

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092615\
 Data File : BF081840.D
 Acq On : 26 Sep 2015 21:28
 Operator : UM/IZ
 Sample : G3785-03
 Misc :
 ALS Vial : 55 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MGP221BR-54-54.5

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_F\METHODS\8270-BF092415.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	2.217	5	7	20	rVB	44998	109315	3.58%	0.380%
2	3.337	103	105	117	rBV2	12367	38769	1.27%	0.135%
3	4.491	203	206	209	rBV	34774	38266	1.25%	0.133%
4	5.097	257	259	260	rBV	99981	107206	3.51%	0.373%
5	5.143	260	263	265	rVB	1035467	1480711	48.46%	5.148%
6	5.543	295	298	300	rBV	2699638	2913355	95.35%	10.129%
7	6.560	384	387	390	rBV	2130591	2748818	89.97%	9.557%
8	6.709	397	400	402	rBV	2772569	3043960	99.63%	10.583%
9	6.937	418	420	422	rBV	839864	678596	22.21%	2.359%
10	7.097	431	434	436	rVB	2489004	2296041	75.15%	7.983%
11	7.509	467	470	472	rBV	1749180	1992207	65.21%	6.927%
12	8.229	530	533	535	rBV	780939	856131	28.02%	2.977%
13	9.303	624	627	629	rBV	3408262	3055297	100.00%	10.623%
14	9.692	659	661	664	rBV	528029	591773	19.37%	2.057%
15	9.978	684	686	689	rBV	809752	930330	30.45%	3.235%
16	10.400	719	723	725	rBV2	21532	32787	1.07%	0.114%
17	10.766	753	755	758	rBV2	1481515	1938549	63.45%	6.740%
18	10.881	763	765	768	rBB	30257	33966	1.11%	0.118%
19	11.326	802	804	805	rBV	41496	32407	1.06%	0.113%
20	11.463	814	816	819	rBV	659525	869836	28.47%	3.024%
21	12.869	937	939	942	rBV	95136	85916	2.81%	0.299%
22	13.052	953	955	958	rBV	2095487	2749039	89.98%	9.558%
23	13.578	999	1001	1003	rBV	67908	58622	1.92%	0.204%
24	13.944	1031	1033	1039	rBV	271320	288476	9.44%	1.003%
25	14.104	1045	1047	1050	rBV	616054	797805	26.11%	2.774%
26	14.572	1086	1088	1090	rBV	27595	36668	1.20%	0.127%
27	14.869	1111	1114	1120	rBV2	61878	98441	3.22%	0.342%
28	14.961	1120	1122	1124	rVV	48314	51084	1.67%	0.178%
29	15.578	1173	1176	1179	rBV	521231	756294	24.75%	2.629%
30	16.092	1219	1221	1226	rVB	32657	51362	1.68%	0.179%

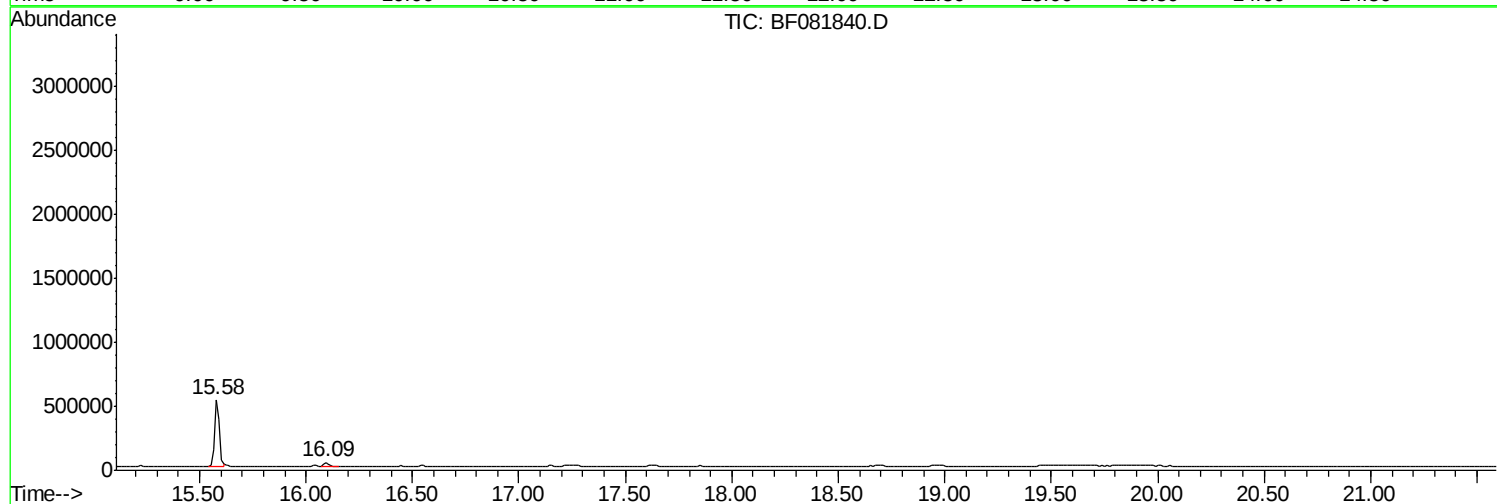
