LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048953.D
Acq On : 14 Jun 2021 17:28
Operator : CG/JU
Sample : M2678-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0207-COMP-G(DISCRETE-CL-07)

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-BG061121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048953.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.167	17	22	34	rVB	271571	421753	17.15%	2.957%
2	3.290	38	43	51	rVB	99714	142167	5.78%	0.997%
3	4.830	300	305	312	rVB2	15251	27533	1.12%	0.193%
4	5.200	363	368	377	rBV	77985	123604	5.03%	0.867%
5	5.664	440	447	455	rVV	780518	1252024	50.92%	8.777%
6	5.740	455	460	472	rVB2	30624	70505	2.87%	0.494%
7	6.974	663	670	677	rBV8	18547	49198	2.00%	0.345%
8	7.262	710	719	728	rBV	771531	1359228	55.28%	9.529%
9	7.515	756	762	767	rBV9	17081	41508	1.69%	0.291%
10	8.120	855	865	872	rBV	143293	248358	10.10%	1.741%
11	9.283	1056	1063	1071	rBV	462375	856338	34.83%	6.003%
12	10.705	1298	1305	1314	rBV	146064	259634	10.56%	1.820%
13	10.940	1338	1345	1354	rBV	183404	338777	13.78%	2.375%
14	13.384	1754	1761	1769	rBV	1120521	1778336	72.33%	12.467%
15	14.101	1876	1883	1889	rBV	130403	181475	7.38%	1.272%
16	14.759	1987	1995	2002	rBV	310330	495124	20.14%	3.471%
17	16.163	2227	2234	2241	rBV	69036	100048	4.07%	0.701%
18	16.246	2241	2248	2260	rBV	962450	1472780	59.90%	10.325%
19	17.509	2456	2463	2470	rBV	399241	621693	25.29%	4.358%
20	17.626	2478	2483	2490	rVB3	81770	116534	4.74%	0.817%
21	18.167	2569	2575	2582	rVB3	61427	98071	3.99%	0.688%
22	18.390	2609	2613	2620	rBV3	53297	84870	3.45%	0.595%
23	19.319	2767	2771	2780	rBV7	21940	42151	1.71%	0.295%
24	19.659	2826	2829	2833	rBV4	22348	28285	1.15%	0.198%
25	20.118	2901	2907	2913	rBV	1924676	2458674	100.00%	17.236%
26	20.876	3033	3036	3040	rBV2	33539	40532	1.65%	0.284%
27	21.440	3129	3132	3142	rVB6	34393	56615	2.30%	0.397%
28	21.692	3170	3175	3181	rVB	57296	91593	3.73%	0.642%
29	21.804	3187	3194	3202	rBV	387443	681020	27.70%	4.774%
30	23.032	3397	3403	3409	rBV7	42587	87537	3.56%	0.614%
31	25.135	3752	3761	3772	rVB2	219668	638520	25.97%	4.476%

