

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
 Data File : BF085898.D
 Acq On : 30 Mar 2016 20:50
 Operator : UM/SJ
 Sample : H2023-02
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-2

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-BF032416.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	4.984	234	236	245	rVB	79988	122177	4.04%	0.483%
2	5.396	270	272	275	rBV	2481105	2639072	87.33%	10.433%
3	6.436	360	363	366	rBV	1993376	2934491	97.10%	11.601%
4	6.573	372	375	377	rBV	2201390	3022076	100.00%	11.947%
5	6.801	393	395	397	rBV	518481	620930	20.55%	2.455%
6	6.950	406	408	411	rBV	2027286	2175660	71.99%	8.601%
7	7.362	442	444	447	rBV	1448099	1892866	62.63%	7.483%
8	8.082	505	507	510	rBV	959327	830804	27.49%	3.284%
9	9.167	599	602	604	rBV	2140936	2891885	95.69%	11.432%
10	9.556	634	636	638	rBV	513637	410783	13.59%	1.624%
11	9.773	653	655	656	rBV	70168	58548	1.94%	0.231%
12	9.807	656	658	659	rVV	51217	47684	1.58%	0.189%
13	9.842	659	661	663	rVB	693014	819296	27.11%	3.239%
14	9.979	671	673	679	rBV2	70939	130253	4.31%	0.515%
15	10.276	697	699	700	rVB	61667	81792	2.71%	0.323%
16	10.345	703	705	711	rVB	30504	36659	1.21%	0.145%
17	10.493	715	718	721	rBV2	31024	55706	1.84%	0.220%
18	10.630	727	730	732	rBV	1596385	1710225	56.59%	6.761%
19	10.745	738	740	747	rVB	101772	124670	4.13%	0.493%
20	11.190	777	779	780	rBV	47351	39311	1.30%	0.155%
21	11.316	788	790	793	rBV	762790	744763	24.64%	2.944%
22	11.853	834	837	841	rBV	126919	144853	4.79%	0.573%
23	12.905	926	929	931	rBV	2291998	2054830	67.99%	8.123%
24	13.808	1005	1008	1013	rBV	64756	115932	3.84%	0.458%
25	13.956	1018	1021	1023	rBV	611636	581501	19.24%	2.299%
26	14.425	1058	1062	1069	rBV5	8713	37198	1.23%	0.147%
27	14.699	1084	1086	1090	rBV	155800	168720	5.58%	0.667%
28	15.031	1113	1115	1117	rBV	27908	33992	1.12%	0.134%
29	15.374	1142	1145	1151	rBV	478595	622543	20.60%	2.461%
30	15.785	1179	1181	1185	rBV	21365	33010	1.09%	0.130%
31	16.528	1243	1246	1253	rVB2	17144	40314	1.33%	0.159%
