

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041917\
 Data File : BG026665.D
 Acq On : 19 Apr 2017 20:51
 Operator : SJ/MA
 Sample : I2755-06
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 3652

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-BG041817.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	5.127	341	347	356	rBV	99988	154519	1.31%	0.213%
2	5.626	425	432	441	rBV	1176033	1936497	16.46%	2.669%
3	7.230	697	705	716	rBV	697705	1310107	11.14%	1.806%
4	7.577	756	764	781	rBV	2293280	3984671	33.88%	5.493%
5	8.029	832	841	848	rBV	564643	942311	8.01%	1.299%
6	8.352	888	896	906	rBV	2287223	3929843	33.41%	5.417%
7	9.128	1022	1028	1033	rBV	359108	614890	5.23%	0.848%
8	9.187	1033	1038	1048	rVB	1660992	2974199	25.28%	4.100%
9	10.826	1309	1317	1334	rVB	798339	1479267	12.58%	2.039%
10	13.264	1725	1732	1742	rBV	5235303	8473100	72.03%	11.679%
11	14.087	1865	1872	1879	rBV	102260	166084	1.41%	0.229%
12	14.639	1958	1966	1975	rBV2	1409822	2202475	18.72%	3.036%
13	16.126	2212	2219	2231	rBV	4177942	6351725	54.00%	8.755%
14	16.325	2246	2253	2256	rBV2	70430	122725	1.04%	0.169%
15	17.371	2424	2431	2437	rBV2	1848494	2864941	24.36%	3.949%
16	18.259	2577	2582	2596	rBV5	135656	426376	3.62%	0.588%
17	19.522	2793	2797	2808	rBV3	145986	392528	3.34%	0.541%
18	19.974	2867	2874	2880	rBV	8545341	11762794	100.00%	16.214%
19	20.415	2939	2949	2958	rBV2	1079470	4543743	38.63%	6.263%
20	20.503	2960	2964	2966	rBV2	646858	940791	8.00%	1.297%
21	21.455	3115	3126	3128	rBV4	402479	1284345	10.92%	1.770%
22	21.531	3130	3139	3147	rVV	1396530	5408760	45.98%	7.456%
23	21.613	3148	3153	3171	rVB	2838387	6872301	58.42%	9.473%
24	24.786	3685	3693	3706	rVB2	1248059	3408140	28.97%	4.698%

