

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102116\
 Data File : BF090781.D
 Acq On : 22 Oct 2016 23:49
 Operator : UM/SJ
 Sample : H5343-12
 Misc :
 ALS Vial : 62 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RMAB-SB07-12.0-12.5

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_F\METHODS\8270-BF102116.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	5.057	236	238	247	rBV	746506	1184955	19.07%	2.227%
2	5.469	272	274	277	rBV	3619817	5037513	81.07%	9.466%
3	6.497	361	364	366	rBV	4062641	4939792	79.50%	9.283%
4	6.623	372	375	378	rBV	4525971	5077351	81.71%	9.541%
5	6.852	393	395	406	rBV	1221441	1338071	21.53%	2.514%
6	7.012	406	409	411	rBV	4355933	4527859	72.87%	8.509%
7	7.423	441	445	447	rBV	2349785	3278850	52.77%	6.161%
8	7.515	451	453	461	rVB	49884	123921	1.99%	0.233%
9	8.143	505	508	510	rBV	1131539	1617674	26.03%	3.040%
10	9.218	598	602	604	rBV	5758043	6213504	100.00%	11.676%
11	9.332	610	612	615	rVB	110088	114596	1.84%	0.215%
12	9.606	634	636	639	rBV	1115227	1486182	23.92%	2.793%
13	9.892	658	661	663	rBV	2237136	2079281	33.46%	3.907%
14	10.326	698	699	701	rVB	110234	83498	1.34%	0.157%
15	10.543	715	718	721	rBV	37576	65522	1.05%	0.123%
16	10.681	727	730	733	rBV	3145199	3710457	59.72%	6.973%
17	10.795	739	740	747	rVB	121020	194027	3.12%	0.365%
18	11.252	777	780	781	rBV	65446	86509	1.39%	0.163%
19	11.378	788	791	793	rBV	1822561	1718289	27.65%	3.229%
20	11.606	808	811	815	rBV	483321	495592	7.98%	0.931%
21	12.418	880	882	885	rBV	1251334	1694584	27.27%	3.184%
22	12.966	927	930	932	rBV	5299627	5223342	84.06%	9.815%
23	13.172	946	948	952	rBV2	42601	73396	1.18%	0.138%
24	13.412	967	969	971	rBV	239982	215101	3.46%	0.404%
25	13.858	1006	1008	1018	rBV	341259	455244	7.33%	0.855%
26	14.018	1018	1022	1024	rBV	831802	1236324	19.90%	2.323%