32	18.208	1389	1393	1402	rVB6	17302	72975	2.41%	0.288%

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Instrument :
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ClientSampleId :
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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

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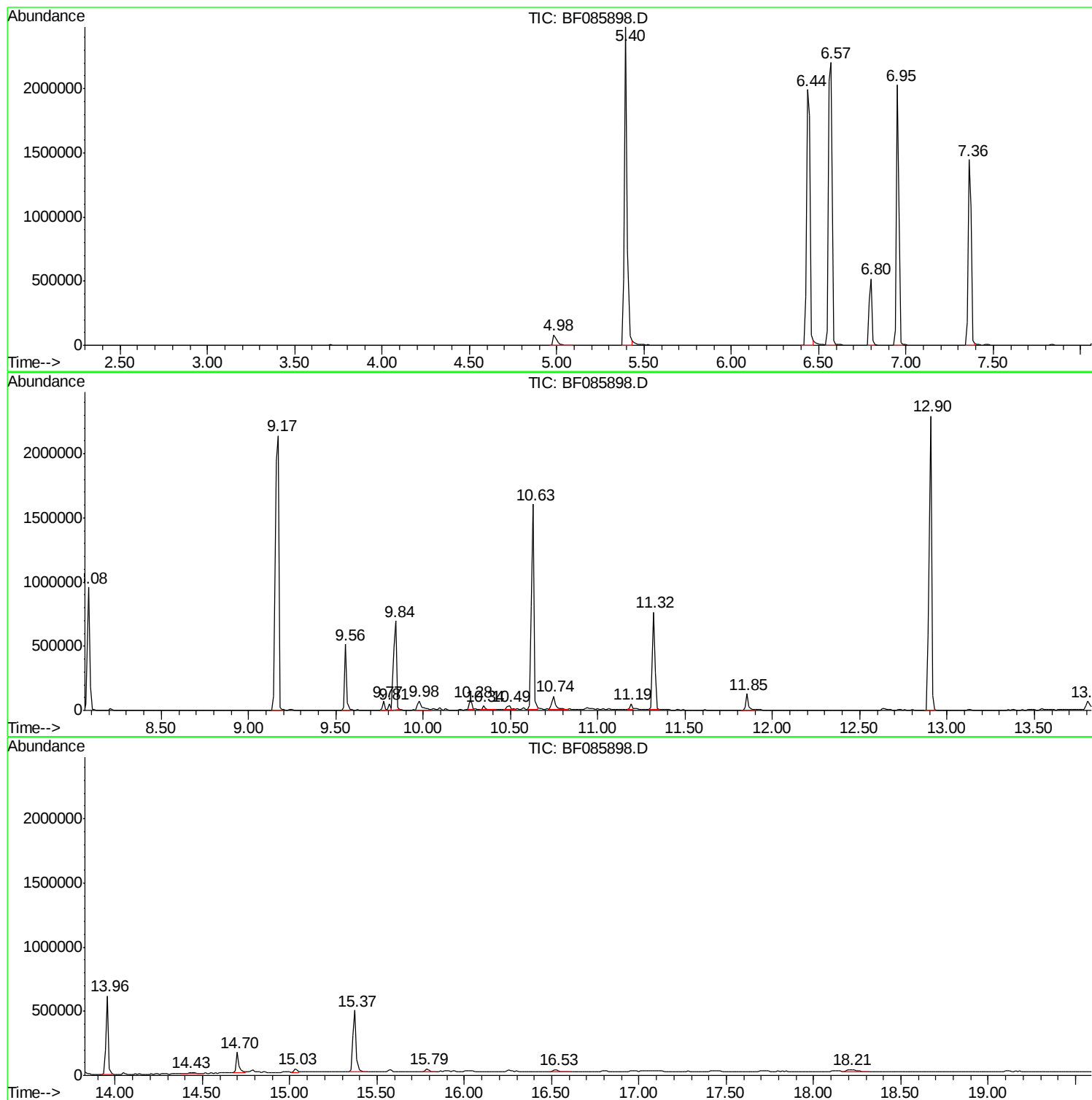
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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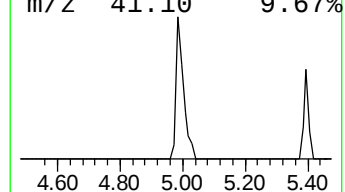
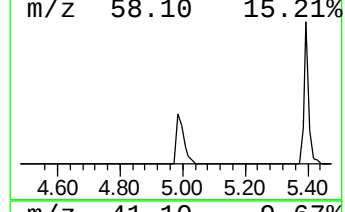
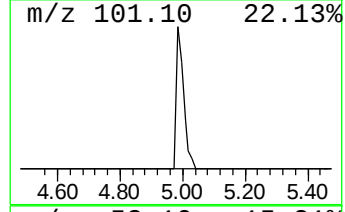
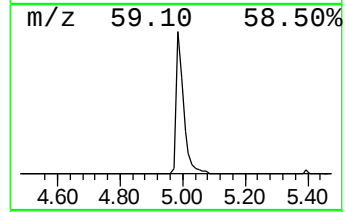
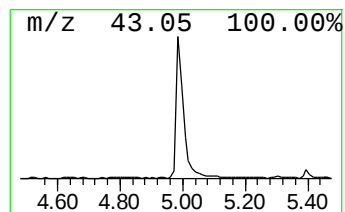
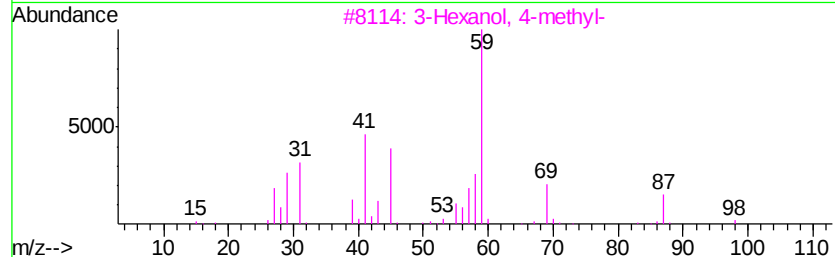
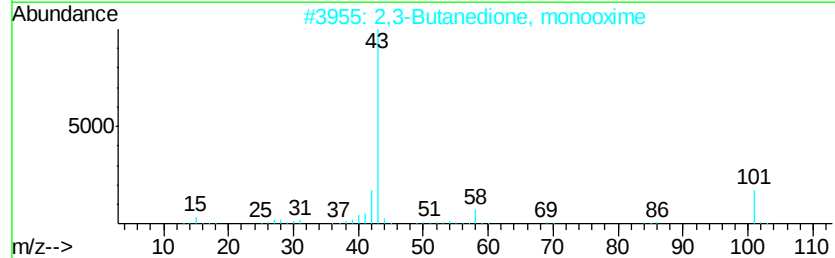
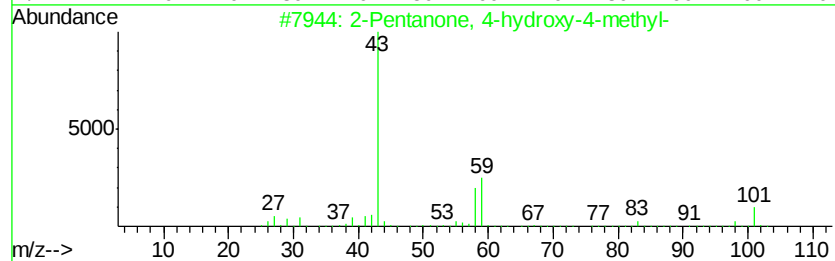
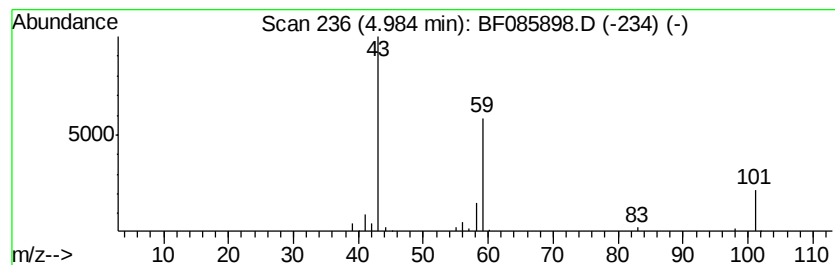
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	3.94 ng	122177	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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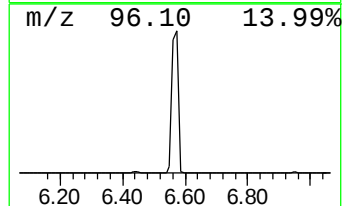
