

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120618\
 Data File : BF111158.D
 Acq On : 7 Dec 2018 00:28
 Operator : JU/SJ
 Sample : J6202-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SAMPLE-1

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-BF120518.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	3.863	298	302	309	rVB	111436	161726	1.57%	0.173%
2	4.387	385	391	396	rVB2	131028	150269	1.46%	0.160%
3	5.016	489	498	506	rVB	518747	704921	6.83%	0.752%
4	5.422	562	567	570	rBV	9905186	9288568	89.95%	9.914%
5	6.434	733	739	743	rBV	9887539	10325866	100.00%	11.021%
6	6.575	758	763	766	rBV	10568162	9582582	92.80%	10.228%
7	6.804	798	802	805	rBV	3774896	2960641	28.67%	3.160%
8	6.963	825	829	832	rVB	8704280	7314579	70.84%	7.807%
9	7.363	892	897	900	rBV	7159292	6241146	60.44%	6.661%
10	8.087	1016	1020	1023	rBV	4842817	3902483	37.79%	4.165%
11	9.163	1198	1203	1206	rBV	11632423	10202871	98.81%	10.890%
12	9.551	1266	1269	1272	rBV	990461	799371	7.74%	0.853%
13	9.839	1314	1318	1322	rVB	5235452	4294273	41.59%	4.583%
14	10.622	1447	1451	1455	rBV	6490130	6040407	58.50%	6.447%
15	11.322	1566	1570	1573	rBV	4849497	3915108	37.92%	4.179%
16	11.857	1657	1661	1671	rBV	1685059	1613553	15.63%	1.722%
17	12.639	1791	1794	1806	rBV	739305	822933	7.97%	0.878%
18	12.910	1835	1840	1843	rBV	7657655	7054949	68.32%	7.530%
19	13.810	1989	1993	2001	rBV	1596912	1635078	15.83%	1.745%
20	13.951	2013	2017	2021	rBV	2751506	2594358	25.12%	2.769%
21	14.445	2098	2101	2106	rBV	305558	340400	3.30%	0.363%
22	14.745	2150	2152	2155	rBV	120811	111188	1.08%	0.119%
23	14.821	2162	2165	2167	rVB	139504	128597	1.25%	0.137%
24	15.080	2205	2209	2216	rBV2	137862	218188	2.11%	0.233%
25	15.392	2257	2262	2267	rBV	2248408	2574334	24.93%	2.748%
26	15.445	2269	2271	2275	rVB	140359	156696	1.52%	0.167%
27	15.874	2341	2344	2347	rBV2	112341	131533	1.27%	0.140%
28	15.921	2348	2352	2357	rVV2	262605	425326	4.12%	0.454%

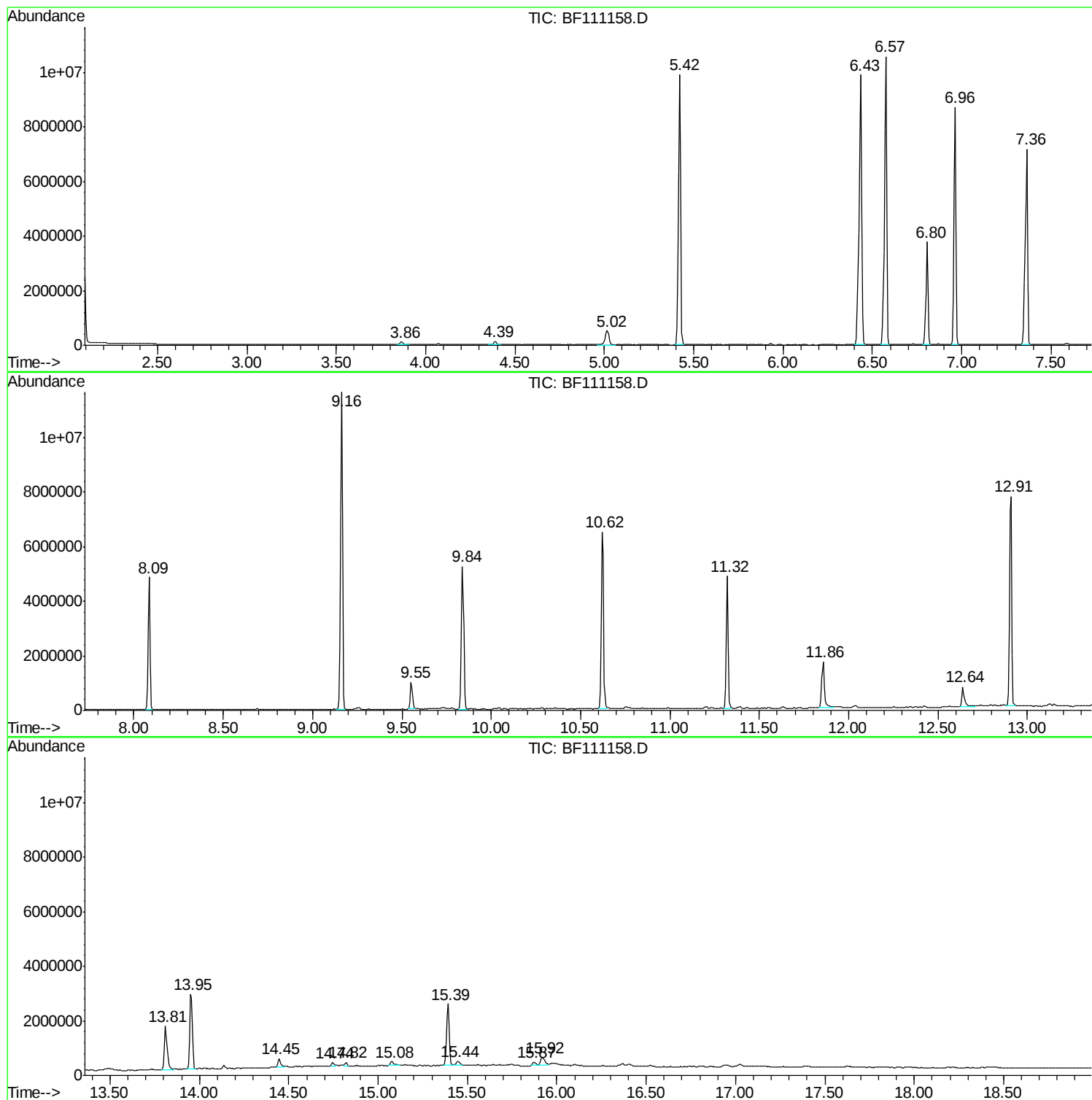
