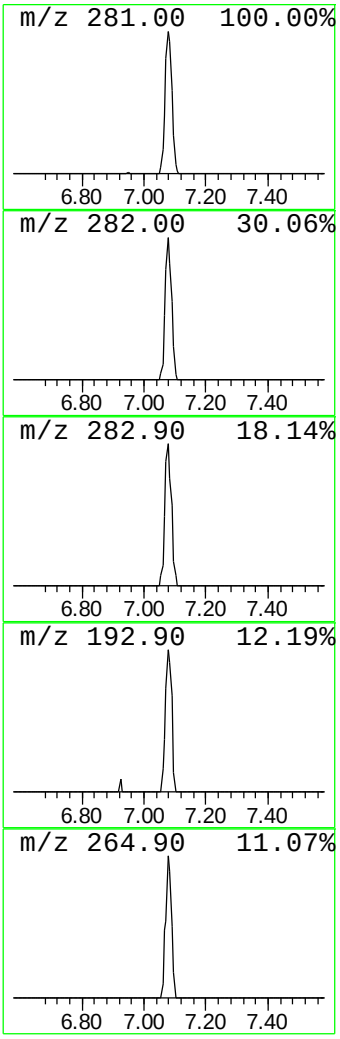
Peak Number 2 Cyclotetrasiloxane, octamet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.08	6.36 ng	65463	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetrasiloxane, octamethyl-	296	C8H24O4Si4	000556-67-2	90
2	4H-1,2,4-Triazole-3-thiol, 4-all...	281	C16H15N3S	031803-13-1	50
3	trans-4-Dimethylamino-4'-methoxy...	281	C18H19NO2	052119-37-6	47
4	4-Amino-5-(4-acetylphenylazo)ben...	281	C14H11N5O2	166766-09-2	47
5	Benzofuran-6-ol-3-one, 2-(4-etho...	310	C18H14O5	1000128-64-6	45





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Data File : BG041488.D
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Sample : K3539-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MH-J-A-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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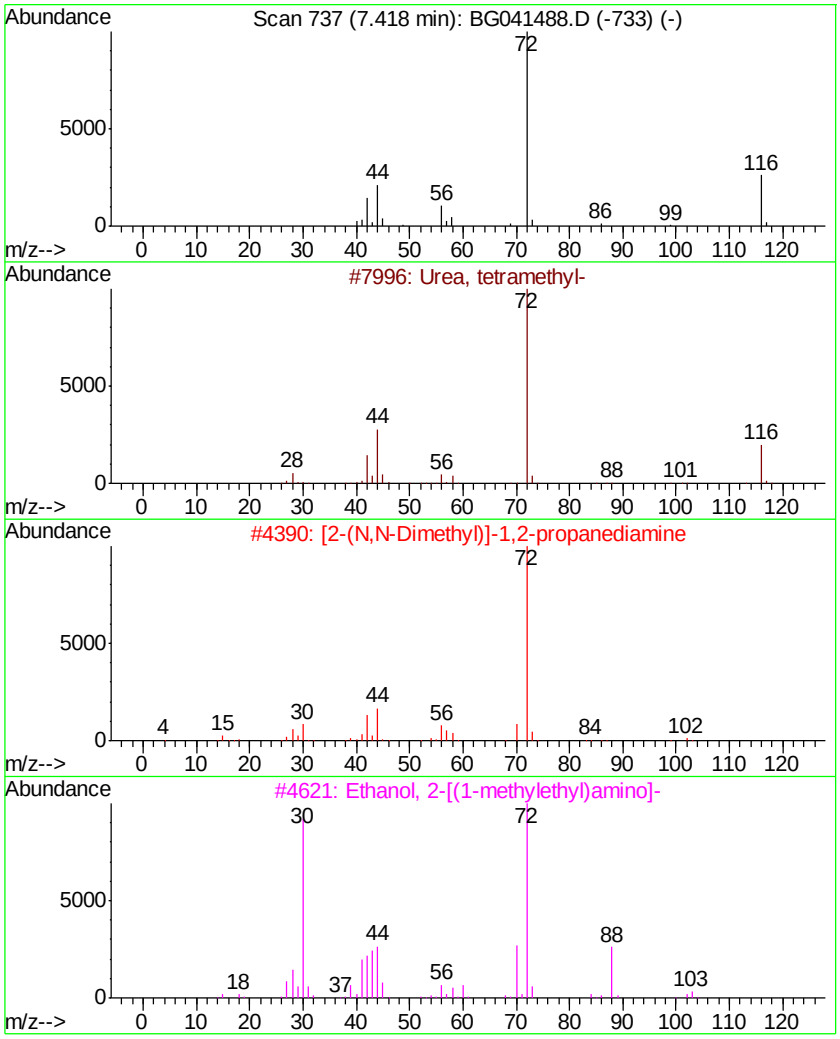
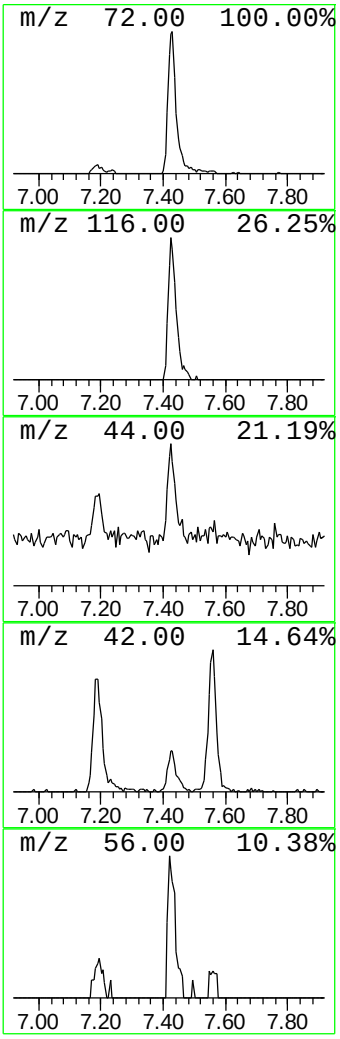
****

