LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138656.D
Acq On : 25 Jul 2024 16:50
Operator : RC/JU
Sample : P3357-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-854-J-SO-2-2.5-072024

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_F\Methods\8270-BF070924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138656.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	8	16	rVB	857603	1297913	55.19%	8.174%
2	3.375	213	218	234	rBV	19446	61476	2.61%	0.387%
3	5.069	496	506	523	rVB	73679	114180	4.86%	0.719%
4	5.481	570	576	587	rBV	1084947	1457891	62.00%	9.181%
5	6.487	741	747	768	rBV	1185030	1553826	66.08%	9.785%
6	6.681	775	780	791	rVB	36163	50826	2.16%	0.320%
7	6.851	804	809	814	rBV	387886	470410	20.00%	2.962%
8	7.416	898	905	915	rBV	739715	994172	42.28%	6.261%
9	8.134	1021	1027	1034	rBV	502026	628966	26.75%	3.961%
10	8.445	1075	1080	1085	rBV	68052	93769	3.99%	0.591%
11	9.204	1203	1209	1214	rBV	1316818	1650230	70.18%	10.393%
12	9.886	1319	1325	1334	rBV	558328	691839	29.42%	4.357%
13	9.986	1334	1342	1357	rBV	1441115	2351555	100.00%	14.809%
14	10.675	1454	1459	1474	rBV	761340	990853	42.14%	6.240%
15	11.369	1572	1577	1586	rBV	501006	656268	27.91%	4.133%
16	11.892	1660	1666	1674	rBV4	16438	32324	1.37%	0.204%
17	12.463	1759	1763	1770	rVB3	18018	26786	1.14%	0.169%
18	12.951	1841	1846	1851	rBV	941644	1181237	50.23%	7.439%
19	13.857	1995	2000	2014	rBV	31150	74651	3.17%	0.470%
20	14.010	2018	2026	2033	rVV	259273	356002	15.14%	2.242%
21	14.974	2184	2190	2196	rBV	556149	758709	32.26%	4.778%
22	15.468	2269	2274	2287	rBV	235193	385159	16.38%	2.426%