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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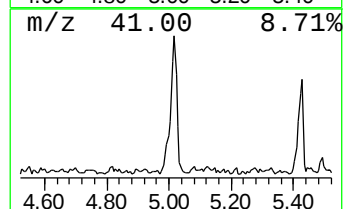
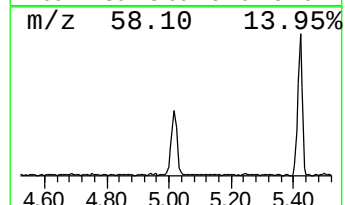
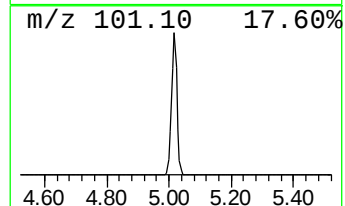
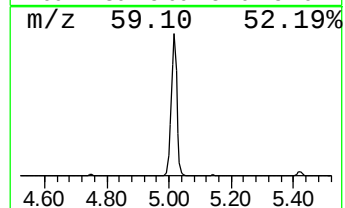
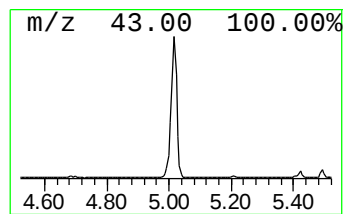
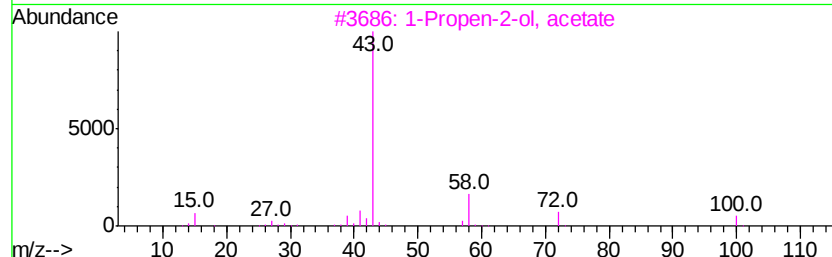
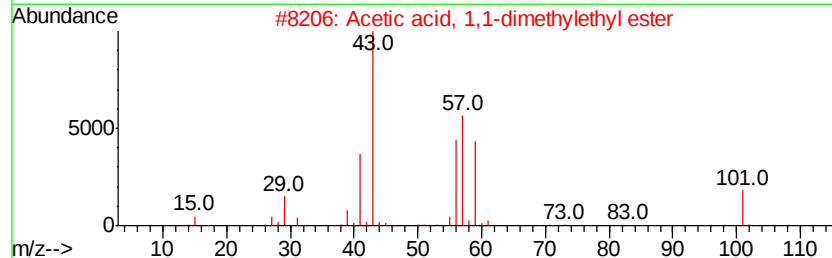
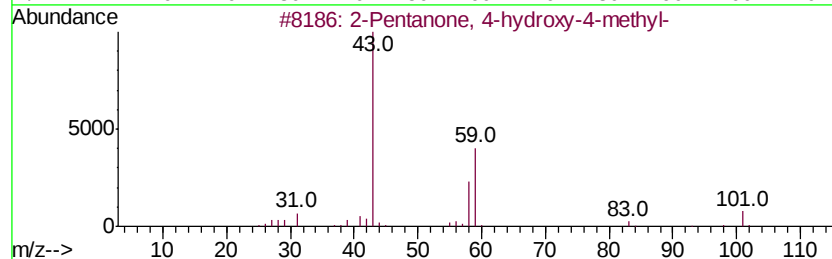
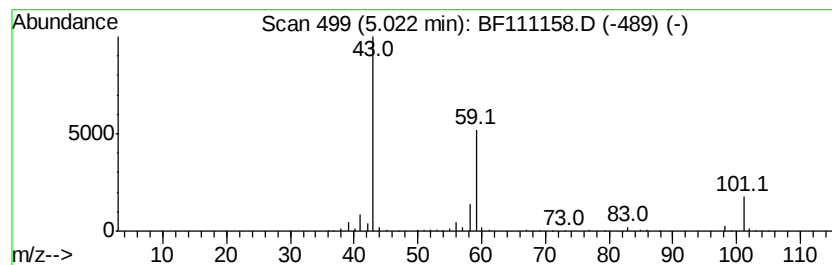
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	4.76 ng	704921	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	45
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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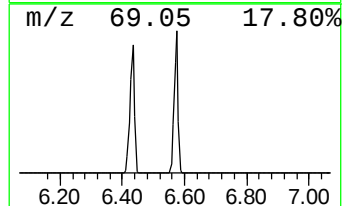
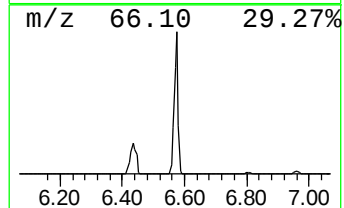
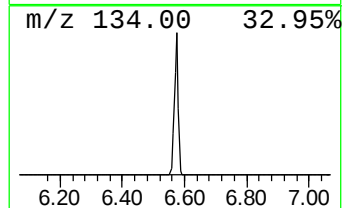
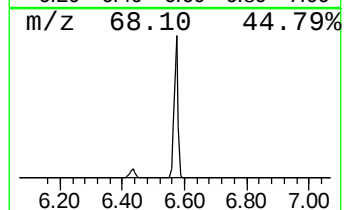
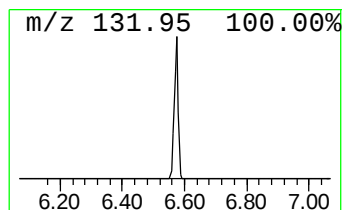
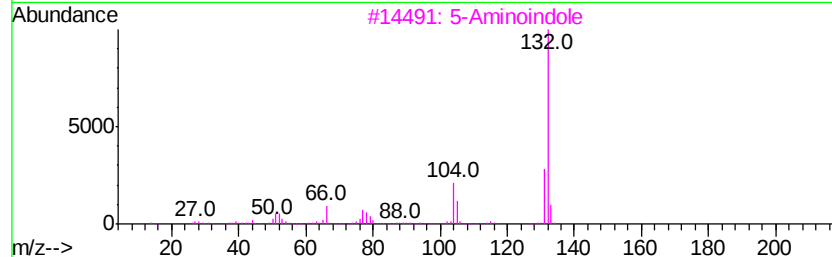
