

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
 Data File : BG019905.D
 Acq On : 4 Dec 2015 13:28
 Operator : UM/NP
 Sample : G4609-04
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 CF-1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.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	2.990	21	26	46	rVV	1627793	2276644	75.48%	12.158%
2	3.137	46	51	60	rVV3	37251	74560	2.47%	0.398%
3	3.220	60	65	75	rVB	83659	124490	4.13%	0.665%
4	5.194	395	401	409	rVB	137328	206961	6.86%	1.105%
5	5.664	474	481	490	rBV	626807	988199	32.76%	5.277%
6	7.268	745	754	766	rBV	676380	1180840	39.15%	6.306%
7	7.650	807	819	830	rBV	644072	1119231	37.11%	5.977%
8	8.120	892	899	905	rBV	105463	171257	5.68%	0.915%
9	8.443	947	954	962	rVB	450805	796909	26.42%	4.256%
10	9.289	1089	1098	1107	rBV	416005	741789	24.59%	3.961%
11	9.383	1107	1114	1119	rBV2	20611	35196	1.17%	0.188%
12	10.940	1371	1379	1386	rBV	150561	265472	8.80%	1.418%
13	13.372	1785	1793	1804	rVB	1185018	1859260	61.65%	9.929%
14	14.195	1925	1933	1942	rBV	343134	502107	16.65%	2.681%
15	14.747	2021	2027	2040	rVB2	264439	425587	14.11%	2.273%
16	16.228	2271	2279	2294	rBV	1074288	1663979	55.17%	8.886%
17	16.445	2312	2316	2319	rBV	27156	34129	1.13%	0.182%
18	17.238	2445	2451	2456	rBV2	21997	30778	1.02%	0.164%
19	17.491	2488	2494	2500	rBV	367819	540774	17.93%	2.888%
20	18.366	2638	2643	2650	rBV	103470	149633	4.96%	0.799%
21	19.536	2836	2842	2849	rVB3	20144	35375	1.17%	0.189%
22	19.636	2854	2859	2866	rBV2	40823	69035	2.29%	0.369%