Sum of corrected areas: 15879042

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
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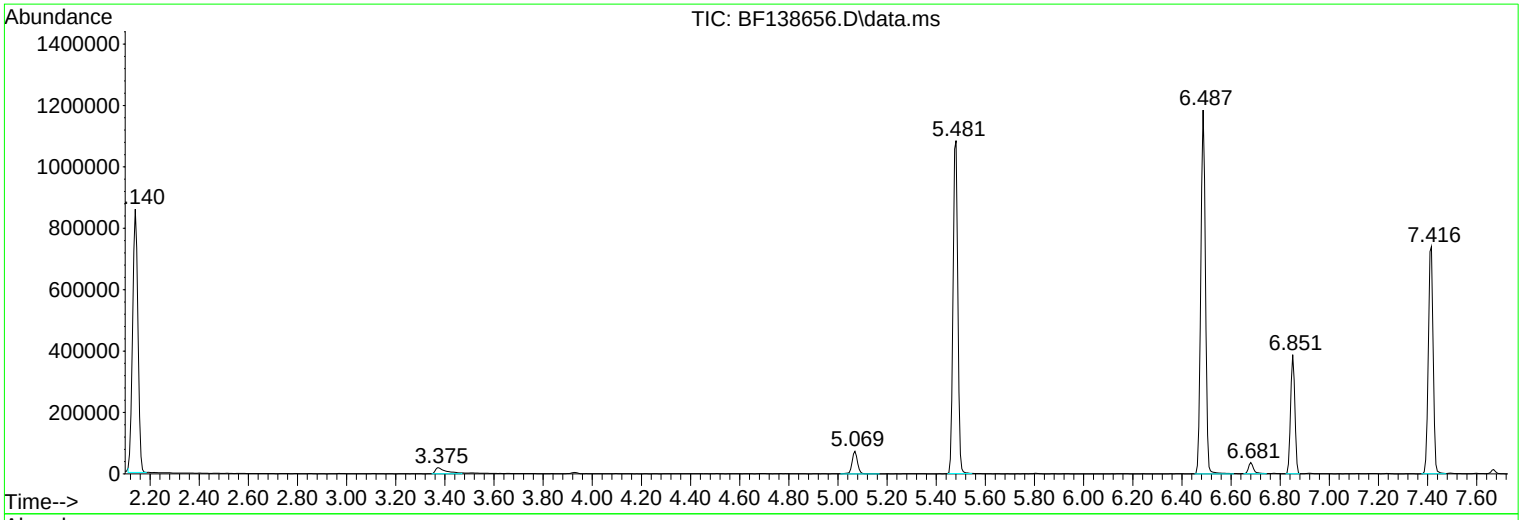
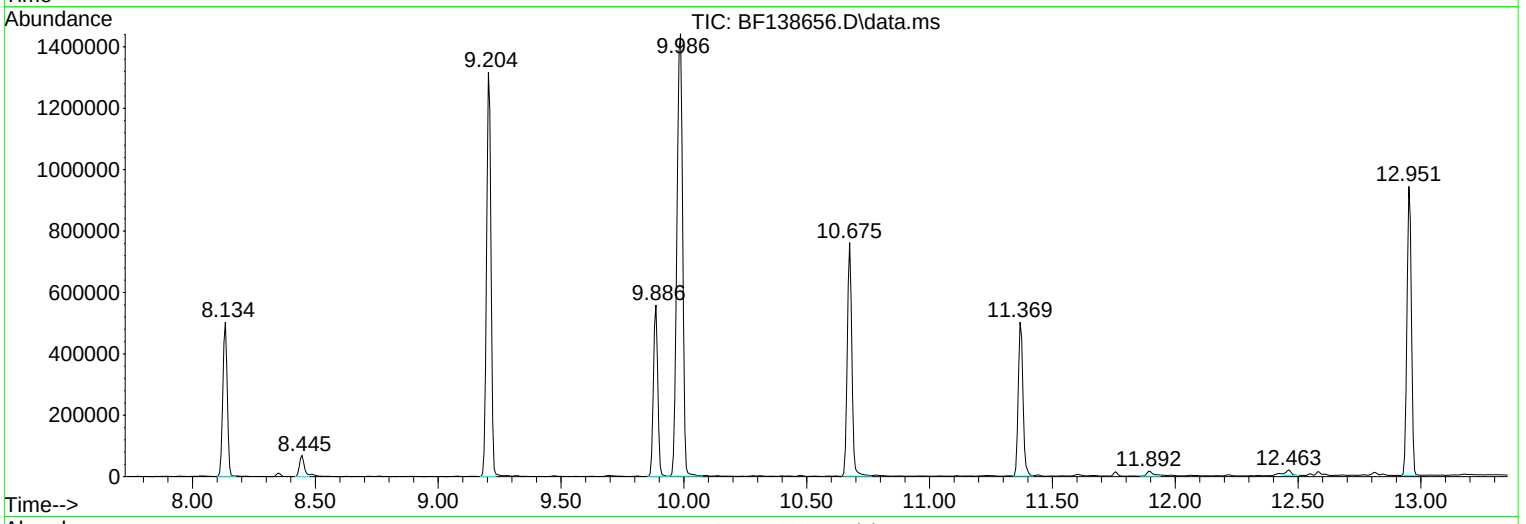
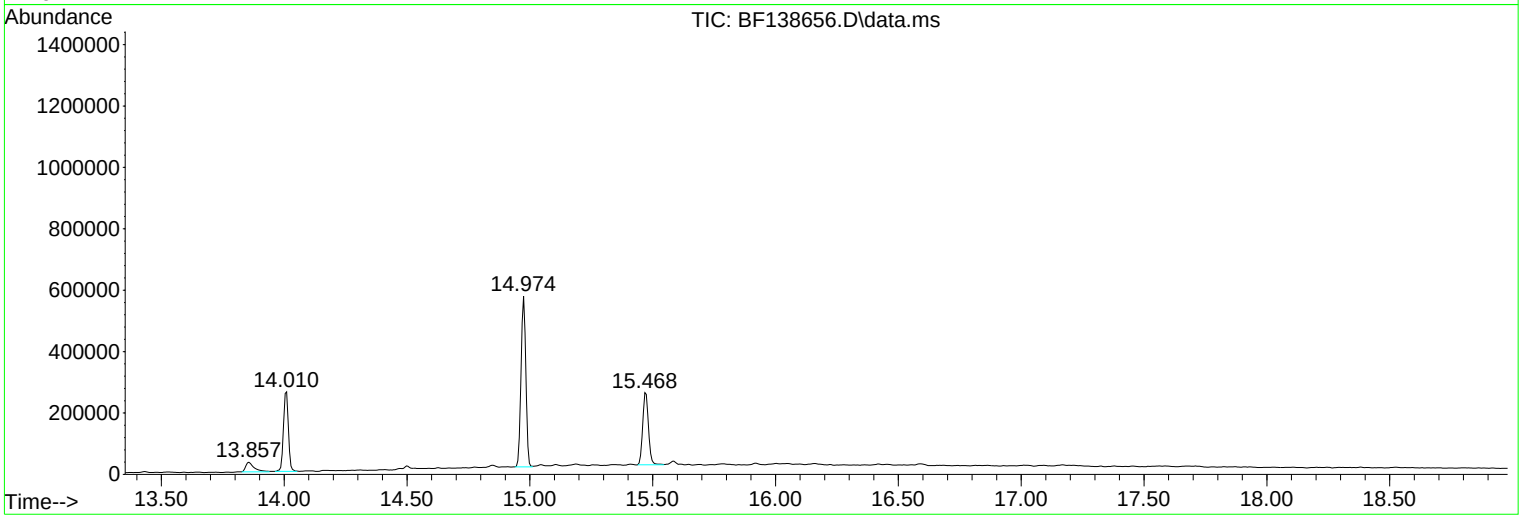
BNA_F
ClientSampleId :
S-854-J-SO-2-2.5-072024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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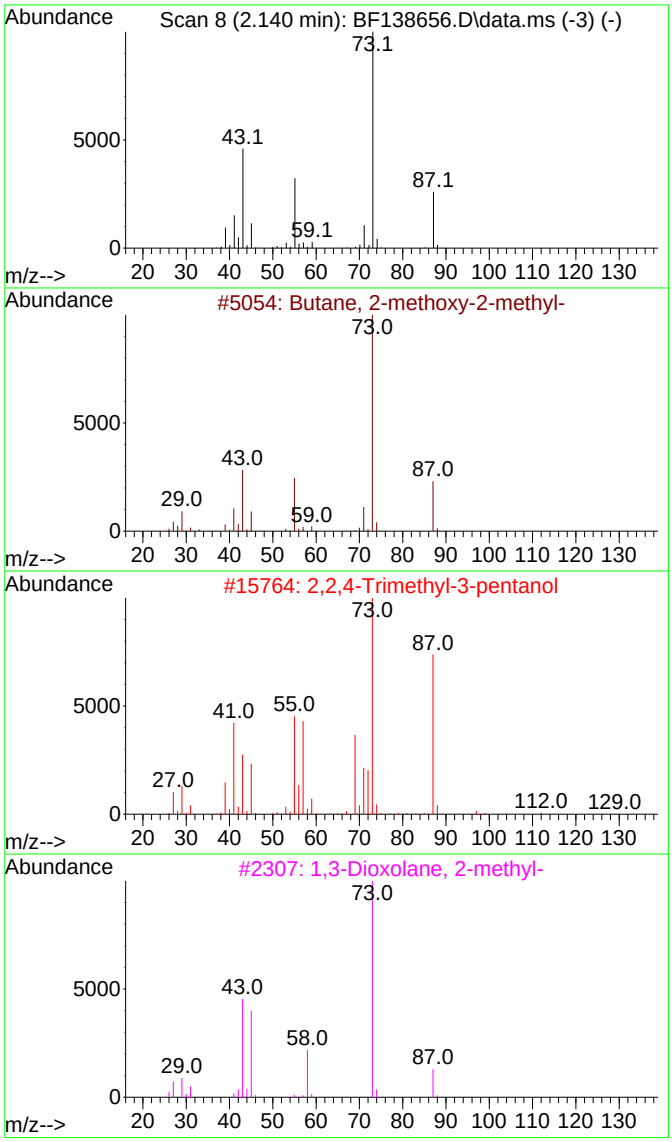