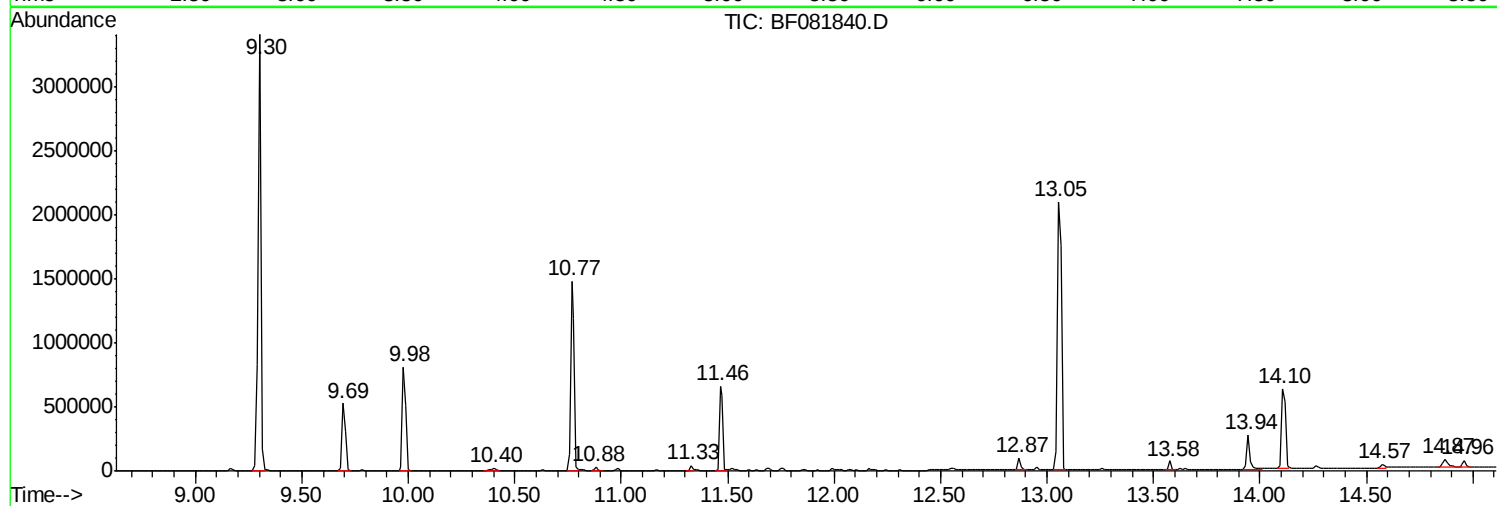
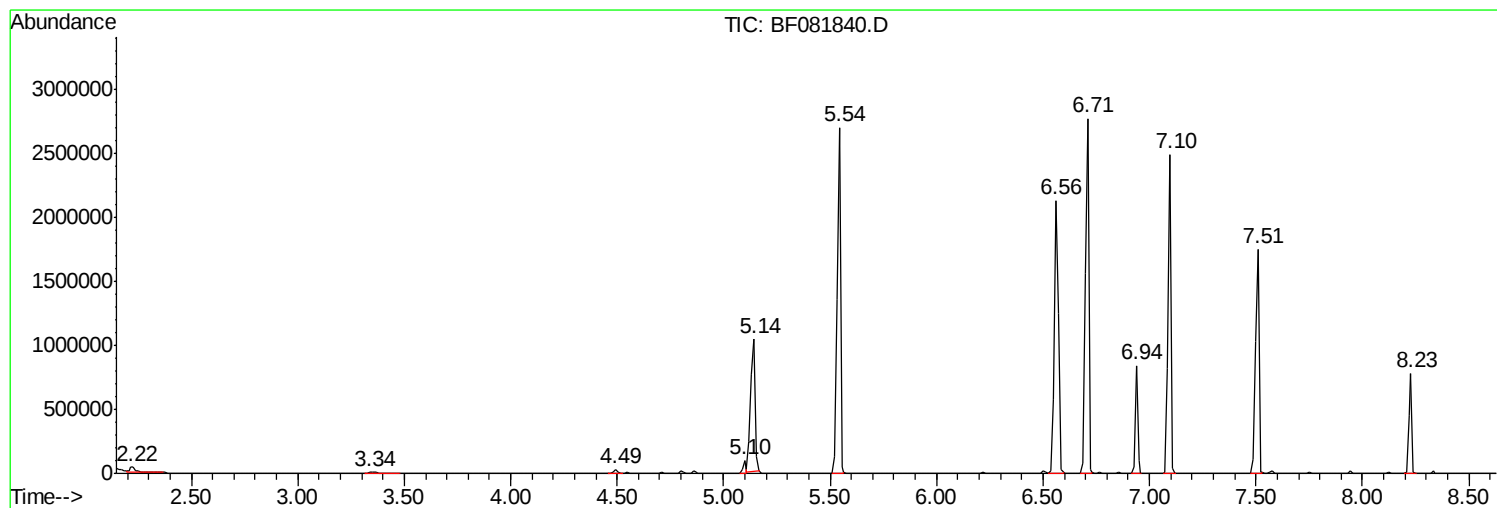
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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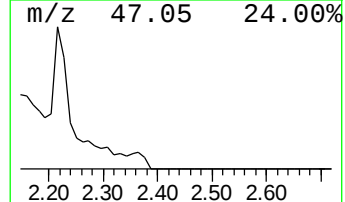
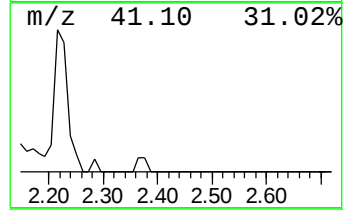
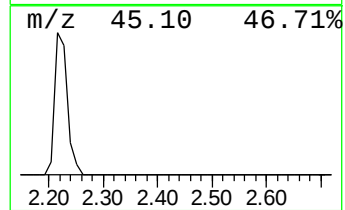
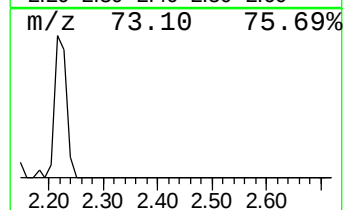
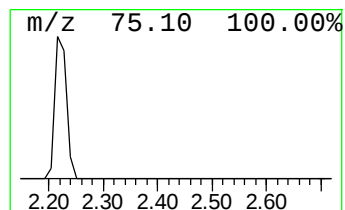
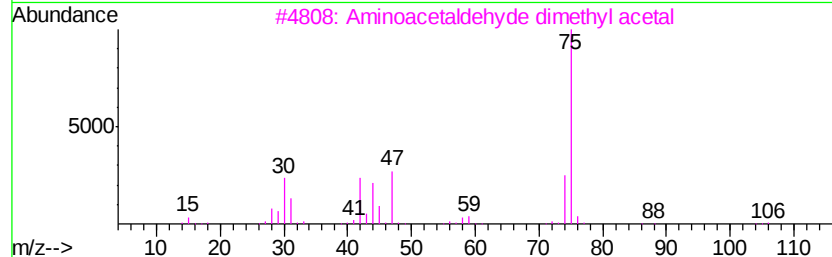
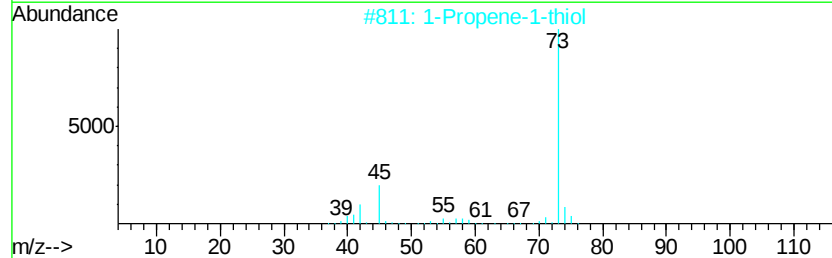
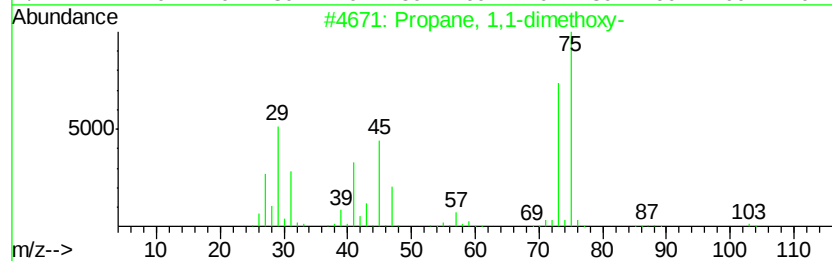
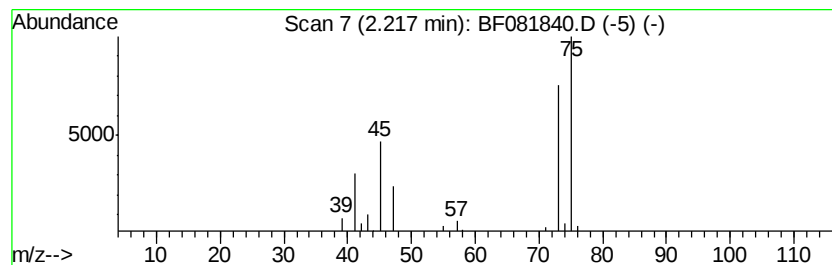
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	3.22 ng	109315	1,4-Dichlorobenzene-d4	6.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2		1-Propene-1-thiol	74	C3H6S	000925-89-3	9
3		Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9



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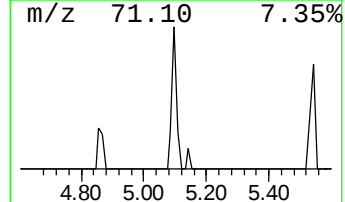
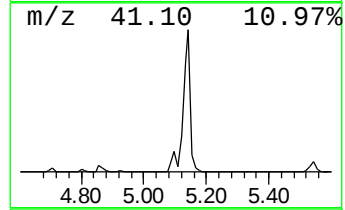
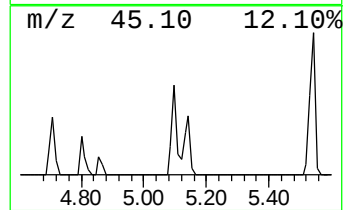
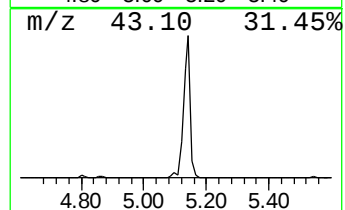