Sum of corrected areas: 14264485

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Misc :
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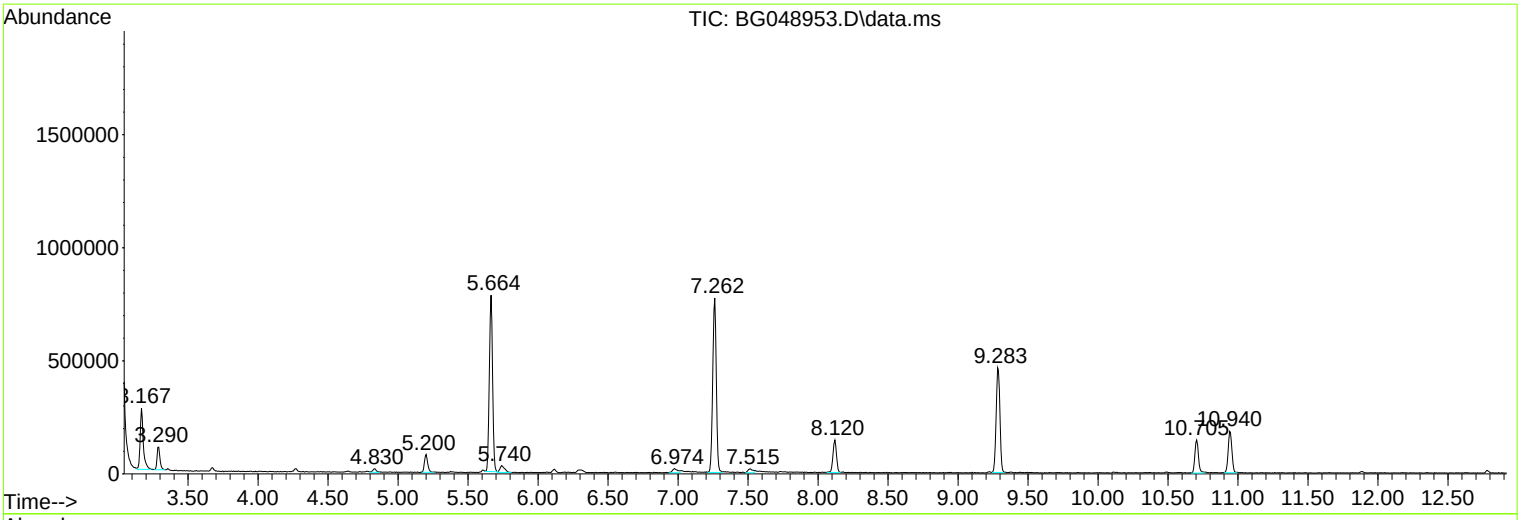
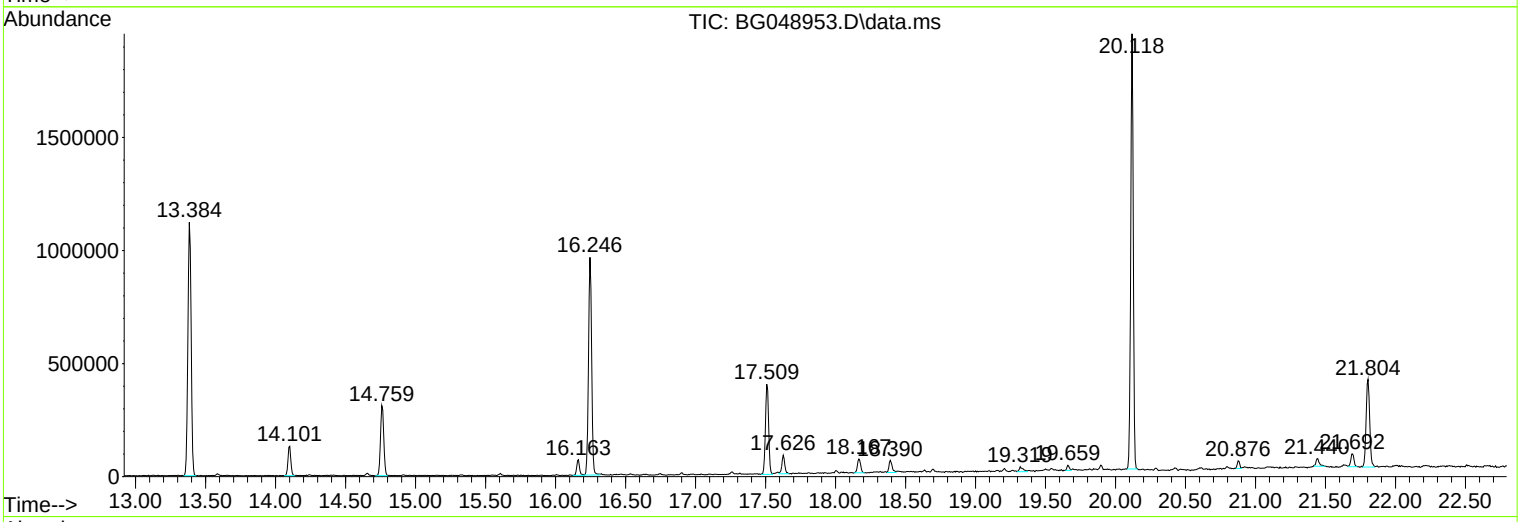
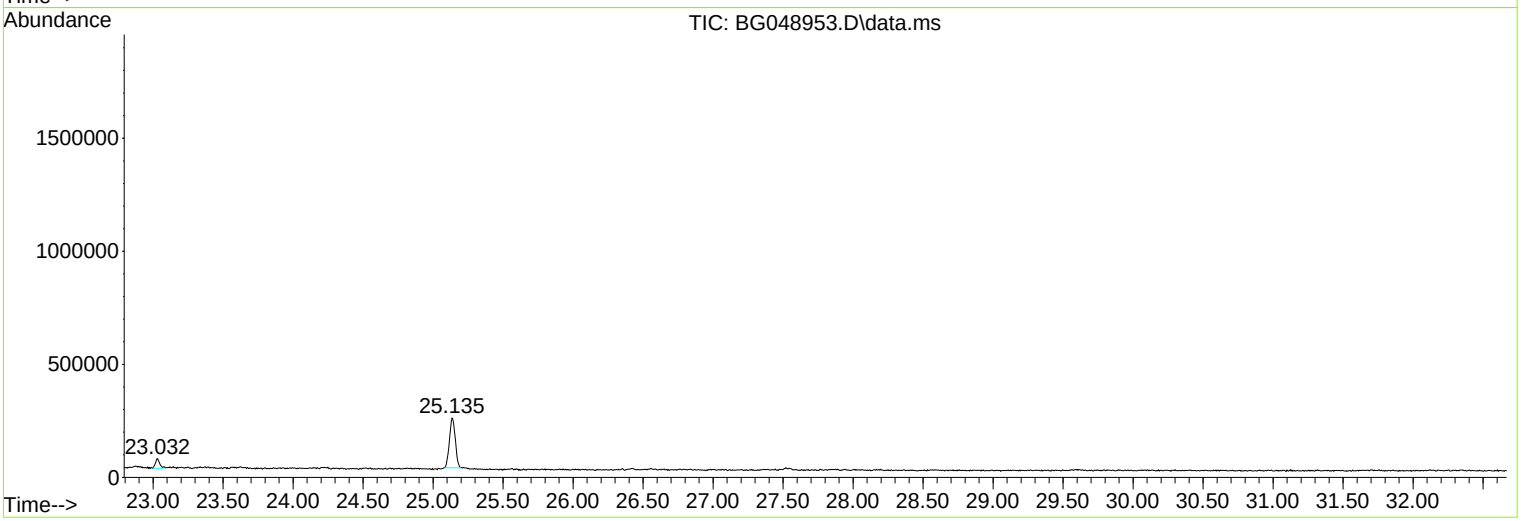
Instrument :
BNA_G
ClientSampleId :
0207-COMP-G(DISCRETE-CL-07)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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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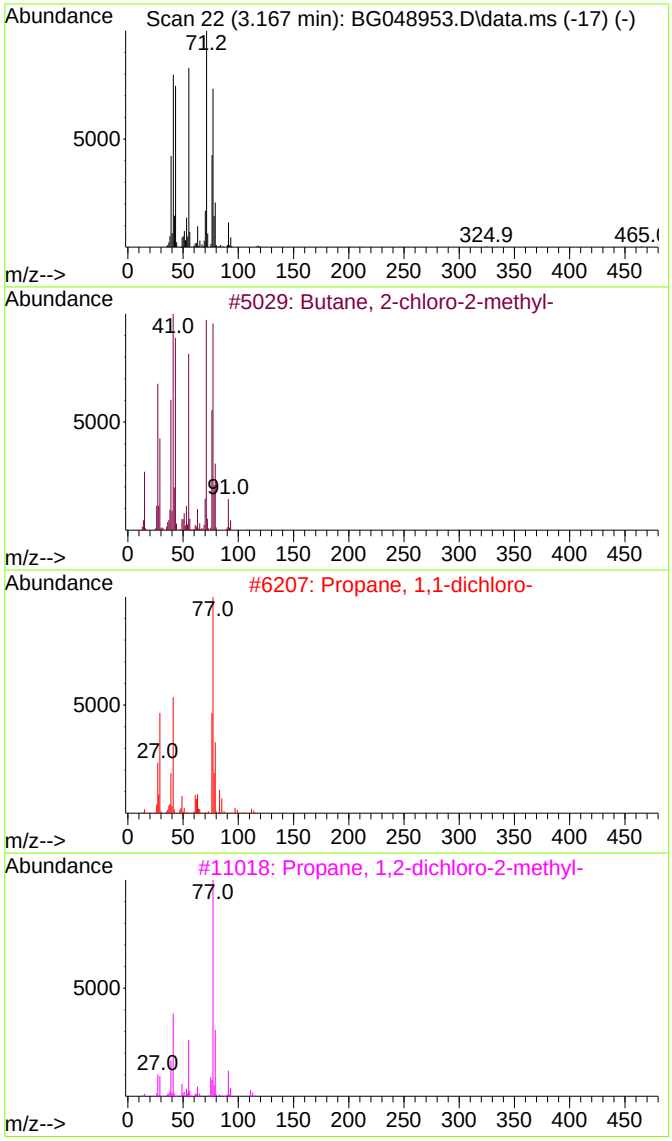
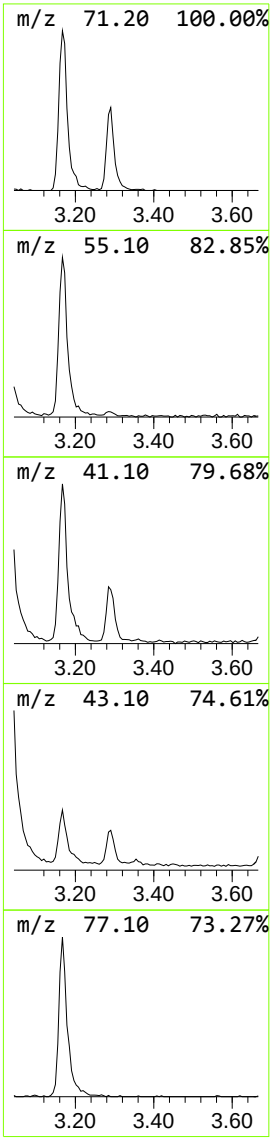
****

Peak Number 1 Butane, 2-chloro-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.167	33.96 ng	421753	1,4-Dichlorobenzene-d4	8.120

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	64
2	Propane, 1,1-dichloro-	112	C3H6Cl2	000078-99-9	32
3	Propane, 1,2-dichloro-2-methyl-	126	C4H8Cl2	000594-37-6	27
4	2-Butene, 1-methoxy-, (Z)-	86	C5H10O	010034-16-9	16
5	2-Penten-1-ol, 2-methyl-, (E)-	100	C6H12O	016958-19-3	16