Peak Number 3 Urea, tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	6.55 ng	67411	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	[2-(N,N-Dimethyl)]-1,2-propanedi...	102	C5H14N2	1000133-38-7	50
3	Ethanol, 2-[(1-methylethyl)amino]-	103	C5H13NO	000109-56-8	50
4	2-Pentanamine, N-ethyl-4-methyl-	129	C8H19N	042966-64-3	38
5	DL-Norvaline	117	C5H11NO2	000760-78-1	38





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Acq On : 27 Jun 2019 13:06
Operator : HP/JU
Sample : K3539-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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

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

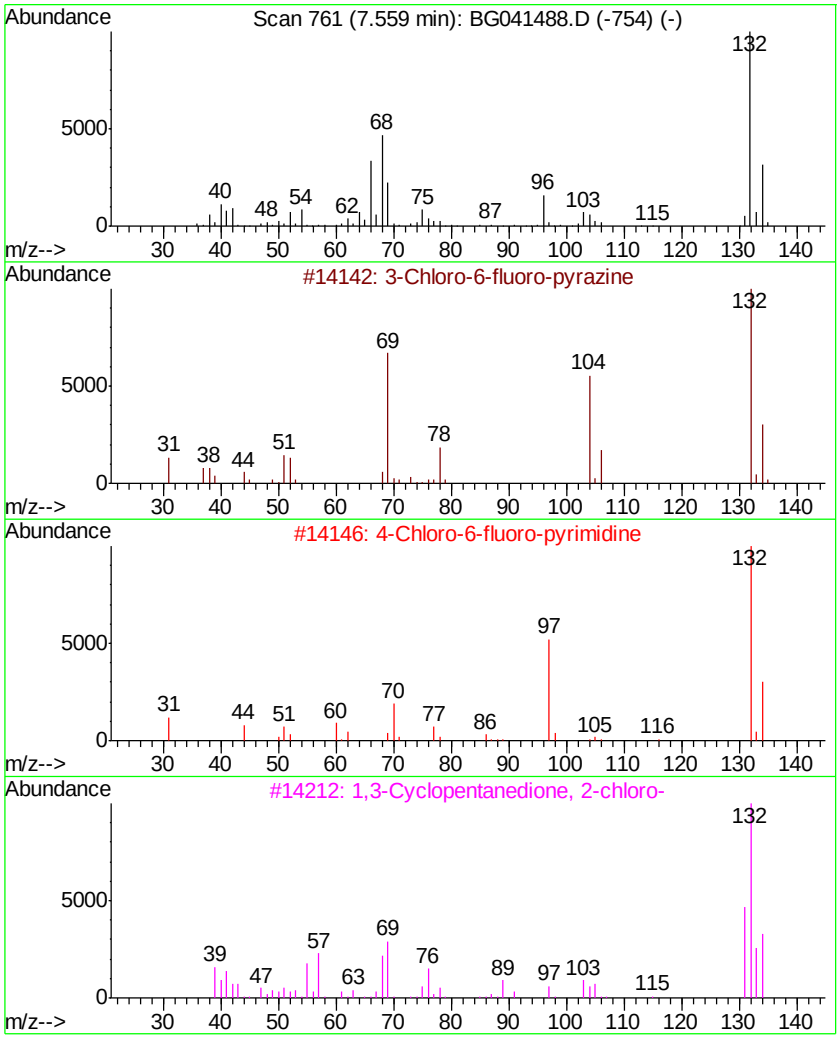
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

