

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
 Data File : BG048330.D
 Acq On : 4 Mar 2021 16:04
 Operator : CG/JU
 Sample : M1545-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MH-20A

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-BG021021.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048330.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.393	680	690	699	rBV	3061025	5559556	1.08%	0.481%
2	8.221	815	831	853	rBV	2259518	15416744	3.01%	1.333%
3	8.427	853	866	902	rVB4	897213	6315529	1.23%	0.546%
4	10.178	1095	1164	1166	rBV6	29897653	482405801	94.13%	41.717%
5	11.100	1300	1321	1325	rBV	10008393	26967377	5.26%	2.332%
6	11.923	1400	1461	1463	rBV10	37049535	512508946	100.00%	44.320%
7	12.299	1514	1525	1530	rBV3	27661201	75334365	14.70%	6.515%
8	12.704	1550	1594	1595	rBV	3306855	26032567	5.08%	2.251%
9	13.521	1722	1733	1737	rBV	2479270	5841685	1.14%	0.505%

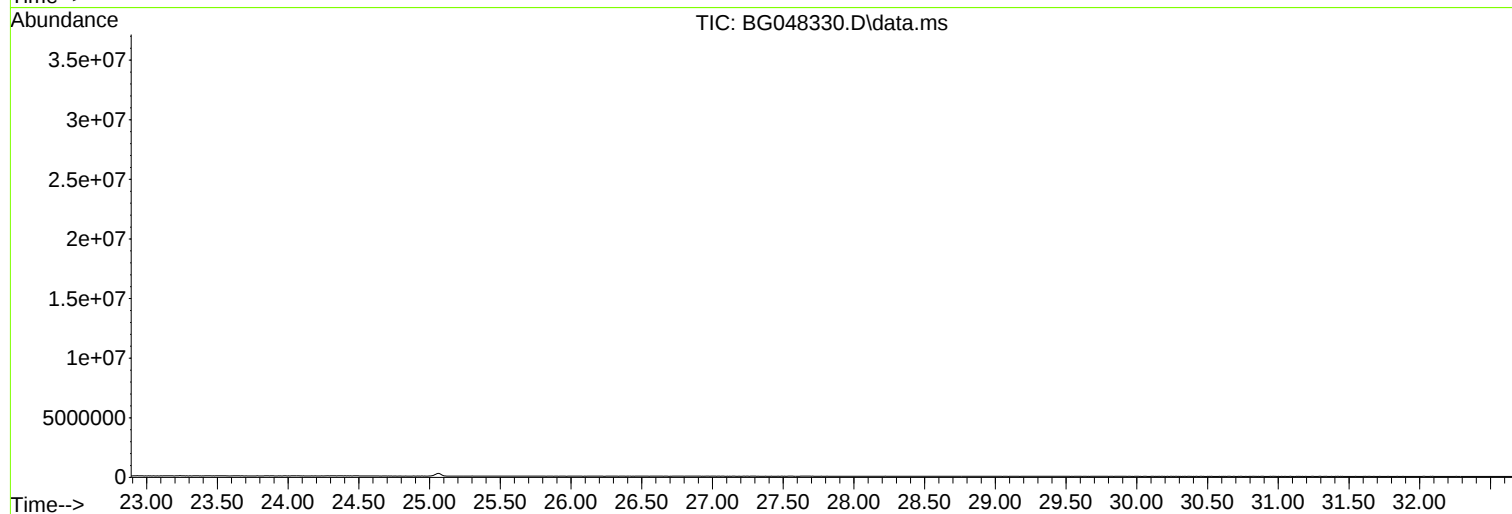
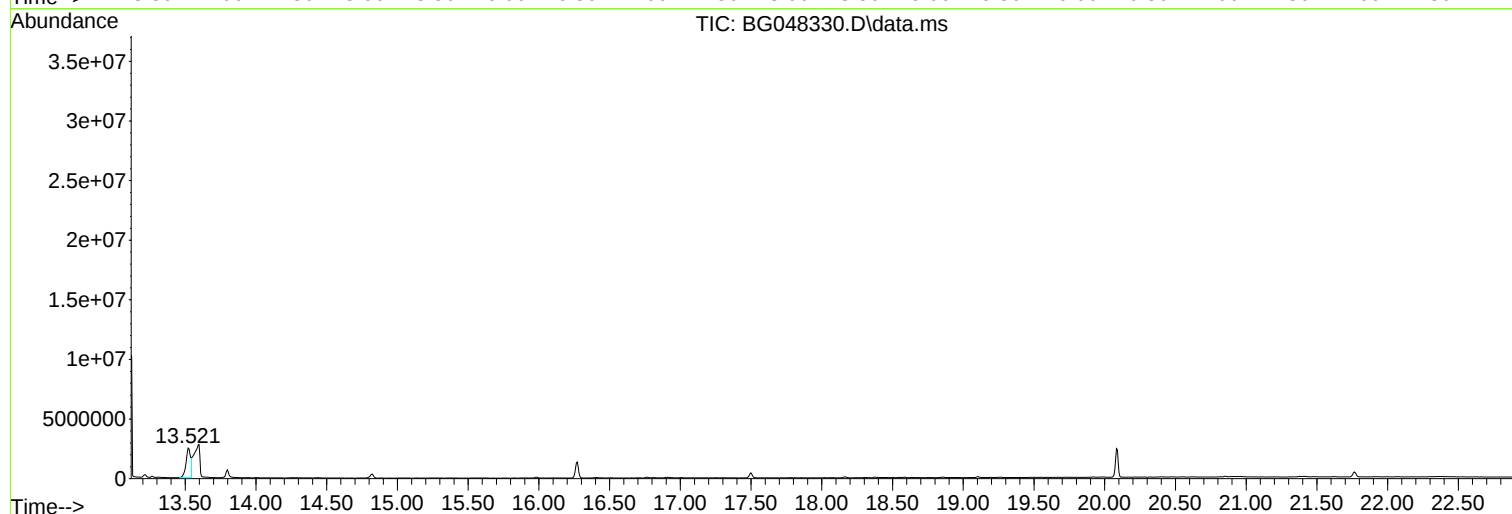