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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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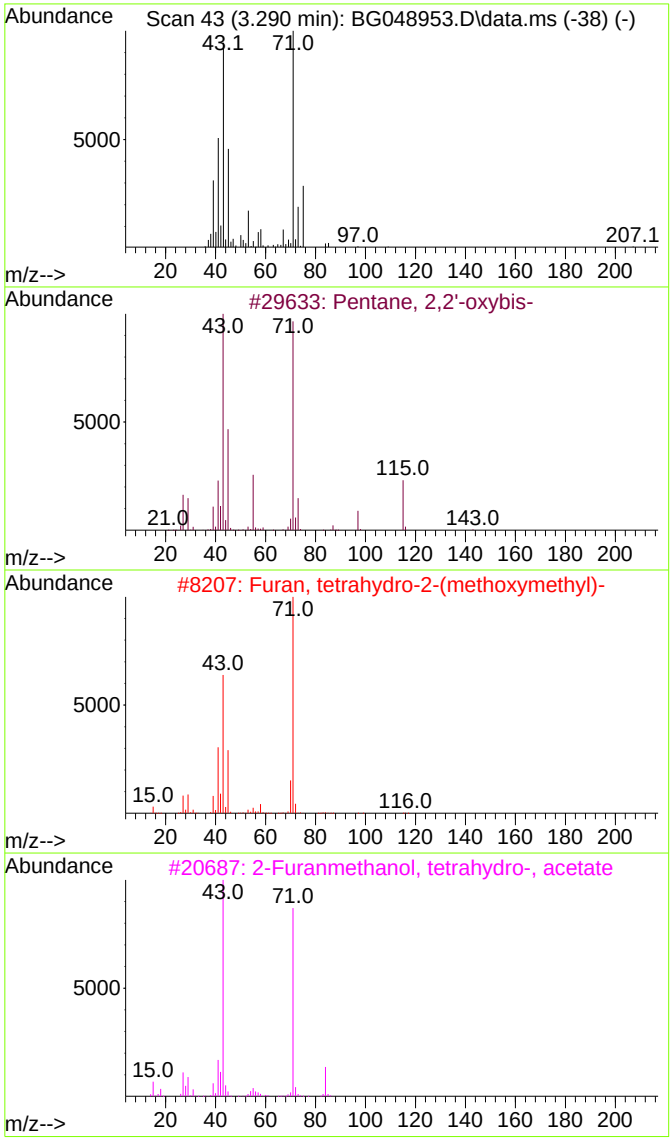
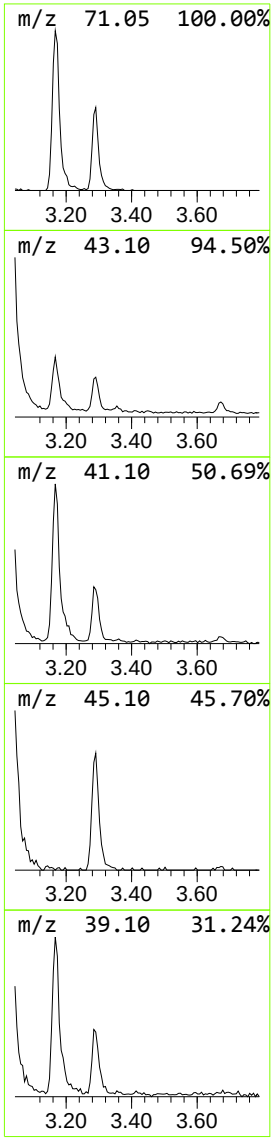
****

Peak Number 2 Pentane, 2,2'-oxybis- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.290	11.45 ng	142167	1,4-Dichlorobenzene-d4	8.120

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2'-oxybis-	158	C10H22O	056762-00-6	64
2	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	53
3	2-Furanmethanol, tetrahydro-, ac...	144	C7H12O3	000637-64-9	38
4	3-Penten-2-ol	86	C5H10O	001569-50-2	38
5	Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	38





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Operator : CG/JU
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0207-COMP-G(DISCRETE-CL-07)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
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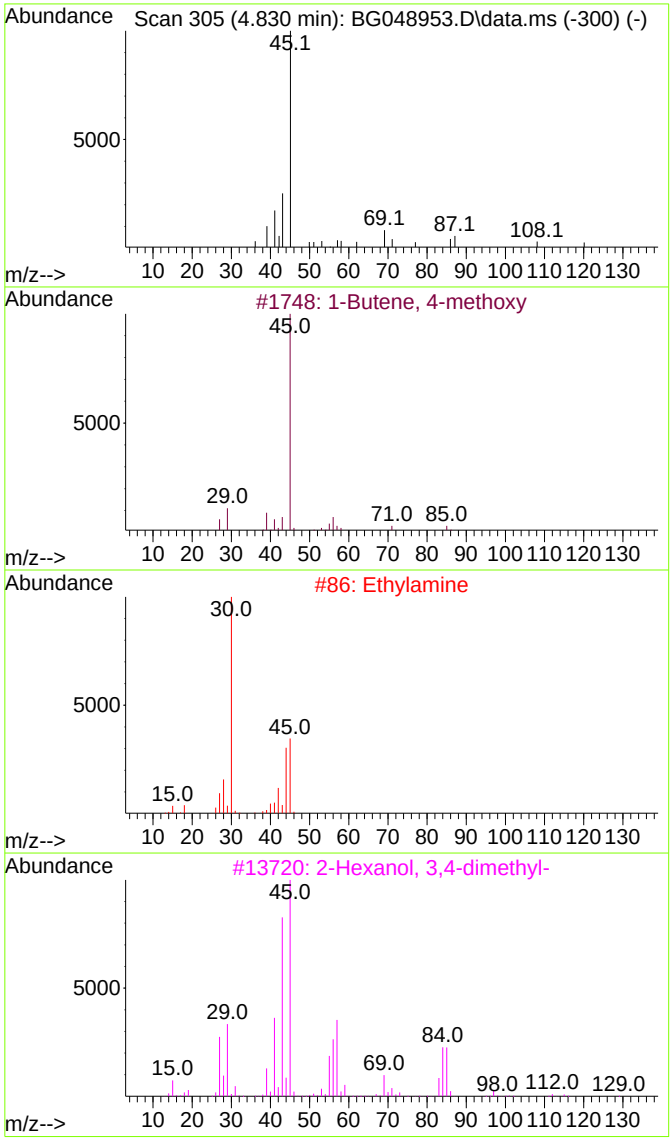
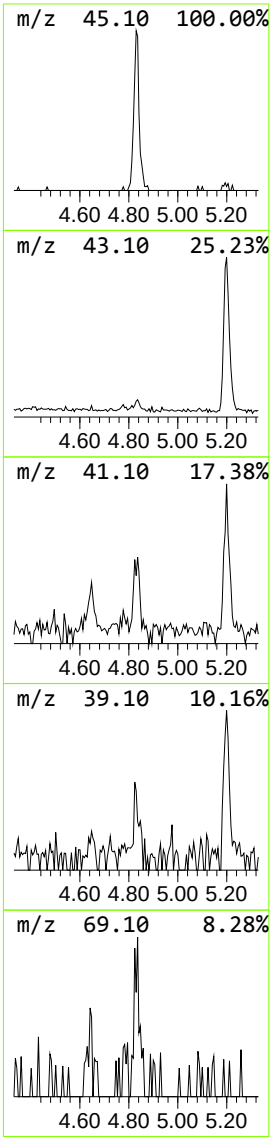
****

Peak Number 3 unknown4.830 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.830	2.22 ng	27533	1,4-Dichlorobenzene-d4	8.120

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene, 4-methoxy	86	C5H10O	004696-30-4	9
2	Ethylamine	45	C2H7N	000075-04-7	4
3	2-Hexanol, 3,4-dimethyl-	130	C8H18O	019550-05-1	4
4	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	4
5	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	4