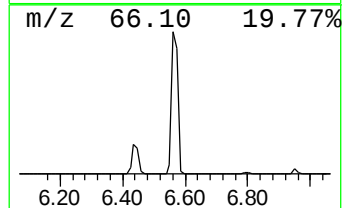
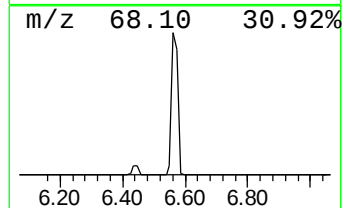
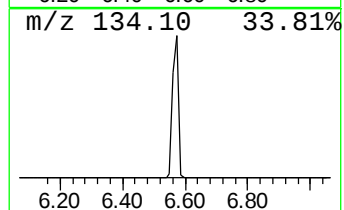
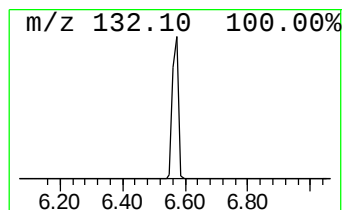
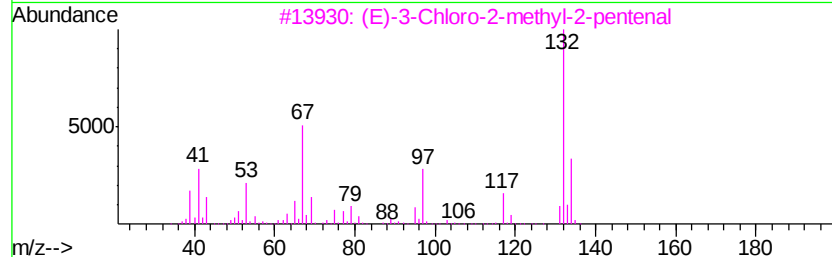
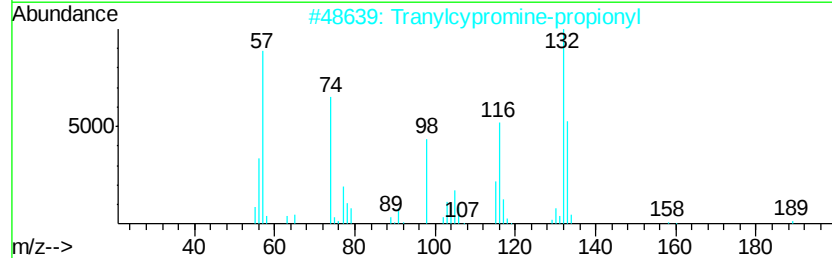
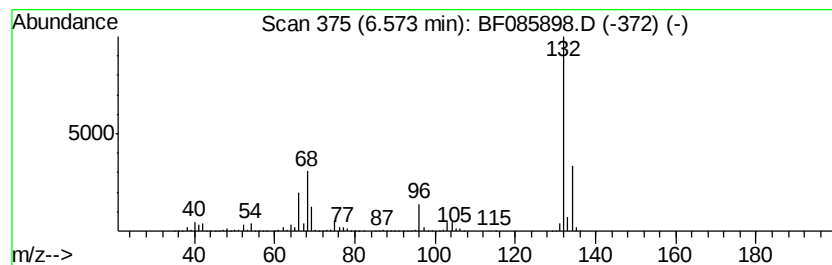
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	97.34 ng	3022080	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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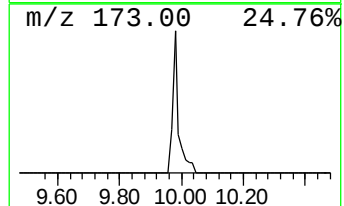
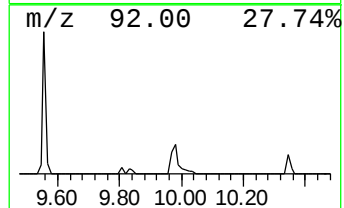
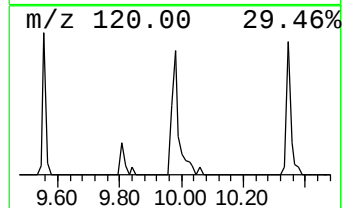
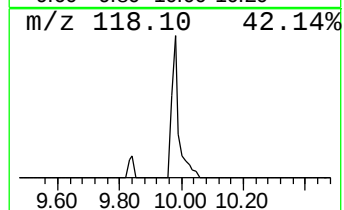
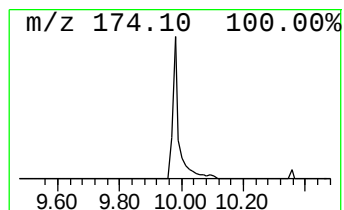
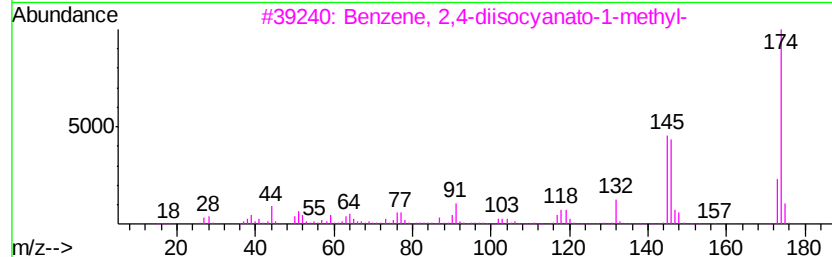
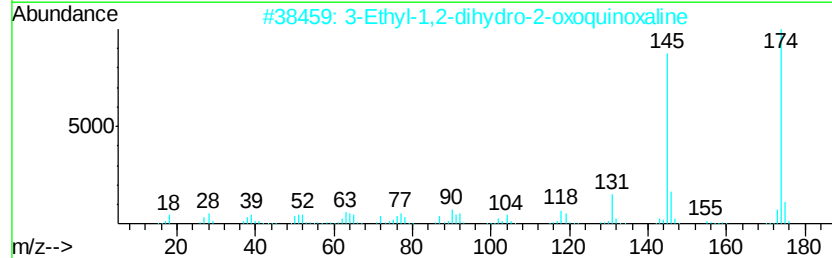
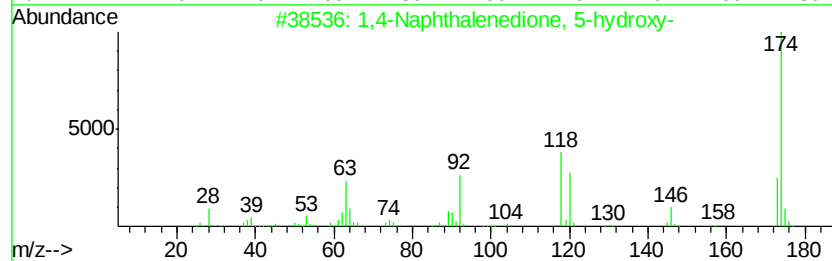
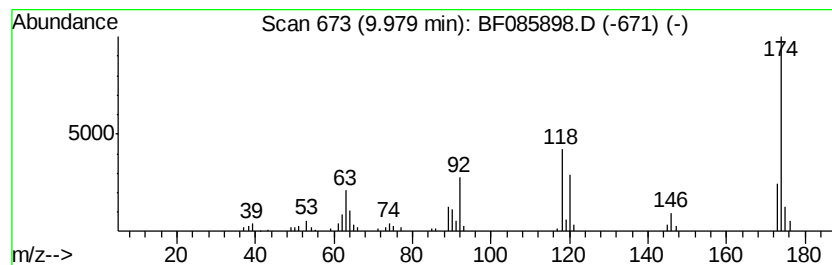