27	15.447	1144	1147	1154	rBV	710847	943992	15.19%	1.774%

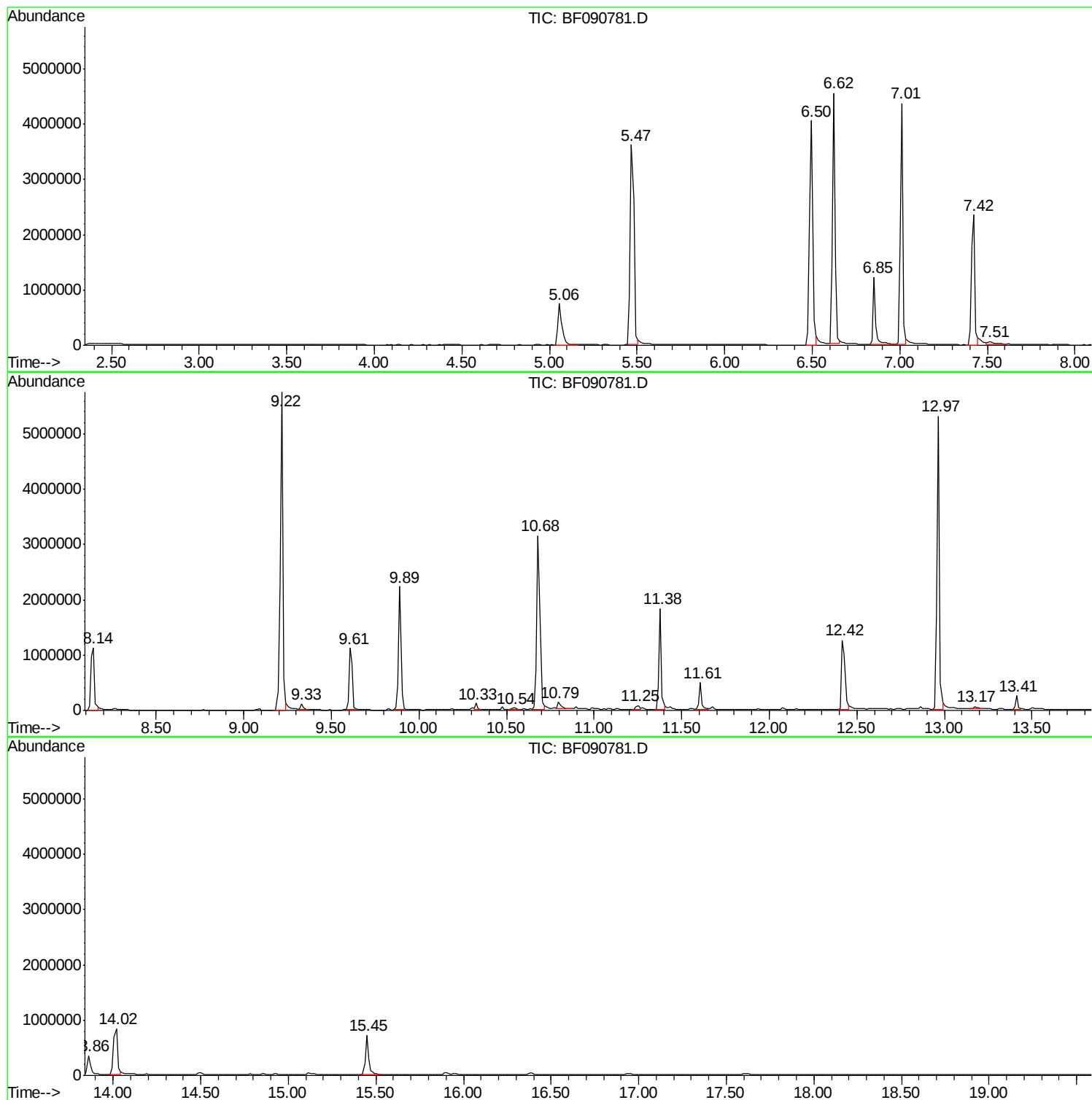
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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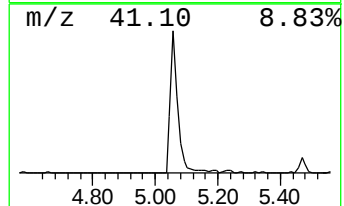
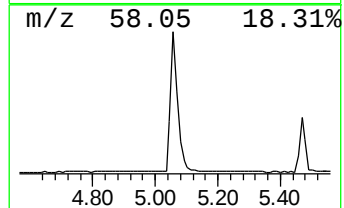
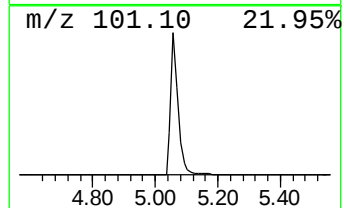
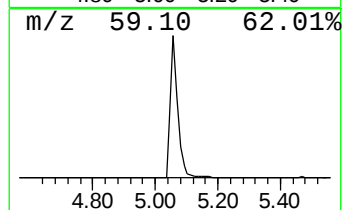
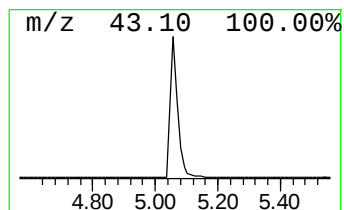
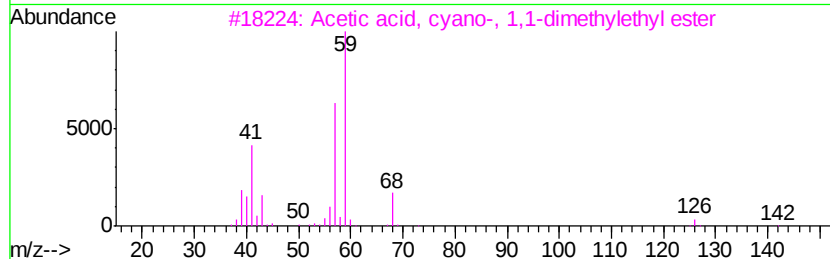
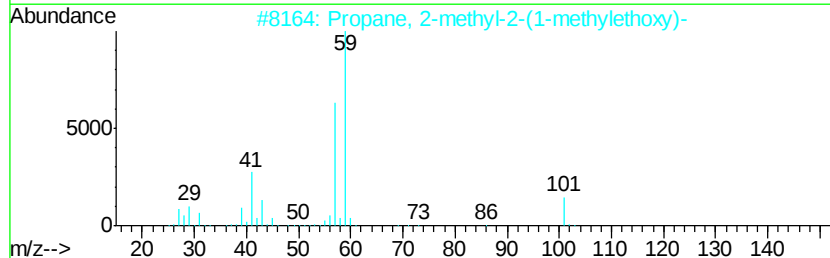
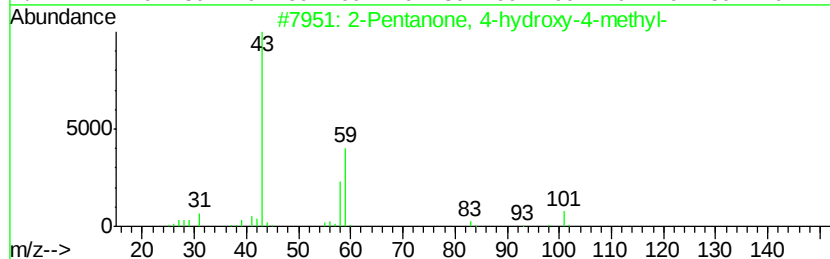
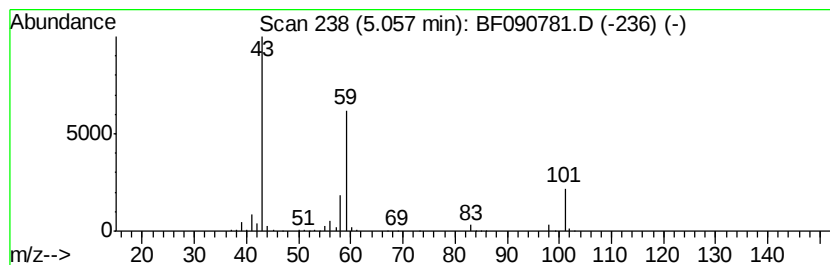
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	17.71 ng	1184960	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	53
3		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Acetone	58	C3H6O	000067-64-1	9



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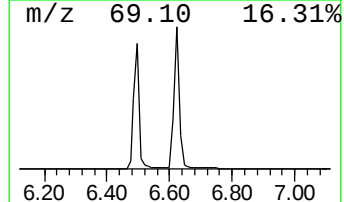