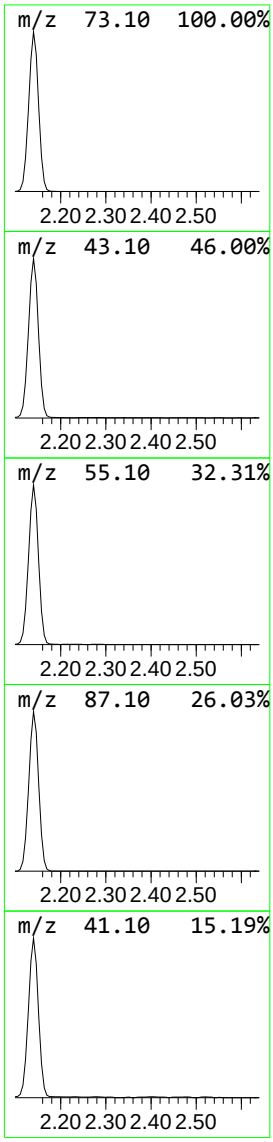
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	55.18 ng	1297910	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Data File : BF138656.D
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Operator : RC/JU
Sample : P3357-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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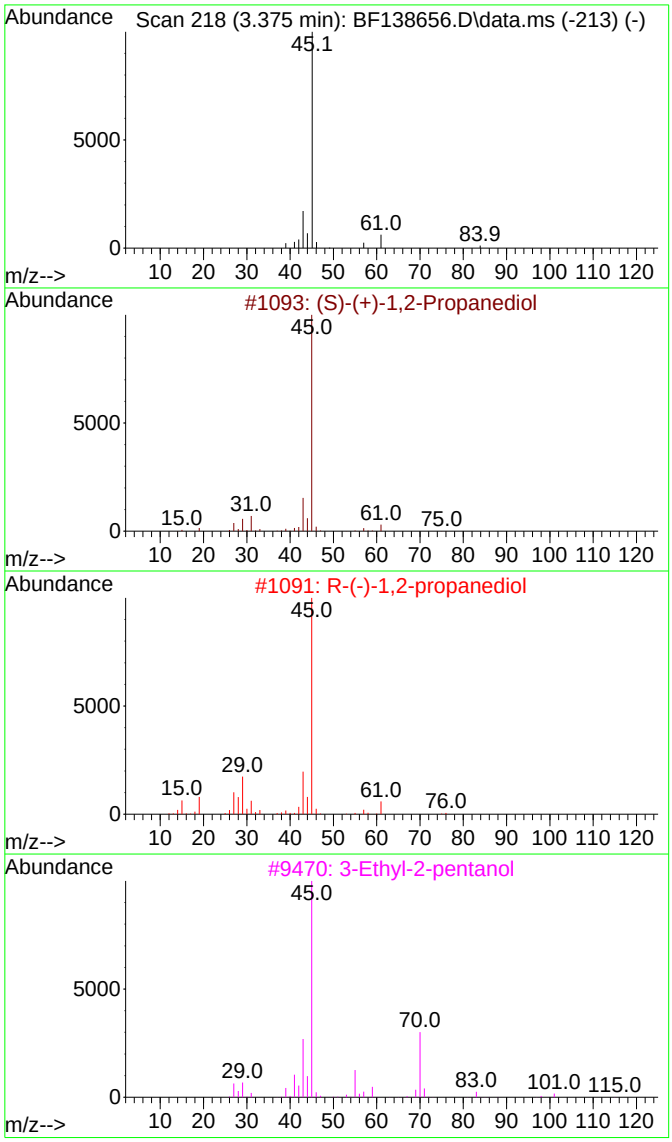
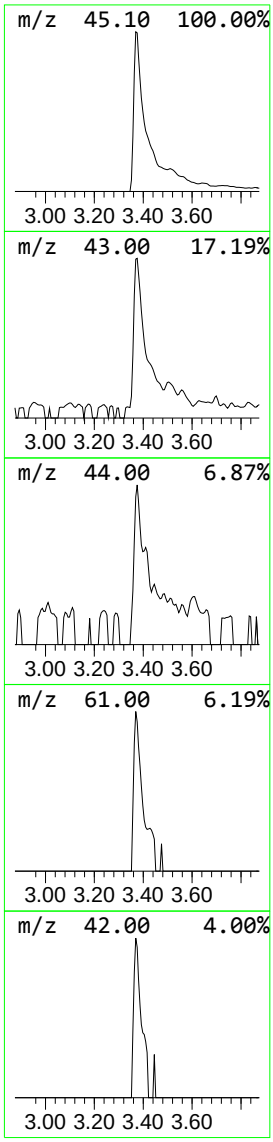
****