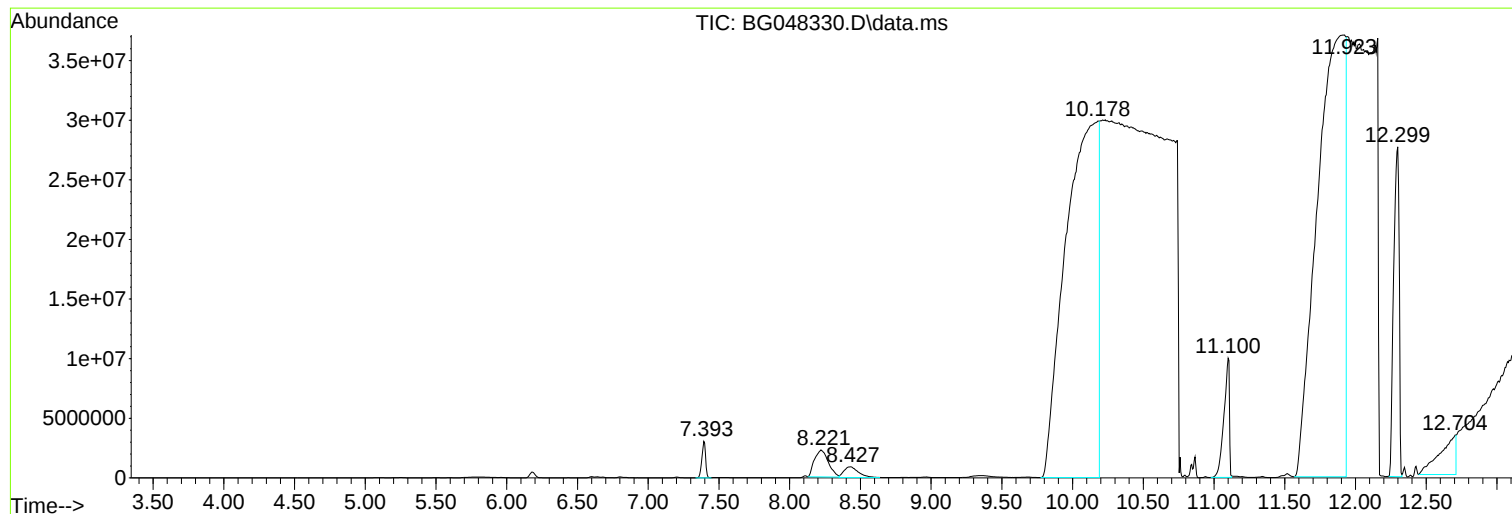
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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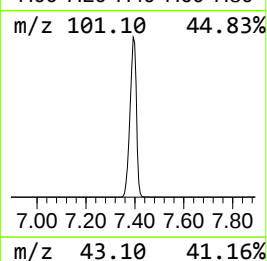
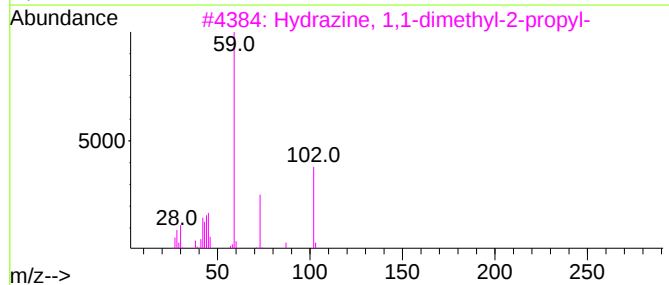
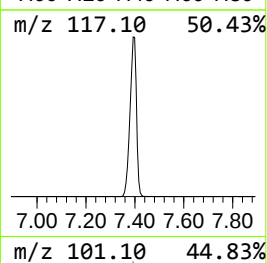
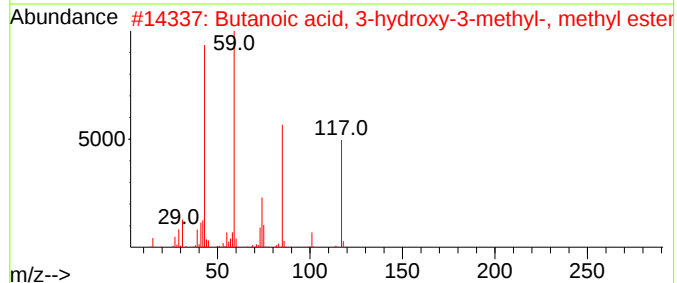
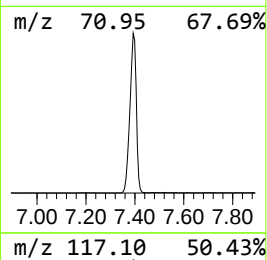
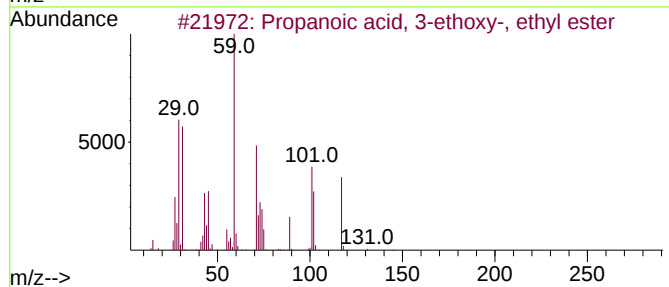
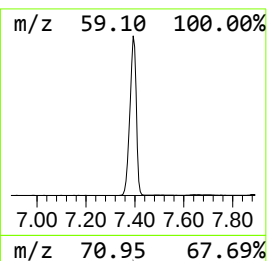
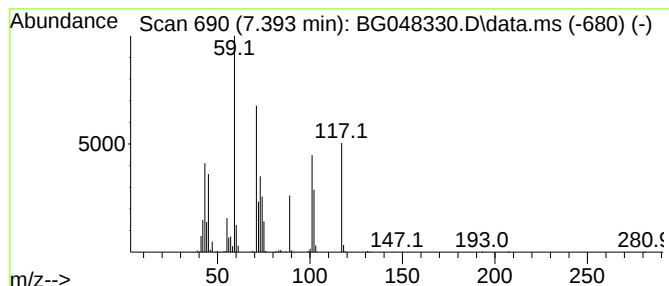
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Peak Number 1 Propanoic acid, 3-ethoxy-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.393	7.21 ng	5559560	1,4-Dichlorobenzene-d4	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 3-ethoxy-, ethyl...	146	C7H14O3	000763-69-9	90
2			Butanoic acid, 3-hydroxy-3-methyl...	132	C6H12O3	006149-45-7	32
3			Hydrazine, 1,1-dimethyl-2-propyl-	102	C5H14N2	052728-54-8	27
4			Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	25
5			Ethanol, 2-ethoxy-	90	C4H10O2	000110-80-5	14