23	19.900	2900	2904	2910	rVB2	31361	48649	1.61%	0.260%
24	20.094	2931	2937	2943	rBV	2323989	3016073	100.00%	16.107%
25	20.781	3050	3054	3059	rVB	48556	65322	2.17%	0.349%
26	20.858	3061	3067	3073	rVB5	27575	55309	1.83%	0.295%
27	20.993	3086	3090	3095	rBV	34045	56001	1.86%	0.299%
28	21.046	3095	3099	3103	rVV	66513	91763	3.04%	0.490%
29	21.110	3107	3110	3116	rVB	29360	40802	1.35%	0.218%
30	21.398	3155	3159	3167	rVB	92389	134408	4.46%	0.718%
31	21.557	3182	3186	3190	rVB	46633	65015	2.16%	0.347%
32	21.627	3195	3198	3210	rVB3	26545	56684	1.88%	0.303%
33	21.762	3215	3221	3230	rVB	428384	703529	23.33%	3.757%
34	22.109	3275	3280	3288	rBV	20806	35264	1.17%	0.188%

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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:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	22.738	3382	3387	3393	rBV2	20433	35471	1.18%	0.189%
36	23.090	3444	3447	3453	rVB3	23484	35806	1.19%	0.191%
37	23.278	3472	3479	3495	rVB	131435	280423	9.30%	1.498%
38	23.507	3513	3518	3526	rVB2	35840	73040	2.42%	0.390%
39	25.053	3771	3781	3792	rBV	230245	639803	21.21%	3.417%

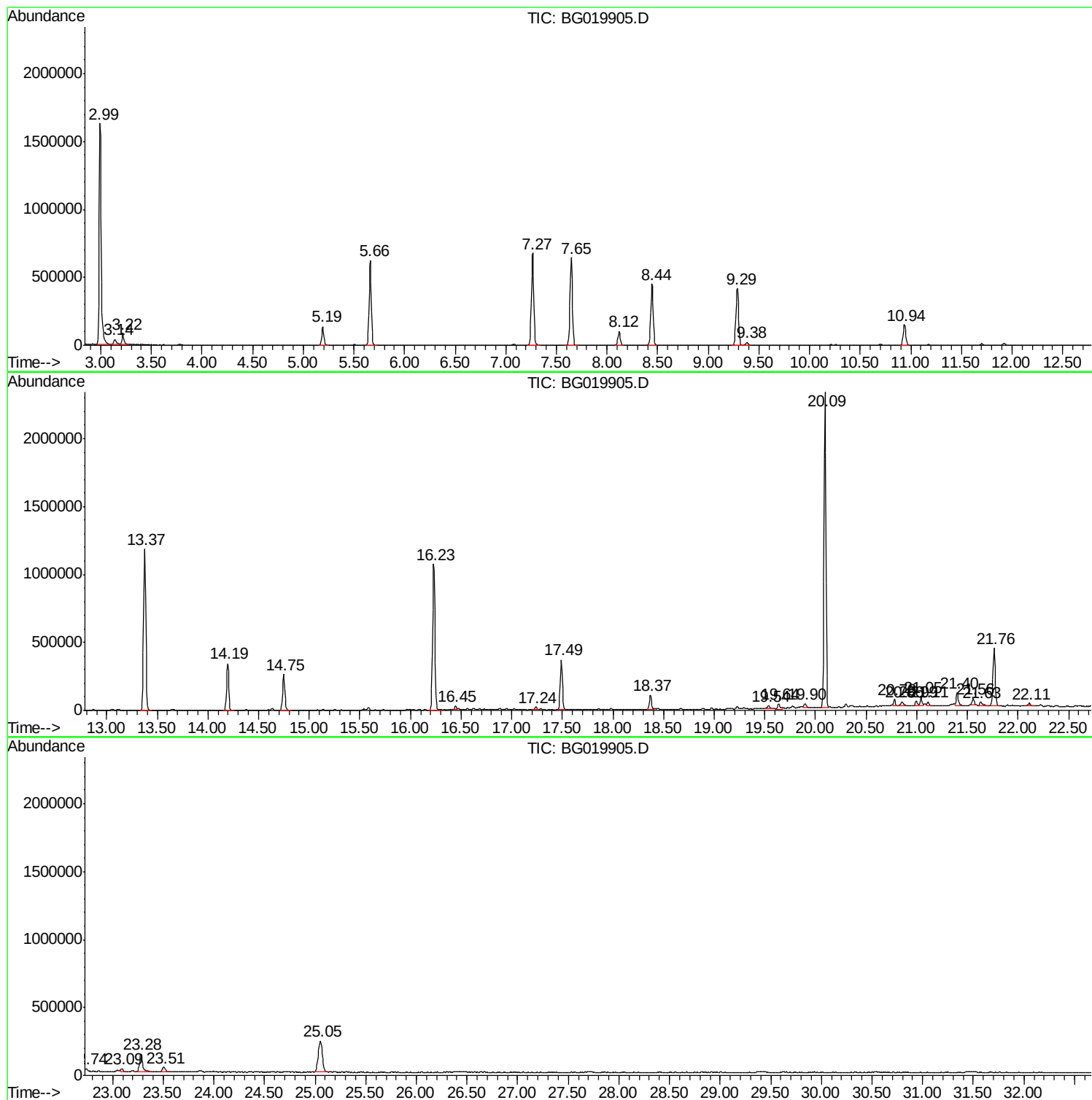
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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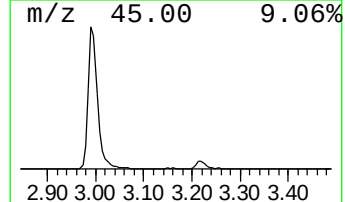
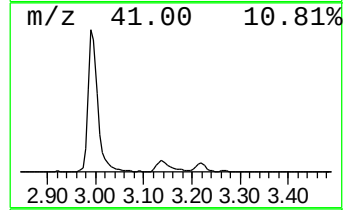
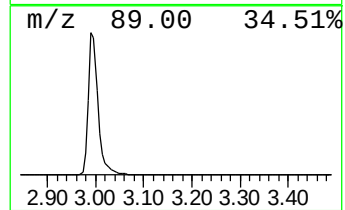
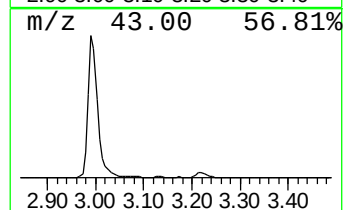
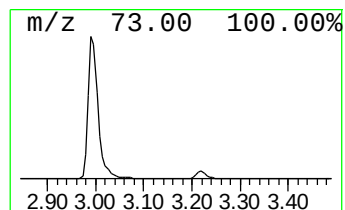
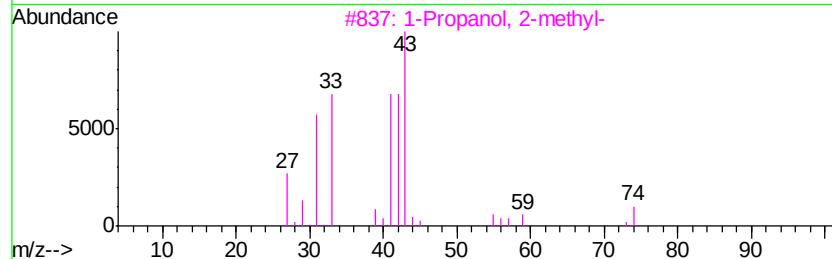