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.375	2.61 ng	61476	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3	3-Ethyl-2-pentanol	116	C7H16O	000609-27-8	9
4	2-Heptanol	116	C7H16O	000543-49-7	9
5	Propylene Glycol	76	C3H8O2	000057-55-6	9





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Sample : P3357-08
Misc :
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Instrument :
BNA_F
ClientSampleId :
S-854-J-SO-2-2.5-072024

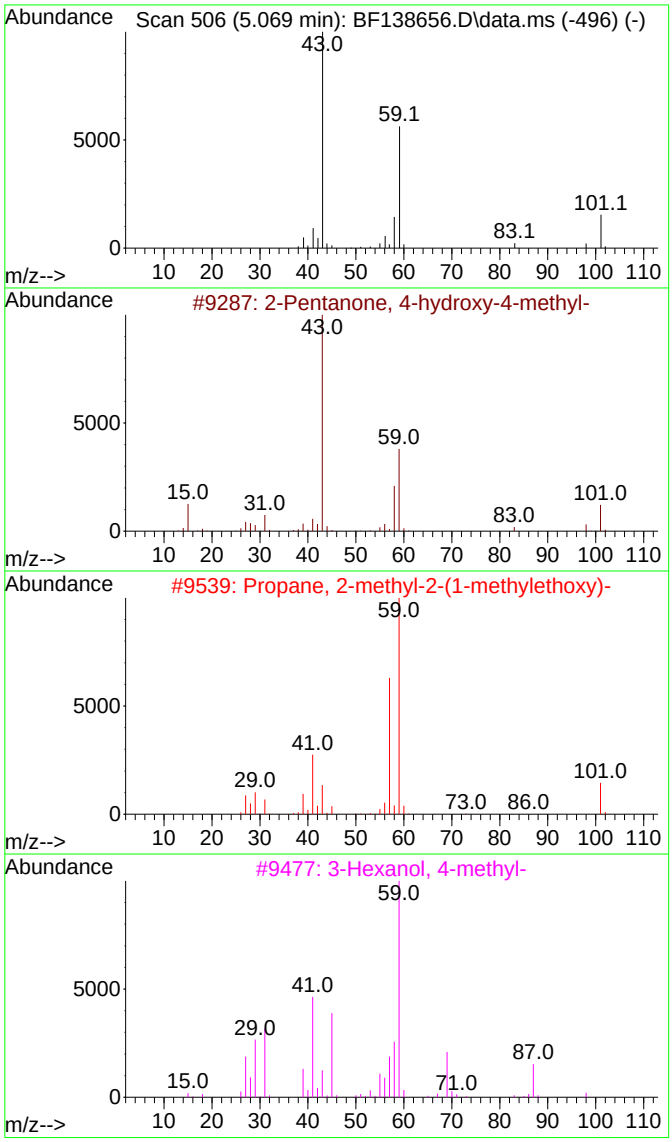
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