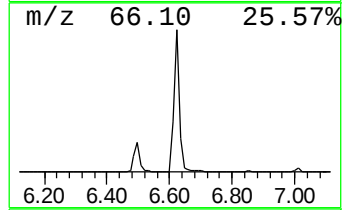
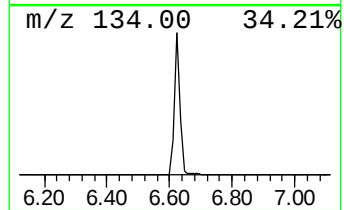
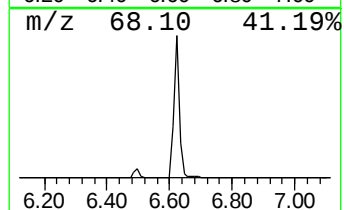
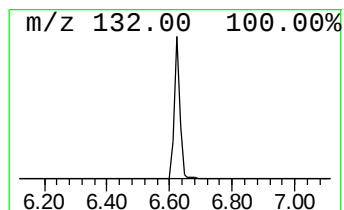
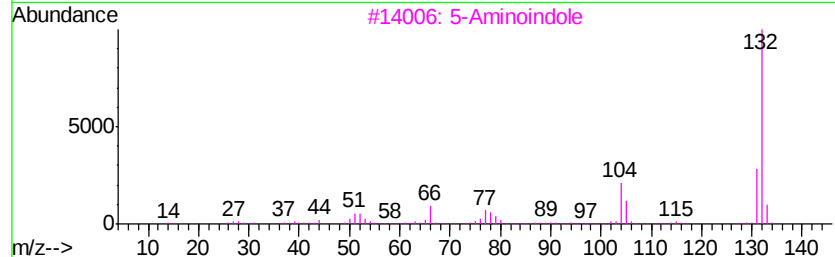
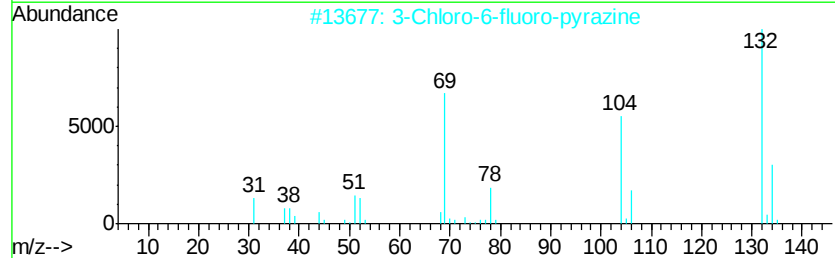
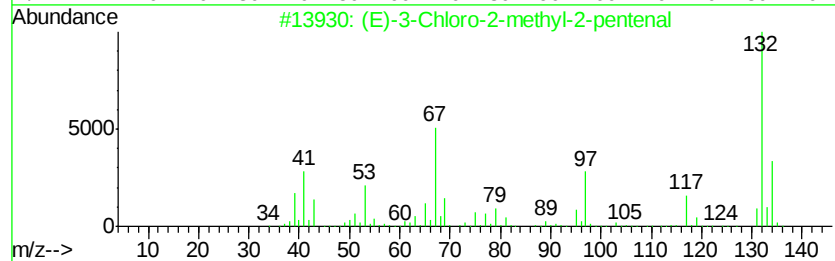
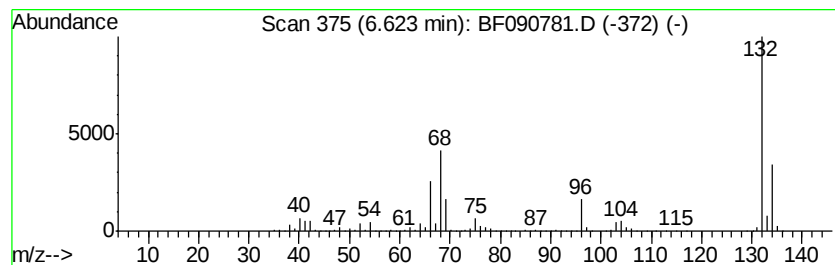
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	75.89 ng	5077350	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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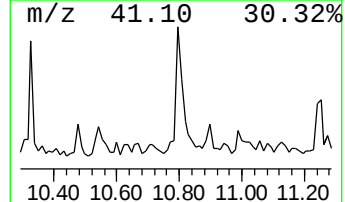
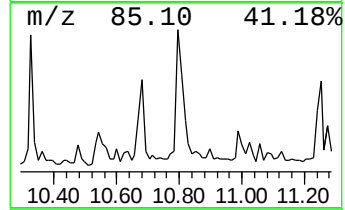
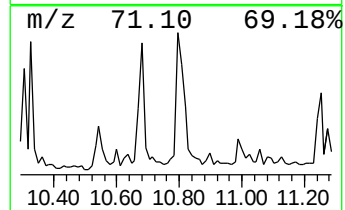
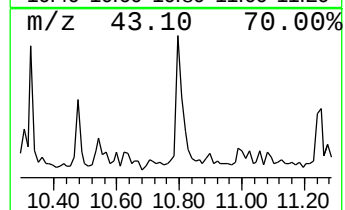
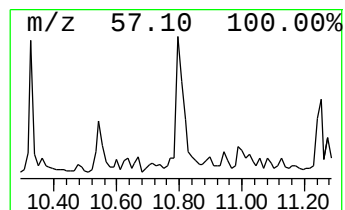
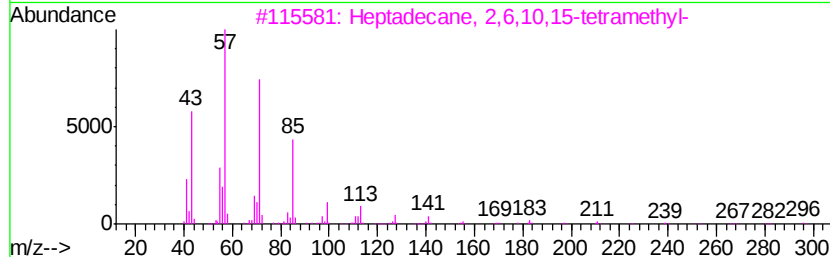
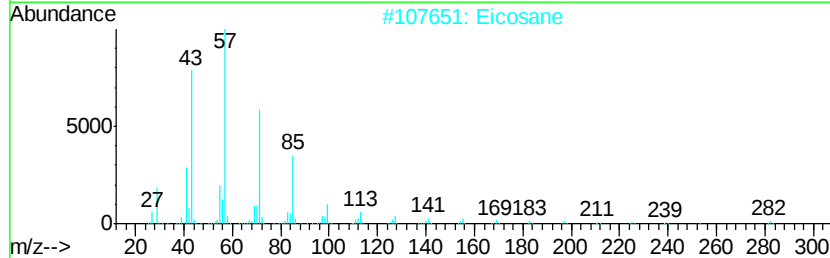
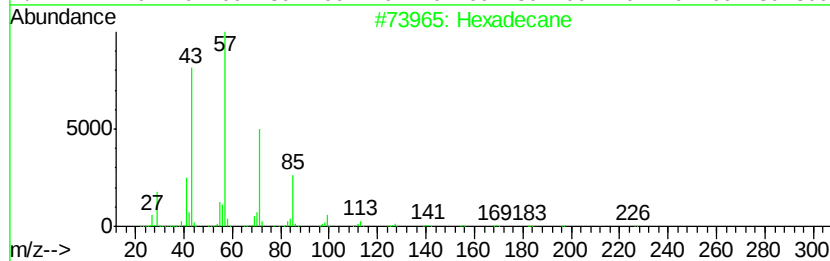
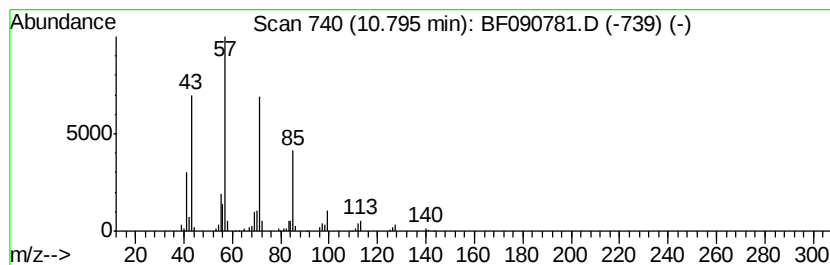