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,4-Naphthalenedione, 5-hyd... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.98	3.18 ng	130253	Acenaphthene-d10	9.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Naphthalenedione, 5-hydroxy-	174	C10H6O3	000481-39-0	97
2		3-Ethyl-1,2-dihydro-2-oxoquinoxaline	174	C10H10N2O	013297-35-3	43
3		Benzene, 2,4-diisocyanato-1-methyl-	174	C9H6N2O2	000584-84-9	43
4		2-Fluoro-5-phenylpyrimidine	174	C10H7FN2	062850-13-9	38
5		2,3-Dimethylchromone	174	C11H10O2	017584-90-6	37



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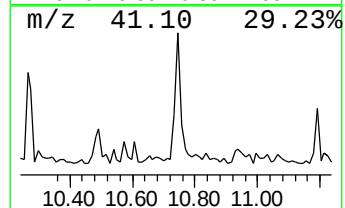
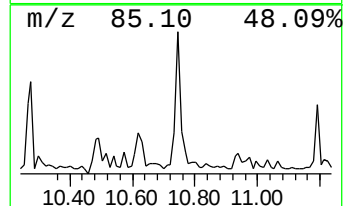
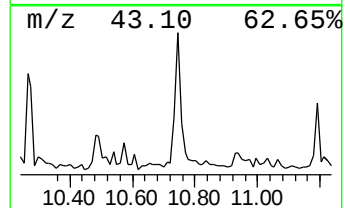
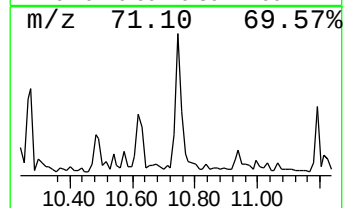
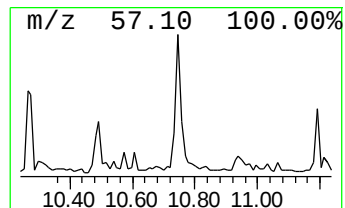
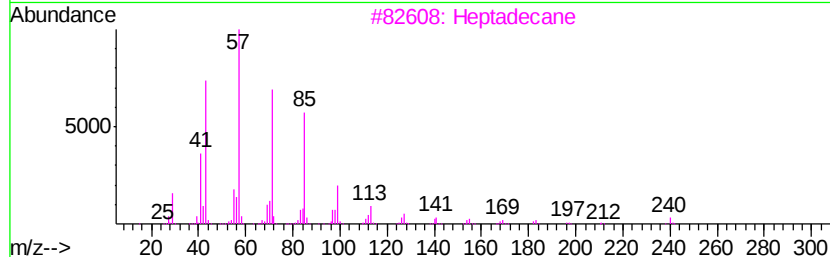
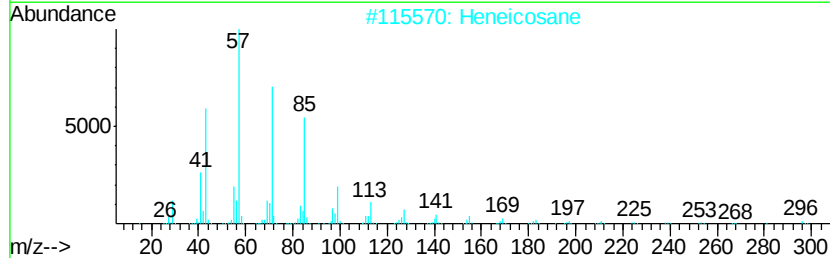
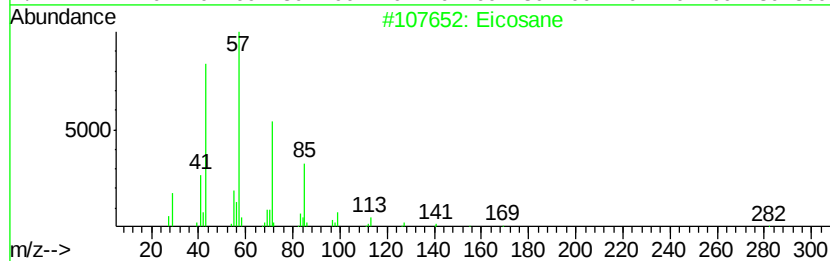
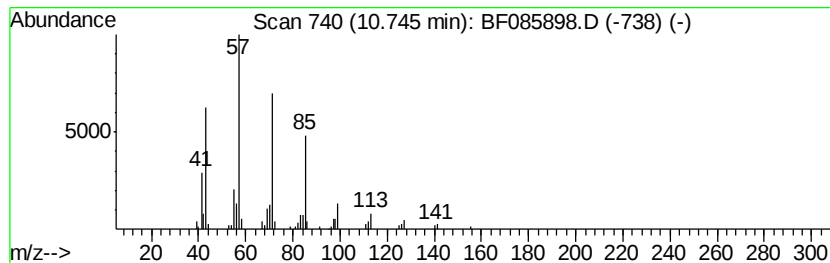
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	3.35 ng	124670	Phenanthrene-d10	11.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Heptadecane		240	C17H36	000629-78-7	91
