

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080816\
 Data File : BF089663.D
 Acq On : 8 Aug 2016 16:01
 Operator : UM/SJ
 Sample : H4351-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CORE-E

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-BF080416.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	4.638	263	267	282	rBV	141916	367567	19.15%	2.441%
2	5.313	324	326	358	rBV	881900	1504830	78.42%	9.994%
3	6.959	467	470	477	rBV	778027	1551132	80.83%	10.301%
4	7.073	477	480	496	rVB	1168905	1701702	88.68%	11.301%
5	7.416	508	510	522	rBV	130711	240995	12.56%	1.600%
6	7.656	528	531	548	rBV	908226	1215450	63.34%	8.072%
7	8.330	587	590	612	rBV	580470	979964	51.07%	6.508%
8	9.450	685	688	698	rBV	202474	343617	17.91%	2.282%
9	11.233	840	844	846	rBV	1231324	1918986	100.00%	12.744%
10	11.919	901	904	910	rBV	208348	280419	14.61%	1.862%
11	12.262	931	934	937	rBV	266221	418782	21.82%	2.781%
12	12.308	937	938	943	rVB	16844	23111	1.20%	0.153%
13	13.131	1006	1010	1012	rBV	30393	38997	2.03%	0.259%
14	13.485	1034	1041	1045	rBV	8517	25668	1.34%	0.170%
15	13.565	1045	1048	1055	rVV	591940	1034684	53.92%	6.871%
16	13.897	1074	1077	1082	rBV	32009	51035	2.66%	0.339%
17	14.662	1142	1144	1151	rVB	295493	429729	22.39%	2.854%
18	15.668	1229	1232	1242	rBV	25156	48933	2.55%	0.325%
19	16.777	1324	1329	1337	rBV	69071	134400	7.00%	0.893%
20	17.028	1348	1351	1354	rBV	1132118	1847510	96.28%	12.269%
21	18.286	1458	1461	1465	rBV2	89661	158164	8.24%	1.050%
22	18.354	1465	1467	1474	rVB	238179	384684	20.05%	2.555%
23	19.520	1566	1569	1572	rBV	48128	53232	2.77%	0.354%
24	20.023	1611	1613	1621	rBV	205155	279839	14.58%	1.858%
25	20.537	1656	1658	1664	rBV3	10704	24616	1.28%	0.163%

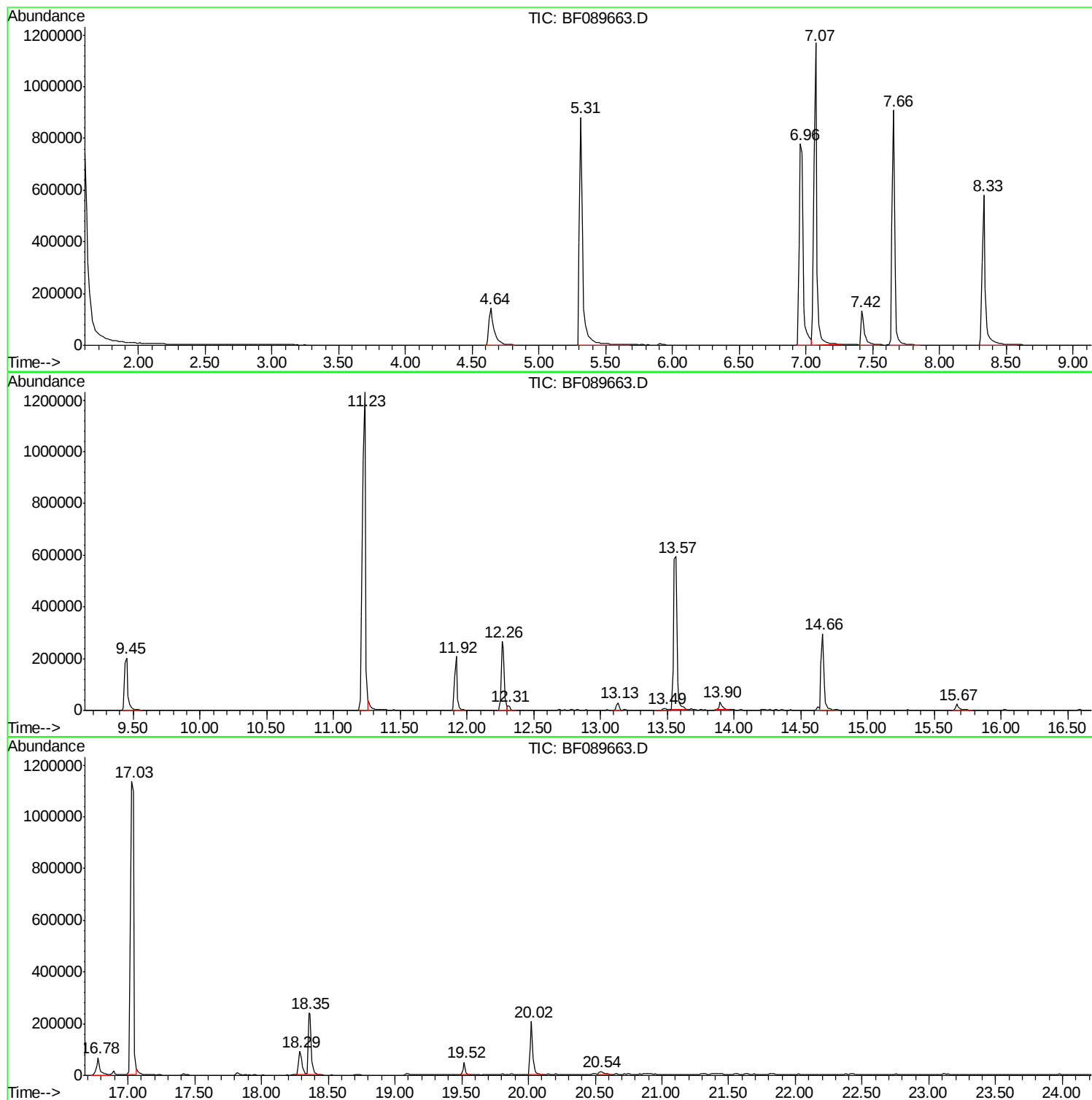
Sum of corrected areas: 15058046

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080816\