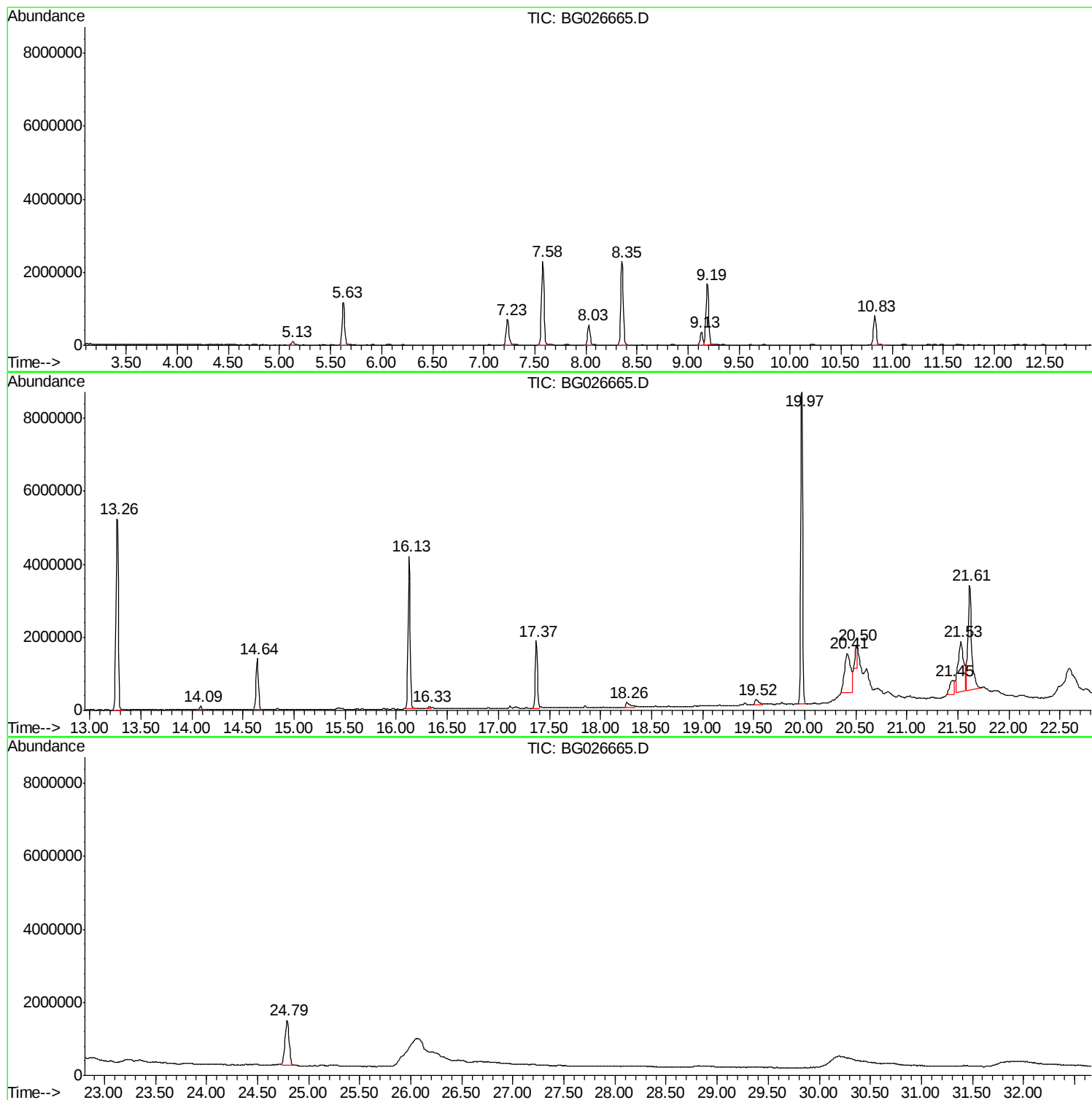
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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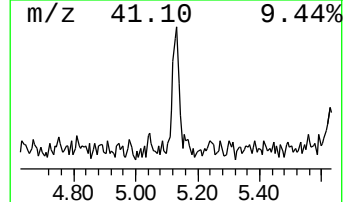
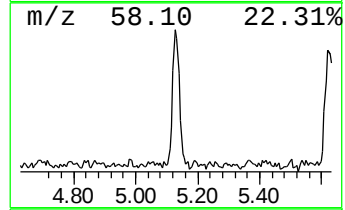
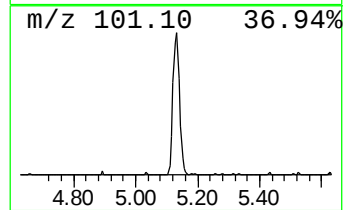
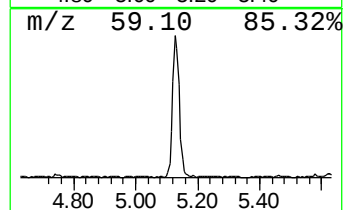
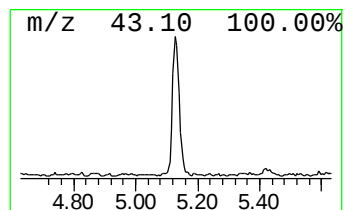
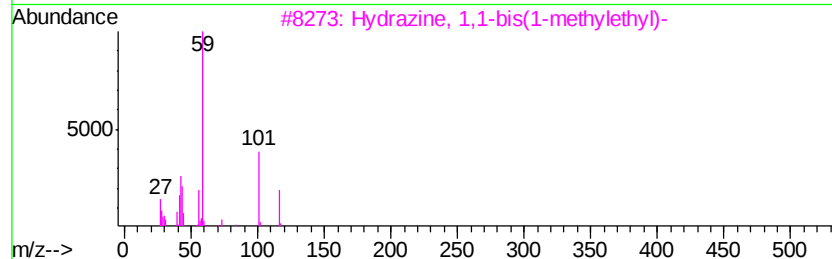
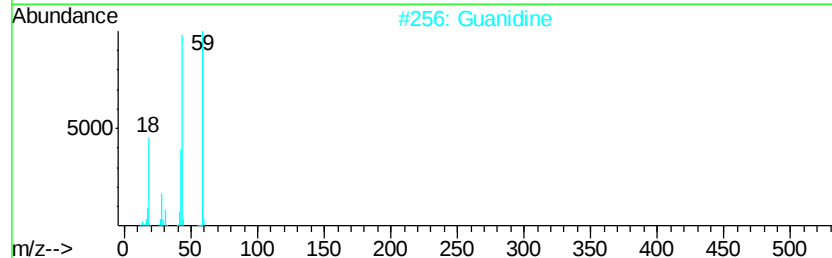
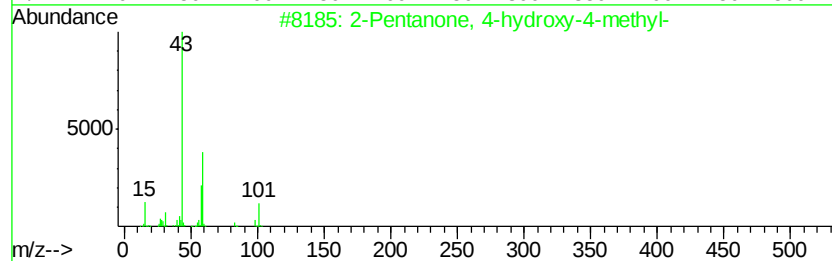
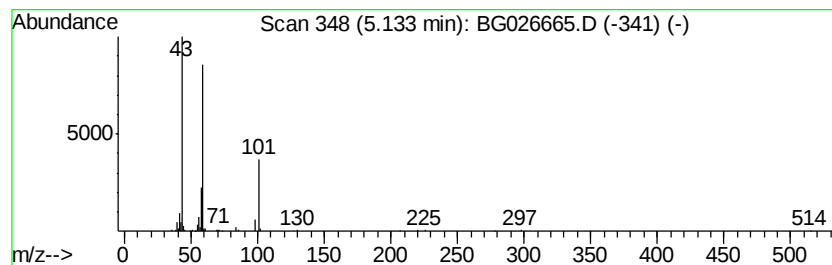
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	3.28 ng	154519	1,4-Dichlorobenzene-d4	8.03