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
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0207-COMP-G(DISCRETE-CL-07)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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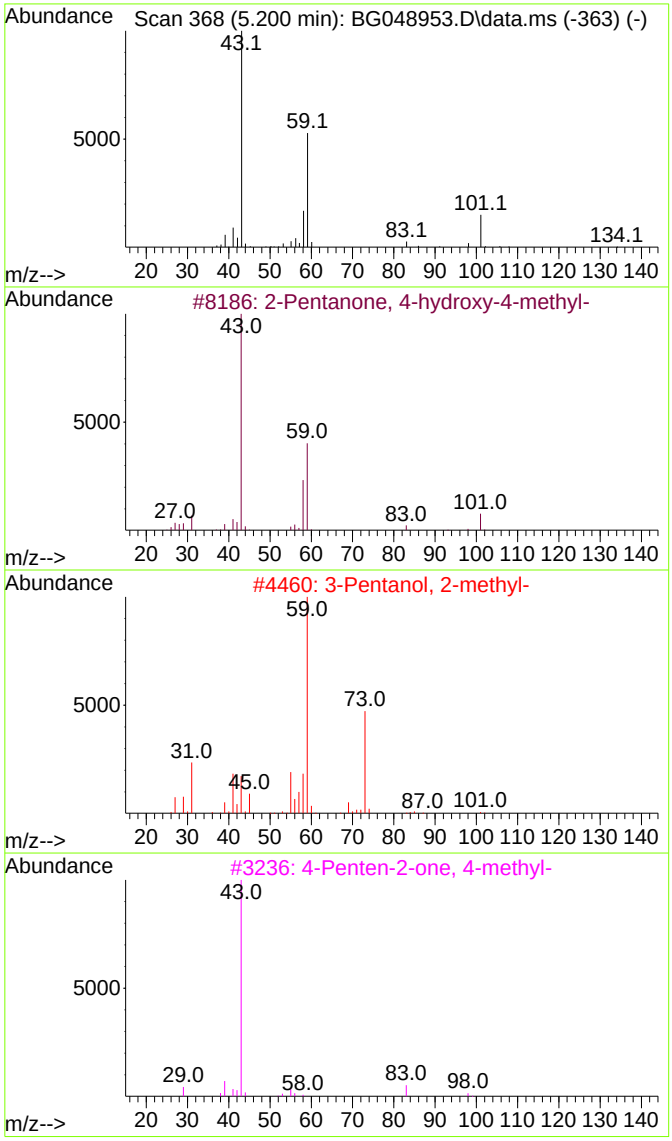
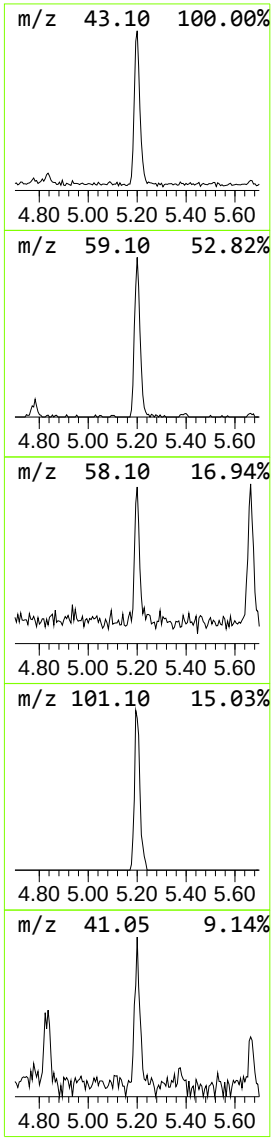
****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.200	9.95 ng	123604	1,4-Dichlorobenzene-d4	8.120

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	28
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	14
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Oxirane-2-carboxylic acid, methy...	102	C4H6O3	004538-50-5	9





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Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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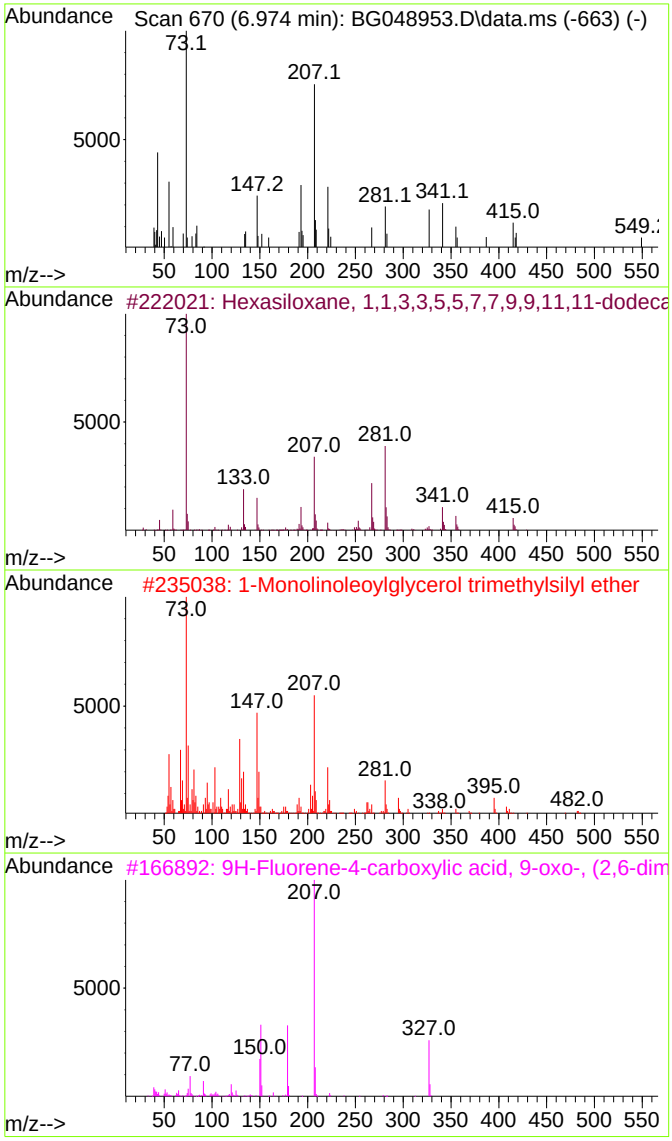
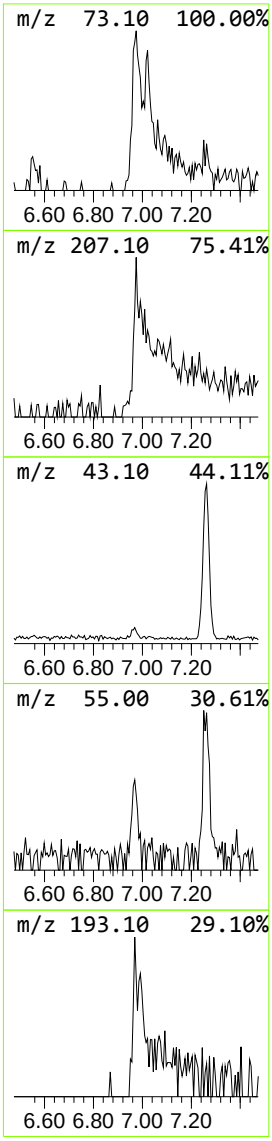
****

Peak Number 6 unknown6.974 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.974	3.96 ng	49198	1,4-Dichlorobenzene-d4	8.120

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexasiloxane, 1,1,3,3,5,5,7,7,9,...	430	C12H38O5Si6	000995-82-4	40
2	1-Monolinoleoylglycerol trimethy...	498	C27H54O4Si2	054284-45-6	38
3	9H-Fluorene-4-carboxylic acid, 9...	327	C22H17NO2	1000304-78-2	38
4	Acetic acid, [4-(1,1-dimethyleth...	222	C13H18O3	088530-52-3	38
5	1,4-Bis(trimethylsilyl)benzene	222	C12H22Si2	013183-70-5	38