Data File : BF089663.D
Acq On : 8 Aug 2016 16:01
Operator : UM/SJ
Sample : H4351-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CORE-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080816\
Data File : BF089663.D
Acq On : 8 Aug 2016 16:01
Operator : UM/SJ
Sample : H4351-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CORE-E

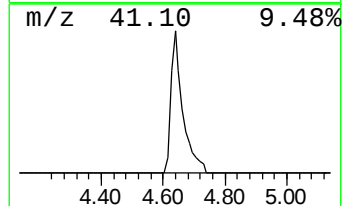
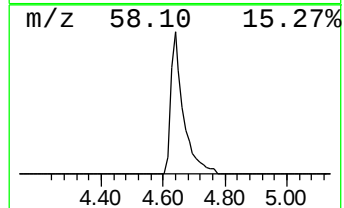
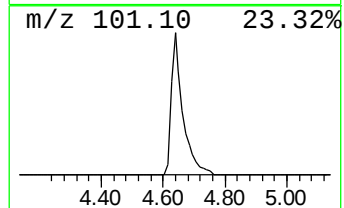
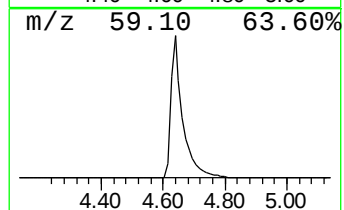
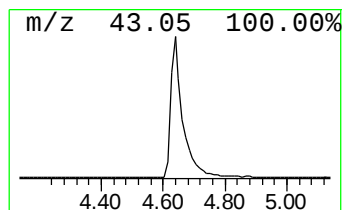
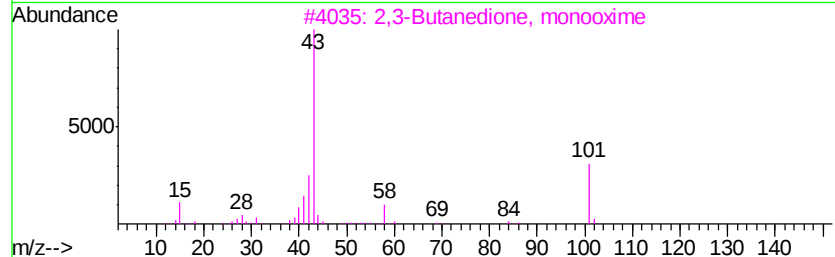
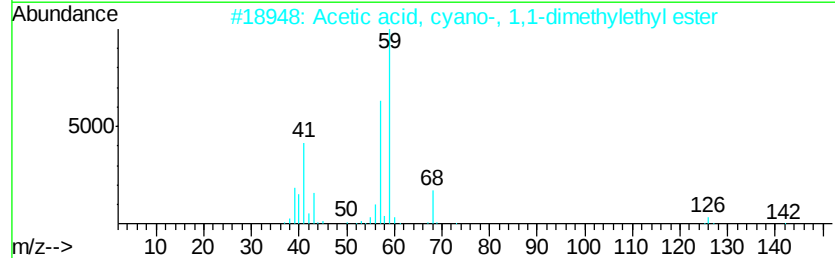
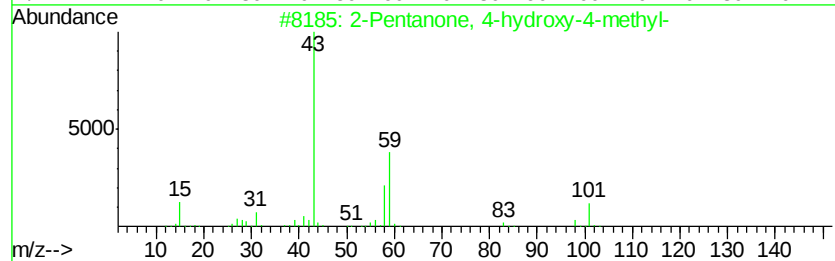
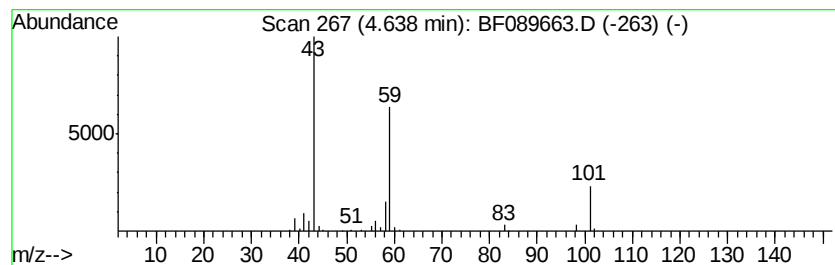
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.64	30.50 ng	367567	1,4-Dichlorobenzene-d4	7.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080816\