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Guanidine	59	CH5N3	000113-00-8	50
3			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	36
4			4-Ethyl-3-octanol	158	C10H22O	019781-26-1	33
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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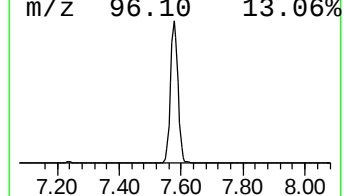
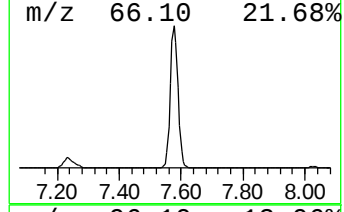
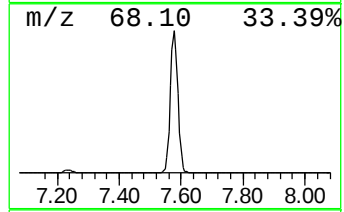
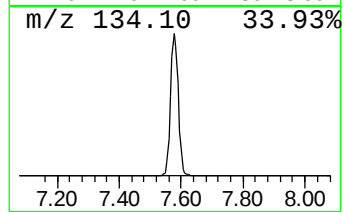
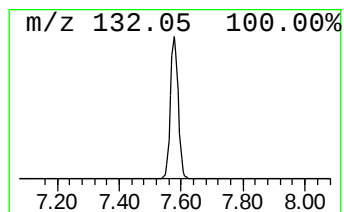
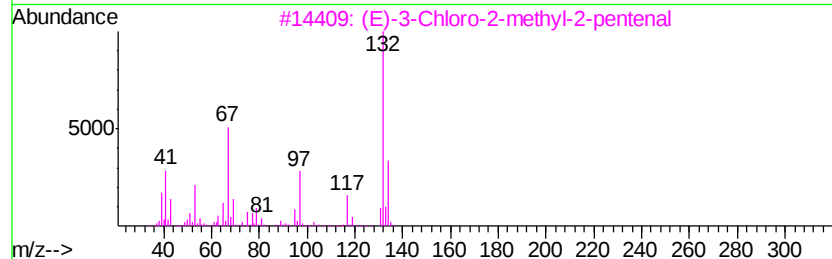
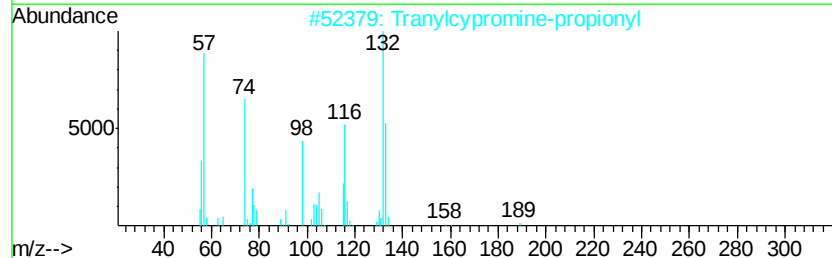
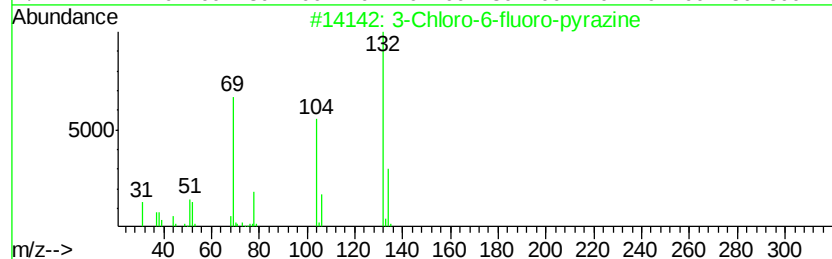
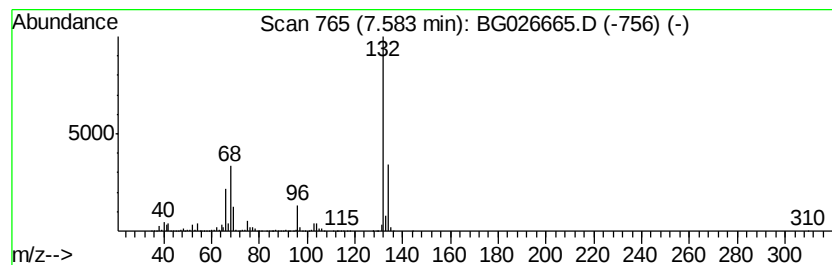
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	84.57 ng	3984670	1,4-Dichlorobenzene-d4	8.03