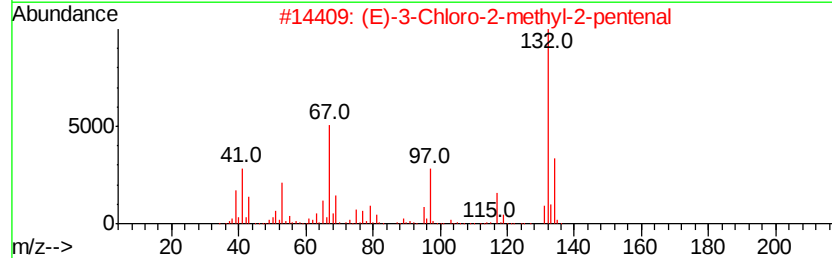
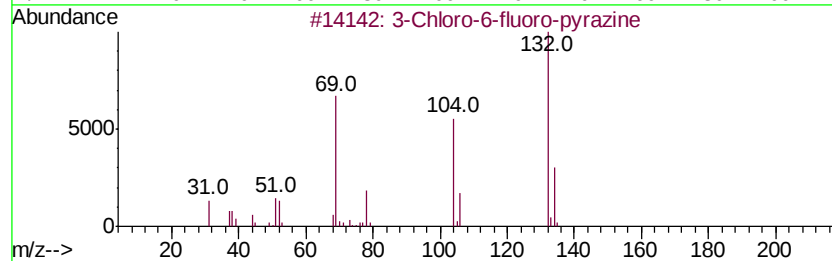
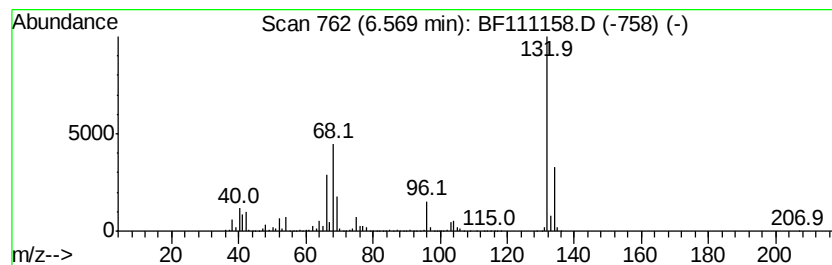
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	64.73 ng	9582580	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	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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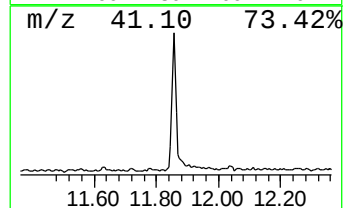
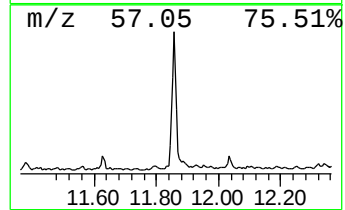
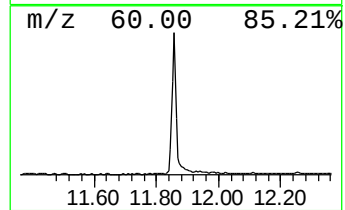
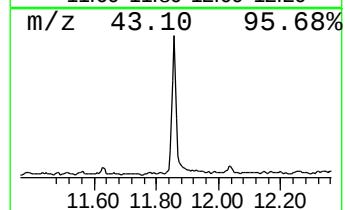
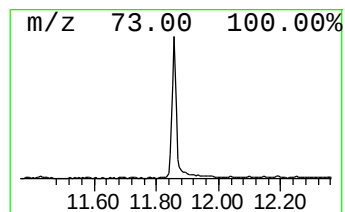
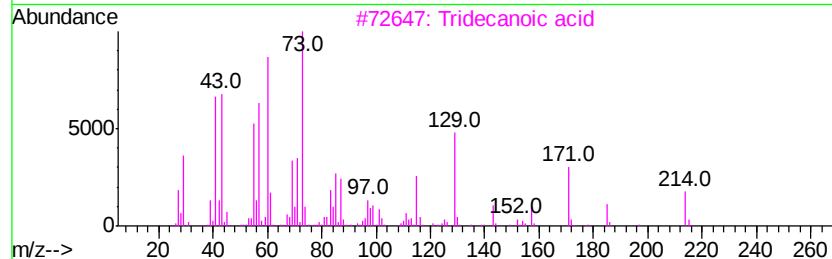
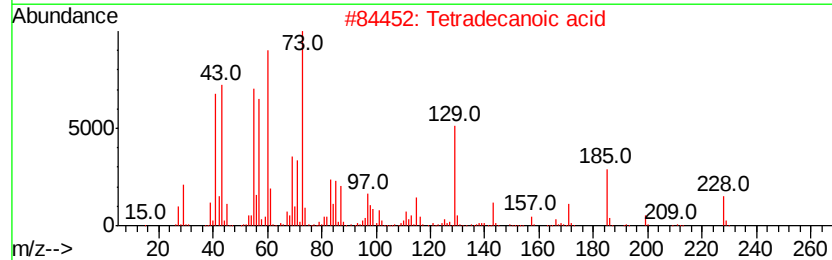
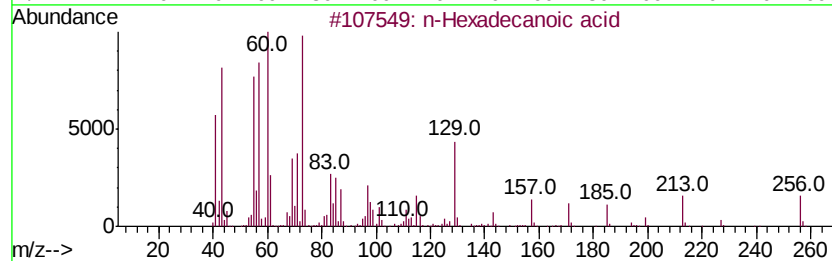
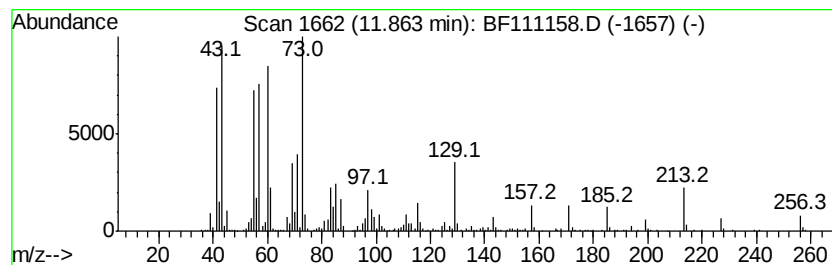
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	8.24 ng	1613550	Phenanthrene-d10	11.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	96
3		Tridecanoic acid	214	C13H26O2	000638-53-9	95
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5		Undecanoic acid	186	C11H22O2	000112-37-8	72