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Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.79	2.26 ng	194027	Phenanthrene-d10	11.38	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Eicosane	282	C20H42	000112-95-8	86
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
4	Octacosane	394	C28H58	000630-02-4	78
5	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	64



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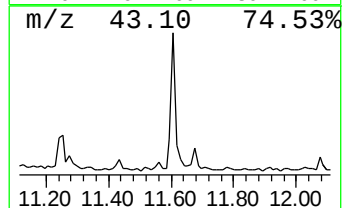
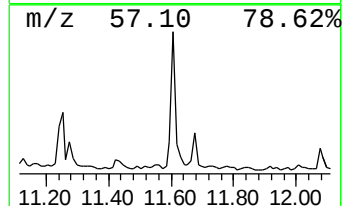
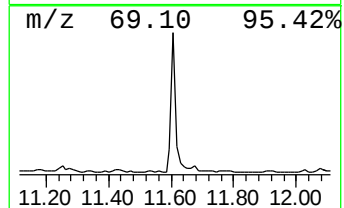
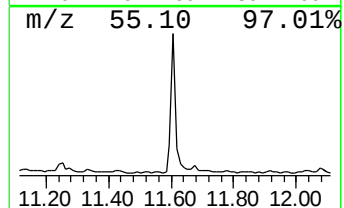
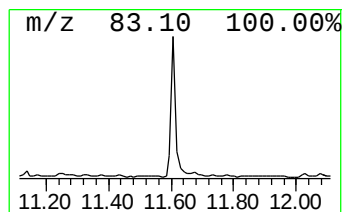
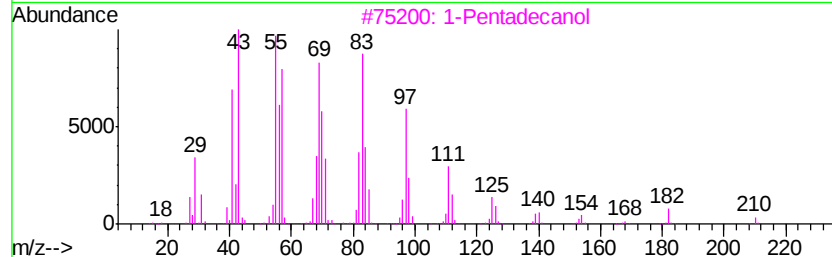
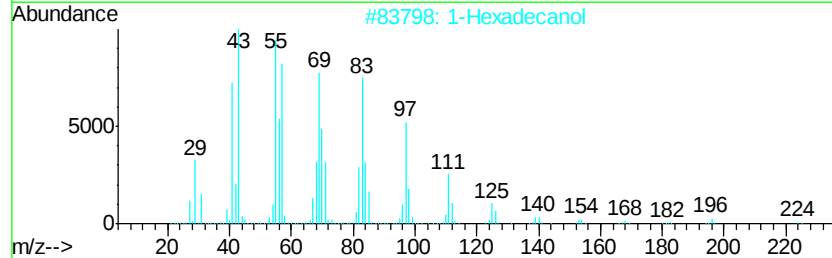
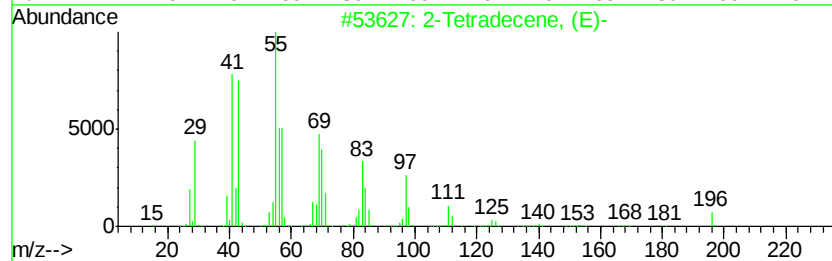
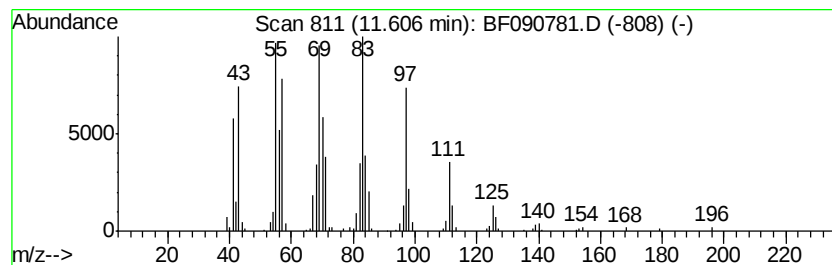
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Tetradecene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.		