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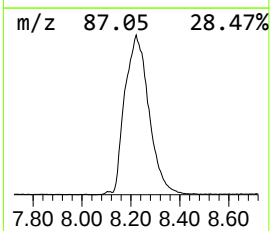
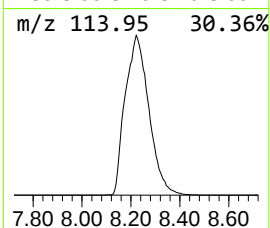
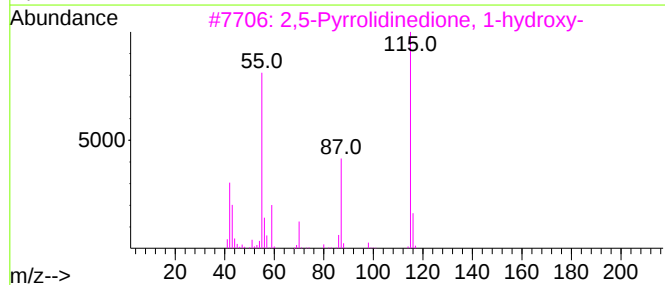
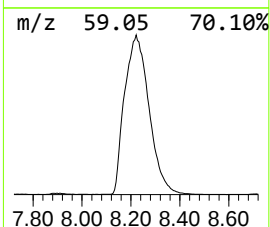
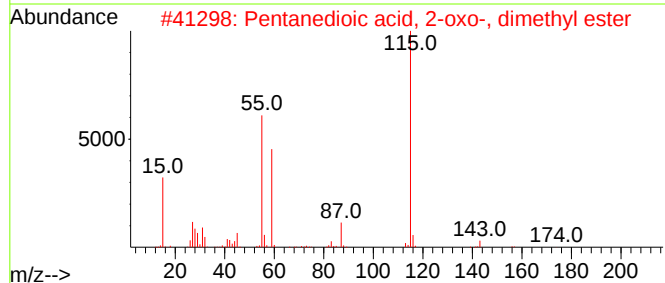
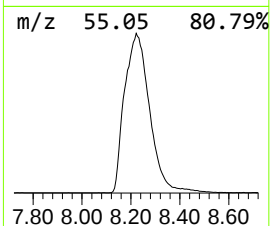
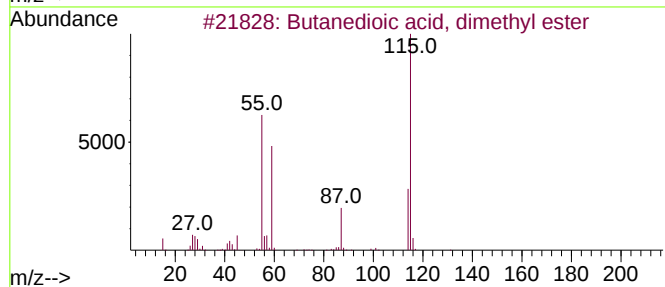
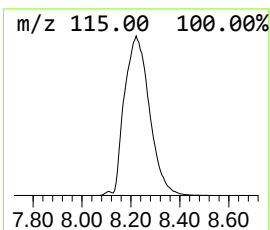
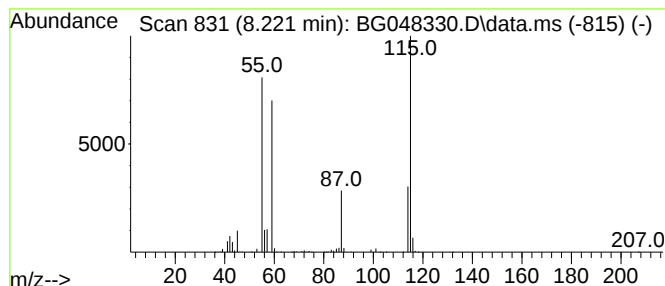
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Peak Number 2 Butanedioic acid, dimethyl ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.221	20.00 ng	15416700	1,4-Dichlorobenzene-d4	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanedioic acid, dimethyl ester	146	C6H10O4	000106-65-0	91
2			Pentanedioic acid, 2-oxo-, dimet...	174	C7H10O5	013192-04-6	64
3			2,5-Pyrrolidinedione, 1-hydroxy-	115	C4H5NO3	006066-82-6	40
4			3-Hexanol, 5-methyl-	116	C7H16O	000623-55-2	10
5			Pentanal, oxime	101	C5H11NO	000628-79-5	10