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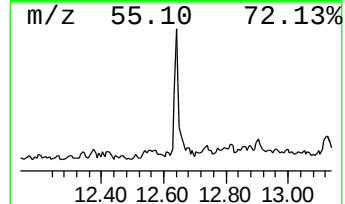
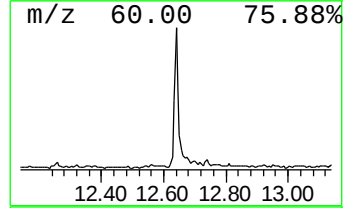
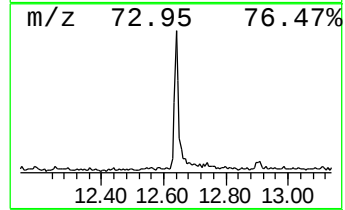
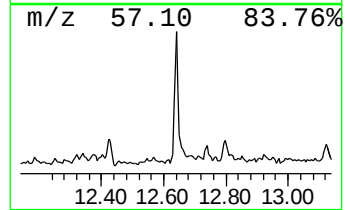
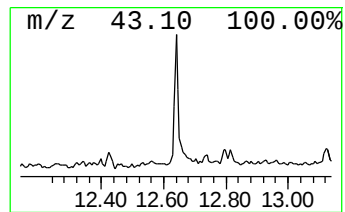
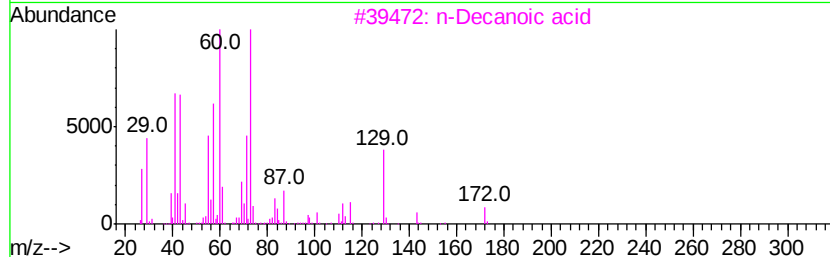
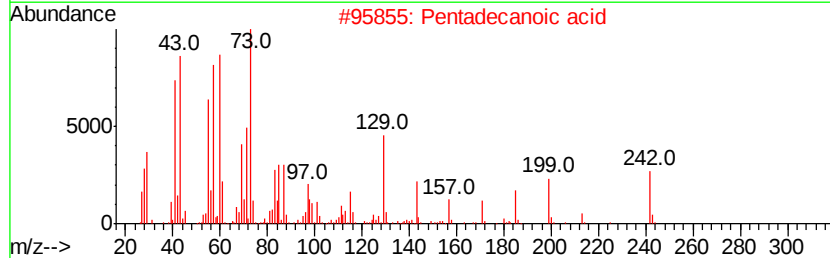
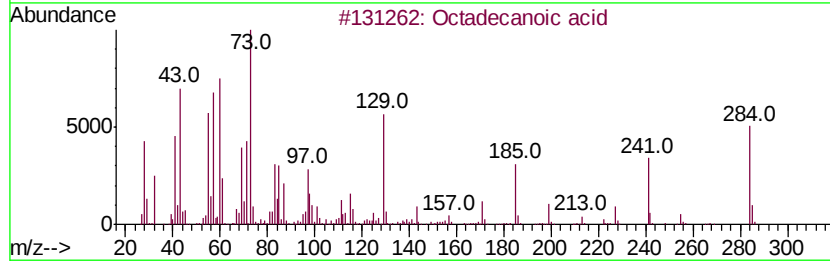
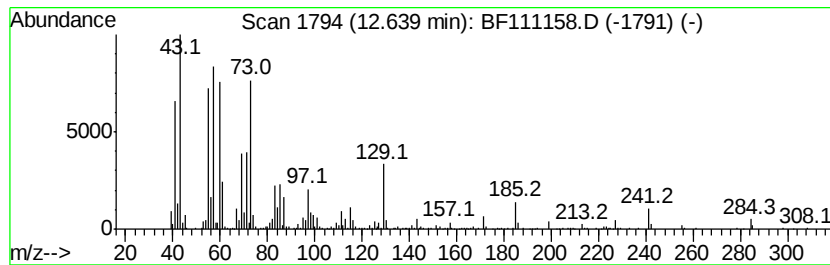
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	4.20 ng	822933	Phenanthrene-d10	11.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		n-Decanoic acid	172	C10H20O2	000334-48-5	70
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	25



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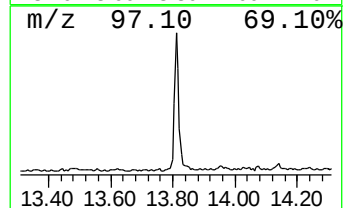
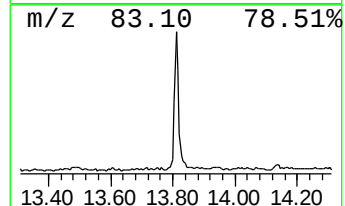
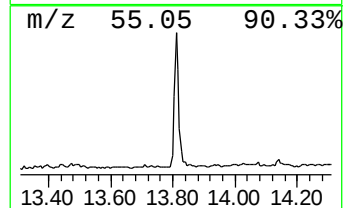
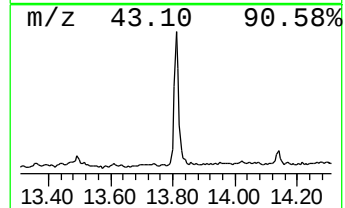
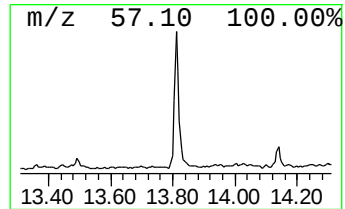