11.61	5.77 ng	495592	Phenanthrene-d10		11.38		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2		Tetradecene, (E)-	196	C14H28	035953-53-8	96
2	1		Hexadecanol	242	C16H34O	036653-82-4	94
3	1		Pentadecanol	228	C15H32O	000629-76-5	91
4	5		Octadecene, (E)-	252	C18H36	007206-21-5	91
5	9		Octadecene, (E)-	252	C18H36	007206-25-9	91



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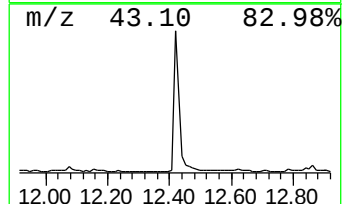
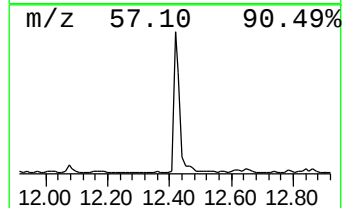
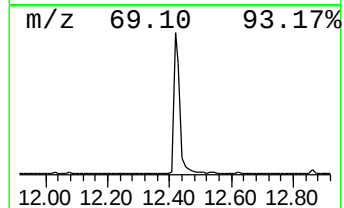
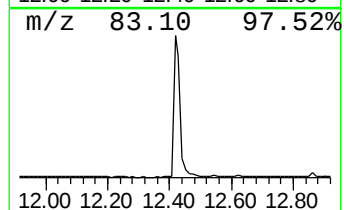
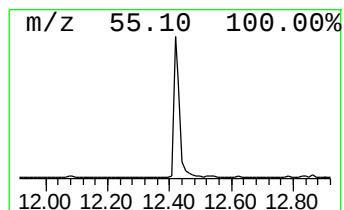
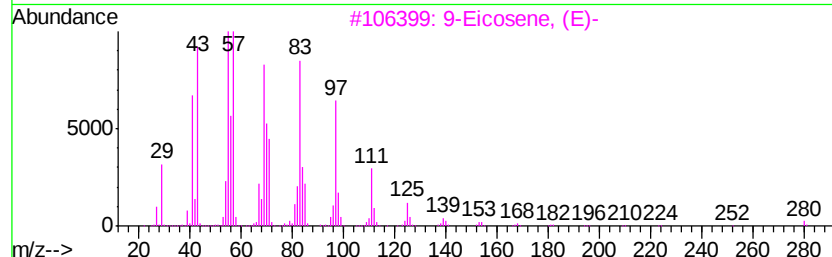
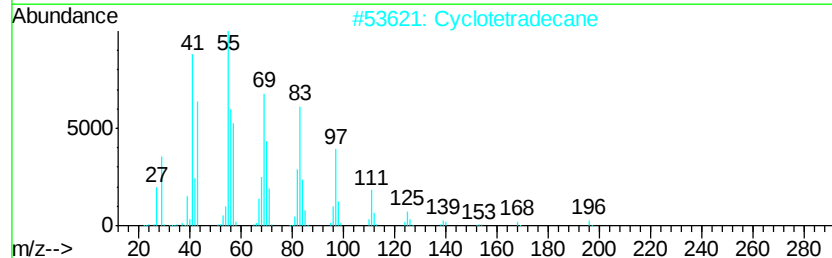
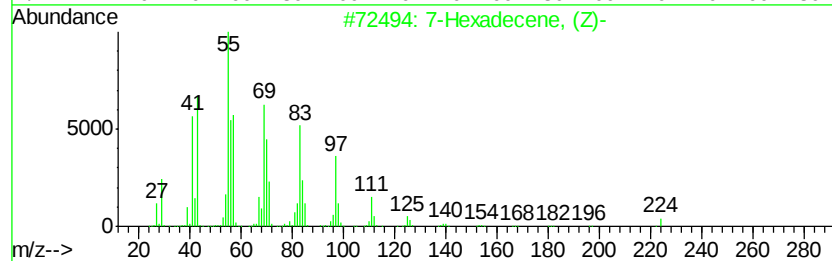
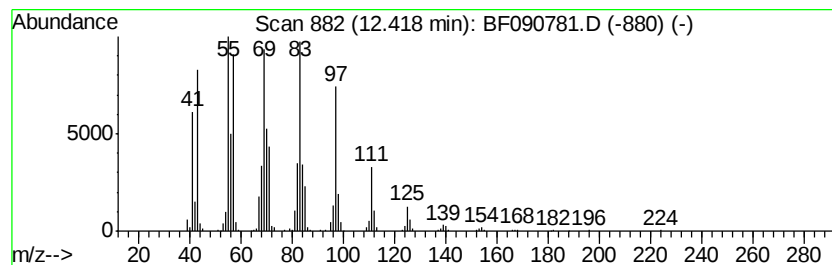
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 7-Hexadecene, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	19.72 ng	1694580	Phenanthrene-d10	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	98
2		Cyclotetradecane	196	C14H28	000295-17-0	98
3		9-Eicosene, (E)-	280	C20H40	074685-29-3	94
4		5-Octadecene, (E)-	252	C18H36	007206-21-5	91
5		1-Nonadecene	266	C19H38	018435-45-5	91