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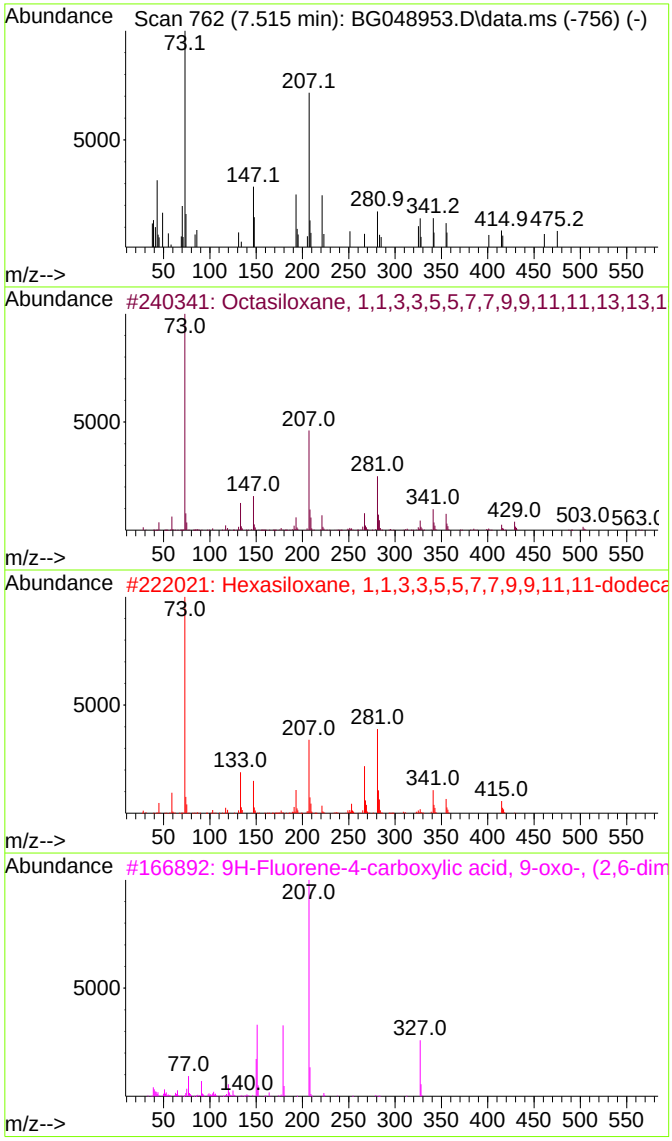
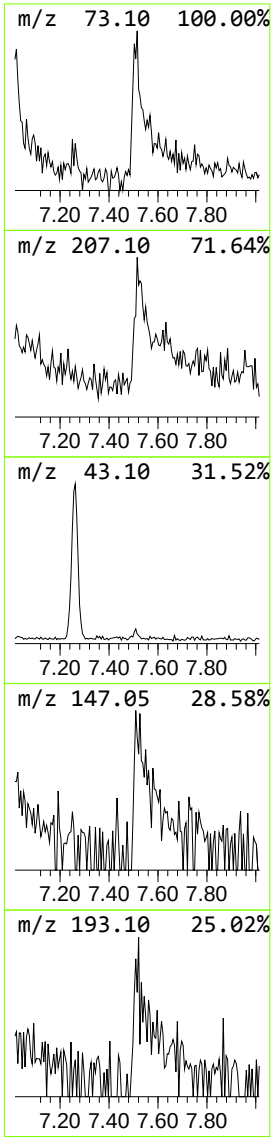
****
Peak Number 7 Octasiloxane, 1,1,3,3,5,5,7... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.515	3.34 ng	41508	1,4-Dichlorobenzene-d4	8.120

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octasiloxane, 1,1,3,3,5,5,7,7,9,...	578	C16H50O7Si8	019095-24-0	53
2	Hexasiloxane, 1,1,3,3,5,5,7,7,9,...	430	C12H38O5Si6	000995-82-4	47
3	9H-Fluorene-4-carboxylic acid, 9...	327	C22H17NO2	1000304-78-2	35
4	Carbonic acid, monoamide, N-(2-e...	207	C12H17NO2	1000340-19-1	22
5	Heptasiloxane, 1,1,3,3,5,5,7,7,9...	504	C14H44O6Si7	019095-23-9	16





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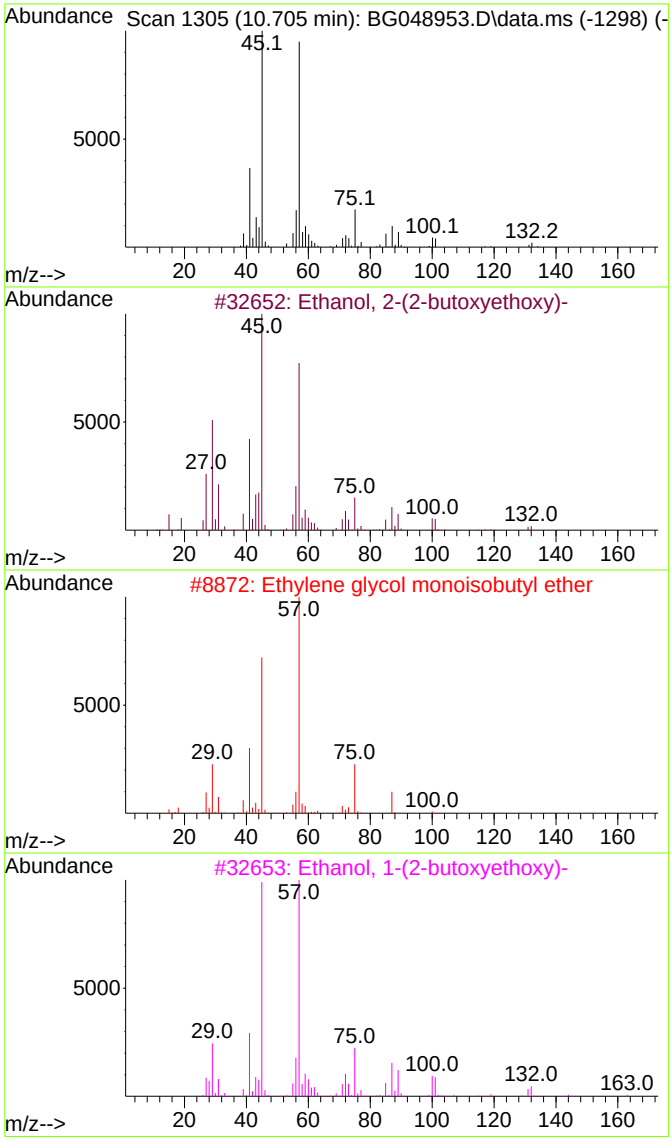
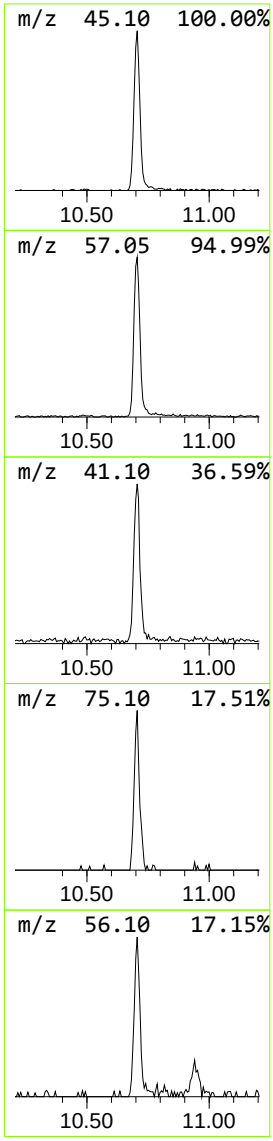
Peak Number 8 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.705	15.33 ng	259634	Naphthalene-d8	10.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
3	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
4	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	47
5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	45





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TIC Library : C:\Database\NIST11.L
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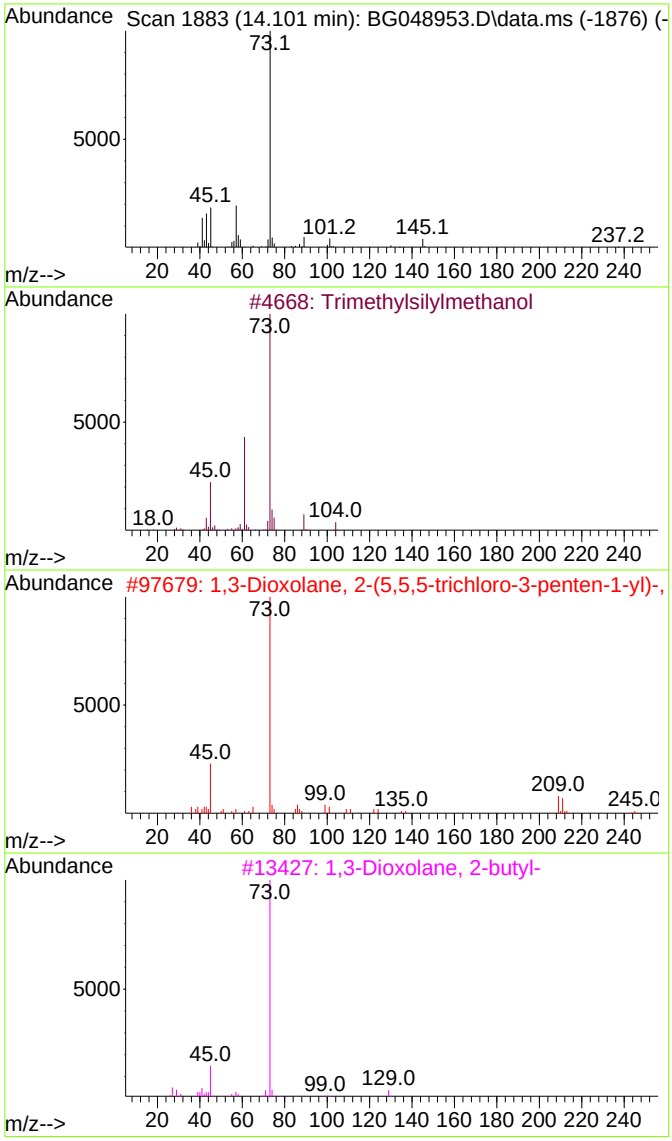
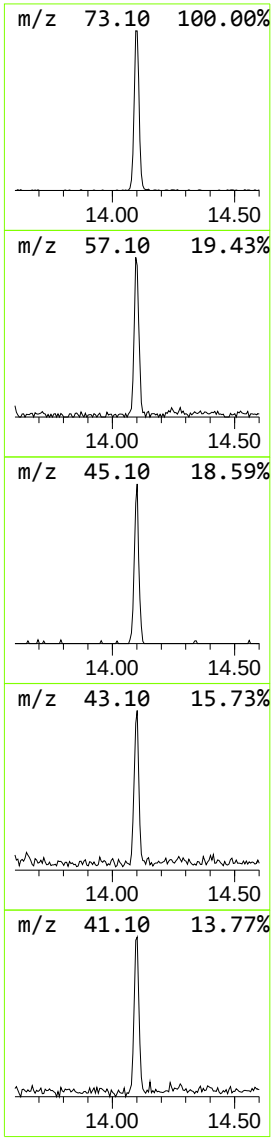
****
Peak Number 9 unknown14.101 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.101	7.33 ng	181475	Acenaphthene-d10	14.759