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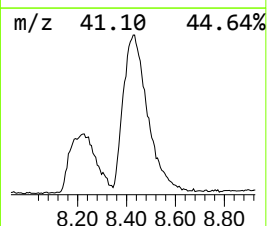
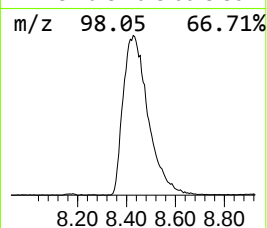
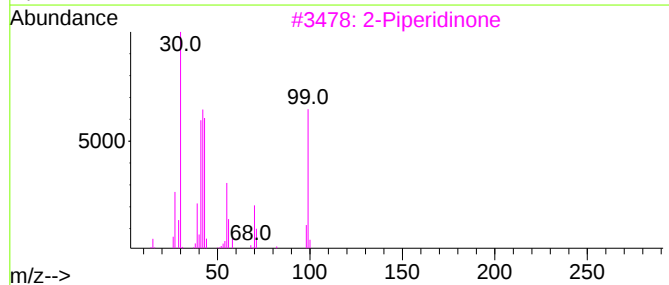
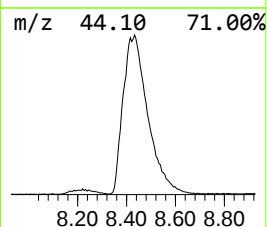
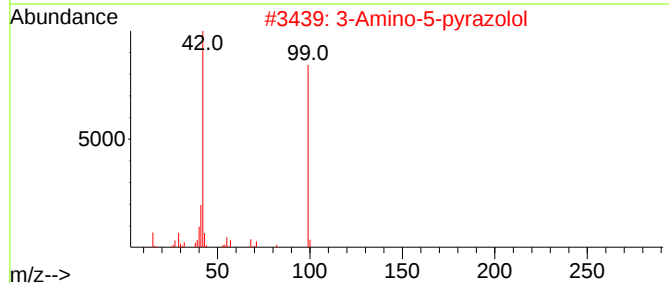
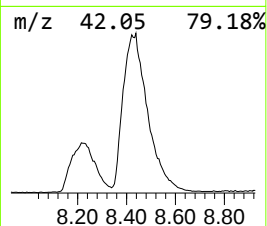
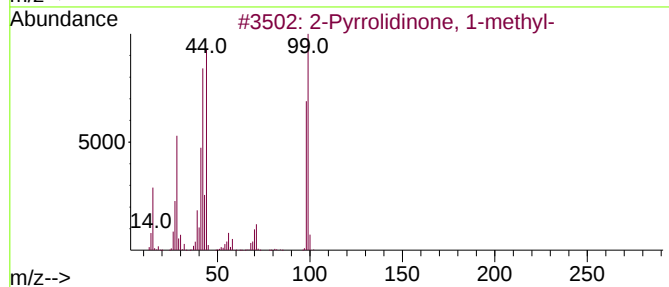
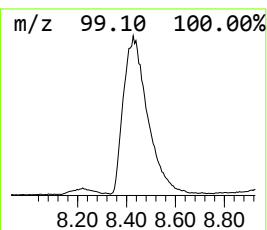
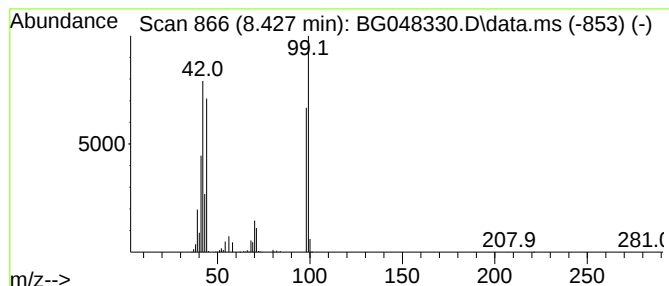
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Peak Number 3 2-Pyrrolidinone, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.427	8.19 ng	6315530	1,4-Dichlorobenzene-d4	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyrrolidinone, 1-methyl-		99	C5H9NO		000872-50-4	94
2	3-Amino-5-pyrazolol		99	C3H5N3O		006126-22-3	47
3	2-Piperidinone		99	C5H9NO		000675-20-7	40
4	4H-1,2,4-Triazol-3-amine, 4-methyl-		98	C3H6N4		016681-76-8	25
5	2-Methyl-3,4,5,6-tetrahydropyrazine		98	C5H10N2		344240-21-7	23