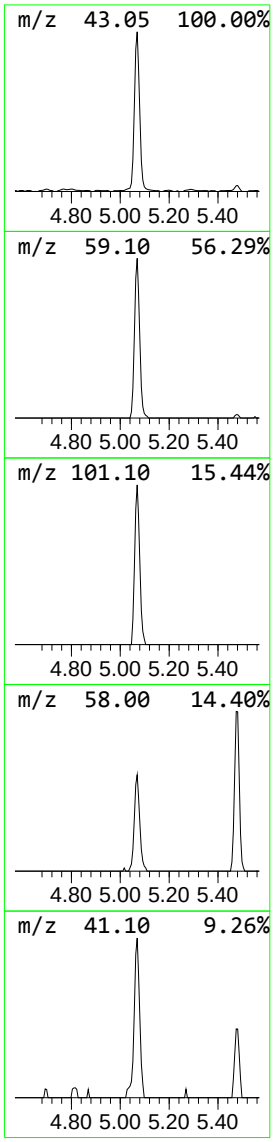
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	4.85 ng	114180	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Sample : P3357-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-854-J-SO-2-2.5-072024

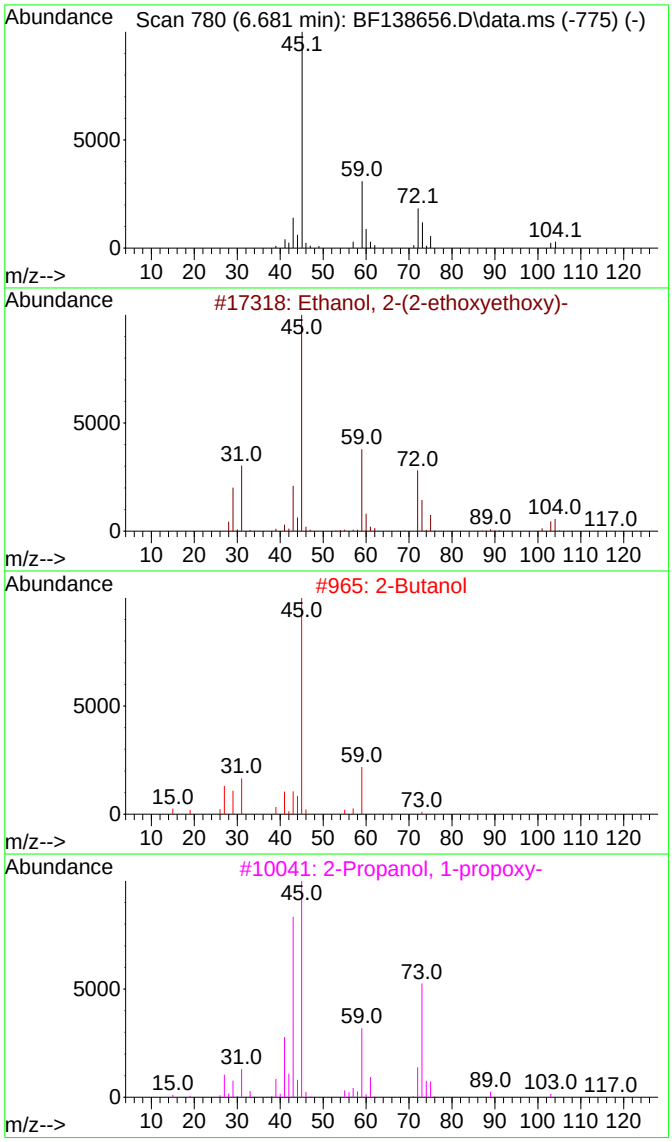
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

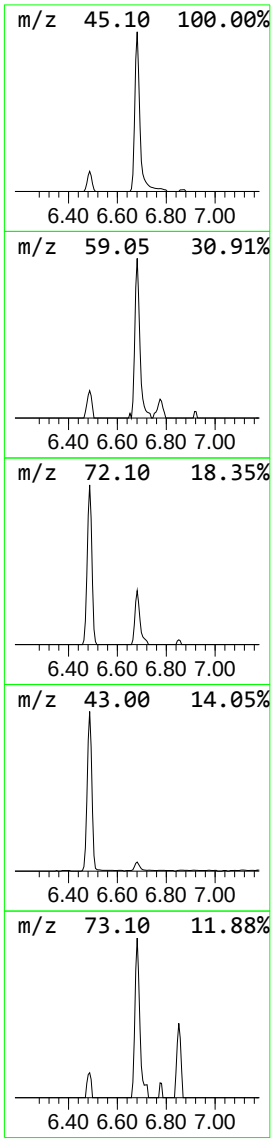
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.681	2.16 ng	50826	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	2-Butanol	74	C4H10O	000078-92-2	45
3	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	39
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	39
5	Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	38