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trimethylsilylmethanol	104	C4H12OSi	003219-63-4	36
2	1,3-Dioxolane, 2-(5,5,5-trichlor...	244	C8H11Cl3O2	1000115-31-1	28
3	1,3-Dioxolane, 2-butyl-	130	C7H14O2	004360-76-3	25
4	2-[2-[2-Methoxyethoxy]ethoxy-1,3...	192	C8H16O5	074733-99-6	25
5	2,2'-Trimethylenebis-1,3-dioxolane	188	C9H16O4	006543-04-0	23





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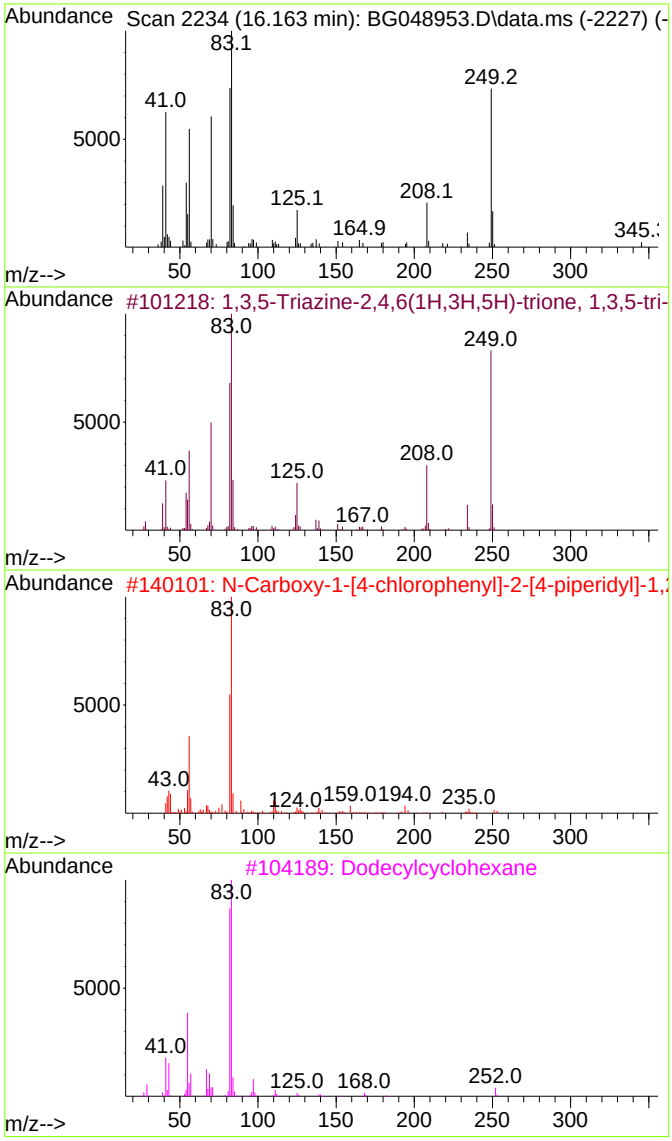
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

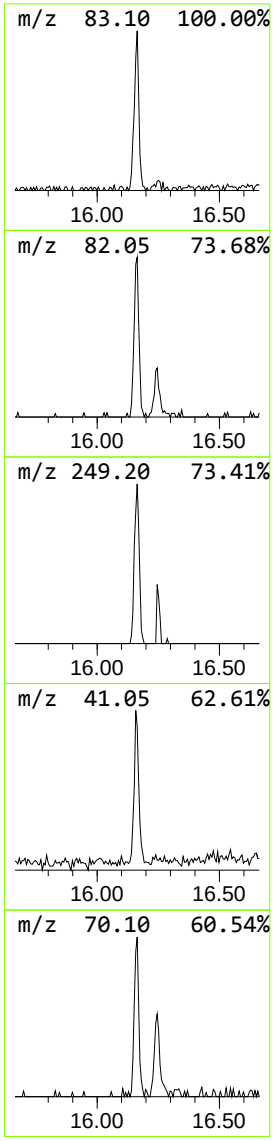
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.163	3.22 ng	100048	Phenanthrene-d10	17.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	249	C12H15N3O3	001025-15-6	95
2	N-Carboxy-1-[4-chlorophenyl]-2-[...	295	C15H18ClNO3	058158-38-6	37
3	Dodecylcyclohexane	252	C18H36	001795-17-1	25
4	Hexane, 1,6-dicyclohexyl-	250	C18H34	001610-23-7	25
5	Acetamide, N-(2-ethoxy-3,6-dihyd...	199	C10H17NO3	056248-08-9	25





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Data File : BG048953.D
Acq On : 14 Jun 2021 17:28
Operator : CG/JU
Sample : M2678-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0207-COMP-G(DISCRETE-CL-07)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

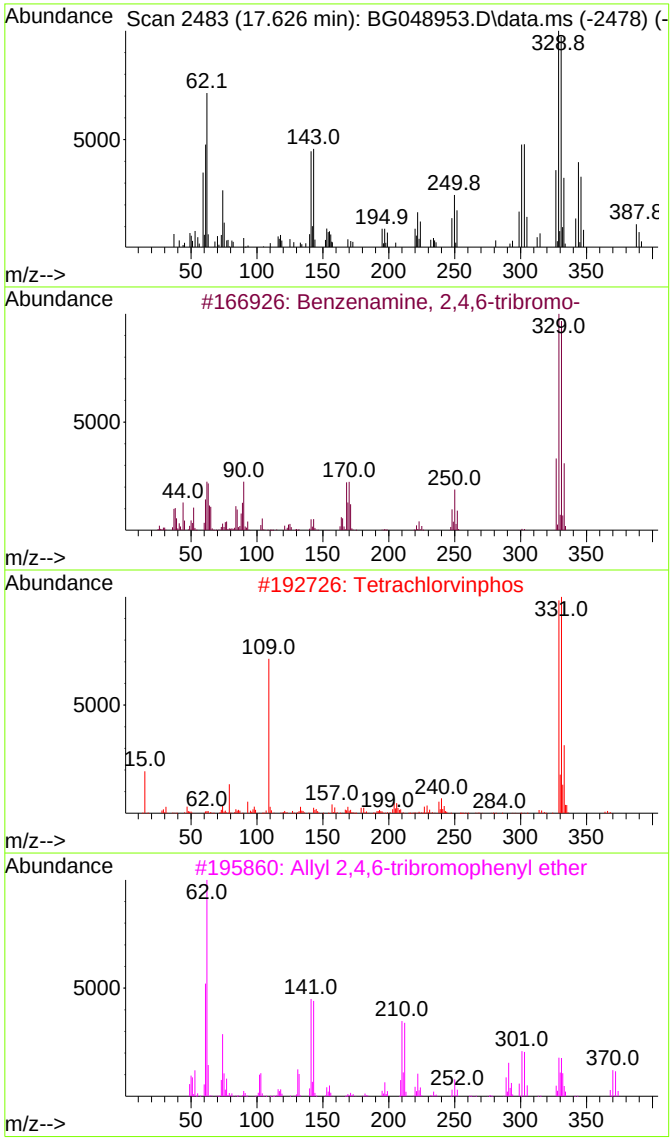
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