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2			Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	12
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4			4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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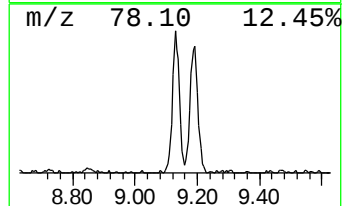
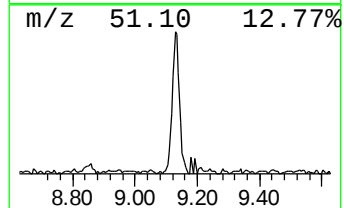
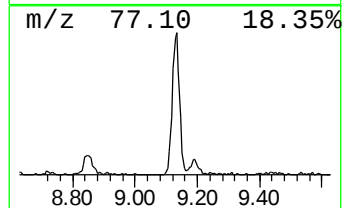
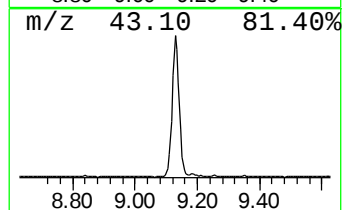
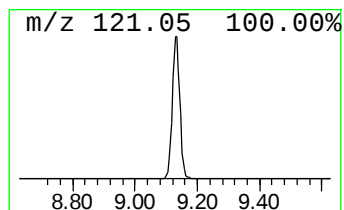
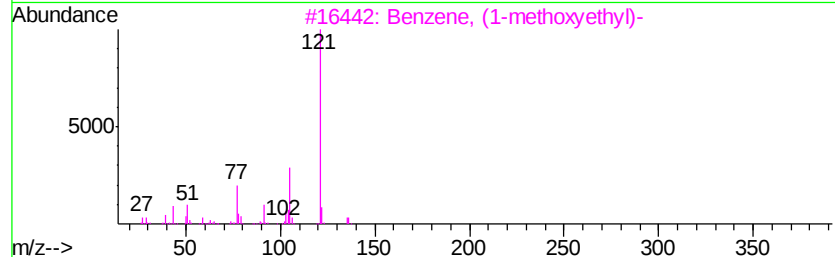
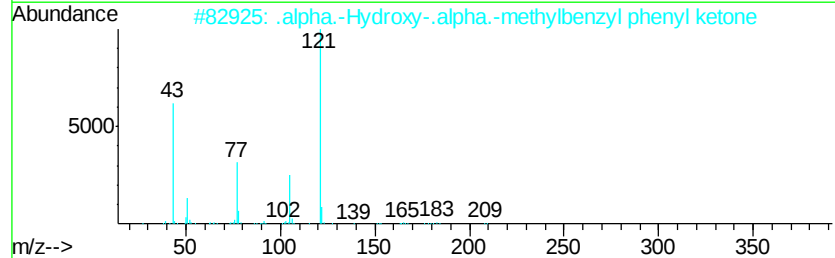
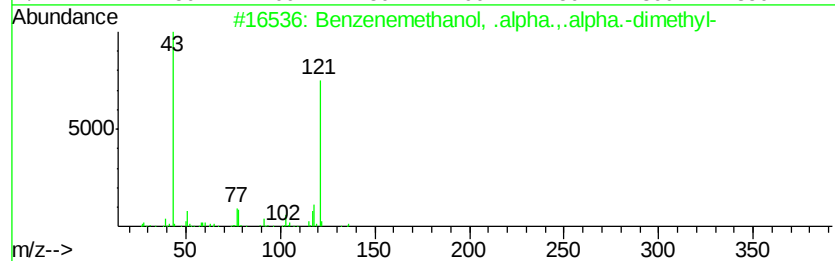
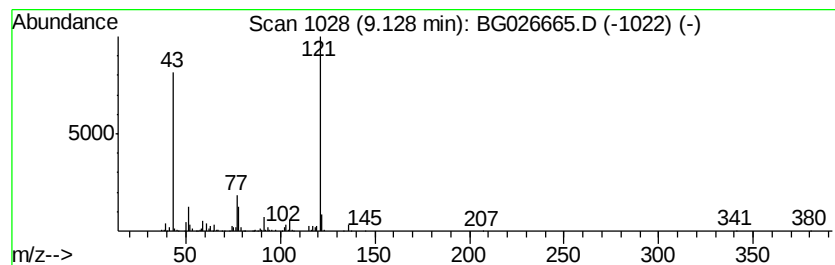
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Peak Number 4 Benzenemethanol, .alpha.,.a... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.13	13.05 ng	614890	1,4-Dichlorobenzene-d4	8.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenemethanol, .alpha.,.alpha....	136	C9H12O	000617-94-7	90
2		.alpha.-Hydroxy-.alpha.-methylbe...	226	C15H14O2	005623-26-7	72
3		Benzene, (1-methoxyethyl)-	136	C9H12O	004013-34-7	64
4		Benzeneacetamide, .alpha.-hydrox...	179	C10H13NO2	002019-70-7	64
5		.alpha.-Ethyl-.alpha.-methylbenz...	150	C10H14O	001565-75-9	64