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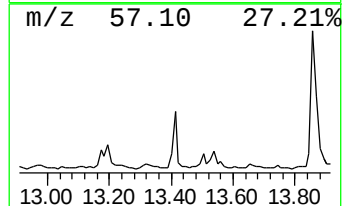
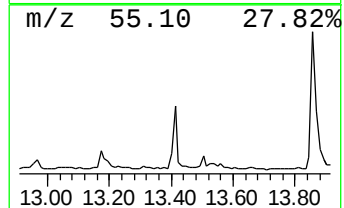
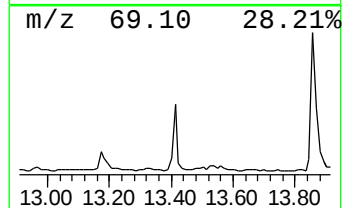
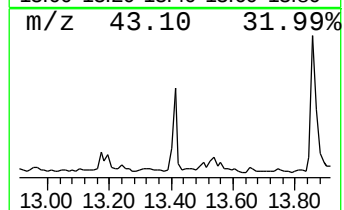
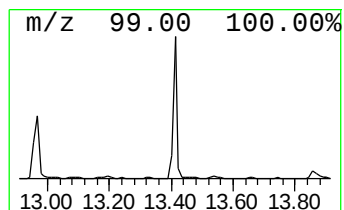
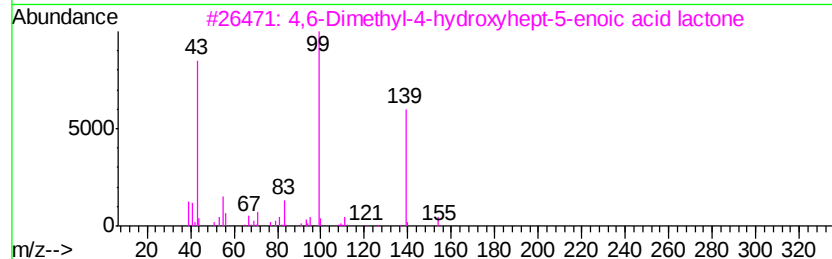
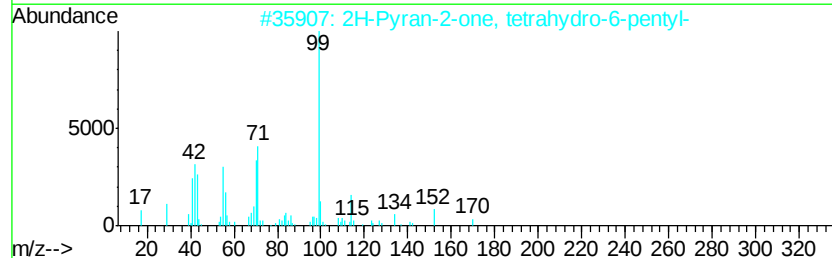
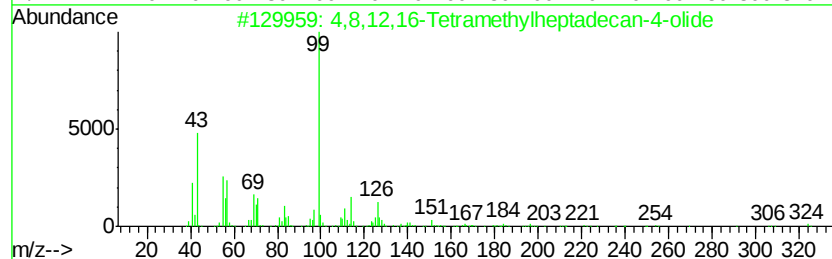
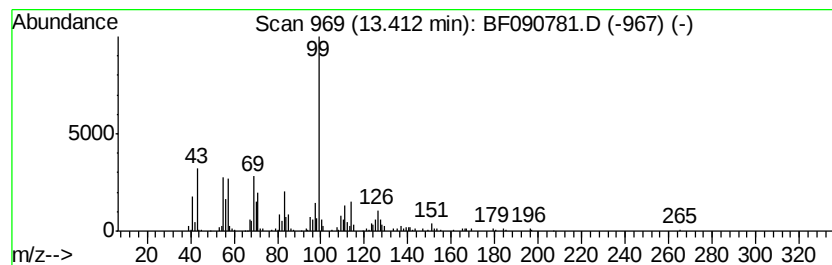
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4,8,12,16-Tetramethylheptad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.41	3.48 ng	215101	Chrysene-d12	14.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	74		
2	2H-Pyran-2-one, tetrahydro-6-pen...	170	C10H18O2	000705-86-2	50		
3	4,6-Dimethyl-4-hydroxyhept-5-eno...	154	C9H14O2	1000122-47-0	50		
4	Acetaldehyde, diethylhydrazone	114	C6H14N2	007422-91-5	50		
5	2(3H)-Furanone, 5-butyldihydro-4...	156	C9H16O2	055013-32-6	47		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102116\
Data File : BF090781.D
Acq On : 22 Oct 2016 23:49
Operator : UM/SJ
Sample : H5343-12
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RMAB-SB07-12.0-12.5

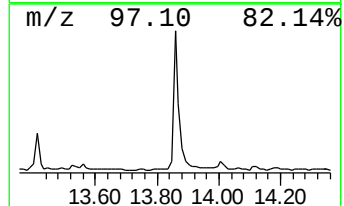
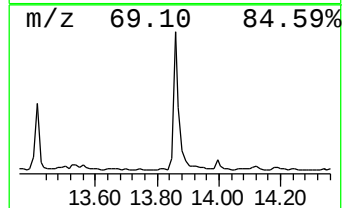