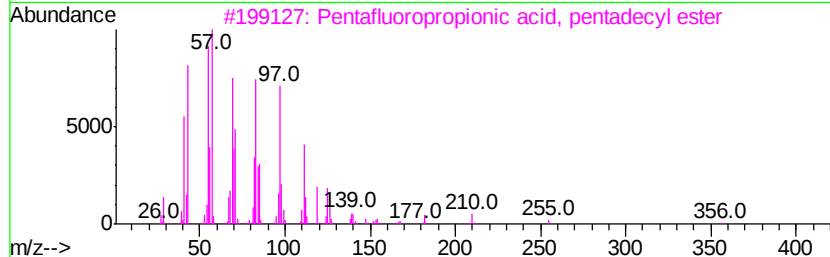
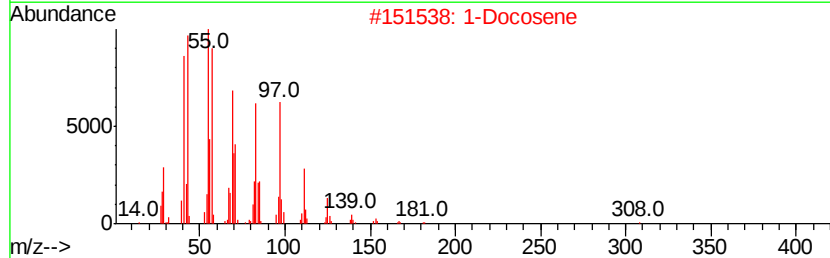
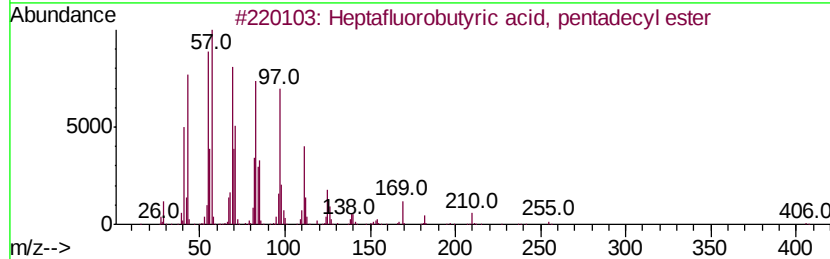
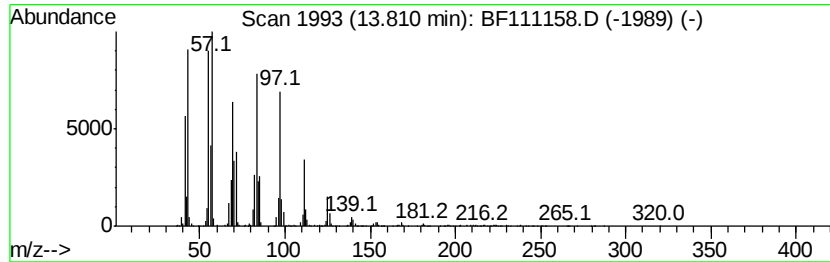
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Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	12.60 ng	1635080	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2		1-Docosene	308	C22H44	001599-67-3	94
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	91



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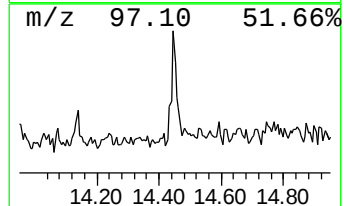
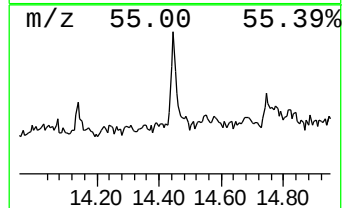
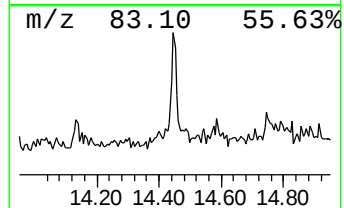
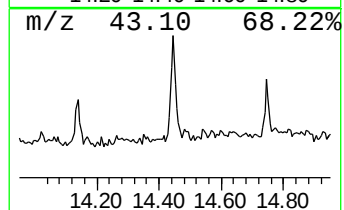
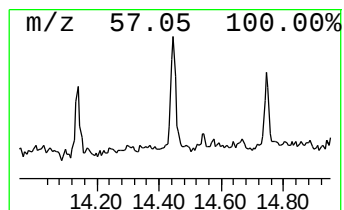
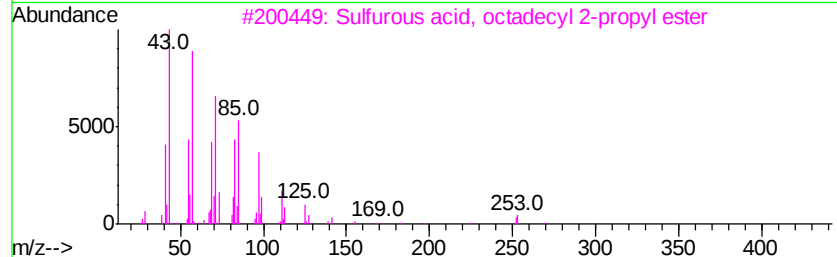
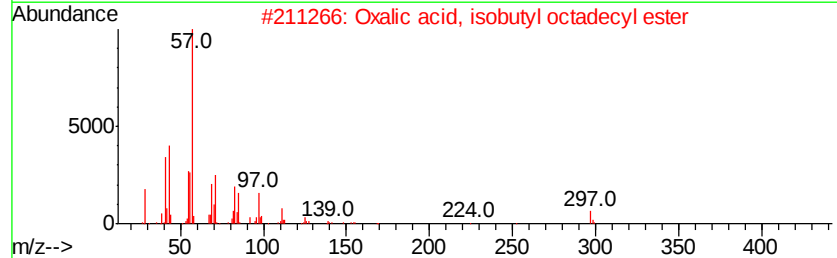
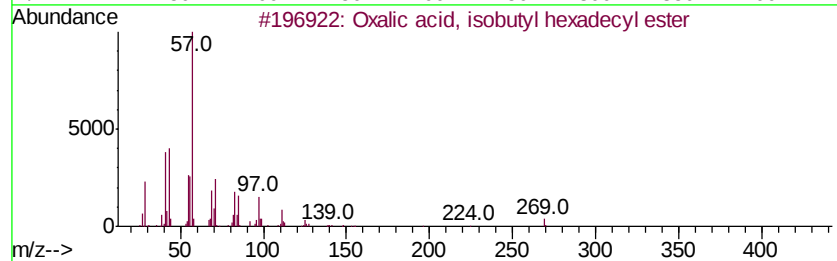
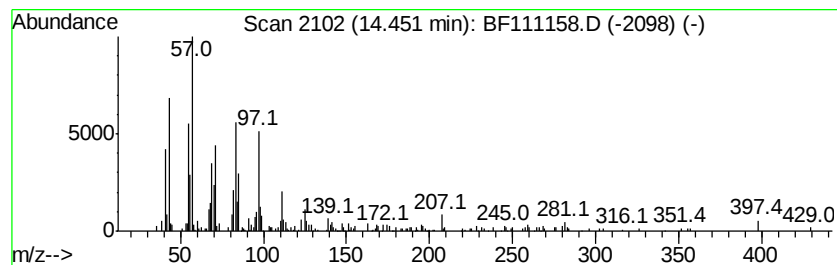