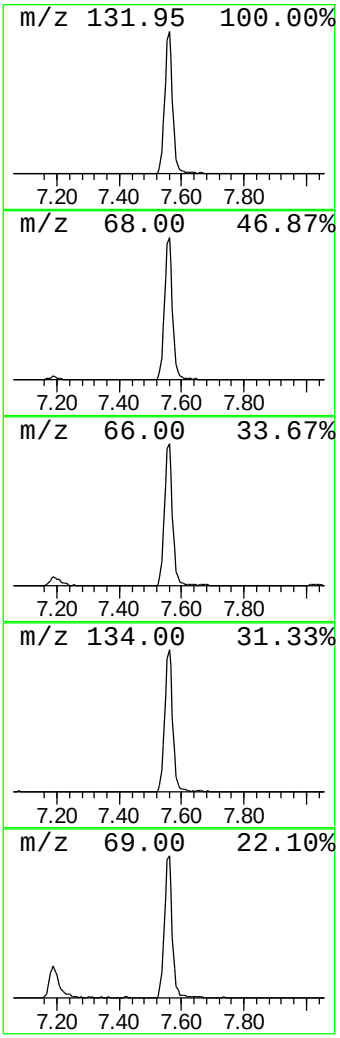
****

Peak Number 4 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	85.02 ng	875572	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	23
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062719\
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Acq On : 27 Jun 2019 13:06
Operator : HP/JU
Sample : K3539-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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

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

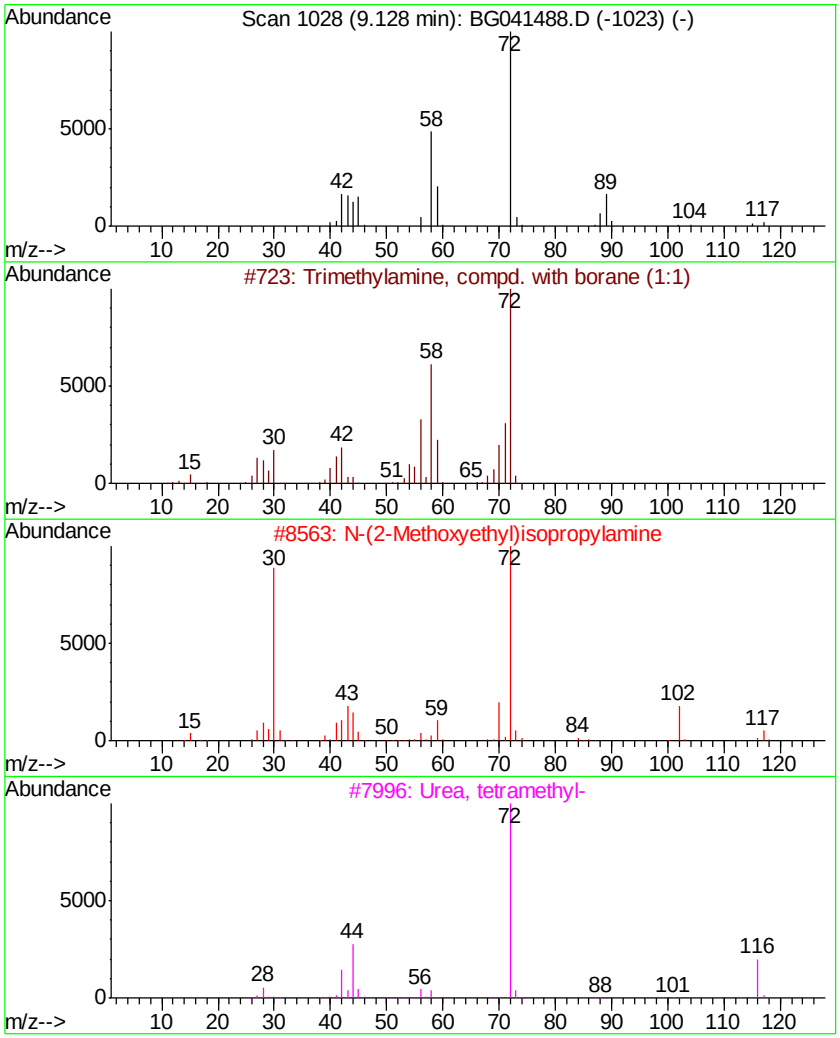
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