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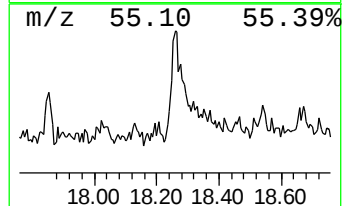
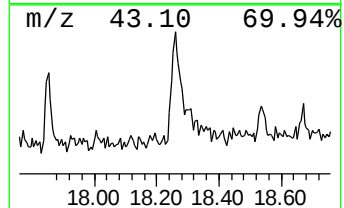
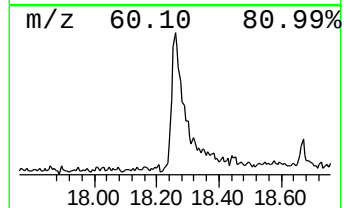
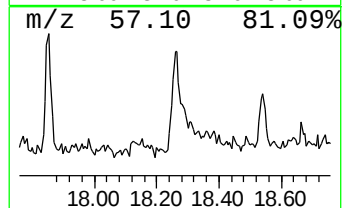
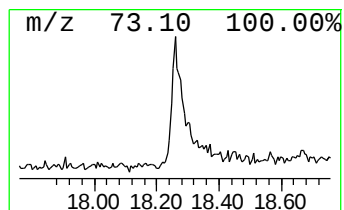
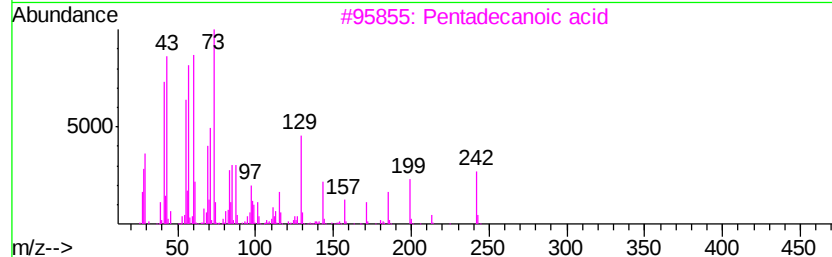
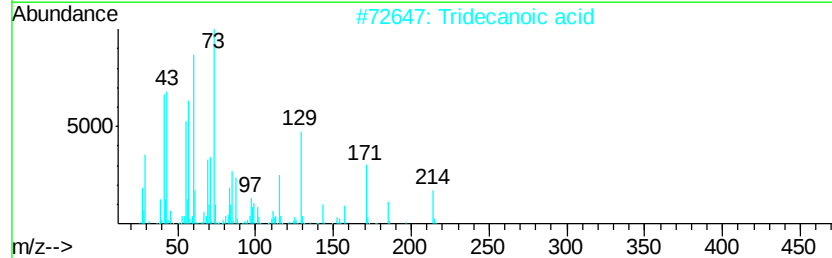
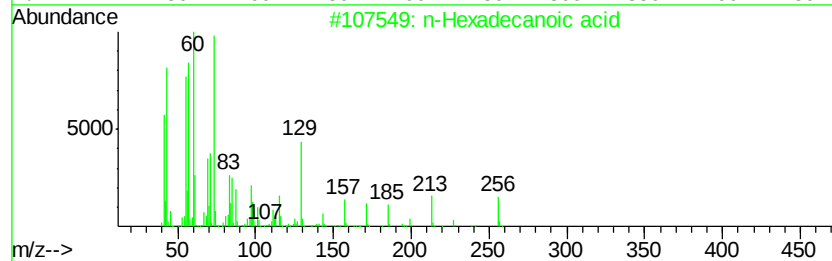
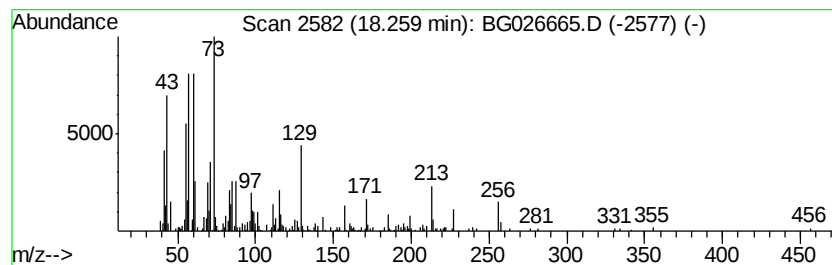
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	2.98 ng	426376	Phenanthrene-d10	17.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		n-Decanoic acid	172	C10H20O2	000334-48-5	70
5		Undecanoic acid	186	C11H22O2	000112-37-8	64