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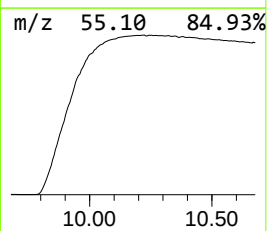
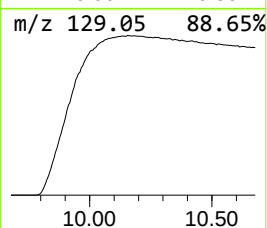
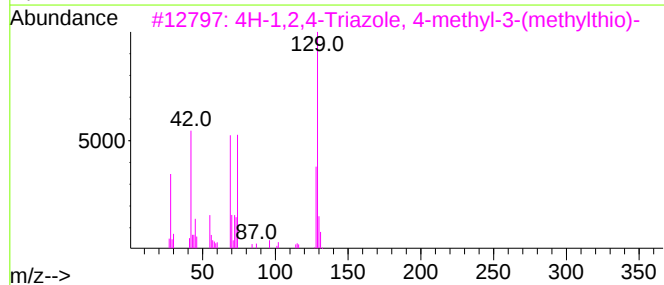
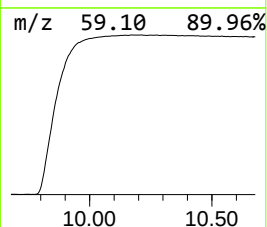
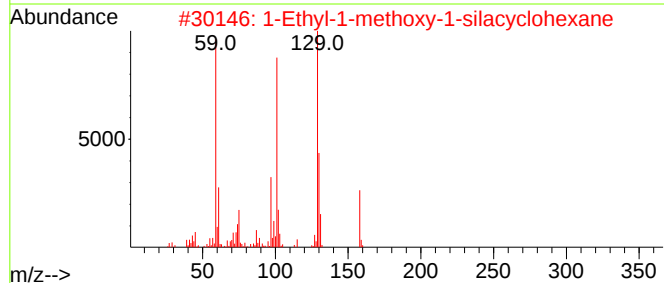
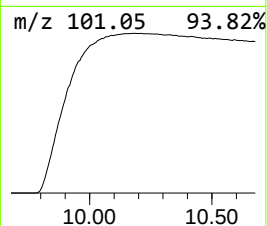
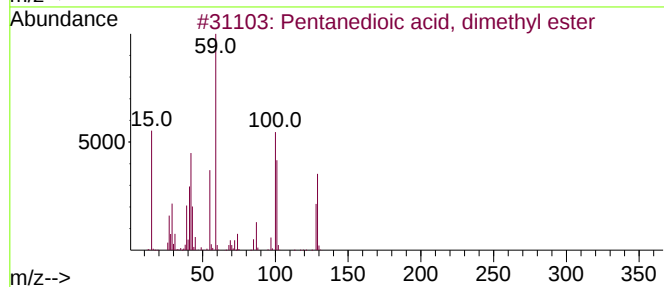
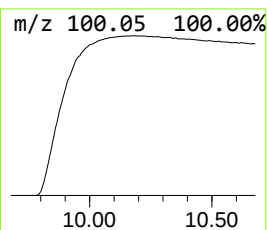
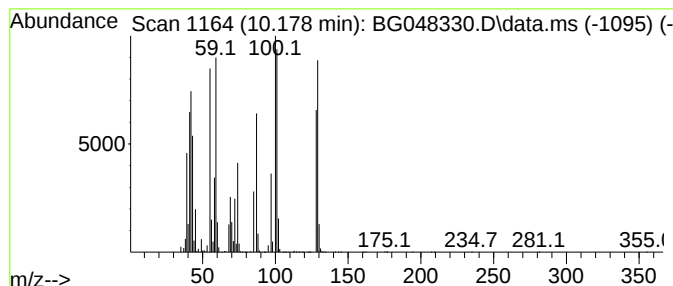
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Peak Number 4 Pentanedioic acid, dimethyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.178	357.77 ng	482406000	Naphthalene-d8	11.153

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	53
2			1-Ethyl-1-methoxy-1-silacyclohexane	158	C8H18OSi	1000279-45-1	35
3			4H-1,2,4-Triazole, 4-methyl-3-(m...	129	C4H7N3S	021094-61-1	27
4			1,2,4-Triazin-5(2H)-one, 3,4-dih...	129	C3H3N3OS	000626-08-4	14
5			Succinic acid, ethyl 4-methoxy-2...	246	C12H22O5	1000330-23-0	14