4	Octadecane		254	C18H38	000593-45-3	90
5	Hexadecane		226	C16H34	000544-76-3	90



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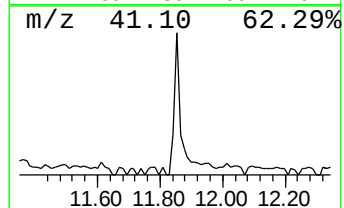
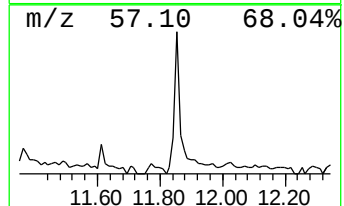
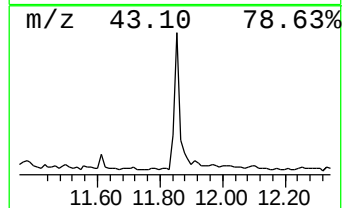
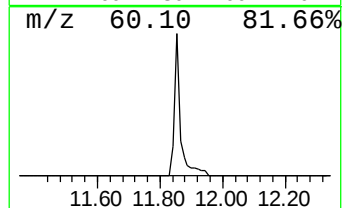
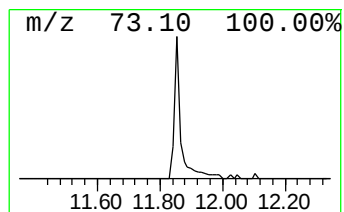
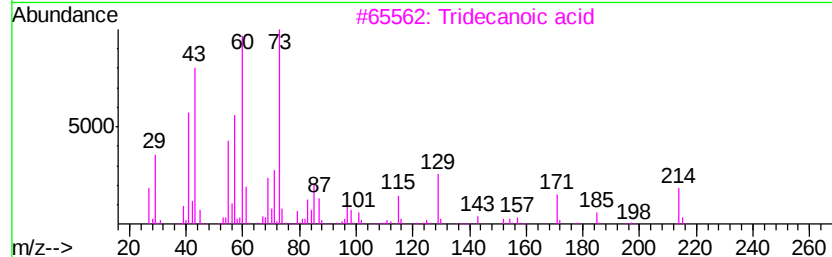
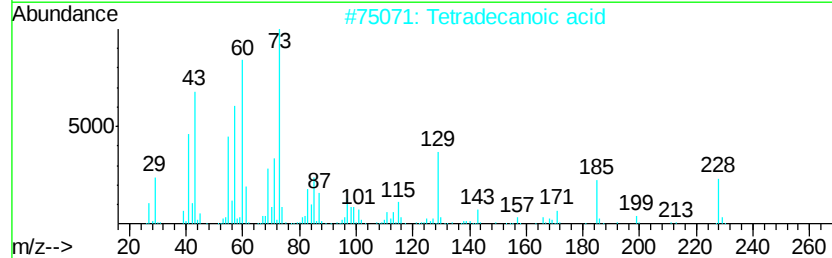
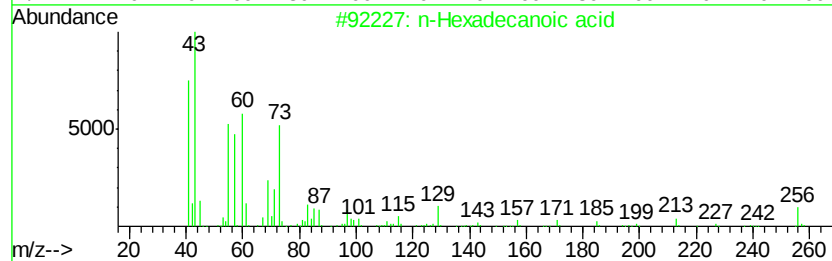
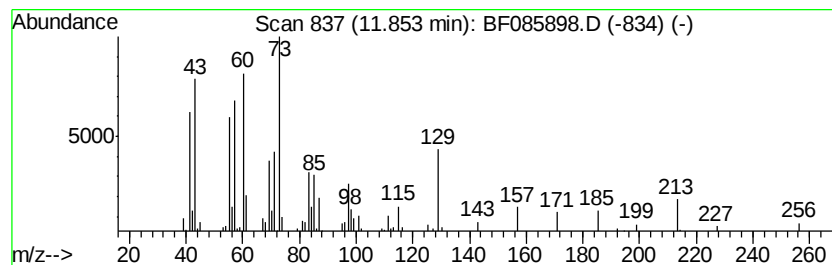
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.85	3.89 ng	144853	Phenanthrene-d10		11.32	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	43
5		N-Acetylisoaxazolidine	115	C5H9NO2	115615-36-6	18



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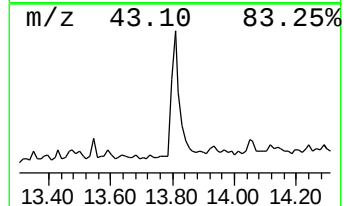
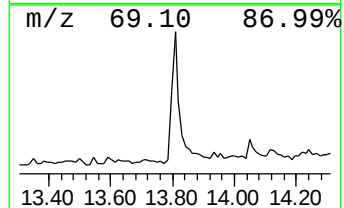
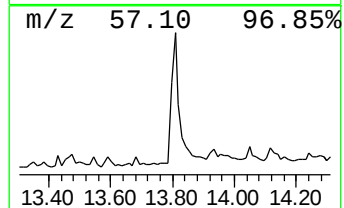
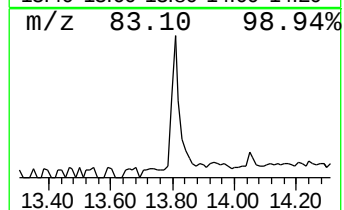
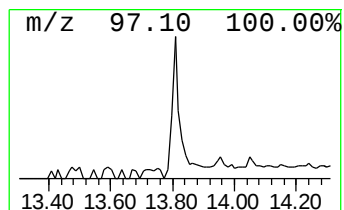