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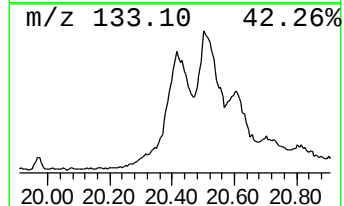
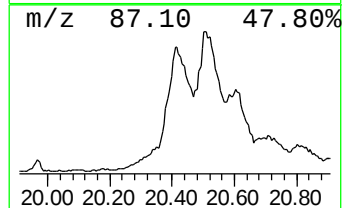
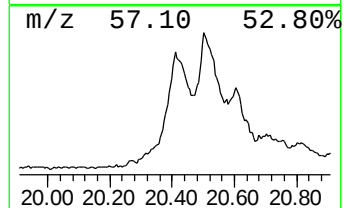
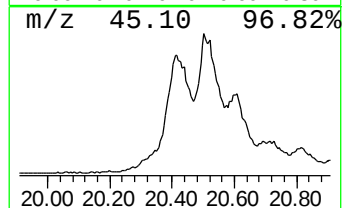
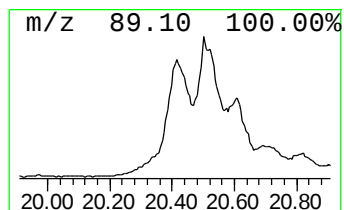
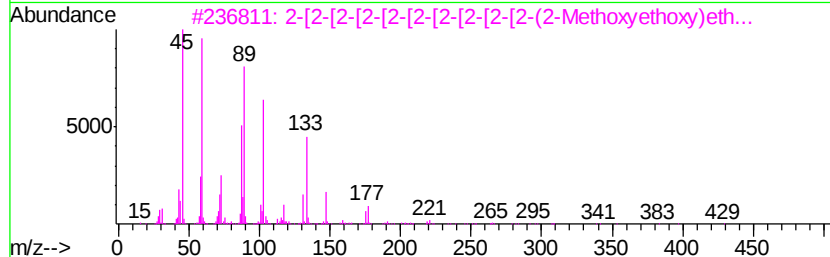
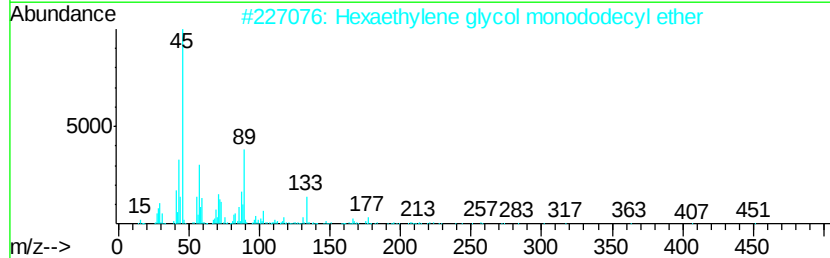
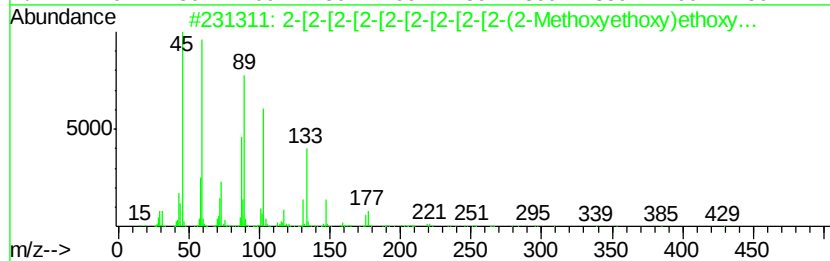
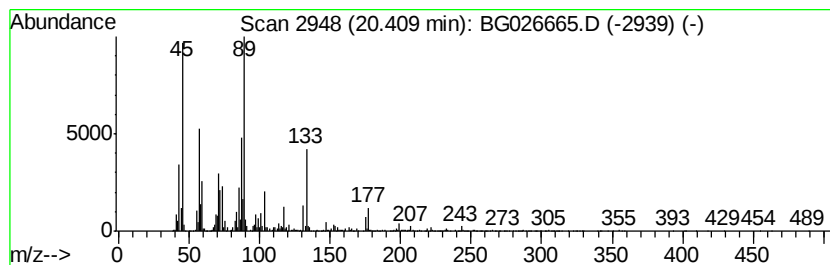
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 2-[2-[2-[2-[2-[2-[2-[2-(... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.41	13.22 ng	4543740	Chrysene-d12	21.61

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual		
1	2	-[2-	-[2-	-[2-	-[2-(2-Met...	472	C21H44O11	1000352-11-2	90
2	Hexaethylene glycol monododecyl			450	C24H50O7	003055-96-7	90		
3	2	-[2-	-[2-	-[2-	-[2-(2-...	516	C23H48O12	1000352-04-4	87
4	3,6,9,12,15-Pentaoxanonadecan-1-ol			294	C14H30O6	001786-94-3	78		
5	2	-[2-	-[2-	-[2-	-[2-(2-...	502	C22H46O12	1000352-13-2	76