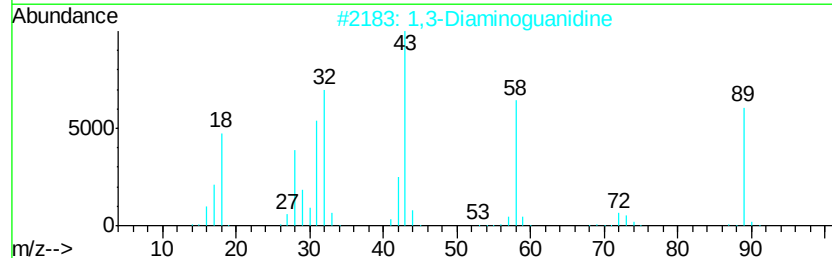
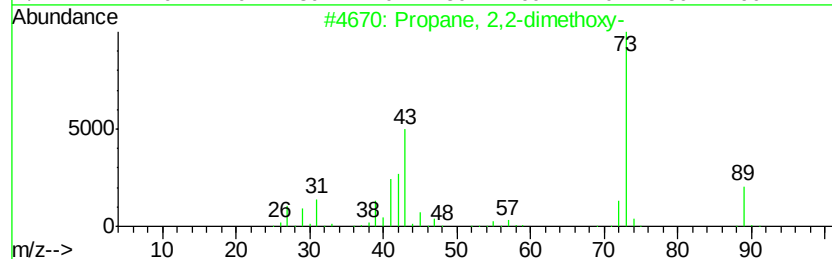
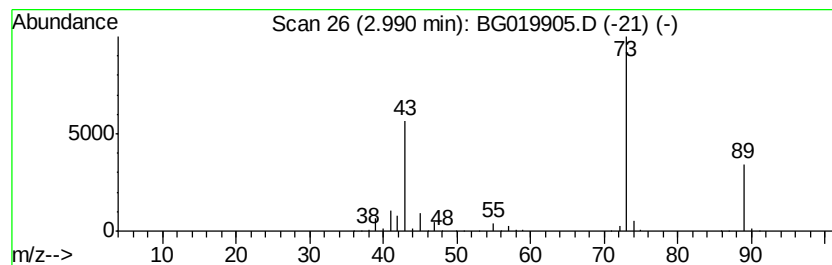
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	265.88 ng	2276640	1,4-Dichlorobenzene-d4	8.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2			1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9



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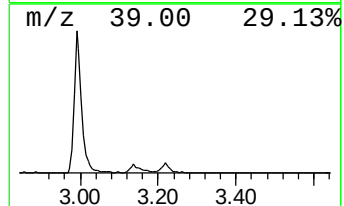
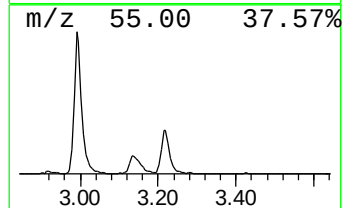
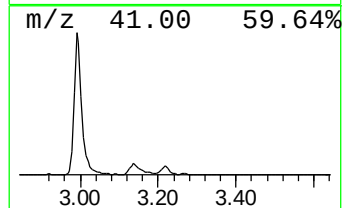
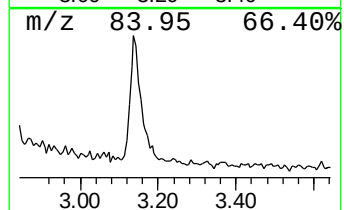
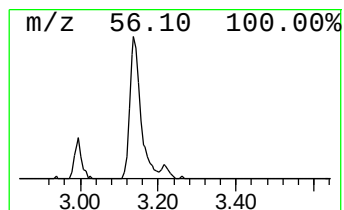
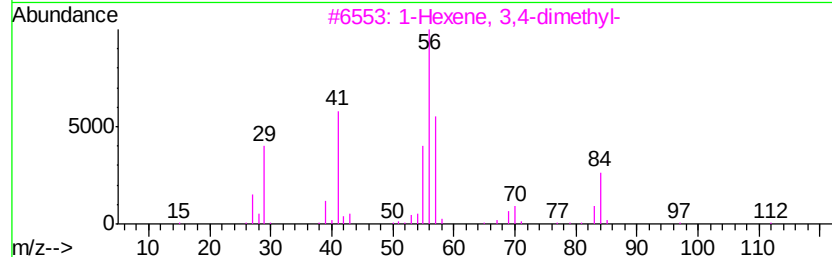
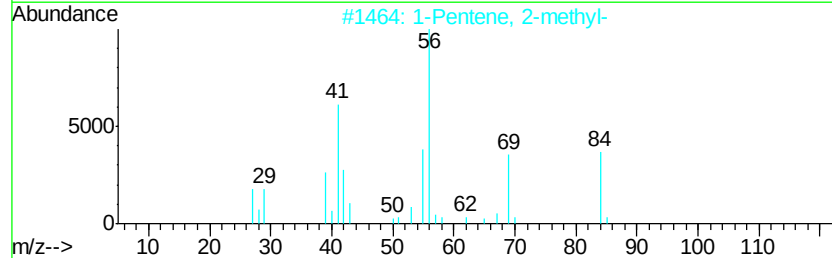
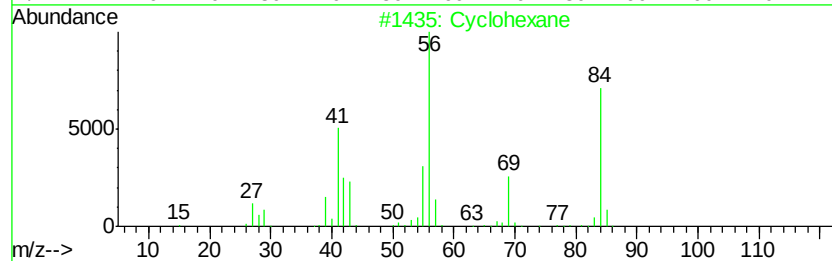
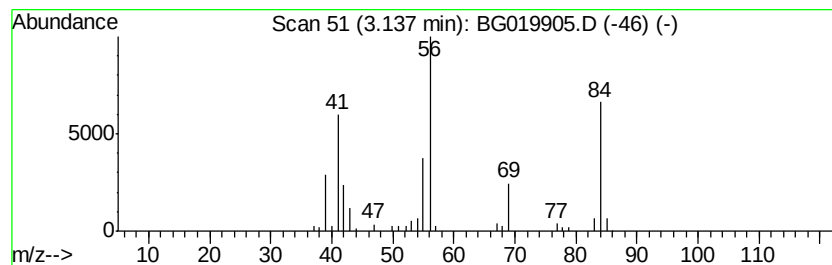
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.14	8.71 ng	74560	1,4-Dichlorobenzene-d4	8.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane	84	C6H12	000110-82-7	91
2		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	56
3		1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1	50
4		Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	42
5		Cyclopropane, propyl-	84	C6H12	002415-72-7	40



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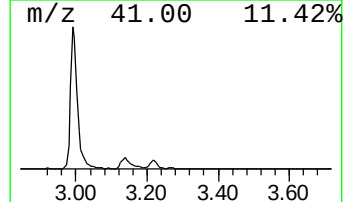
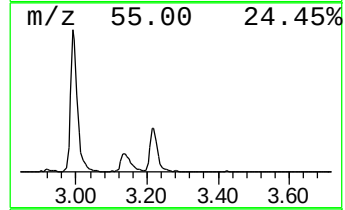
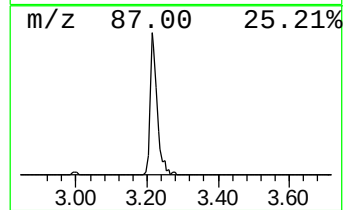
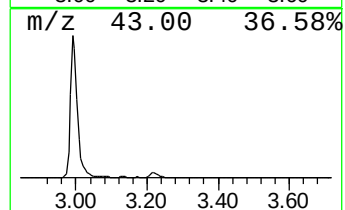
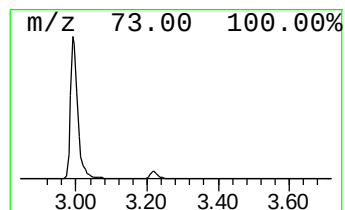
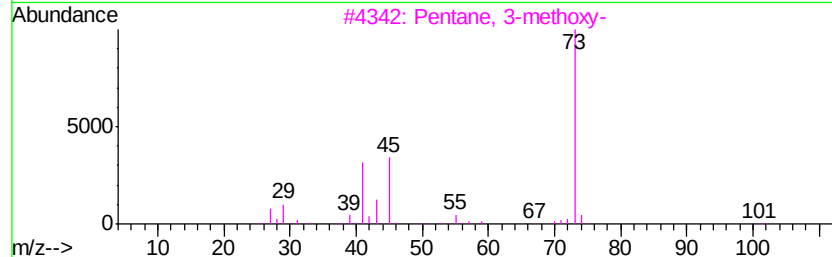
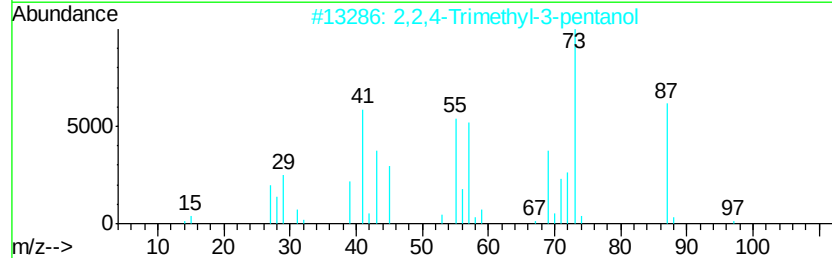