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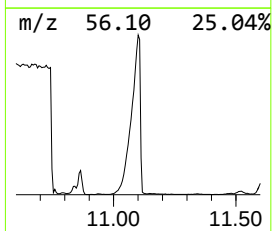
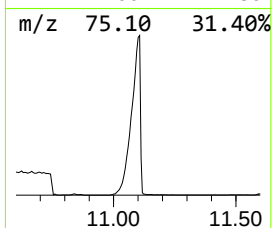
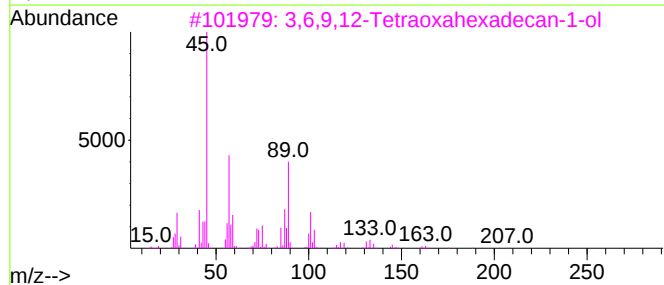
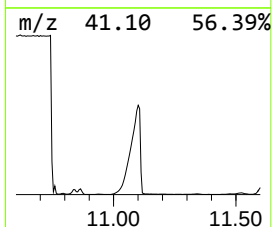
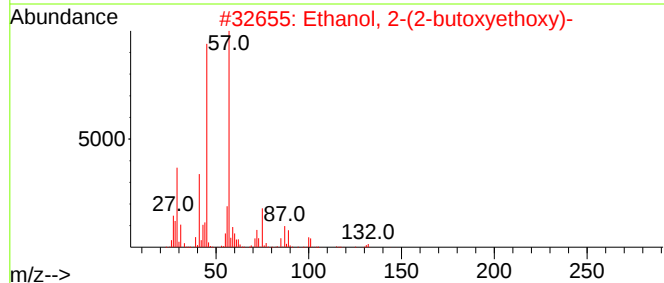
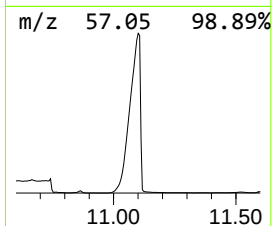
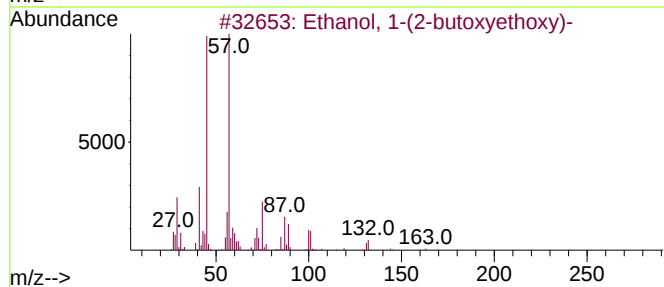
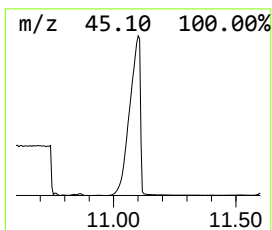
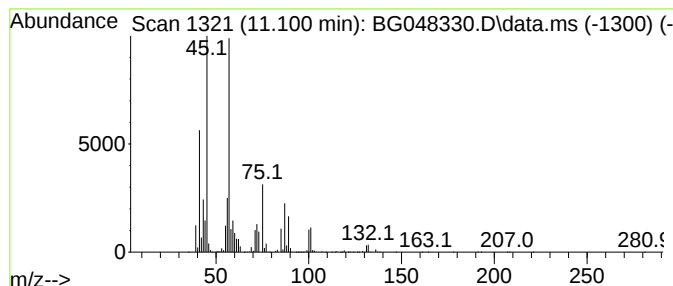
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Peak Number 5 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.100	20.00 ng	26967400	Naphthalene-d8	11.153

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
3			3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	72
4			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	64
5			Butanamide, 3,N-dihydroxy-	119	C4H9NO3	090567-52-5	49



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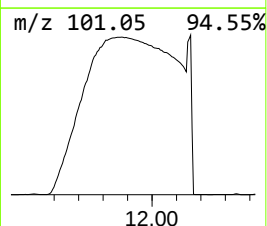
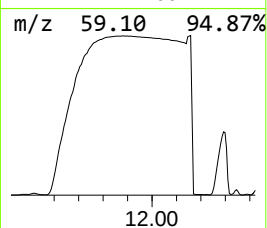
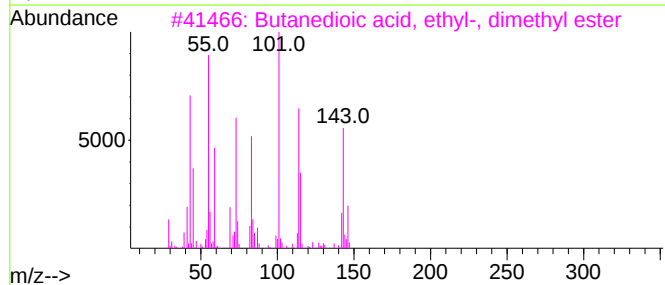
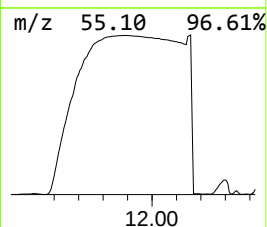
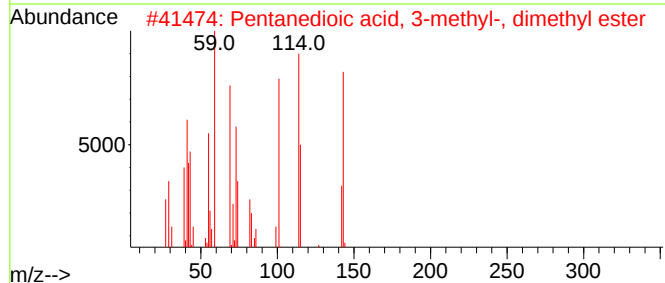
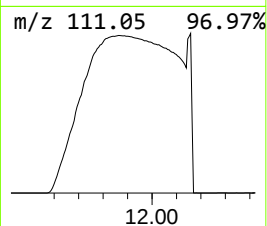
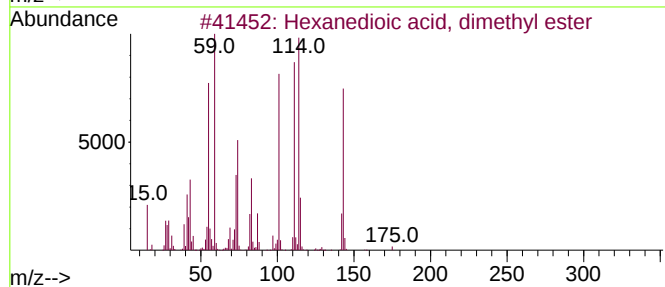
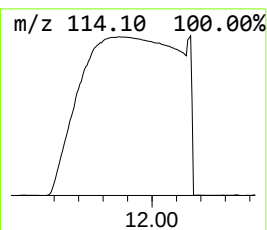
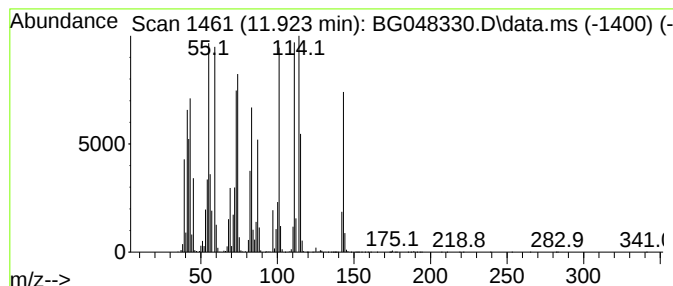
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Peak Number 6 Hexanedioic acid, dimethyl ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.923	380.10 ng	512509000	Naphthalene-d8	11.153