Data File : BF089663.D
Acq On : 8 Aug 2016 16:01
Operator : UM/SJ
Sample : H4351-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CORE-E

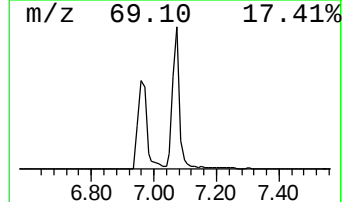
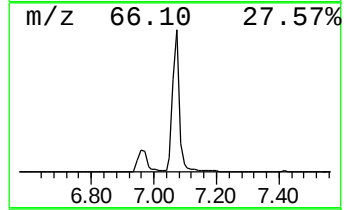
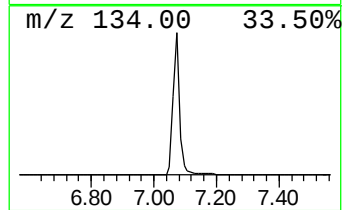
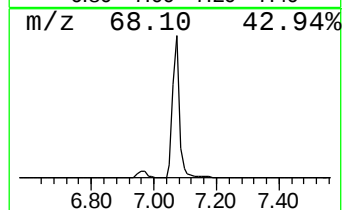
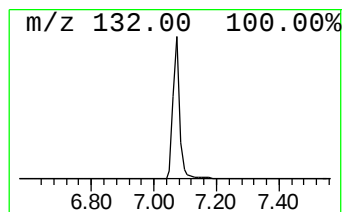
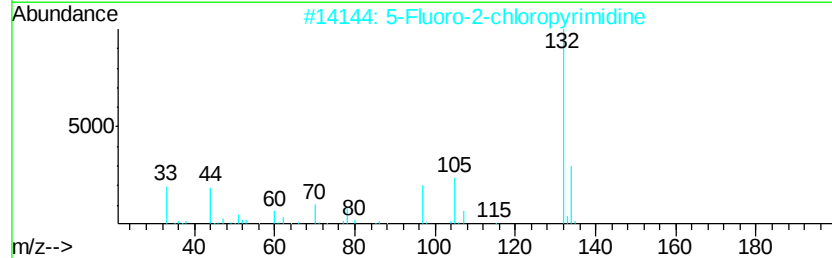
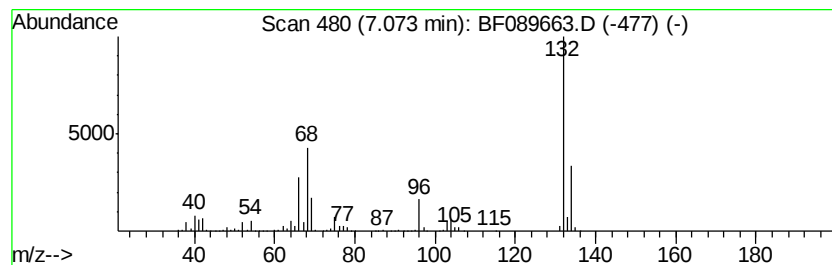
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.07 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	141.22 ng	1701700	1,4-Dichlorobenzene-d4	7.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080816\
Data File : BF089663.D
Acq On : 8 Aug 2016 16:01
Operator : UM/SJ
Sample : H4351-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CORE-E

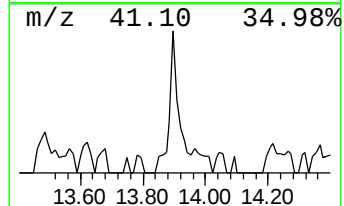
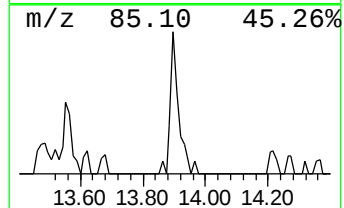
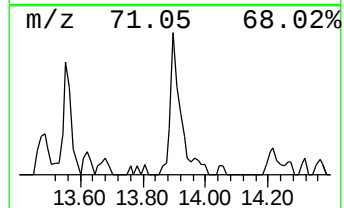