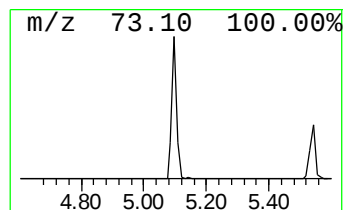
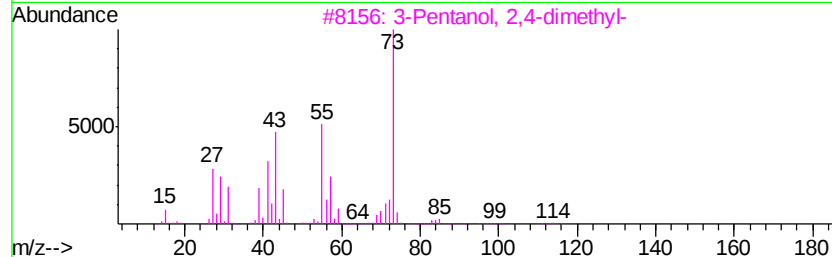
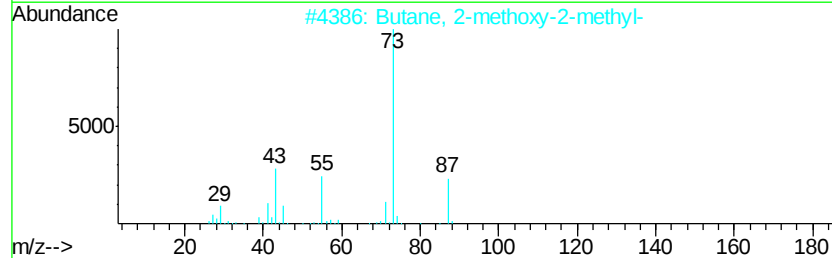
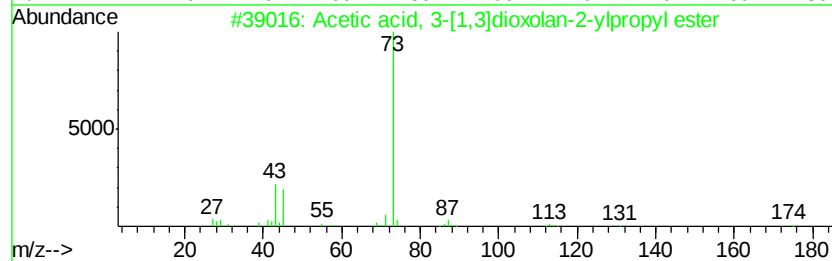
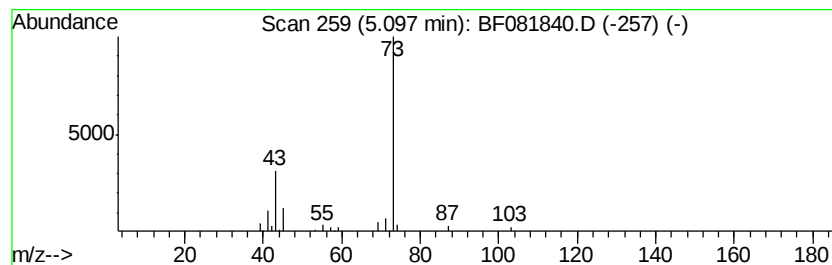
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Peak Number 2 unknown5.10 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	3.16 ng	107206	1,4-Dichlorobenzene-d4	6.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	1000186-02-3	42
2		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	28
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
4		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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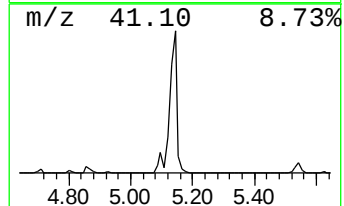
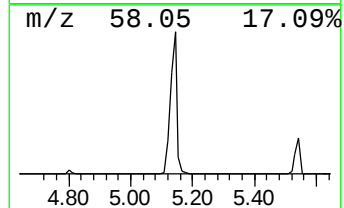
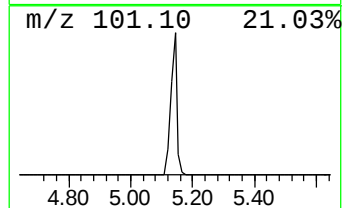
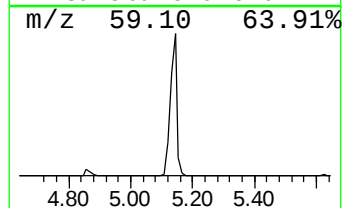
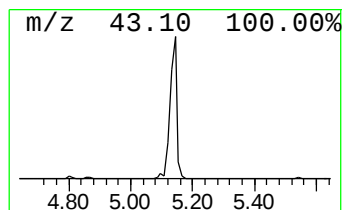
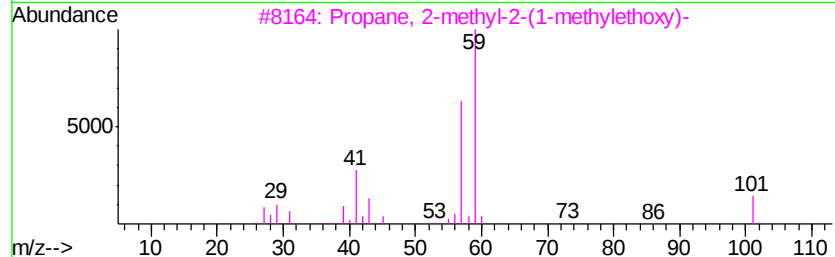
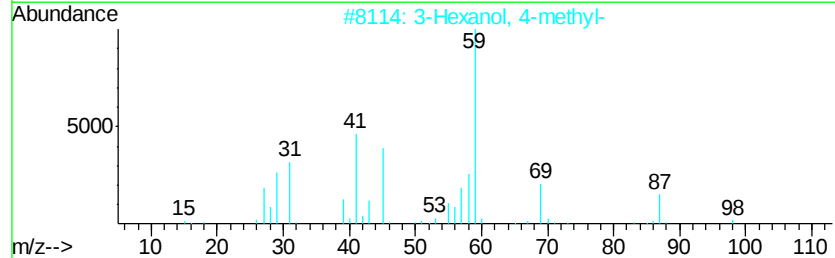
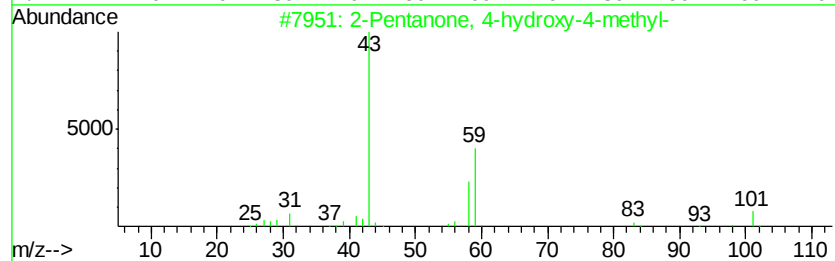