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Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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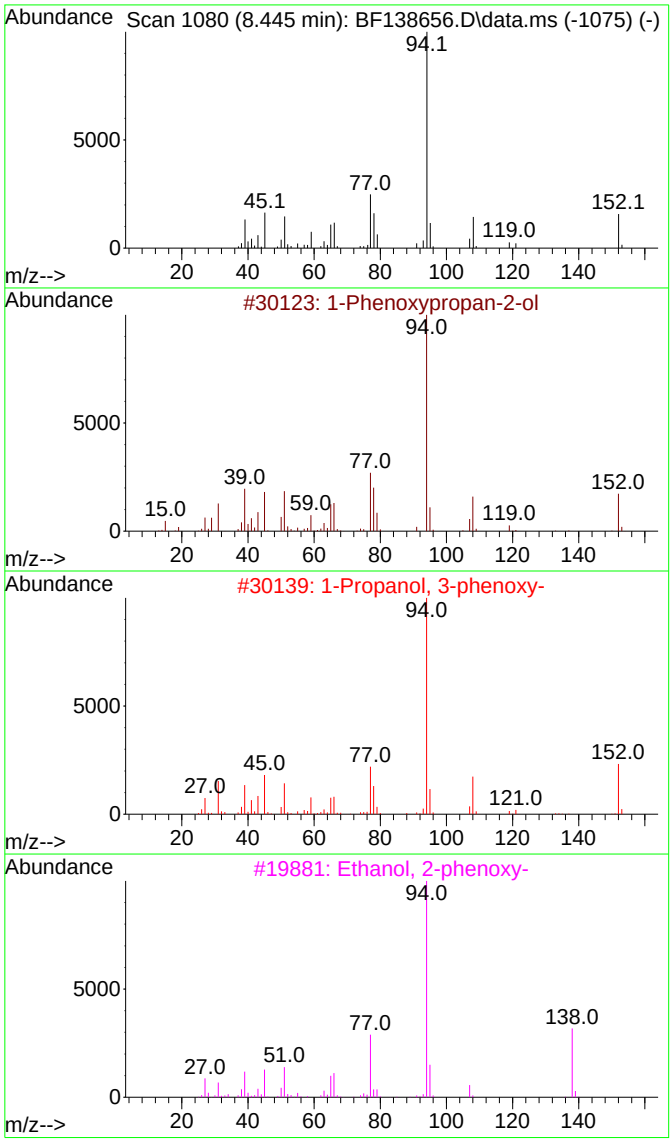
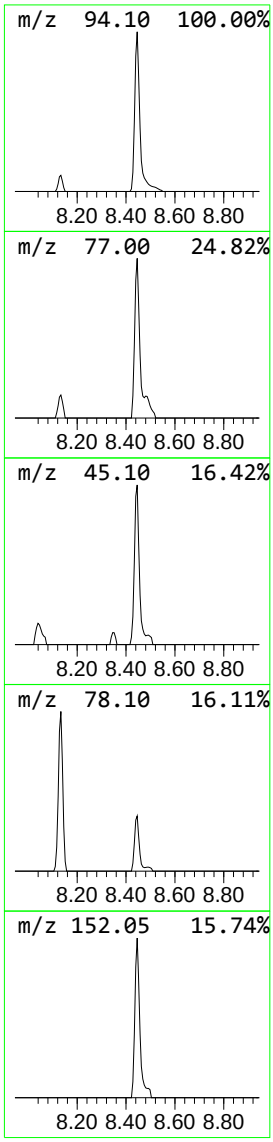
****

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.445	2.98 ng	93769	Naphthalene-d8	8.134

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5	3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59





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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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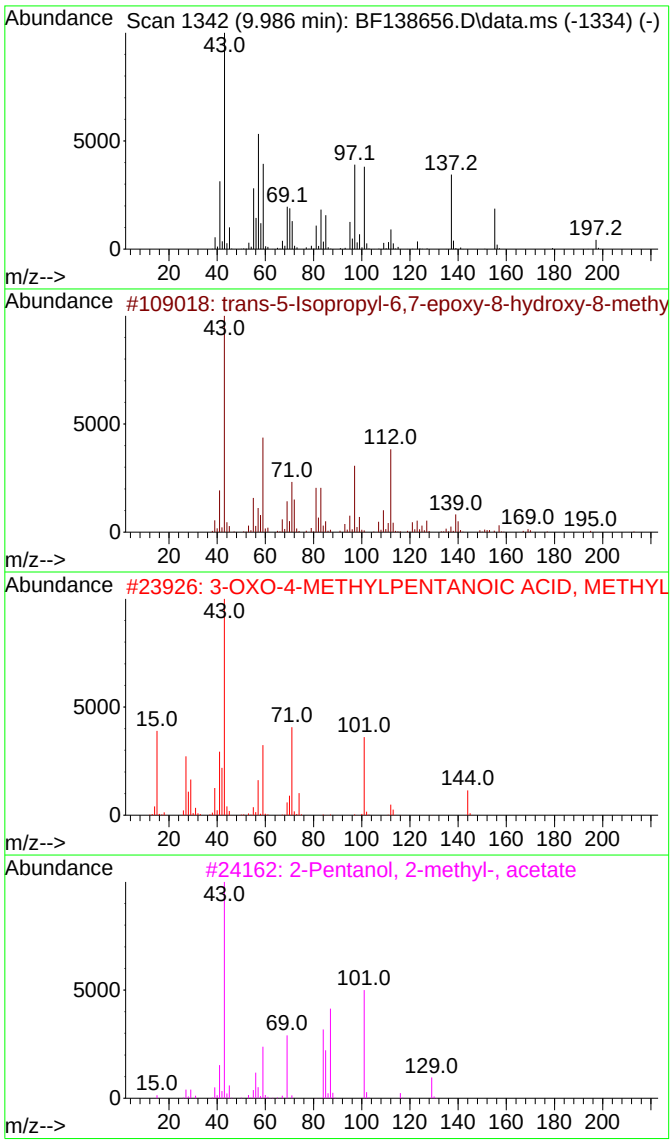
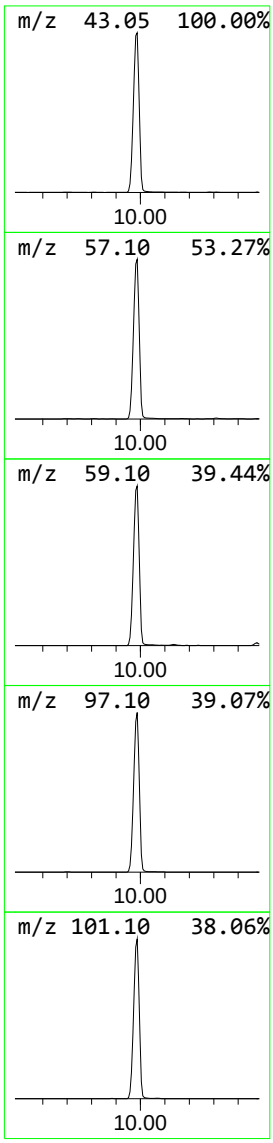
****