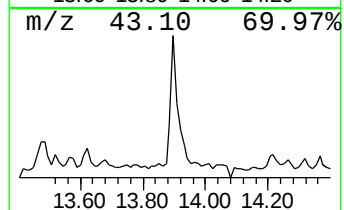
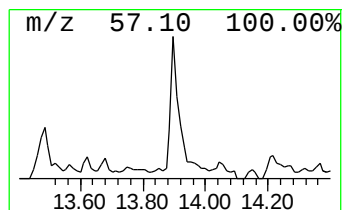
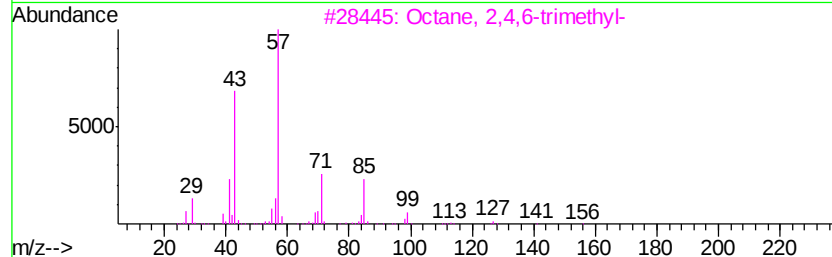
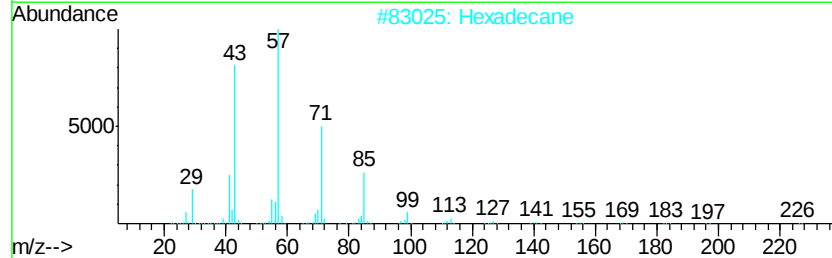
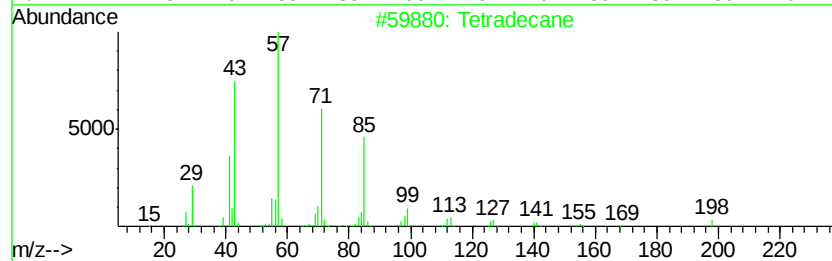
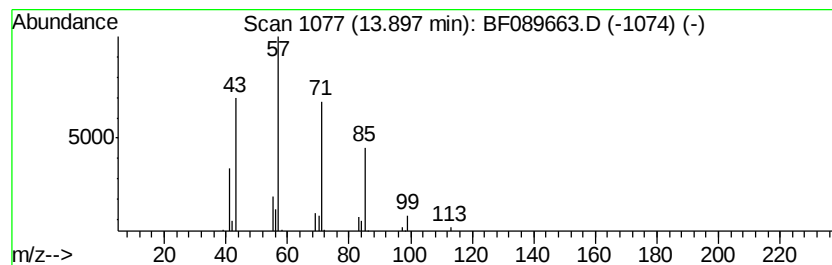
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	2.38 ng	51035	Phenanthrene-d10	14.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	80
2		Hexadecane	226	C16H34	000544-76-3	78
3		Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	72
4		Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	64
5		3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080816\
Data File : BF089663.D
Acq On : 8 Aug 2016 16:01
Operator : UM/SJ
Sample : H4351-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CORE-E

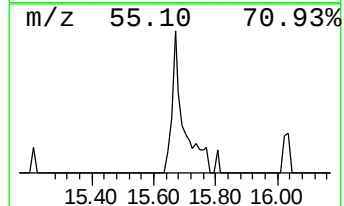
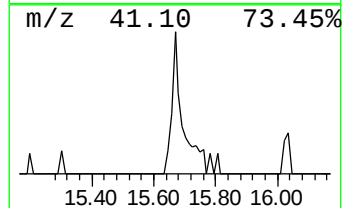
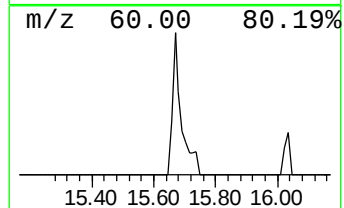
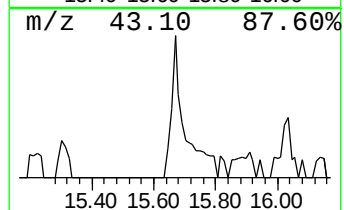