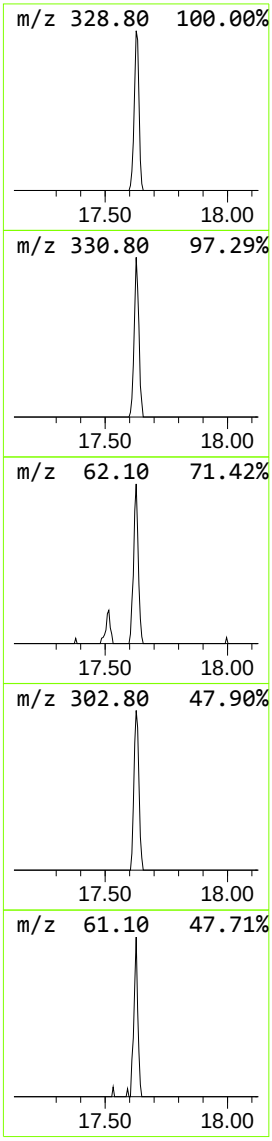
****

Peak Number 11 Benzenamine, 2,4,6-tribromo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.627	3.75 ng	116534	Phenanthrene-d10	17.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	55
2	Tetrachlorvinphos	364	C10H9Cl4O4P	022248-79-9	12
3	Allyl 2,4,6-tribromophenyl ether	368	C9H7Br3O	003278-89-5	12
4	2-Isopropyl-5-methylphenyl 2,2,3...	346	C14H13F7O2	1000366-95-7	10
5	2-(1-Oxo-1H-naphtho[2,1-b]thioph...	329	C20H11NO2S	1000311-45-2	9





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Data File : BG048953.D
Acq On : 14 Jun 2021 17:28
Operator : CG/JU
Sample : M2678-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0207-COMP-G(DISCRETE-CL-07)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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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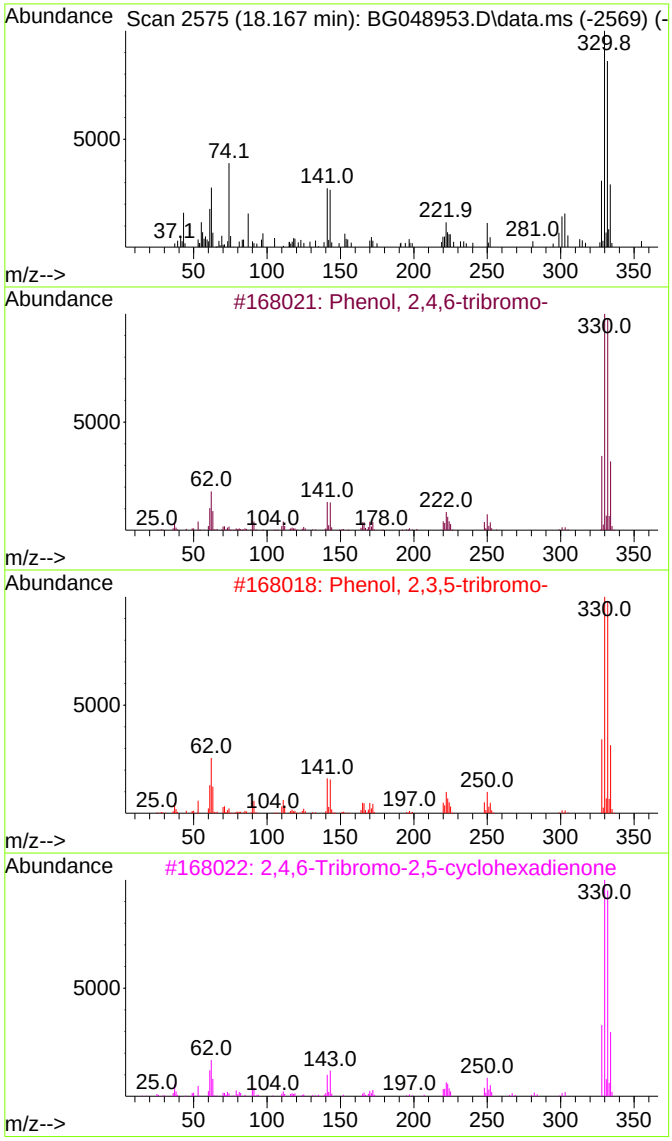
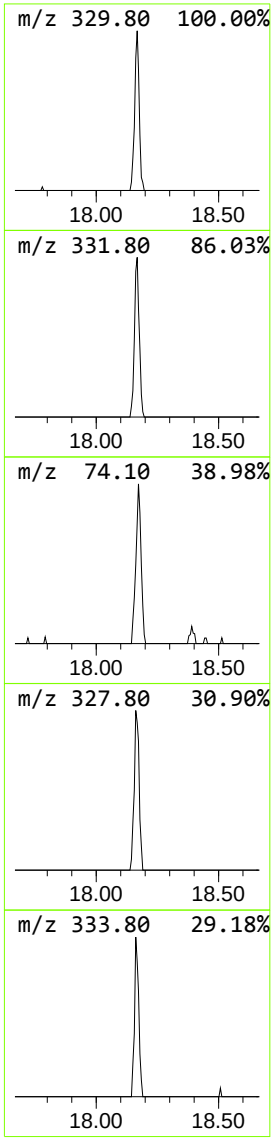
Peak Number 12 Phenol, 2,3,5-tribromo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.167	3.15 ng	98071	Phenanthrene-d10	17.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4,6-tribromo-	328	C6H3Br3O	000118-79-6	99
2	Phenol, 2,3,5-tribromo-	328	C6H3Br3O	057383-81-0	99
3	2,4,6-Tribromo-2,5-cyclohexadienone	328	C6H3Br3O	020244-61-5	96
4	1-Amino-5-morpholin-4-yl-6,7,8,9...	332	C16H20N4O2S	118663-25-5	22
5	2-Amino-3(4-chlorphenyl)-5(4-nit...	330	C16H11ClN2O2S	155243-77-9	10