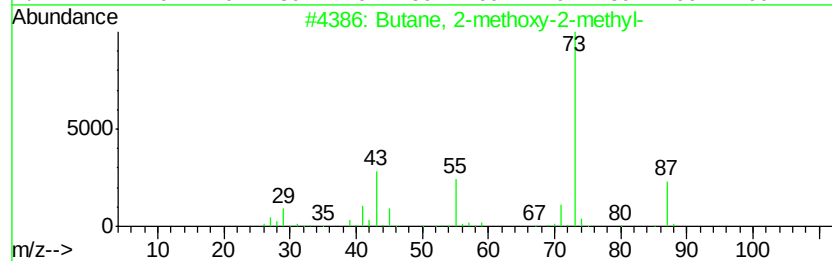
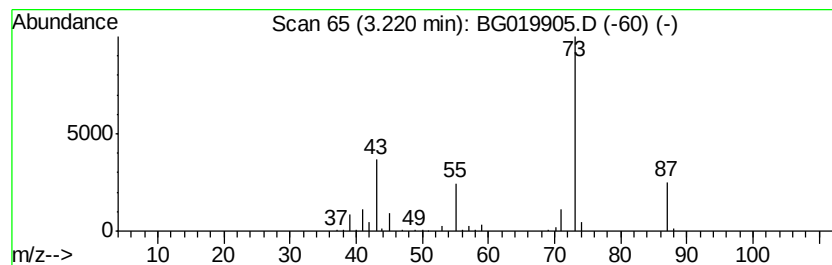
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	14.54 ng	124490	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	64
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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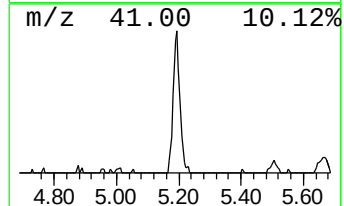
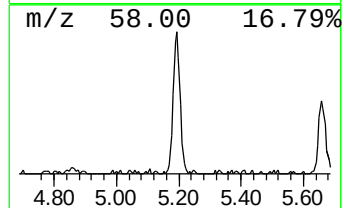
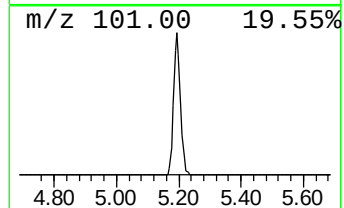
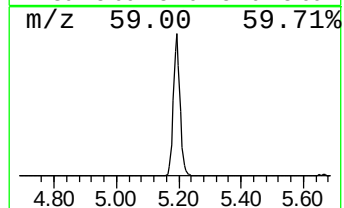
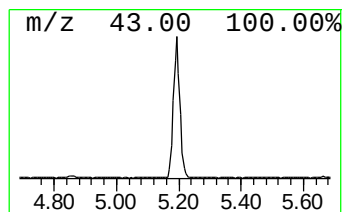
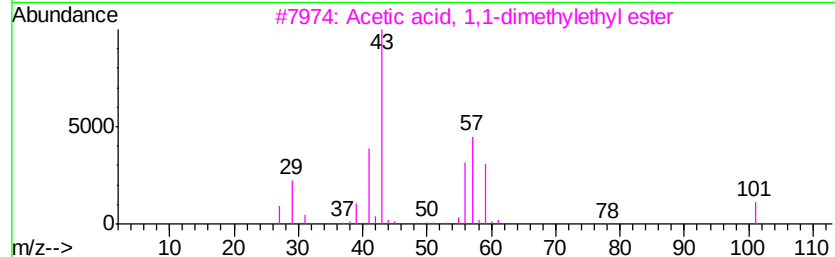
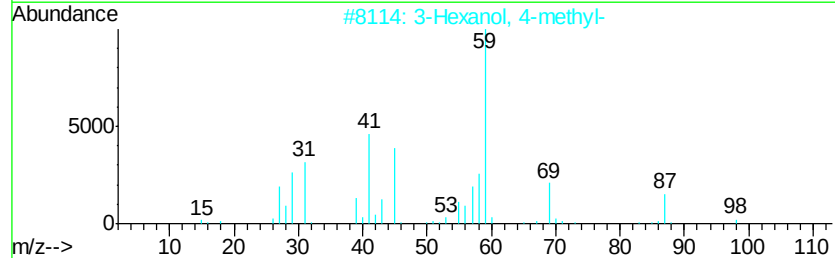
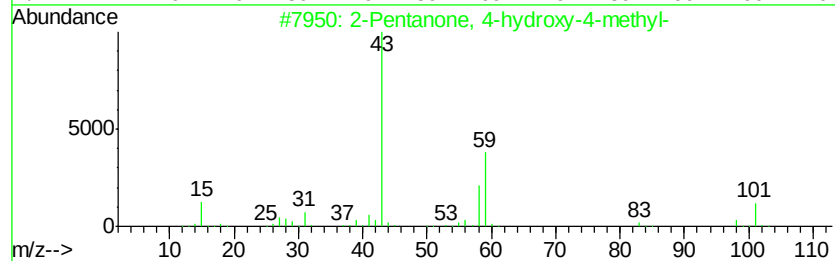
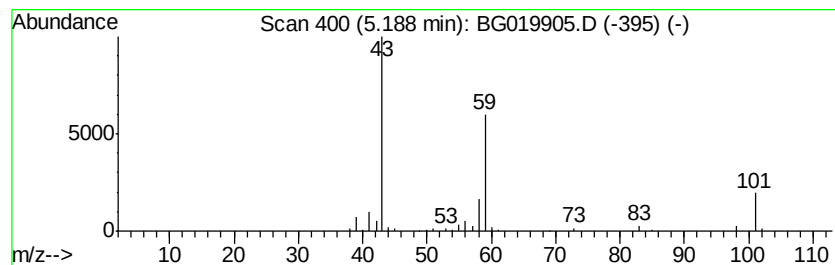
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	24.17 ng	206961	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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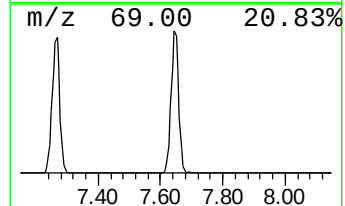
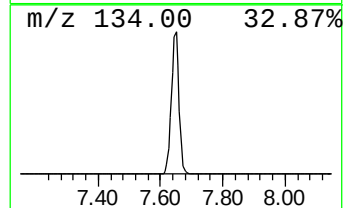
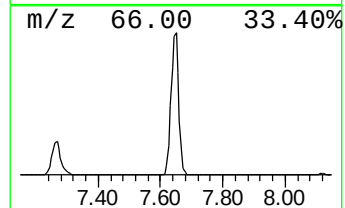
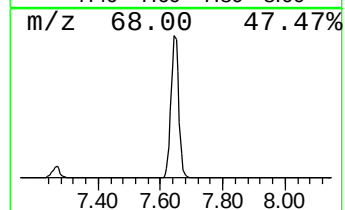
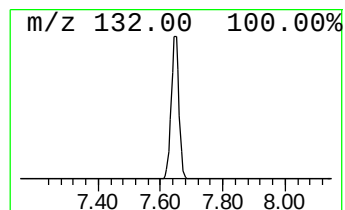
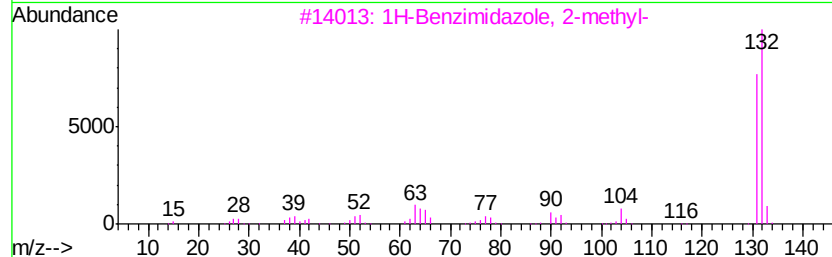
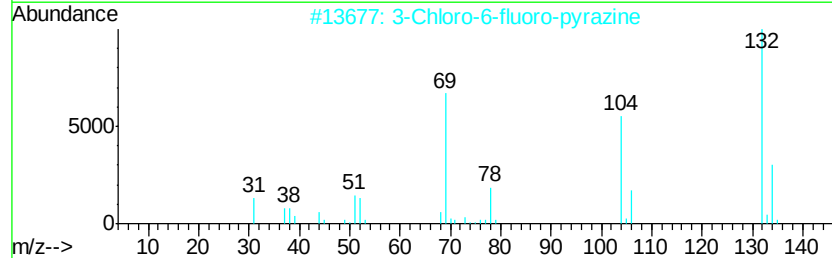
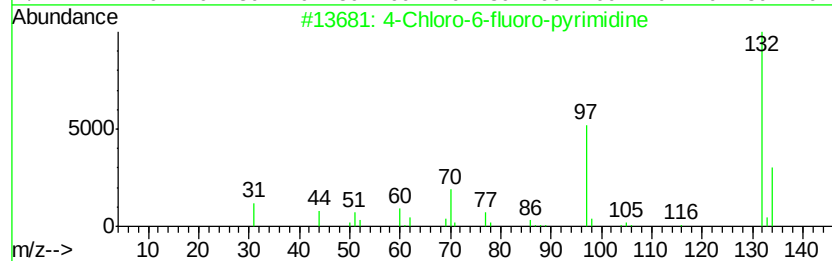
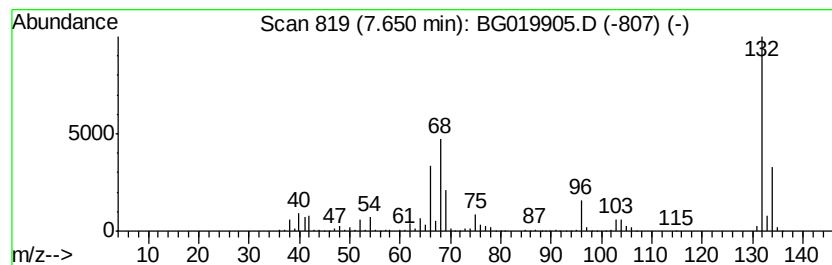
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 unknown7.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	130.71 ng	1119230	1,4-Dichlorobenzene-d4	8.12

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-Aminoindole	132	C8H8N2	005192-03-0	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019905.D