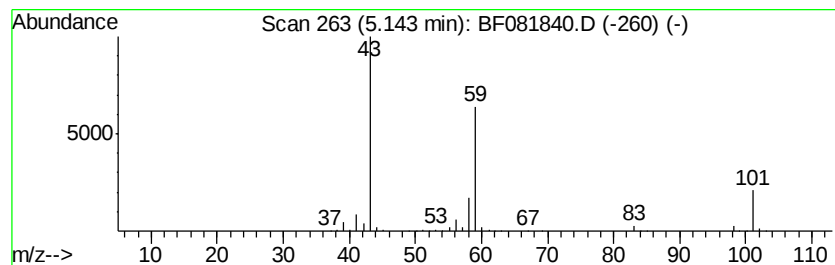
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	43.64 ng	1480710	1,4-Dichlorobenzene-d4	6.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		Acetone	58	C3H6O	000067-64-1	9



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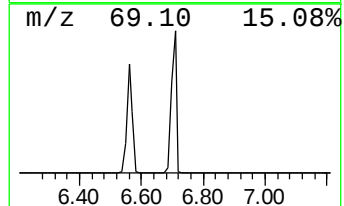
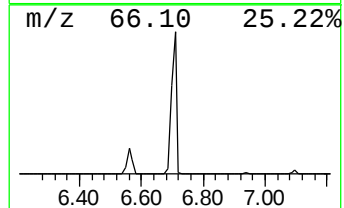
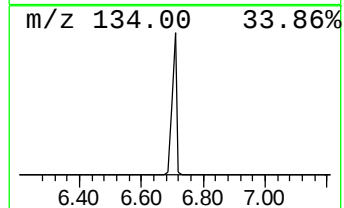
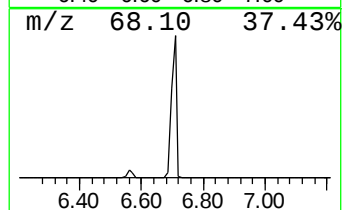
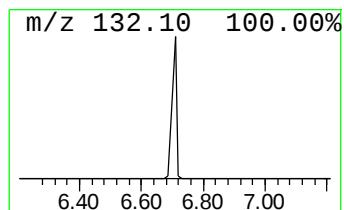
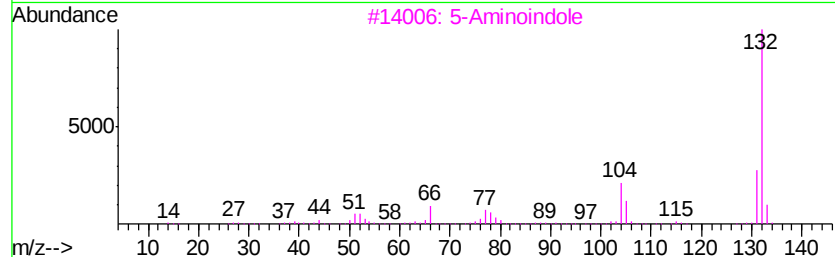
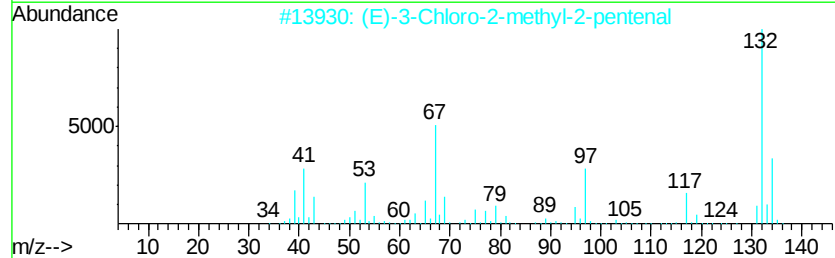
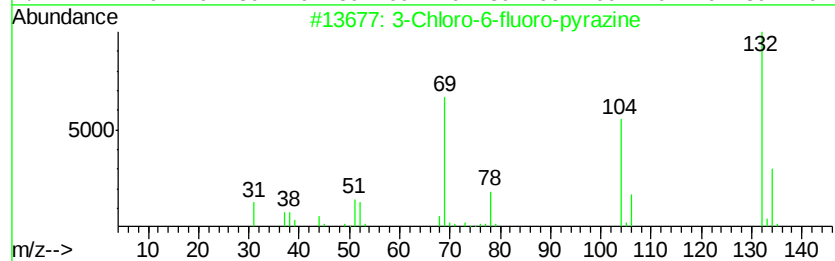
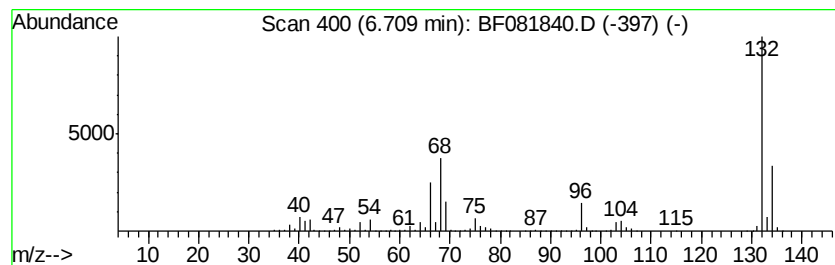
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Peak Number 4 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	89.71 ng	3043960	1,4-Dichlorobenzene-d4	6.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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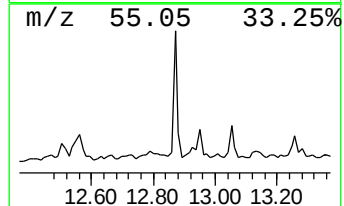
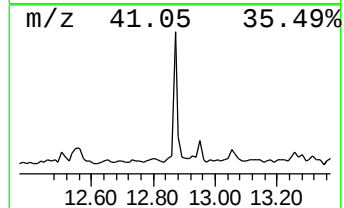