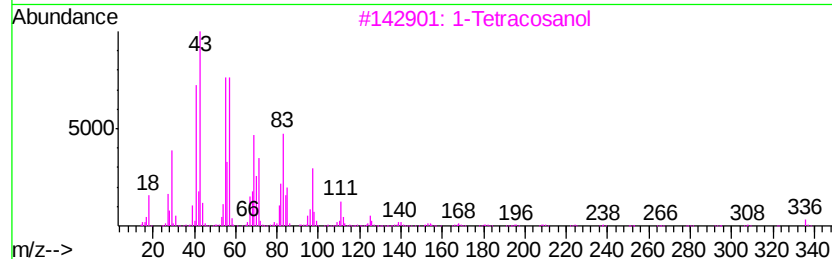
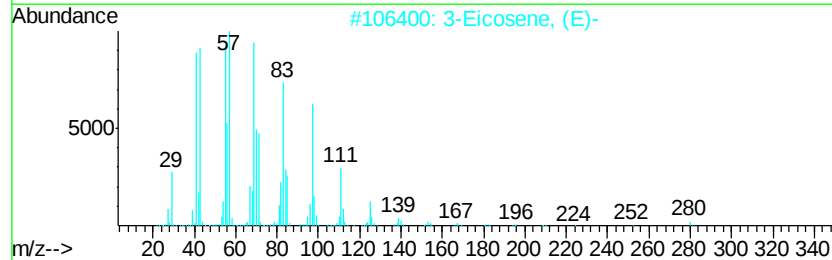
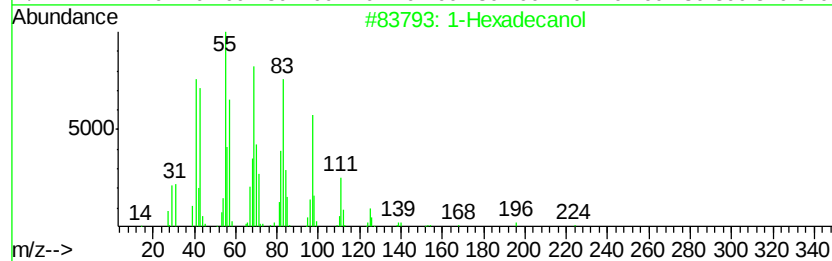
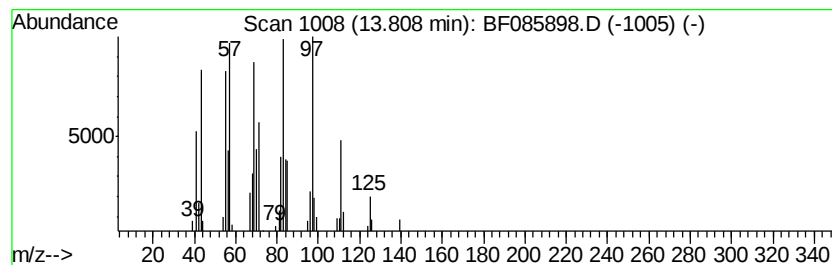
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Hexadecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	3.99 ng	115932	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexadecanol	242	C16H34O	036653-82-4	91
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	90
3		1-Tetracosanol	354	C24H50O	000506-51-4	87
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	81
5		1-Docosene	308	C22H44	001599-67-3	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085898.D
Acq On : 30 Mar 2016 20:50
Operator : UM/SJ
Sample : H2023-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-2

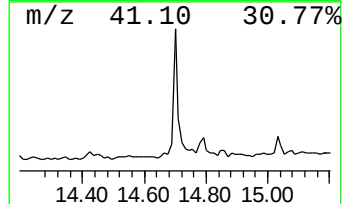
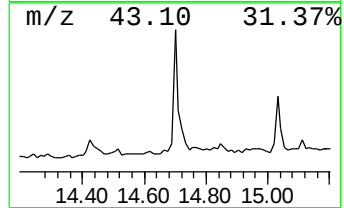
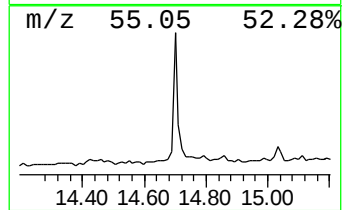
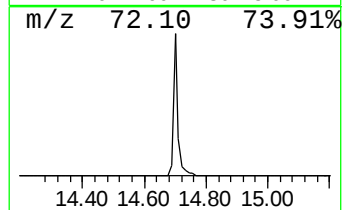
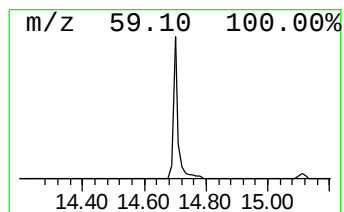
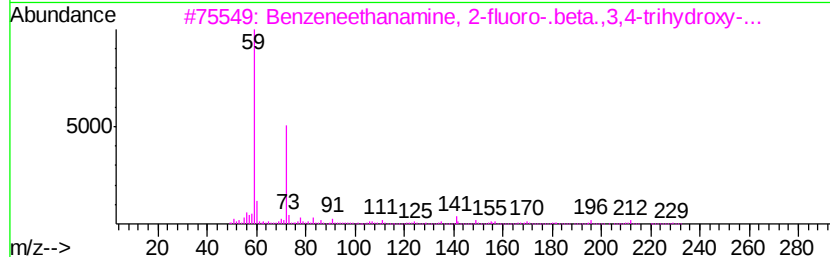