Peak Number 6 unknown9.986 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.986	67.98 ng	2351560	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	32
2	3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	25
3	2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	14
4	1-tert-Butoxy-2-methoxyethane	132	C7H16O2	066728-50-5	10
5	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	10





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ClientSampleId :
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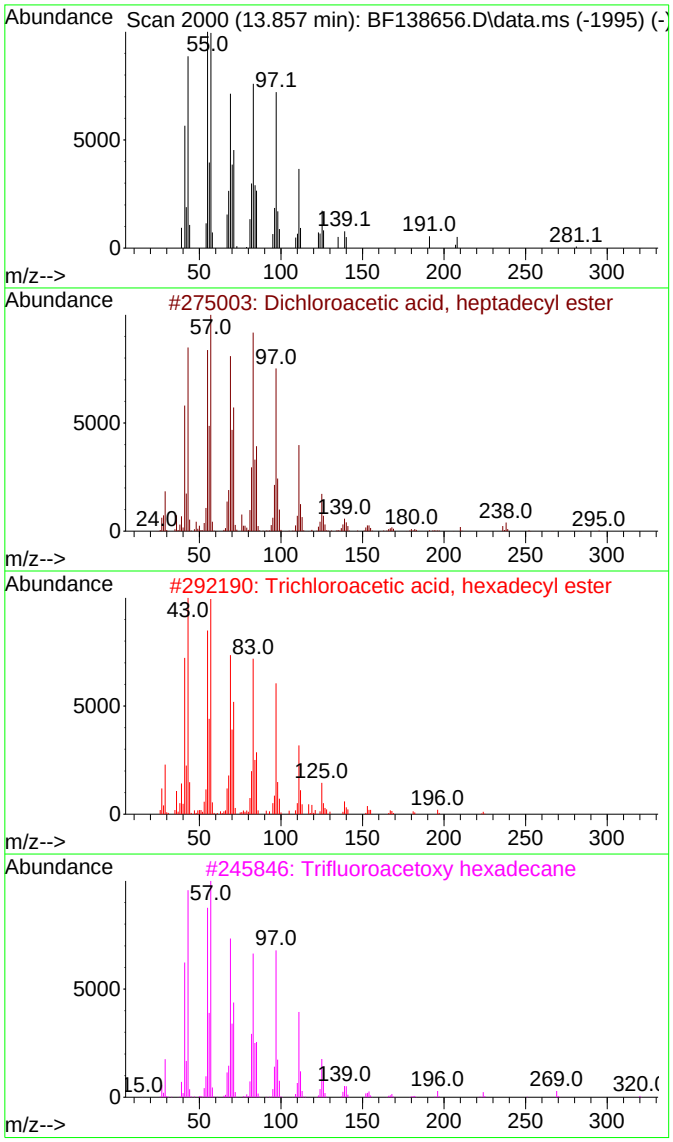
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

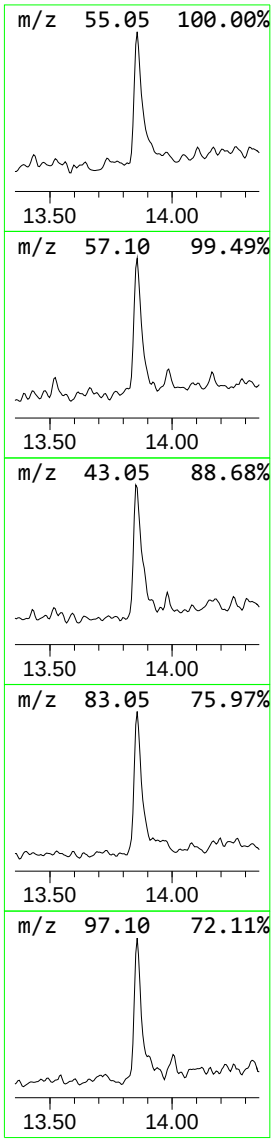
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	4.19 ng	74651	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
5	1-Hexacosene	364	C26H52	018835-33-1	94