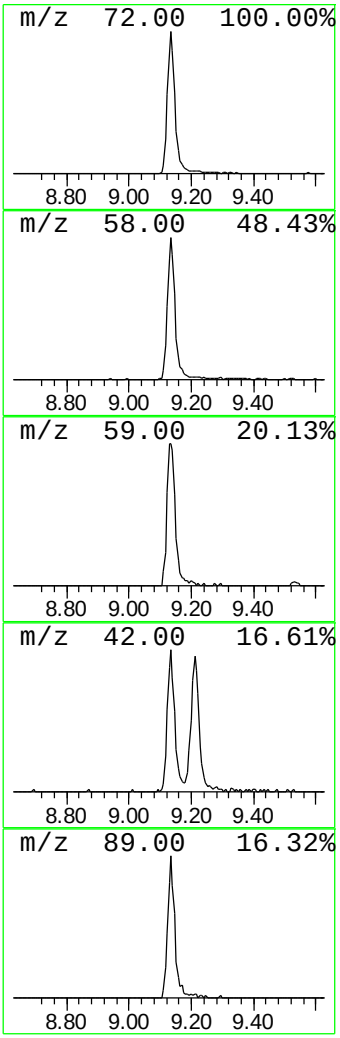
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.13	27.82 ng	286478	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	N-(2-Methoxyethyl)isopropylamine	117	C6H15NO	104678-18-4	33
3	Urea, tetramethyl-	116	C5H12N2O	000632-22-4	25
4	Hexanoic acid, 2-ethoxyethyl ester	188	C10H20O3	1000330-92-9	17
5	Valeric acid, 2-ethoxyethyl ester	174	C9H18O3	1000330-97-5	10





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ClientSampleId : MH-J-A-UNTREATED