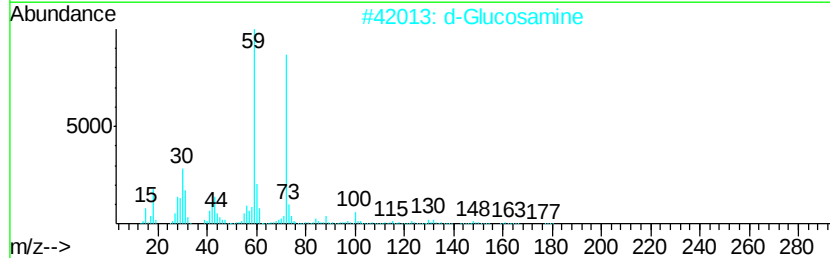
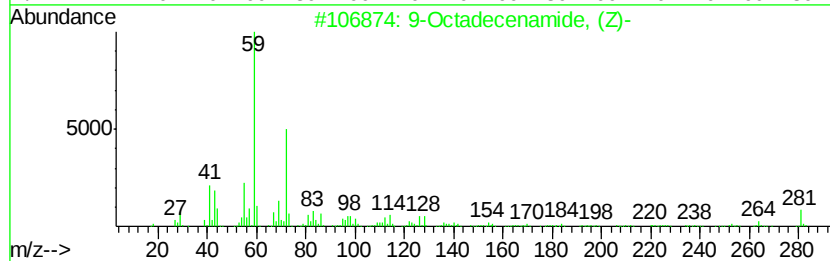
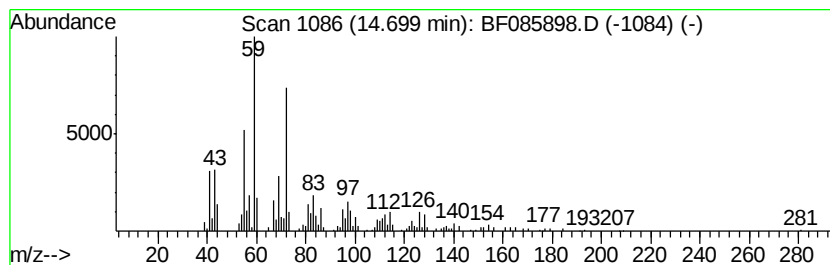
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	5.42 ng	168720	Perylene-d12	15.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		d-Glucosamine	179	C6H13NO5	000090-77-7	59
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
4		Tetradecanamide	227	C14H29NO	000638-58-4	50
5		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085898.D
Acq On : 30 Mar 2016 20:50
Operator : UM/SJ
Sample : H2023-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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...	4.98	3.9	ng	122177	1	6.80	620930	20.0
unknown6.57	6.57	97.3	ng	3022080	1	6.80	620930	20.0
1,4-Naphthalenedi...	9.98	3.2	ng	130253	3	9.84	819296	20.0
Eicosane	10.74	3.4	ng	124670	4	11.32	744763	20.0
n-Hexadecanoic acid	11.85	3.9	ng	144853	4	11.32	744763	20.0
1-Hexadecanol	13.81	4.0	ng	115932	5	13.96	581501	20.0
9-Octadecenamide, ...	14.70	5.4	ng	168720	6	15.37	622543	20.0