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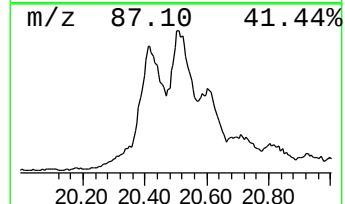
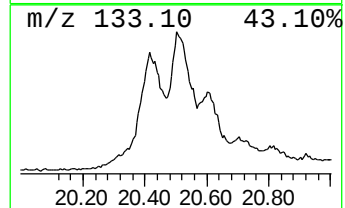
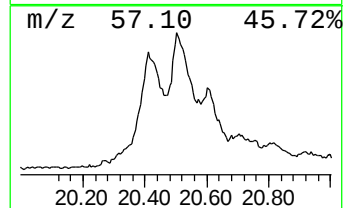
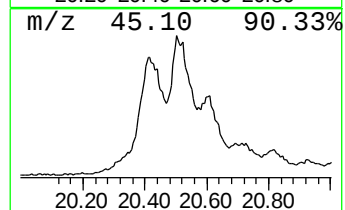
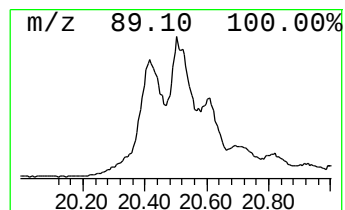
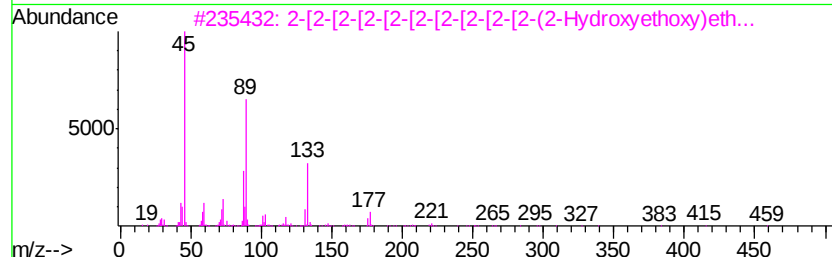
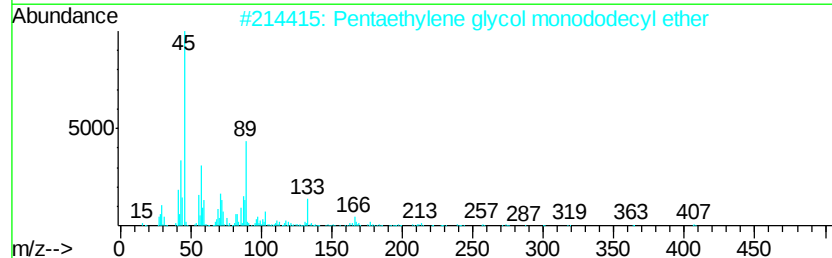
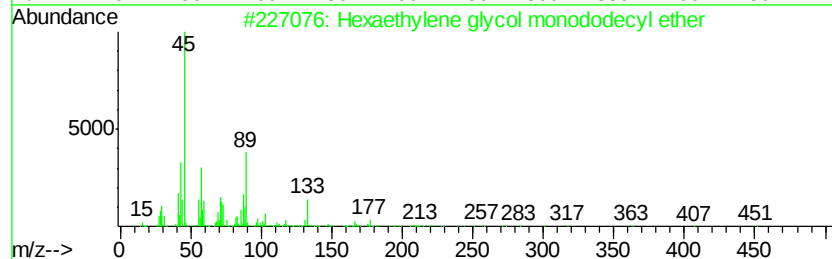
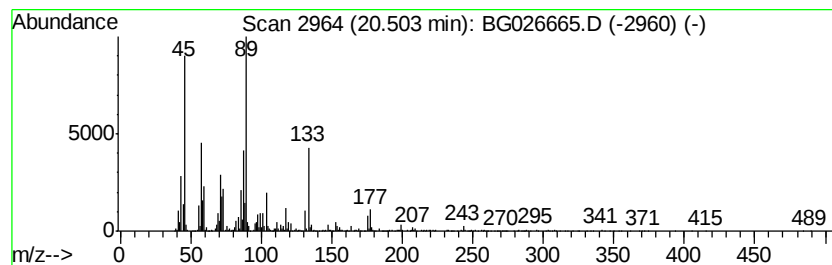
Instrument :
BNA_G
ClientSampleId :
3652

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexaethylene glycol monododecyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.50	2.74 ng	940791	Chrysene-d12	21.61
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexaethylene glycol monododecyl ...	450 C24H50O7	003055-96-7	90
2	Pentaethylene glycol monododecyl...	406 C22H46O6	003055-95-6	83
3	2-[2-[2-[2-[2-[2-[2-[2-(2-...	502 C22H46O12	1000352-13-2	76
4	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414 C18H38O10	1000352-12-5	74
5	Heptaethylene glycol monododecyl...	494 C26H54O8	003055-97-8	72



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041917\
Data File : BG026665.D
Acq On : 19 Apr 2017 20:51
Operator : SJ/MA
Sample : I2755-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