Acq On : 4 Dec 2015 13:28
Operator : UM/NP
Sample : G4609-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
CF-1

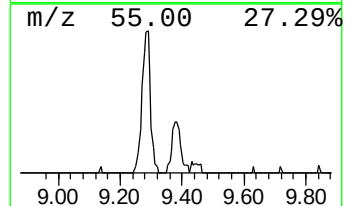
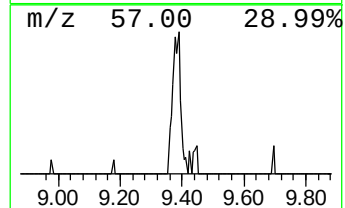
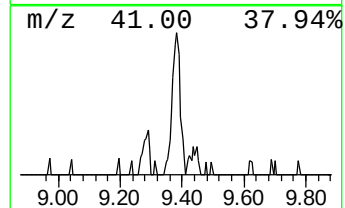
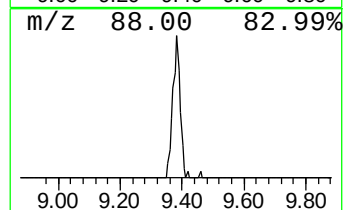
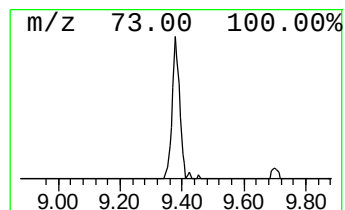
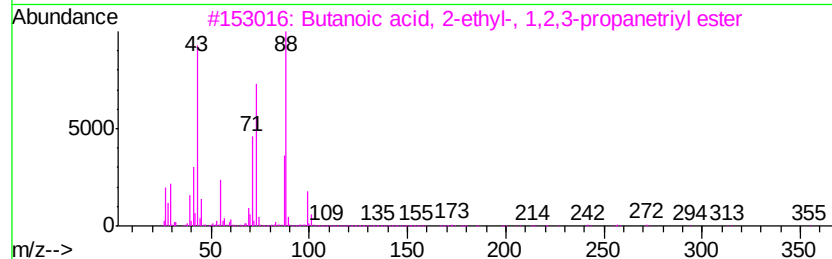
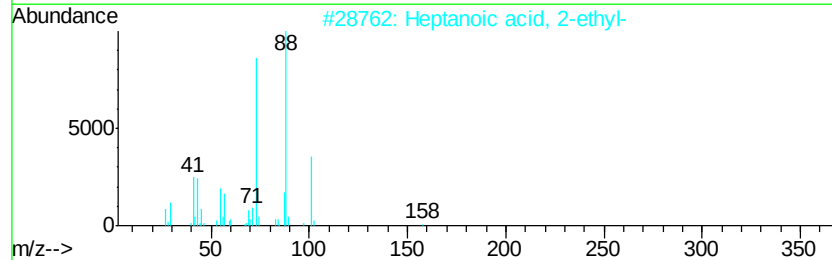
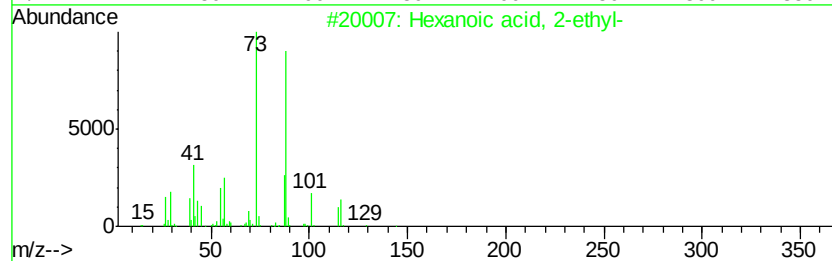
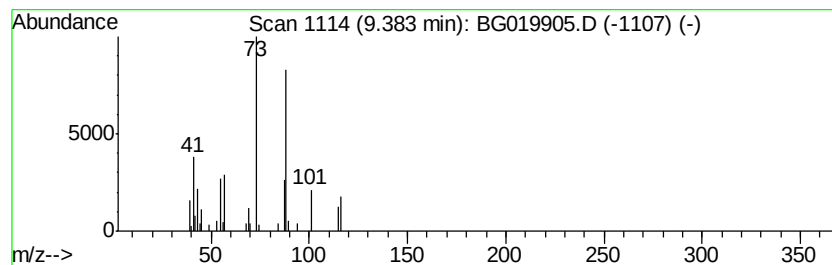
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexanoic acid, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.38	4.11 ng	35196	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78
2		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
3		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	50
4		Heptanoic acid, ethyl ester	158	C9H18O2	000106-30-9	38
5		Hexanamide, 6-(heptyloxy)-	229	C13H27NO2	055191-08-7	28



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019905.D
Acq On : 4 Dec 2015 13:28
Operator : UM/NP
Sample : G4609-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

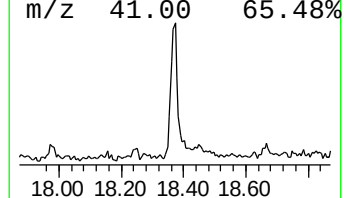
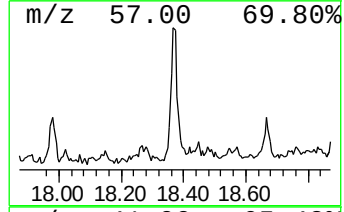
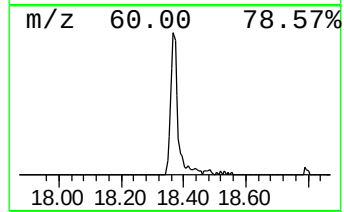
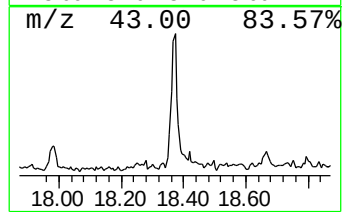
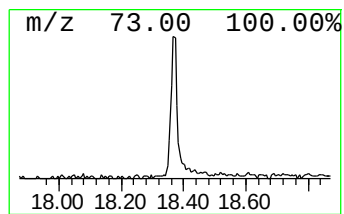
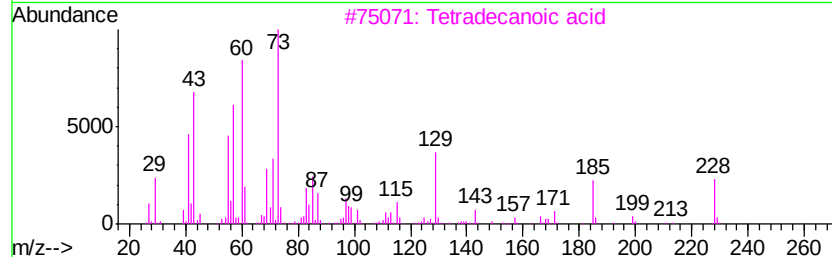
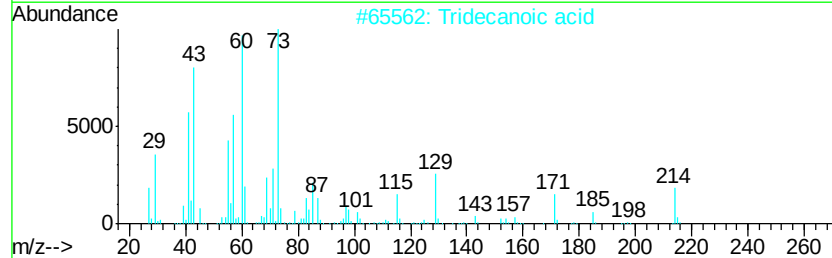
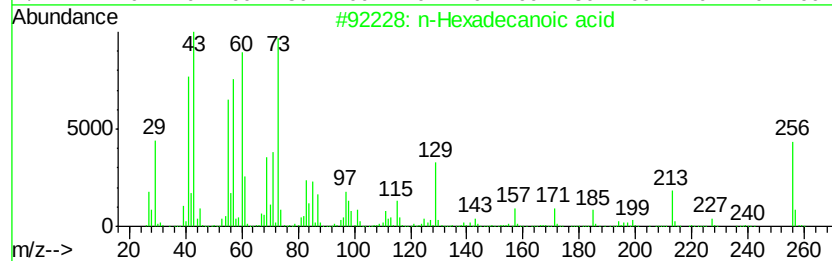
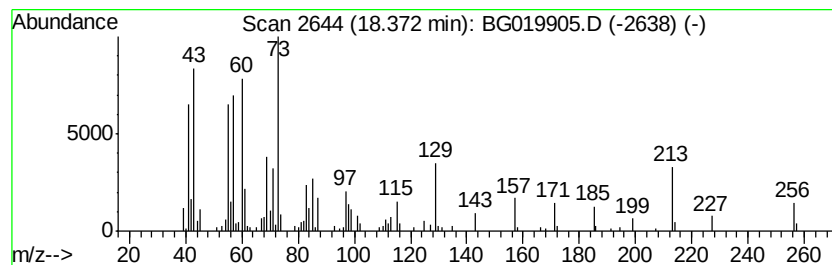
Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.37	5.53 ng	149633	Phenanthrene-d10	17.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019905.D
Acq On : 4 Dec 2015 13:28
Operator : UM/NP
Sample : G4609-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

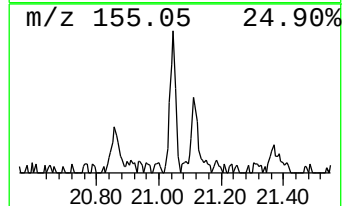
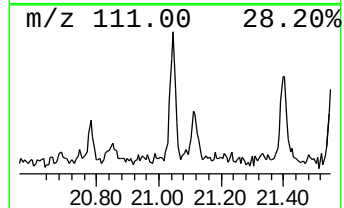
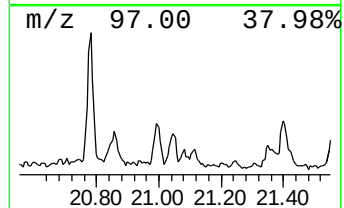
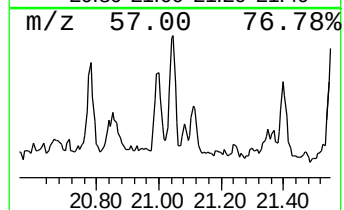
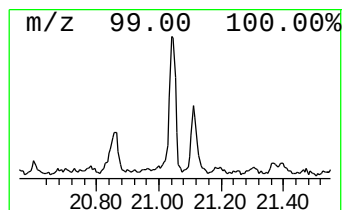
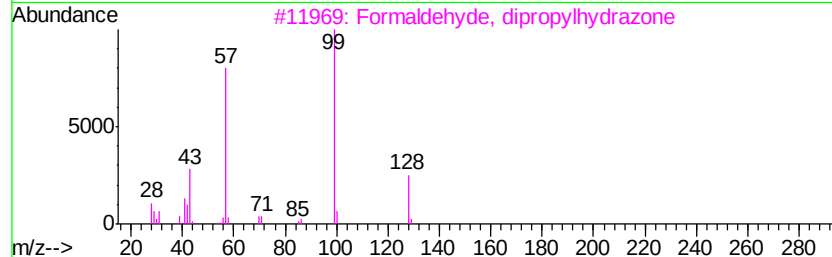
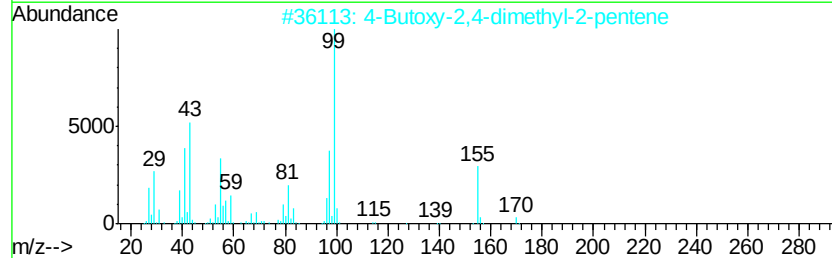
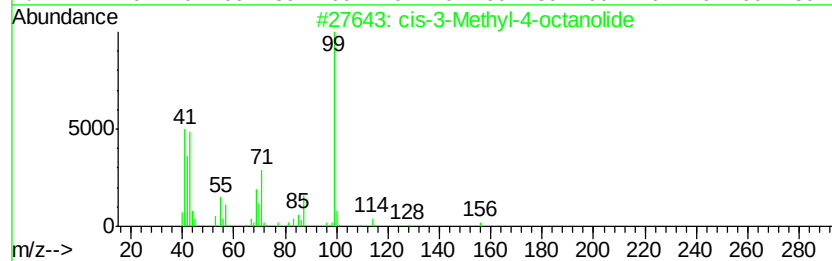
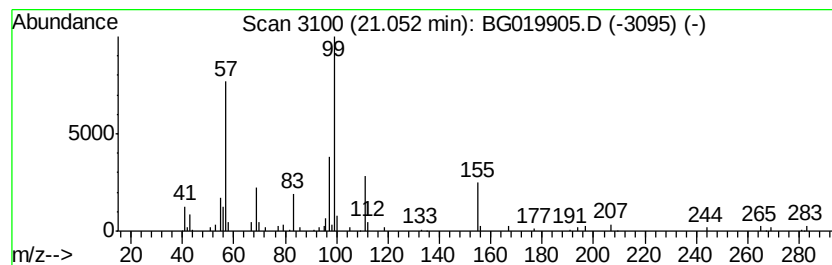
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown21.05 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.05	2.61 ng	91763	Chrysene-d12	21.76	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-3-Methyl-4-octanolide	156	C9H16O2	039638-67-0	43
2	4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	42
3	Formaldehyde, dipropylhydrazine	128	C7H16N2	054253-56-4	38
4	Hexanoic acid, 2-tridecyl ester	298	C19H38O2	055193-20-9	38
5	d-glucose, 2-deoxy-3,5:4,6-di-O-...	240	C10H18B2O5	1000149-94-7	38



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019905.D
Acq On : 4 Dec 2015 13:28
Operator : UM/NP
Sample : G4609-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

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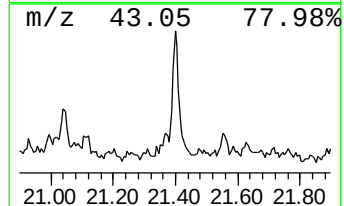
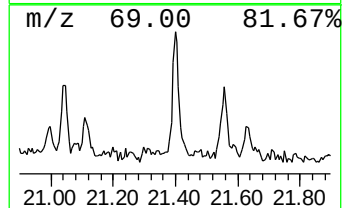