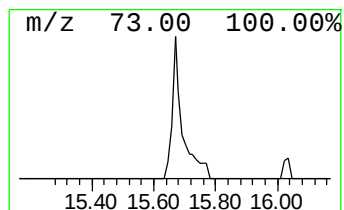
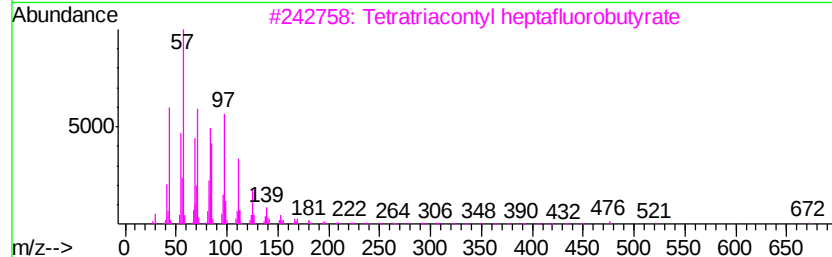
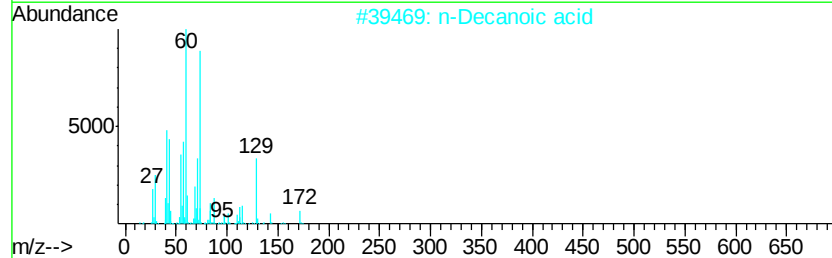
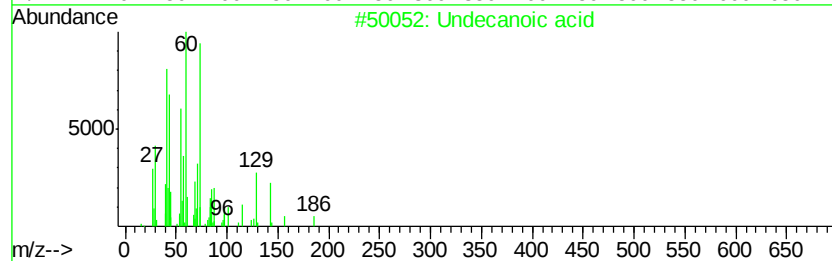
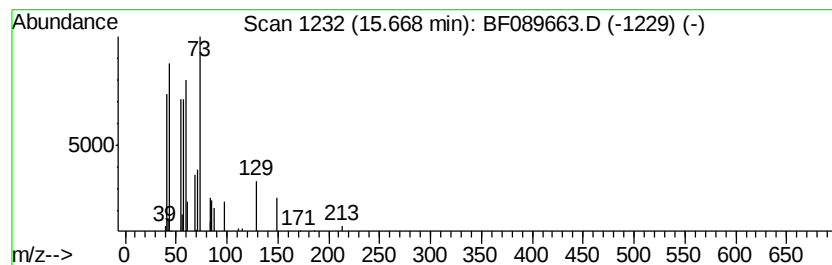
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Undecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	2.28 ng	48933	Phenanthrene-d10	14.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	64	
2	n-Decanoic acid	172	C10H20O2	000334-48-5	53	
3	Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	14	
4	Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	14	
5	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	14	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080816\
Data File : BF089663.D
Acq On : 8 Aug 2016 16:01
Operator : UM/SJ
Sample : H4351-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

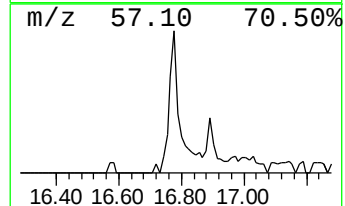