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxalic acid, isobutyl hexadecyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.62 ng	340400	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2		Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
3		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	74
4		Cyclohexane, (1-decylundecyl)-	378	C27H54	006703-99-7	72
5		1-Heptadecene	238	C17H34	006765-39-5	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111158.D
Acq On : 7 Dec 2018 00:28
Operator : JU/SJ
Sample : J6202-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

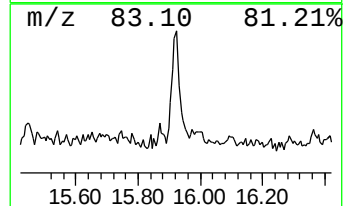
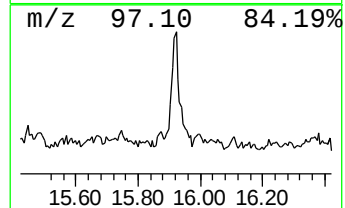
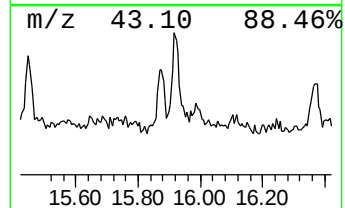
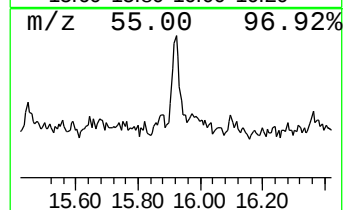
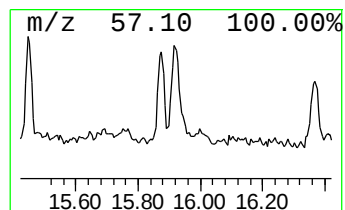
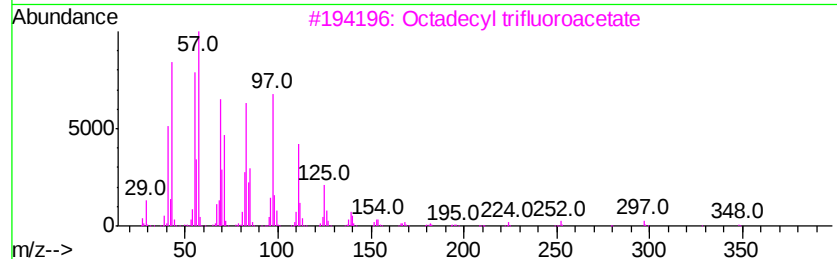
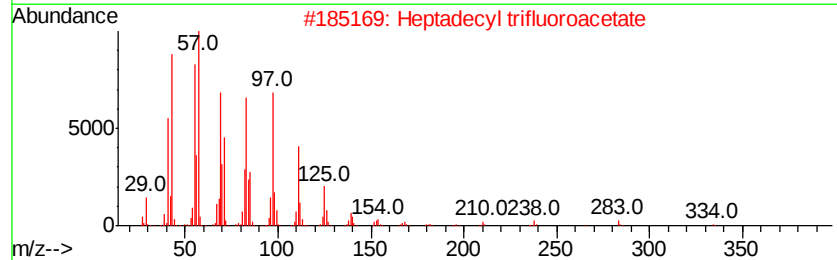
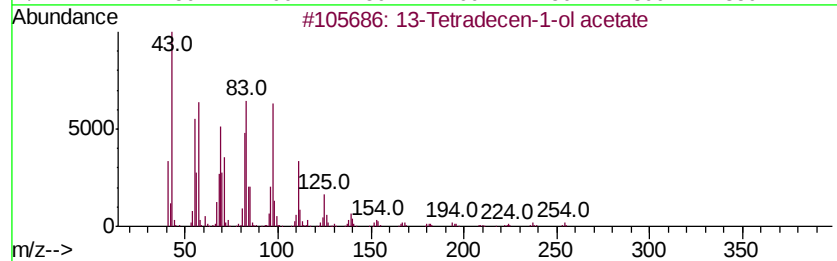
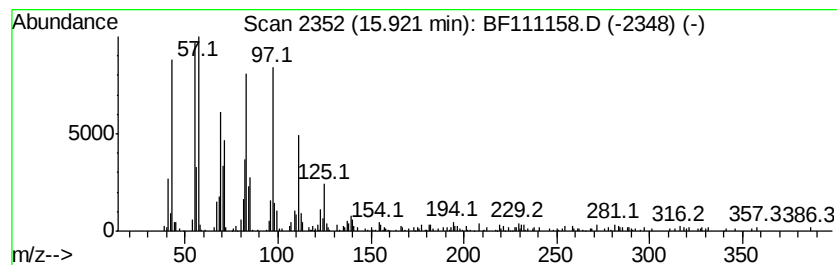
Instrument :
BNA_F
ClientSampleId :
SAMPLE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 13-Tetradecen-1-ol acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.92	3.30 ng	425326	Perylene-d12		15.39	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	95
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
4		1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	91
5		1-Docosene	308	C22H44	001599-67-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120618\
Data File : BF111158.D
Acq On : 7 Dec 2018 00:28
Operator : JU/SJ
Sample : J6202-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.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...	5.02	4.8 ng		704921	1	6.80	2960640	20.0
unknown6.57	6.57	64.7 ng		9582580	1	6.80	2960640	20.0
n-Hexadecanoic acid	11.86	8.2 ng		1613550	4	11.32	3915110	20.0
Octadecanoic acid	12.64	4.2 ng		822933	4	11.32	3915110	20.0
Heptafluorobutyri...	13.81	12.6 ng		1635080	5	13.96	2594360	20.0
Oxalic acid, isob...	14.45	2.6 ng		340400	5	13.96	2594360	20.0
13-Tetradecen-1-o...	15.92	3.3 ng		425326	6	15.39	2574330	20.0