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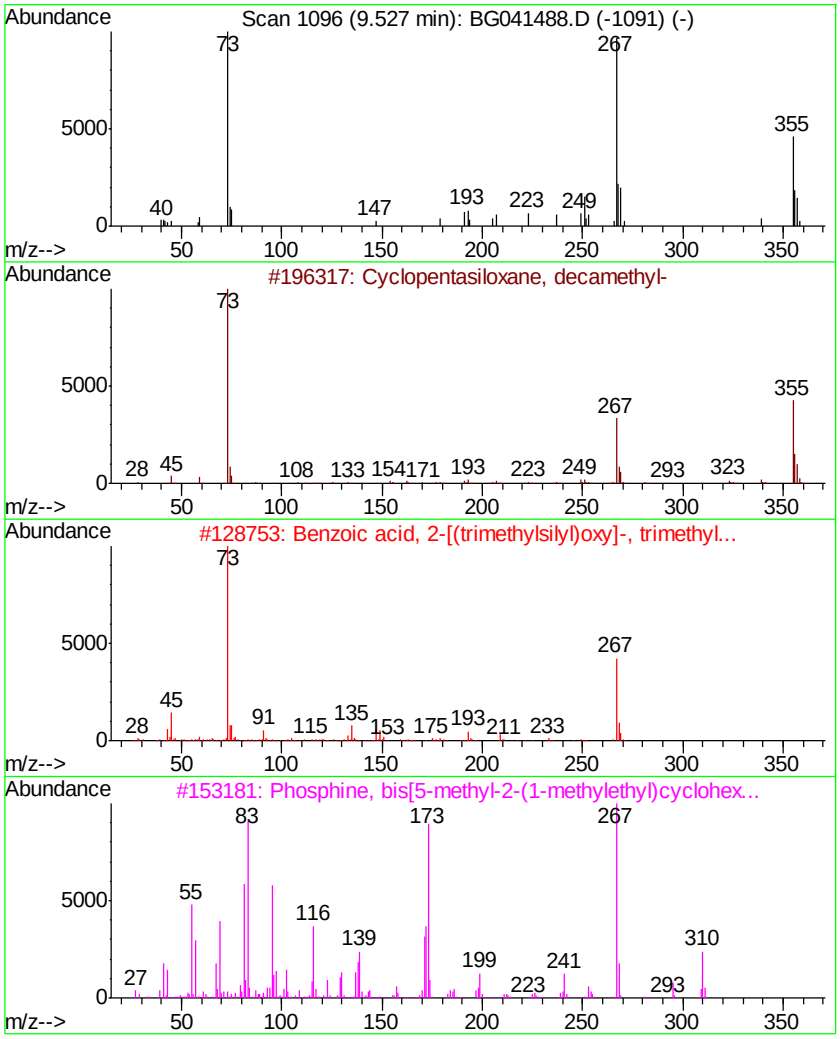
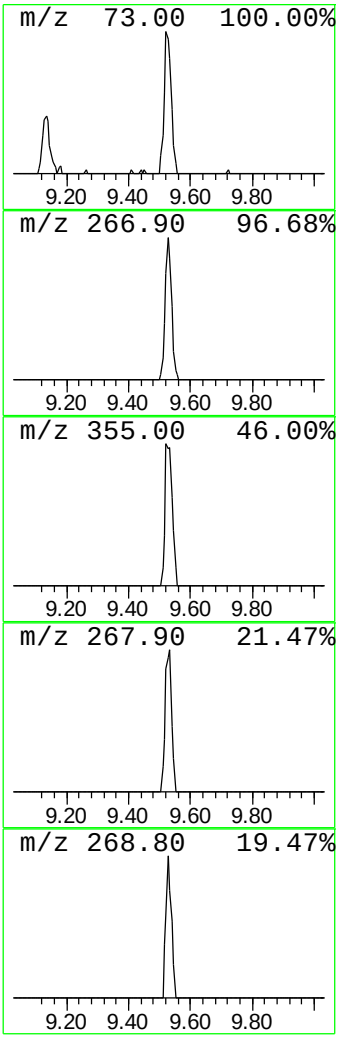
****

Peak Number 7 Cyclopentasiloxane, decamet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.53	3.00 ng	38595	Naphthalene-d8	10.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	83
2	Benzoic acid, 2-[(trimethylsilyl...	282	C13H22O3Si2	003789-85-3	37
3	Phosphine, bis[5-methyl-2-(1-met...	310	C20H39P	062238-19-1	35
4	Benzonitrile, 2-(2-hydroxy-5-nit...	267	C14H9N3O3	303768-30-1	35
5	1H-Trindene, 2,3,4,5,6,7,8,9-oct...	282	C21H30	055682-87-6	35