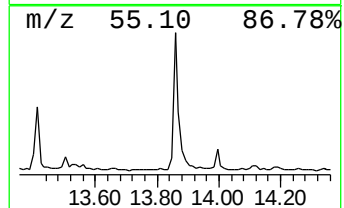
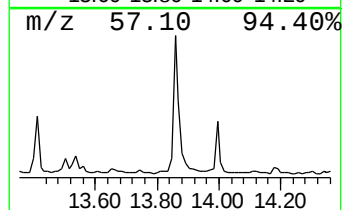
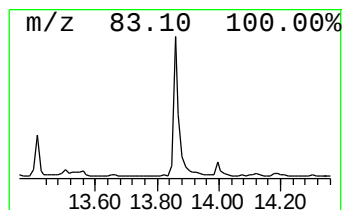
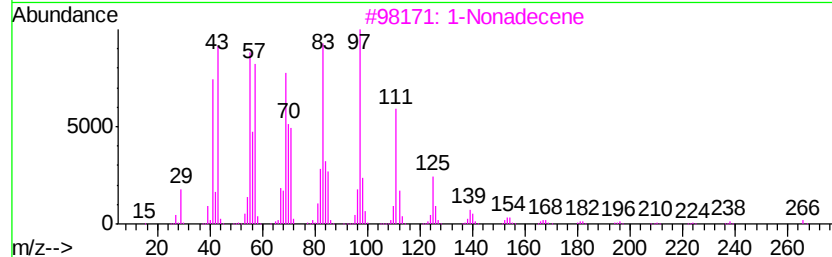
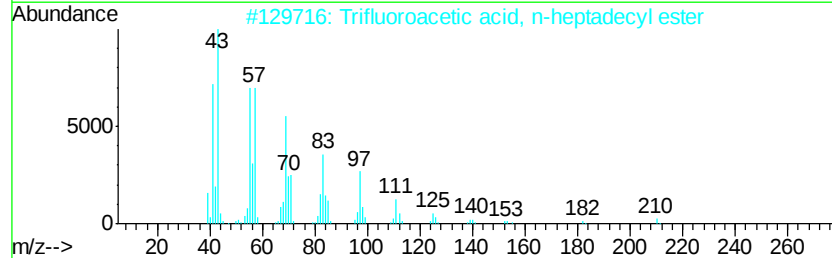
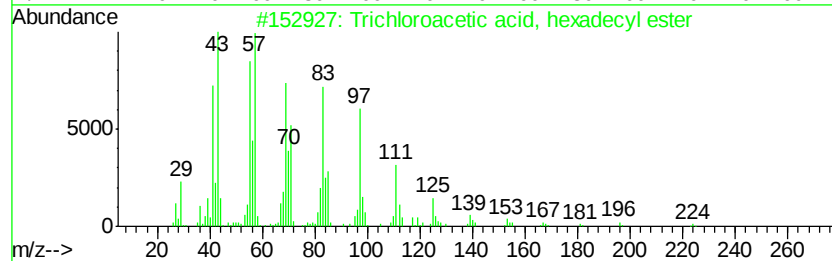
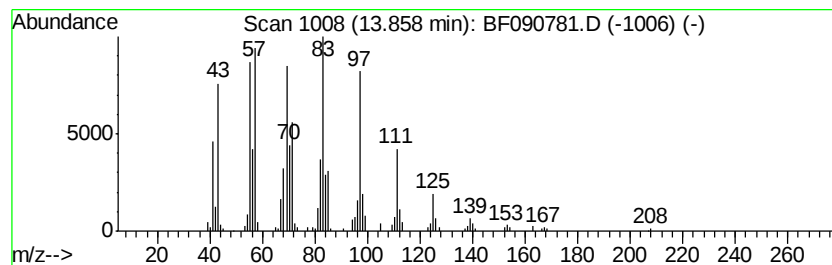
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	7.36 ng	455244	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
3		1-Nonadecene	266	C19H38	018435-45-5	91
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102116\
Data File : BF090781.D
Acq On : 22 Oct 2016 23:49
Operator : UM/SJ
Sample : H5343-12
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RMAB-SB07-12.0-12.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
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
2-Pentanone, 4-hy...	5.06	17.7	ng	1184960	1	6.85	1338070	20.0
unknown6.62	6.62	75.9	ng	5077350	1	6.85	1338070	20.0
Hexadecane	10.79	2.3	ng	194027	4	11.38	1718290	20.0
2-Tetradecene, (E)-	11.61	5.8	ng	495592	4	11.38	1718290	20.0
7-Hexadecene, (Z)-	12.42	19.7	ng	1694580	4	11.38	1718290	20.0
4,8,12,16-Tetrame...	13.41	3.5	ng	215101	5	14.02	1236320	20.0
Trichloroacetic a...	13.86	7.4	ng	455244	5	14.02	1236320	20.0