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Data File : BG048953.D
Acq On : 14 Jun 2021 17:28
Operator : CG/JU
Sample : M2678-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0207-COMP-G(DISCRETE-CL-07)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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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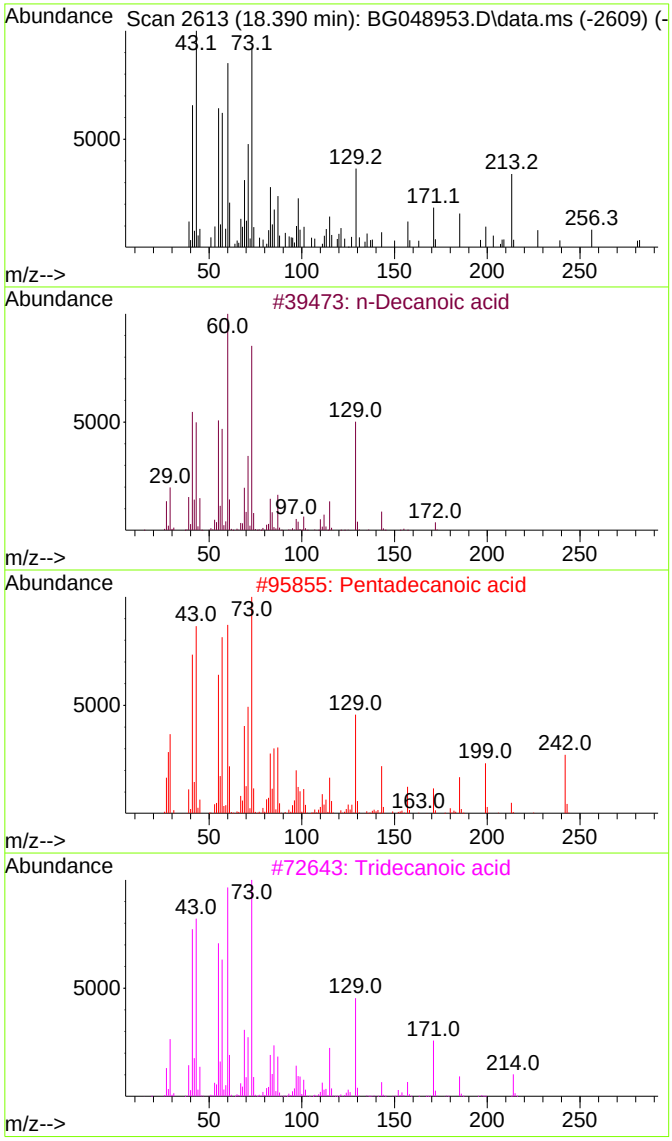
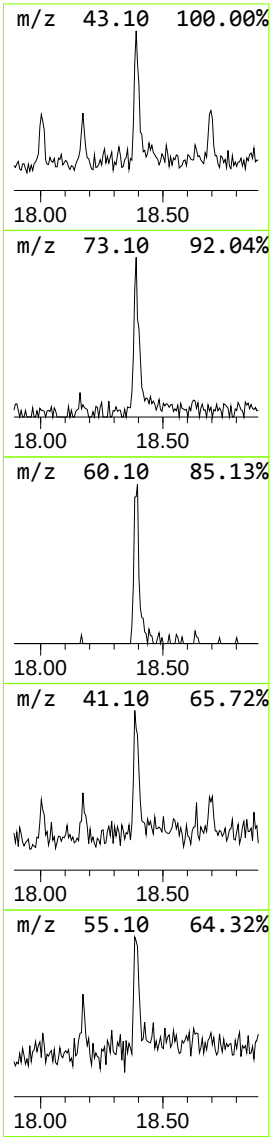
Peak Number 13 n-Decanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.390	2.73 ng	84870	Phenanthrene-d10	17.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	64
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	60
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50





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Acq On : 14 Jun 2021 17:28
Operator : CG/JU
Sample : M2678-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0207-COMP-G(DISCRETE-CL-07)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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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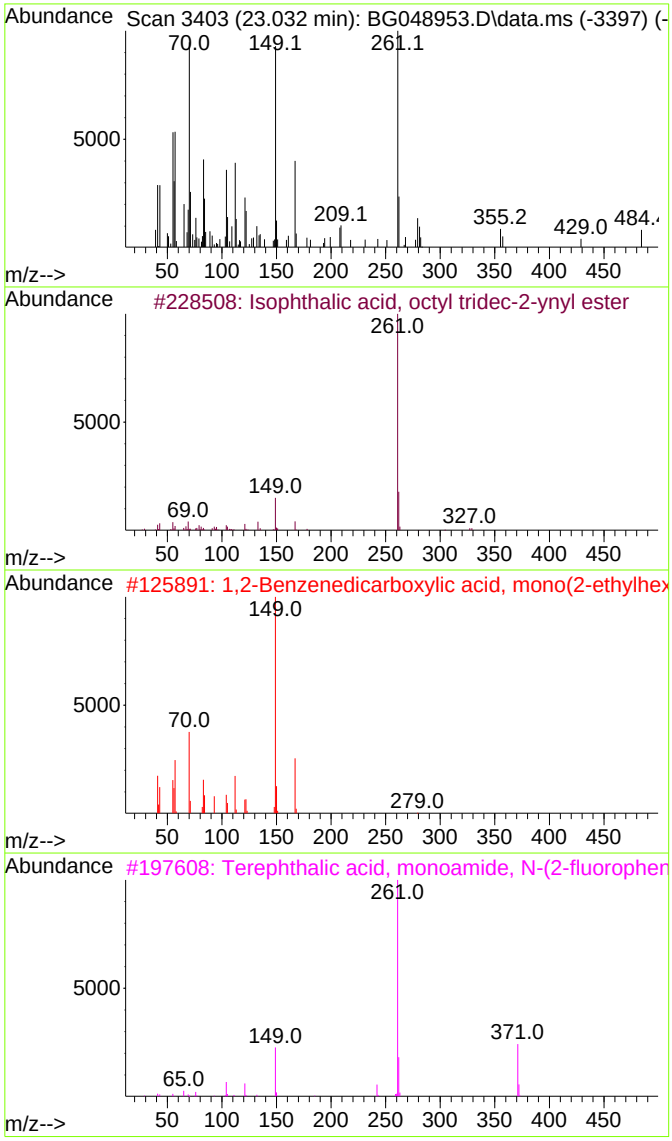
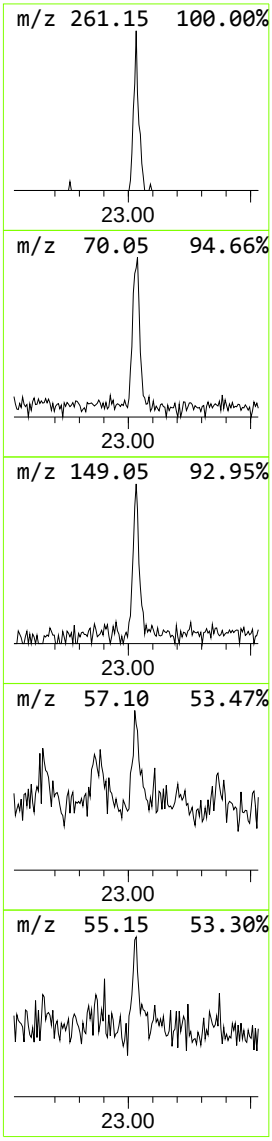
Peak Number 14 unknown23.032 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.032	2.57 ng	87537	Chrysene-d12	21.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isophthalic acid, octyl tridec-2...	456	C29H44O4	1000343-92-0	43
2	1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	004376-20-9	38
3	Terephthalic acid, monoamide, N-...	371	C22H26FNO3	1000324-02-6	35
4	Terephthalic acid, 2-isopropoxyp...	412	C25H32O5	1000324-07-8	35
5	Di-n-octyl phthalate	390	C24H38O4	000117-84-0	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048953.D
Acq On : 14 Jun 2021 17:28
Operator : CG/JU
Sample : M2678-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0207-COMP-G(DISCRETE-CL-07)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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-chlor...	3.167	34.0	ng	421753	1	8.120	248358	20.0
Pentane, 2,2'-o...	3.290	11.4	ng	142167	1	8.120	248358	20.0
unknown4.830	4.830	2.2	ng	27533	1	8.120	248358	20.0
2-Pentanone, 4-...	5.200	9.9	ng	123604	1	8.120	248358	20.0
unknown6.974	6.974	4.0	ng	49198	1	8.120	248358	20.0
Octasiloxane, 1...	7.515	3.3	ng	41508	1	8.120	248358	20.0
Ethanol, 2-(2-b...	10.705	15.3	ng	259634	2	10.946	338777	20.0
unknown14.101	14.101	7.3	ng	181475	3	14.759	495124	20.0
1,3,5-Triazine-...	16.163	3.2	ng	100048	4	17.509	621693	20.0
Benzenamine, 2,...	17.627	3.8	ng	116534	4	17.509	621693	20.0
Phenol, 2,3,5-t...	18.167	3.1	ng	98071	4	17.509	621693	20.0
n-Decanoic acid	18.390	2.7	ng	84870	4	17.509	621693	20.0
unknown23.032	23.032	2.6	ng	87537	5	21.804	681020	20.0