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Instrument : BNA_G
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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
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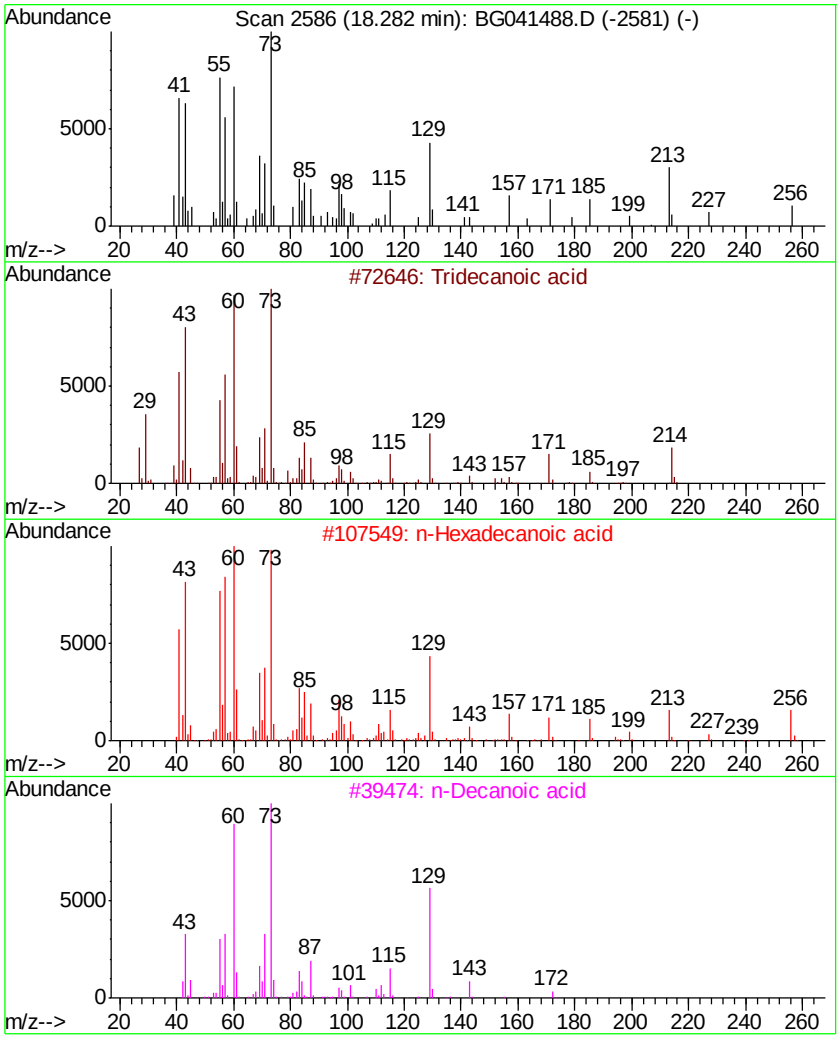
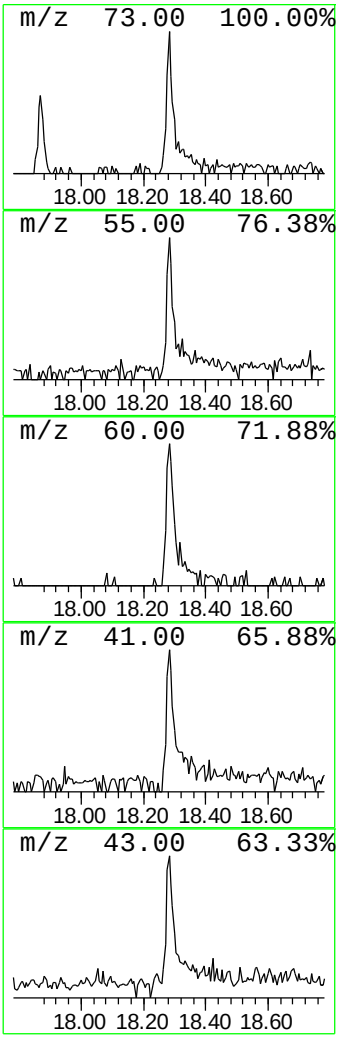
****

Peak Number 8 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	3.07 ng	79997	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	60
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
3	n-Decanoic acid	172	C10H20O2	000334-48-5	47
4	Dodecanoic acid	200	C12H24O2	000143-07-7	35
5	Lactose	342	C12H22O11	000063-42-3	35





Tentatively Identified Compound (LSC) summary

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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	10.1	ng	104311	1	8.03	205970	20.0
Cyclotetrasiloxan...	7.08	6.4	ng	65463	1	8.03	205970	20.0
Urea, tetramethyl-	7.42	6.5	ng	67411	1	8.03	205970	20.0
unknown7.56	7.56	85.0	ng	875572	1	8.03	205970	20.0
Trimethylamine, c...	9.13	27.8	ng	286478	1	8.03	205970	20.0
Cyclopentasiloxan...	9.53	3.0	ng	38595	2	10.86	257221	20.0
Tridecanoic acid	18.28	3.1	ng	79997	4	17.42	520974	20.0