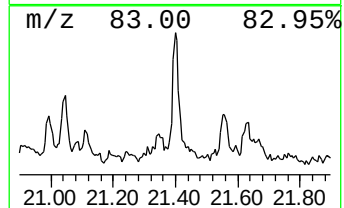
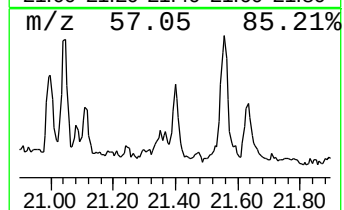
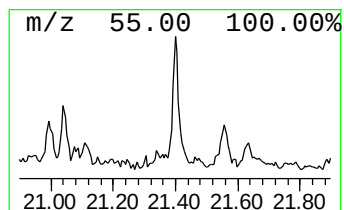
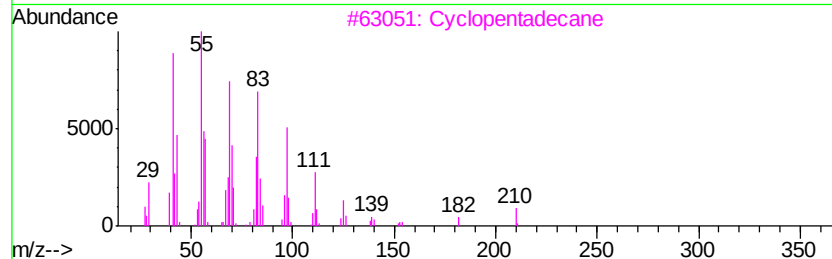
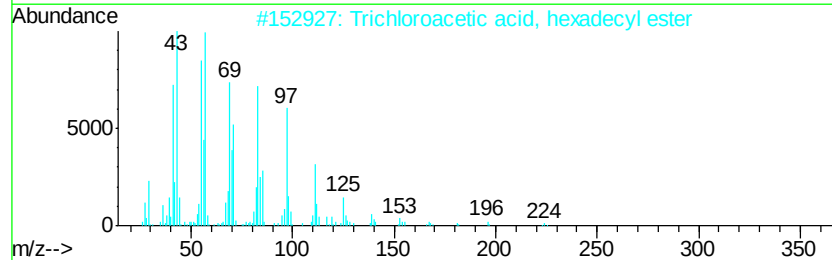
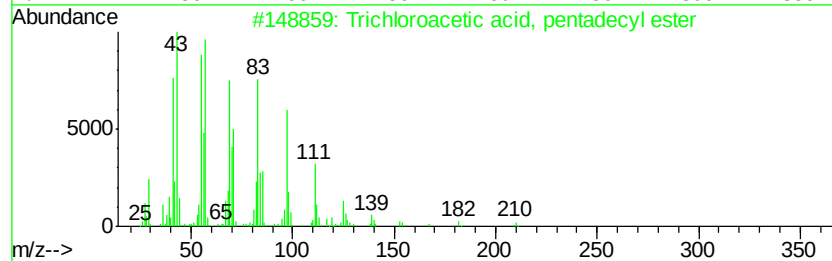
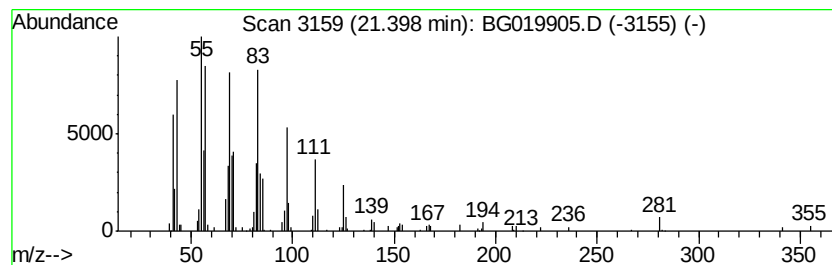
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Trichloroacetic acid, penta... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	3.82 ng	134408	Chrysene-d12	21.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		Cyclopentadecane	210	C15H30	000295-48-7	91
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
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Sample : G4609-04
Misc :
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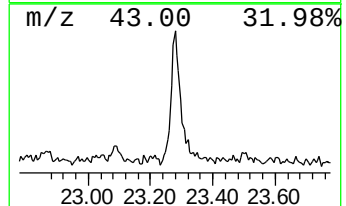
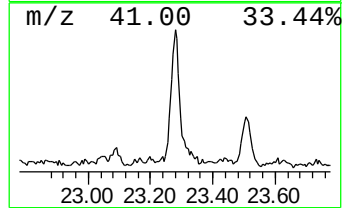
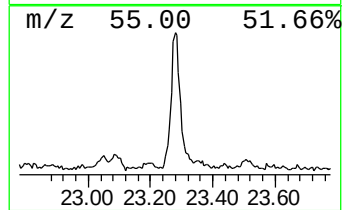
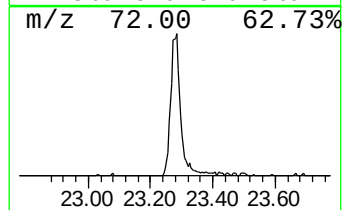
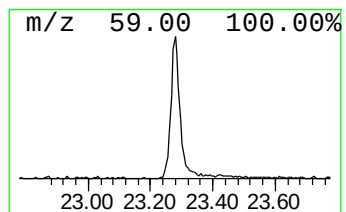
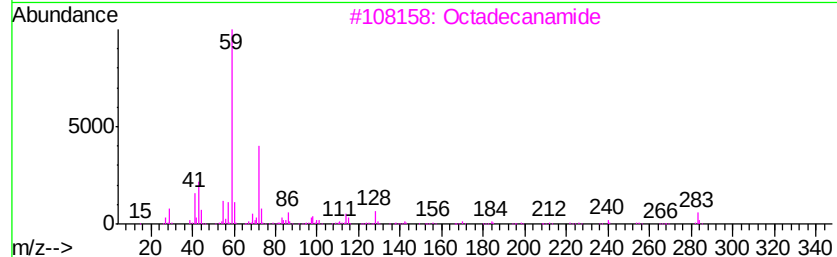
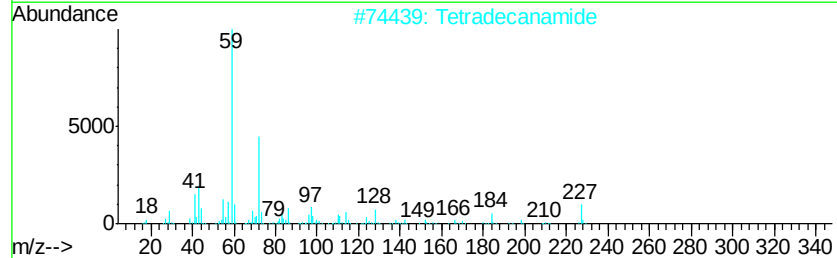
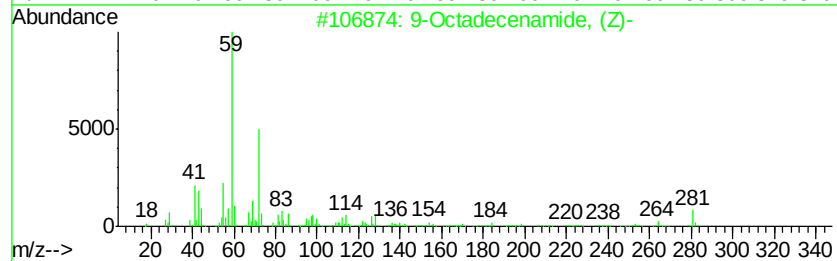
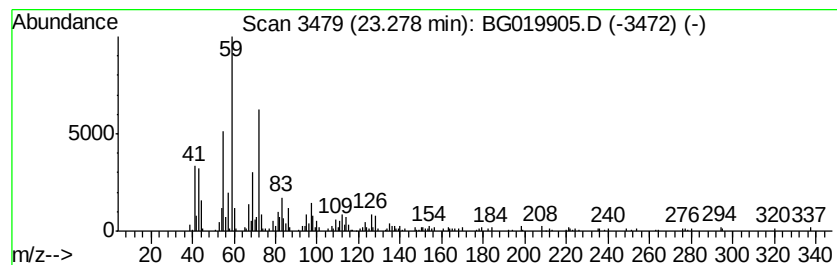
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.28	7.97 ng	280423	Chrysene-d12	21.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		Tetradecanamide	227	C14H29NO	000638-58-4	86
3		Octadecanamide	283	C18H37NO	000124-26-5	64
4		Octanamide	143	C8H17NO	000629-01-6	59
5		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019905.D
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Sample : G4609-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