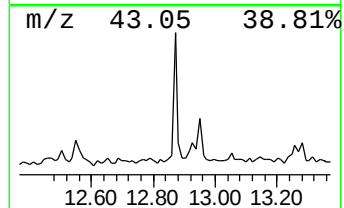
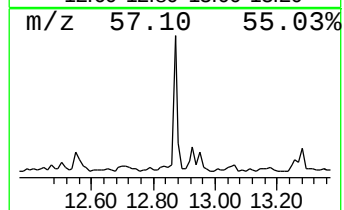
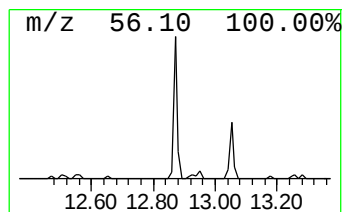
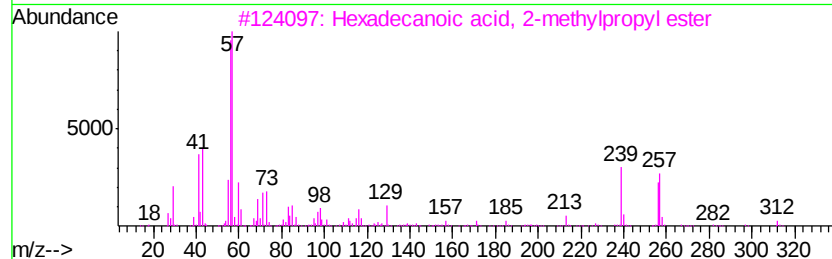
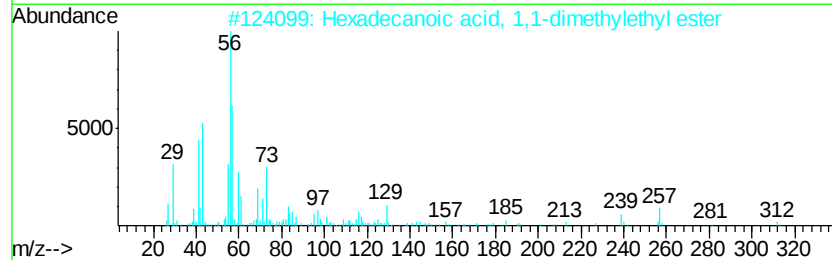
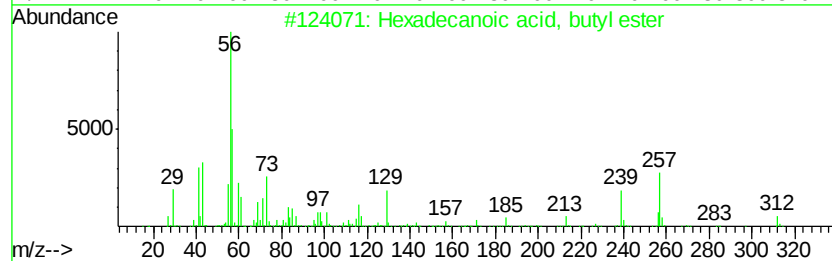
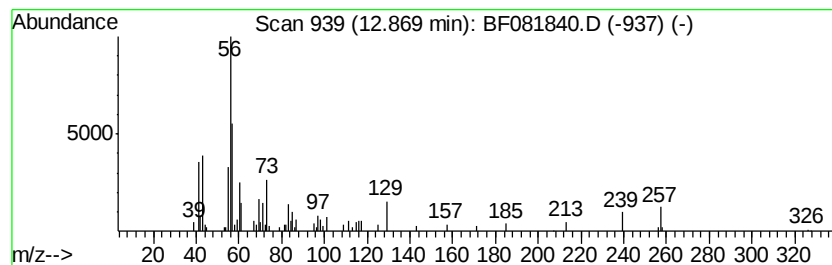
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.87	2.15 ng	85916	Chrysene-d12	14.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	62
3		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	45
4		2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	43
5		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38



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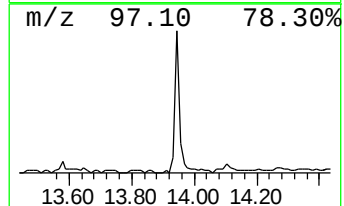
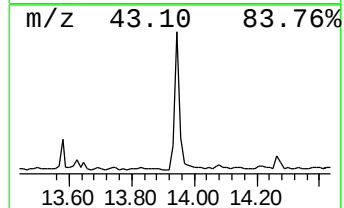
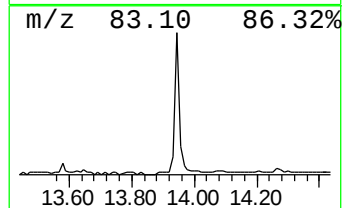
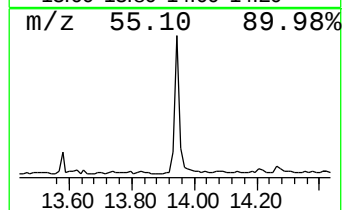
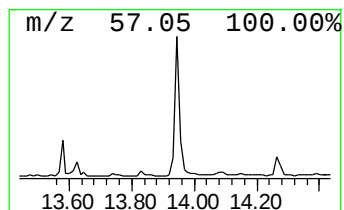
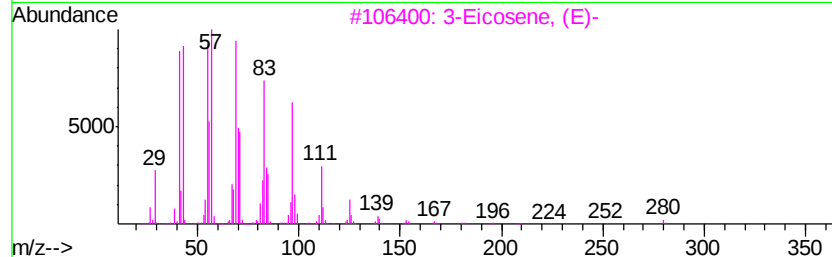
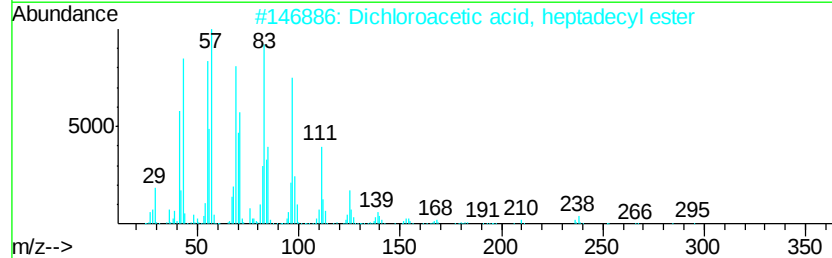
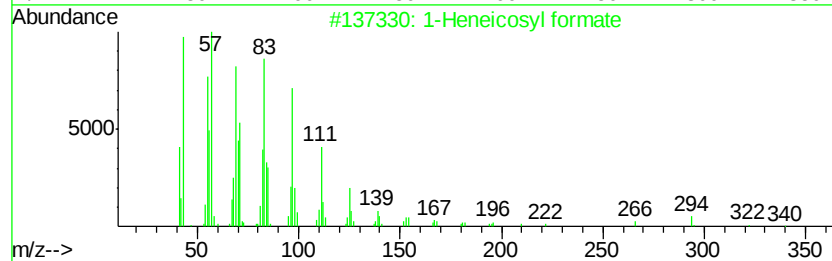