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, dimethyl ester	174	C8H14O4	000627-93-0	64
2			Pentanedioic acid, 3-methyl-, di...	174	C8H14O4	019013-37-7	47
3			Butanedioic acid, ethyl-, dimeth...	174	C8H14O4	014035-95-1	35
4			Hexanedioic acid monochloride mo...	178	C7H11ClO3	035444-44-1	35
5			Heptanedioic acid, dimethyl ester	188	C9H16O4	001732-08-7	27



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Data File : BG048330.D
Acq On : 4 Mar 2021 16:04
Operator : CG/JU
Sample : M1545-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-20A

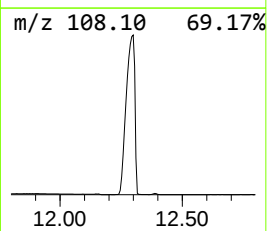
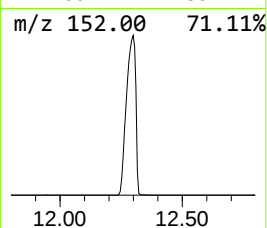
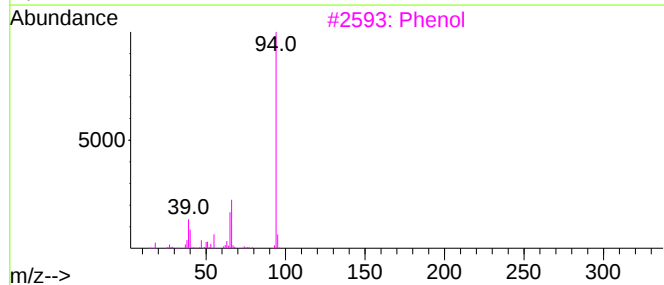
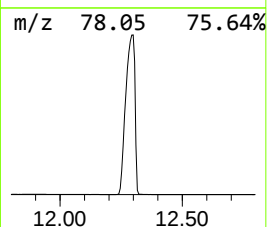
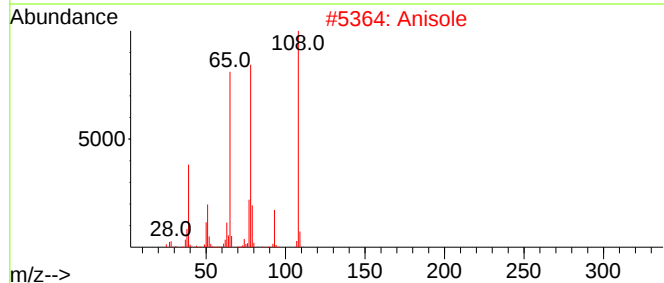
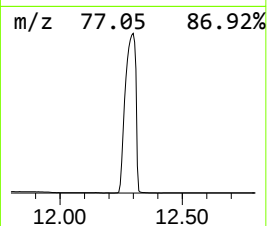
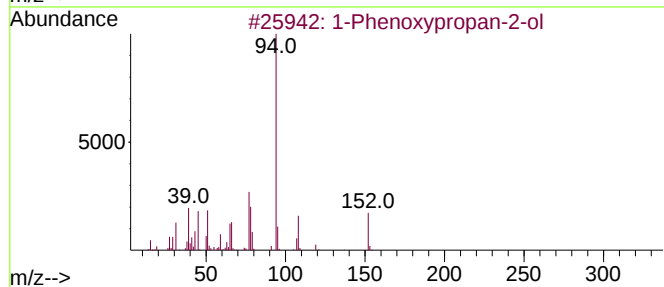
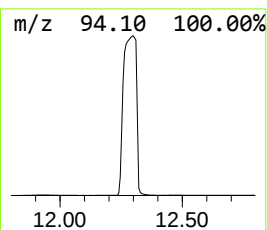
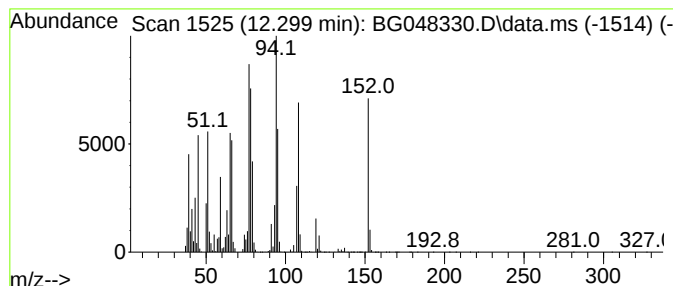
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.299	55.87 ng	75334400	Naphthalene-d8	11.153