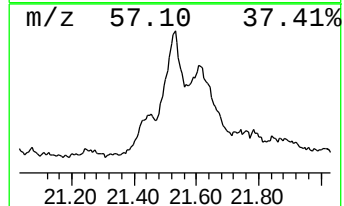
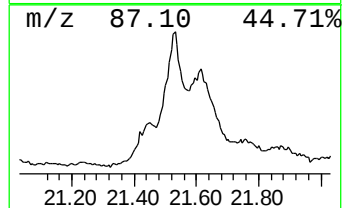
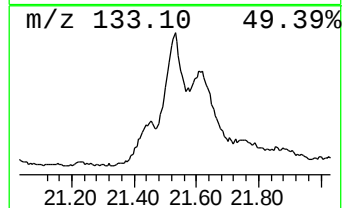
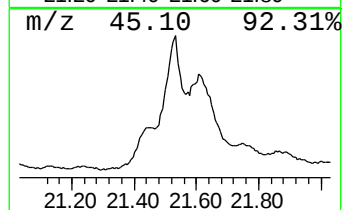
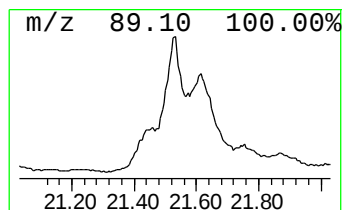
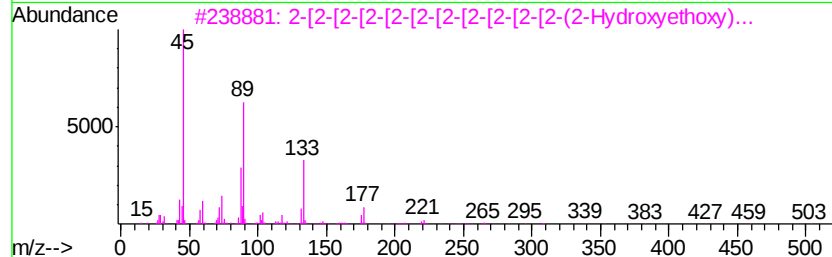
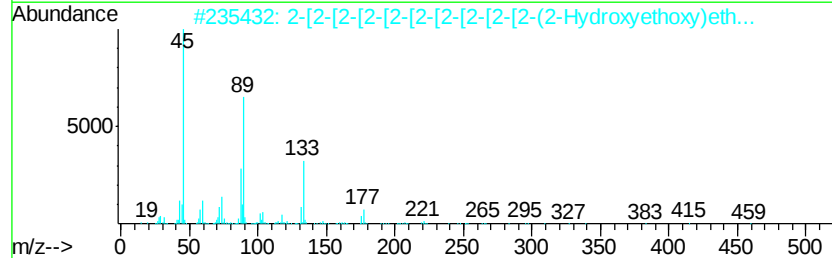
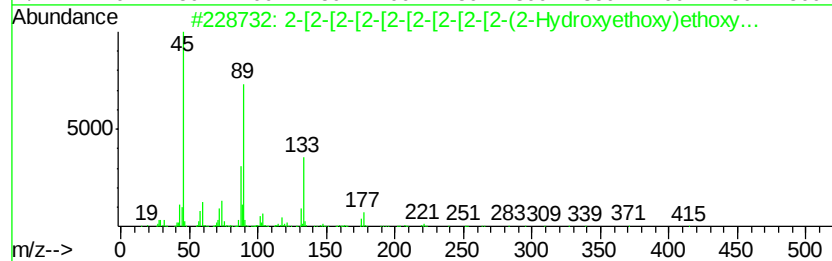
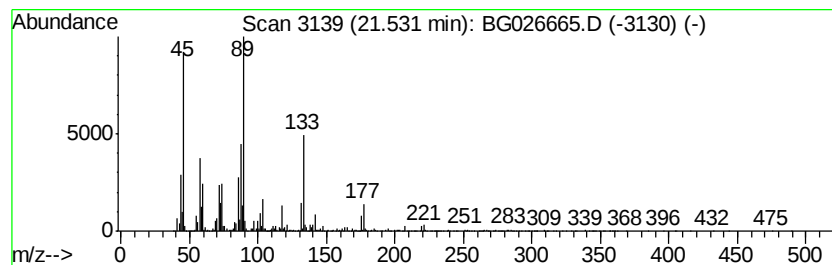
Instrument :
BNA_G
ClientSampleId :
3652

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-[2-[2-[2-[2-[2-[2-[2-(... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.53	15.74 ng	5408760	Chrysene-d12	21.61
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458 C20H42011	1000352-12-6	87
2	2-[2-[2-[2-[2-[2-[2-[2-(2-...	502 C22H46012	1000352-13-2	81
3	2-[2-[2-[2-[2-[2-[2-[2-(2-...	546 C24H50013	1000352-12-7	81
4	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414 C18H38010	1000352-12-5	74
5	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370 C16H3409	005117-19-1	64



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041917\
Data File : BG026665.D
Acq On : 19 Apr 2017 20:51
Operator : SJ/MA
Sample : I2755-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
3652

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041817.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
2-Pentanone, 4-hy...	5.13	3.3	ng	154519	1	8.03	942311	20.0
unknown7.58	7.58	84.6	ng	3984670	1	8.03	942311	20.0
Benzenemethanol, ...	9.13	13.1	ng	614890	1	8.03	942311	20.0
n-Hexadecanoic acid	18.26	3.0	ng	426376	4	17.37	2864940	20.0
2-[2-[2-[2-[2-[2-...	20.41	13.2	ng	4543740	5	21.61	6872300	20.0
Hexaethylene glyc...	20.50	2.7	ng	940791	5	21.61	6872300	20.0
2-[2-[2-[2-[2-[2-...	21.53	15.7	ng	5408760	5	21.61	6872300	20.0