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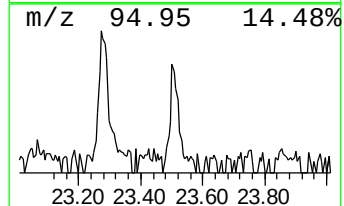
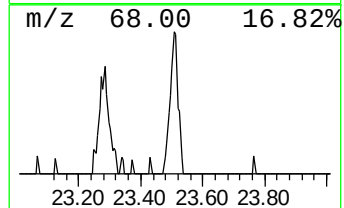
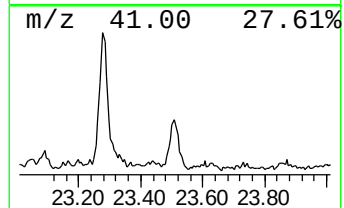
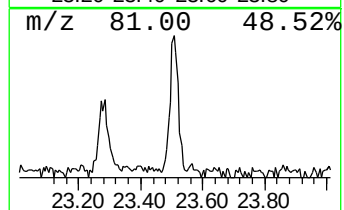
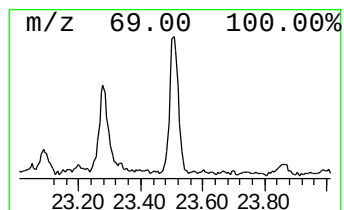
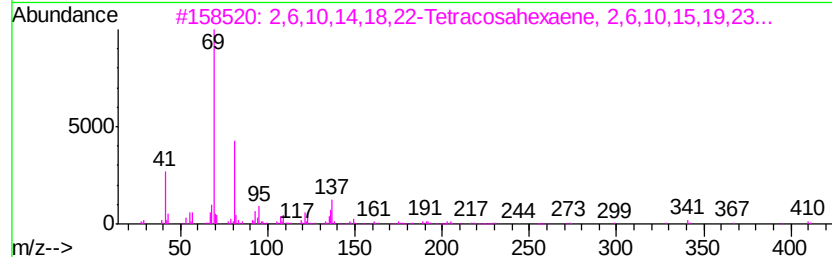
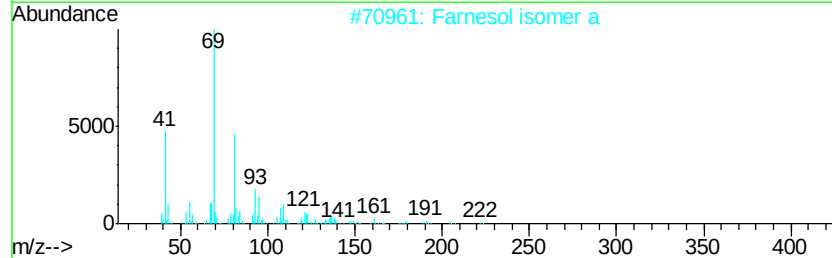
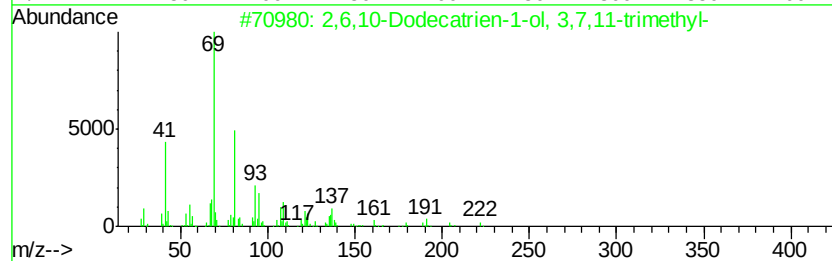
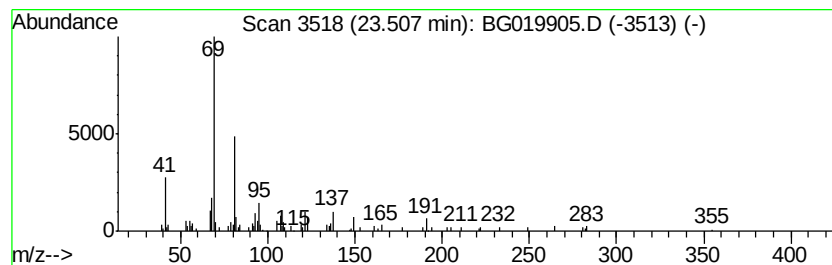
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.51	2.28 ng	73040	Perylene-d12	25.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	93
2		Farnesol isomer a	222	C15H26O	1000108-92-4	87
3		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	72
4		Squalene	410	C30H50	007683-64-9	72
5		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120315\
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	2.99	265.9	ng	2276640	1	8.12	171257	20.0
Cyclohexane	3.14	8.7	ng	74560	1	8.12	171257	20.0
Butane, 2-methoxy...	3.22	14.5	ng	124490	1	8.12	171257	20.0
2-Pentanone, 4-hy...	5.19	24.2	ng	206961	1	8.12	171257	20.0
unknown7.65	7.65	130.7	ng	1119230	1	8.12	171257	20.0
Hexanoic acid, 2-...	9.38	4.1	ng	35196	1	8.12	171257	20.0
n-Hexadecanoic acid	18.37	5.5	ng	149633	4	17.49	540774	20.0
unknown21.05	21.05	2.6	ng	91763	5	21.76	703529	20.0
Trichloroacetic a...	21.40	3.8	ng	134408	5	21.76	703529	20.0
9-Octadecenamide,...	23.28	8.0	ng	280423	5	21.76	703529	20.0
2,6,10-Dodecatric...	23.51	2.3	ng	73040	6	25.05	639803	20.0