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
2			Anisole	108	C7H8O	000100-66-3	46
3			Phenol	94	C6H6O	000108-95-2	30
4			Formic acid phenyl ester	122	C7H6O2	001864-94-4	27
5			2-Propenal, 3-(2-furanyl)-	122	C7H6O2	000623-30-3	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048330.D
Acq On : 4 Mar 2021 16:04
Operator : CG/JU
Sample : M1545-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-20A

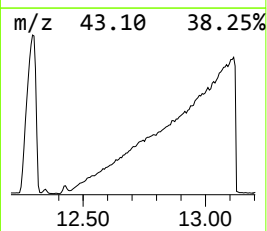
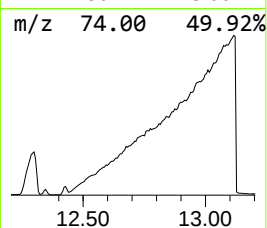
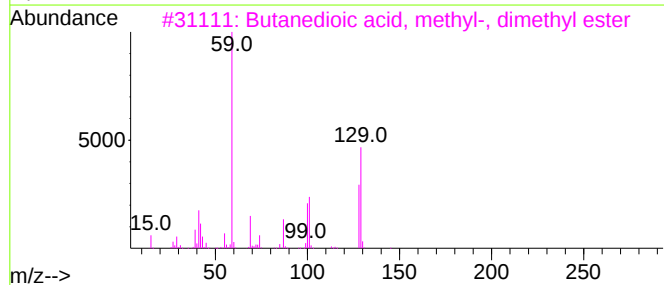
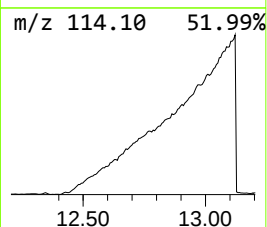
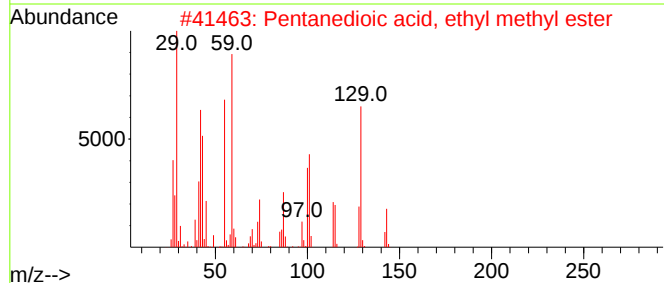
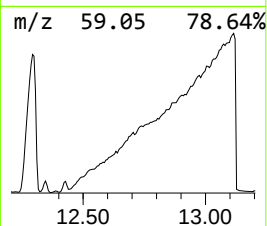
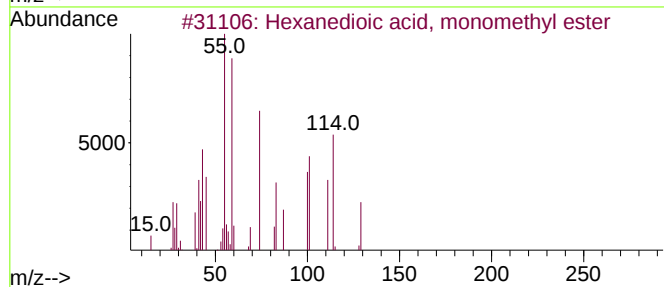
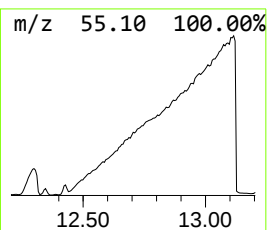
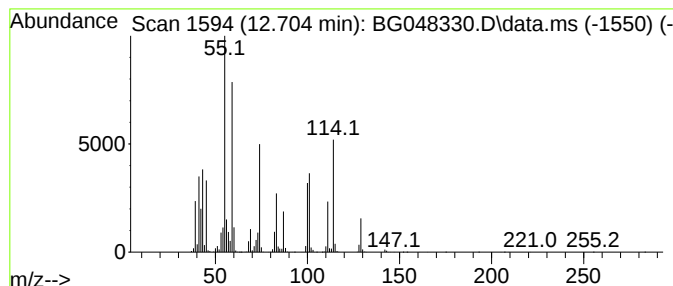
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexanedioic acid, monomethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	19.31 ng	26032600	Naphthalene-d8	11.153

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, monomethyl ester	160	C7H12O4	000627-91-8	91
2			Pentanedioic acid, ethyl methyl ...	174	C8H14O4	051503-30-1	38
3			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	37
4			Ethyl ether	74	C4H10O	000060-29-7	35
5			Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
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Sample : M1545-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-20A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	7.393	7.2	ng	5559560	1	8.110	15416700	20.0
Butanedioic aci...	8.221	20.0	ng	15416700	1	8.110	15416700	20.0
2-Pyrrolidinone...	8.427	8.2	ng	6315530	1	8.110	15416700	20.0
Pentanedioic ac...	10.178	357.8	ng	482406000	2	11.153	26967400	20.0
Ethanol, 1-(2-b...	11.100	20.0	ng	26967400	2	11.153	26967400	20.0
Hexanedioic aci...	11.923	380.1	ng	512509000	2	11.153	26967400	20.0
1-Phenoxypropan...	12.299	55.9	ng	75334400	2	11.153	26967400	20.0
Hexanedioic aci...	12.704	19.3	ng	26032600	2	11.153	26967400	20.0