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TIC Library : C:\Database\NIST20.L
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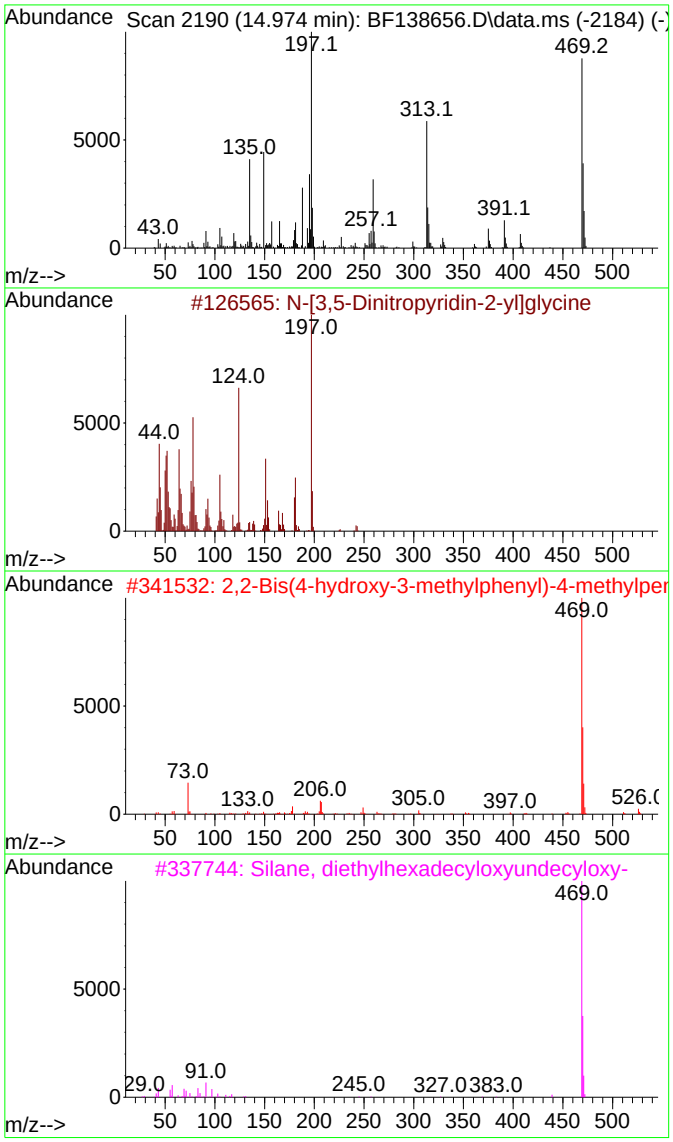
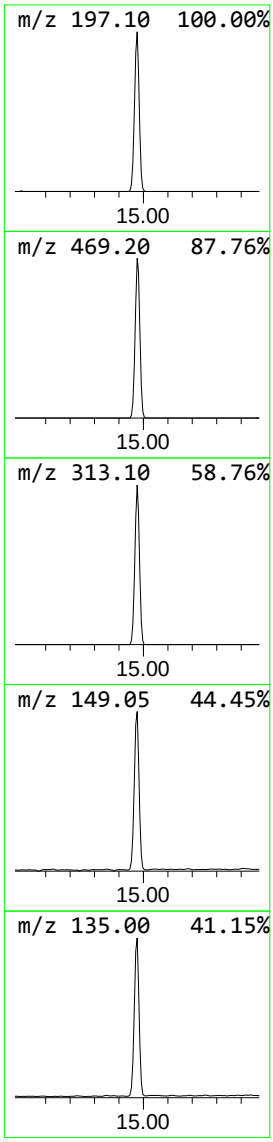
****

Peak Number 8 unknown14.974 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	39.40 ng	758709	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-[3,5-Dinitropyridin-2-yl]glycine	242	C7H6N4O6	003264-08-2	25
2	2,2-Bis(4-hydroxy-3-methylphenyl...	526	C32H54O2Si2	1000462-80-2	22
3	Silane, diethylhexadecyloxyundec...	498	C31H66O2Si	1010363-97-2	12
4	4-Hydrazono-5-hydroxyimino-4,5,6...	197	C6H7N5O3	303194-86-7	11
5	6-(5-Hydroxy-4-methylidenecycloh...	378	C21H38O2Si2	1000495-91-4	11





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.140	55.2	ng	1297910	1	6.851	470410	20.0
(S)-(+)-1,2-Pro...	3.375	2.6	ng	61476	1	6.851	470410	20.0
2-Pentanone, 4-...	5.069	4.8	ng	114180	1	6.851	470410	20.0
Ethanol, 2-(2-e...	6.681	2.2	ng	50826	1	6.851	470410	20.0
1-Phenoxypropan...	8.445	3.0	ng	93769	2	8.134	628966	20.0
unknown9.986	9.986	68.0	ng	2351560	3	9.886	691839	20.0
Dichloroacetic ...	13.857	4.2	ng	74651	5	14.010	356002	20.0
unknown14.974	14.974	39.4	ng	758709	6	15.468	385159	20.0