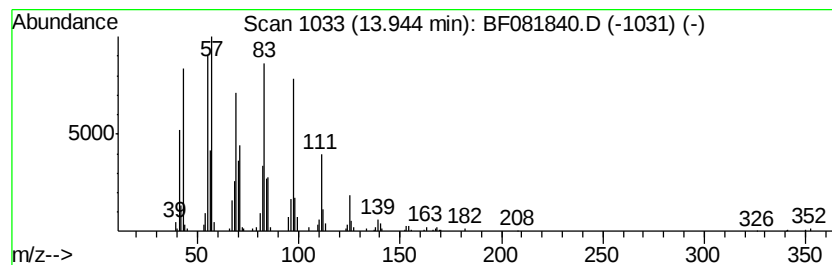
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	7.23 ng	288476	Chrysene-d12	14.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95	
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95	
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91	
4	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91	
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	91	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092615\
Data File : BF081840.D
Acq On : 26 Sep 2015 21:28
Operator : UM/IZ
Sample : G3785-03
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP221BR-54-54.5

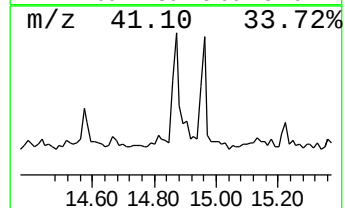
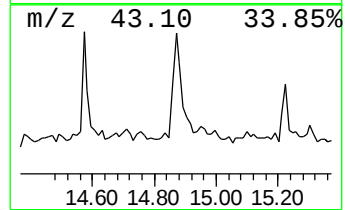
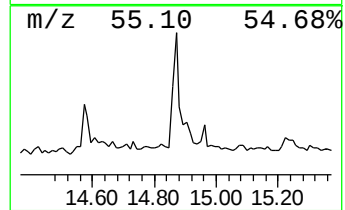
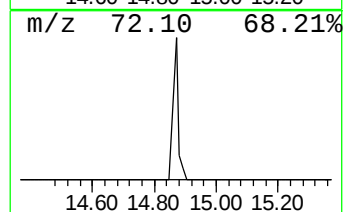
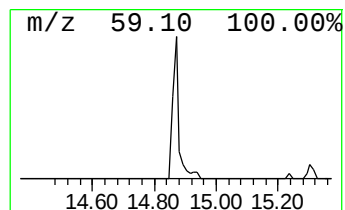
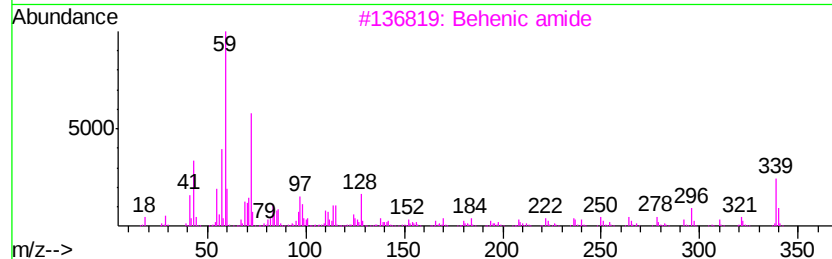
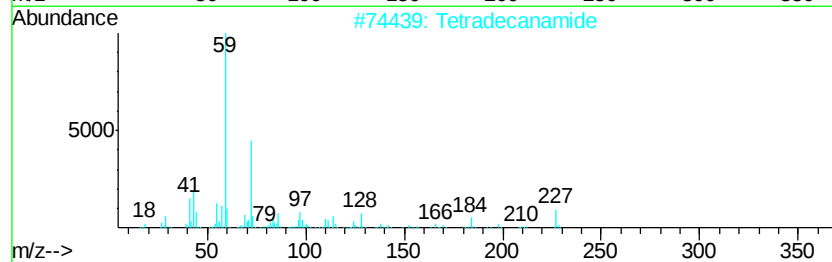
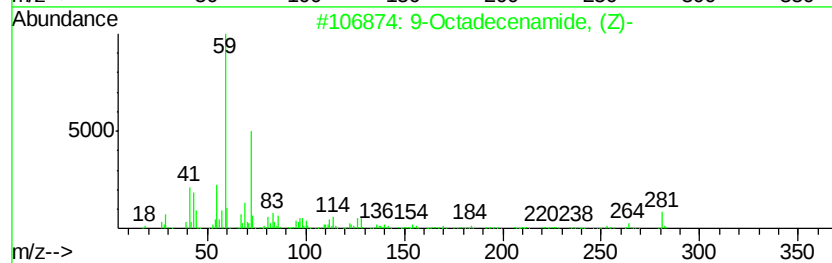
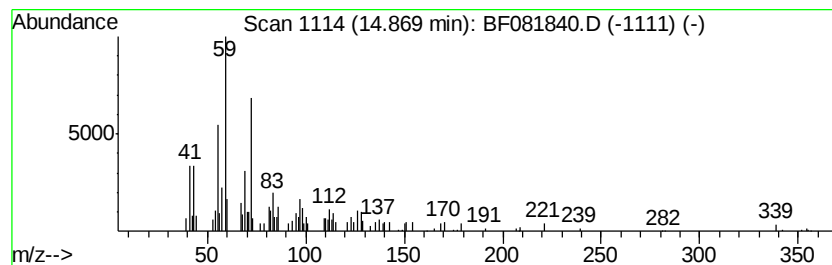
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.60 ng	98441	Perylene-d12	15.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	78
2		Tetradecanamide	227	C14H29NO	000638-58-4	64
3		Behenic amide	339	C22H45NO	003061-75-4	64
4		7-Nonenamide	155	C9H17NO	090949-53-4	59
5		Hexadecanamide	255	C16H33NO	000629-54-9	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092615\
Data File : BF081840.D
Acq On : 26 Sep 2015 21:28
Operator : UM/IZ
Sample : G3785-03
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP221BR-54-54.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.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
Propane, 1,1-dime...	2.22	3.2	ng	109315	1	6.94	678596	20.0
unknown5.10	5.10	3.2	ng	107206	1	6.94	678596	20.0
2-Pentanone, 4-hy...	5.14	43.6	ng	1480710	1	6.94	678596	20.0
unknown6.71	6.71	89.7	ng	3043960	1	6.94	678596	20.0
Hexadecanoic acid...	12.87	2.1	ng	85916	5	14.12	797805	20.0
1-Heneicosyl formate	13.94	7.2	ng	288476	5	14.12	797805	20.0
9-Octadecenamide,...	14.87	2.6	ng	98441	6	15.58	756294	20.0