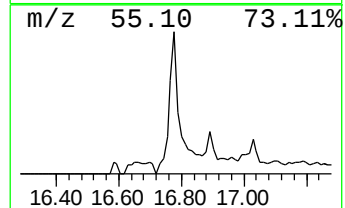
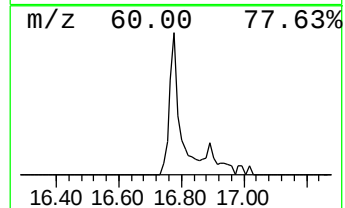
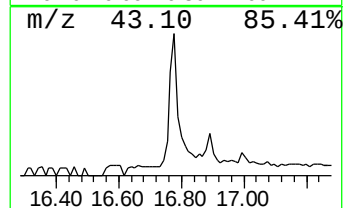
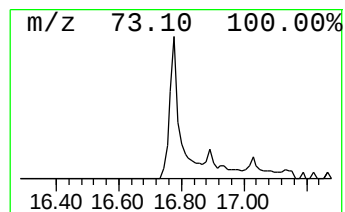
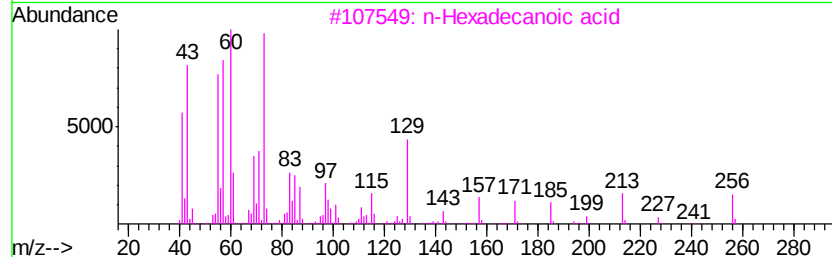
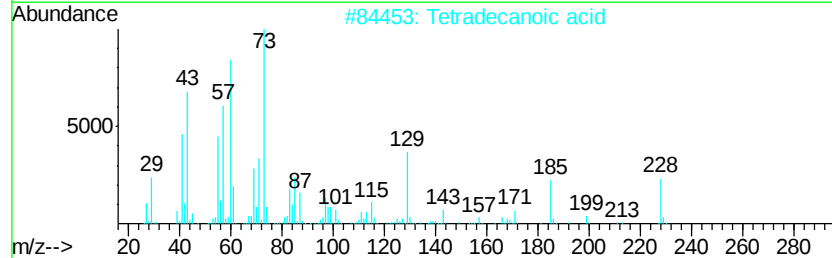
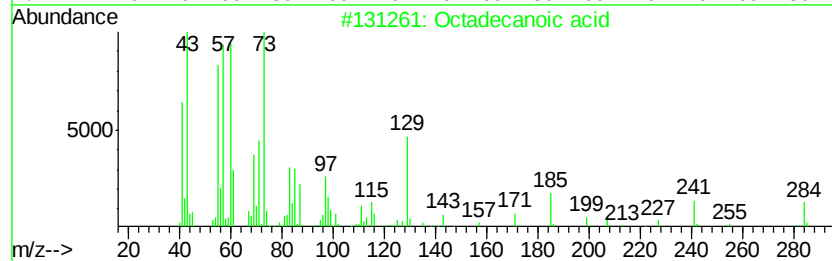
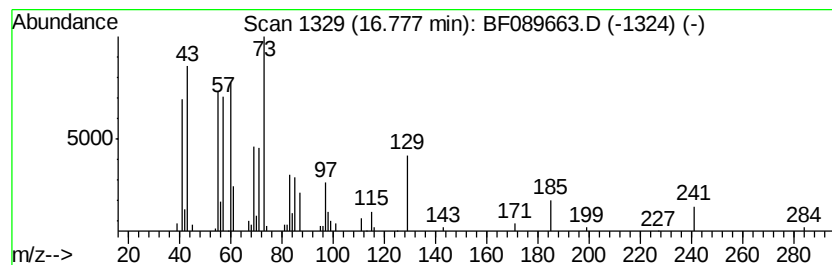
Instrument :
BNA_F
ClientSampleId :
CORE-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.78	6.99 ng	134400	Chrysene-d12	18.37	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080816\
Data File : BF089663.D
Acq On : 8 Aug 2016 16:01
Operator : UM/SJ
Sample : H4351-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CORE-E

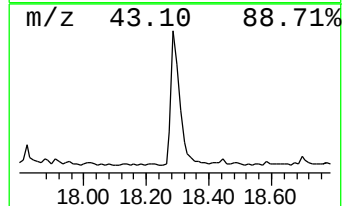
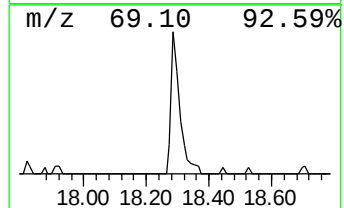
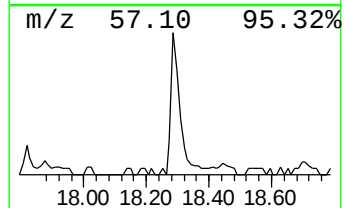
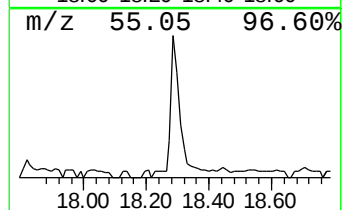
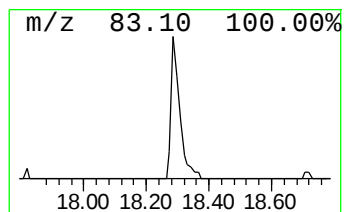
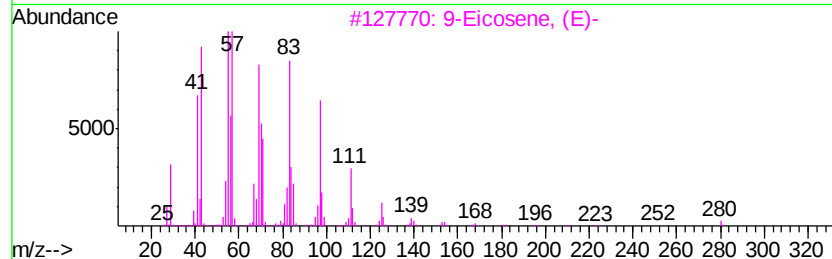
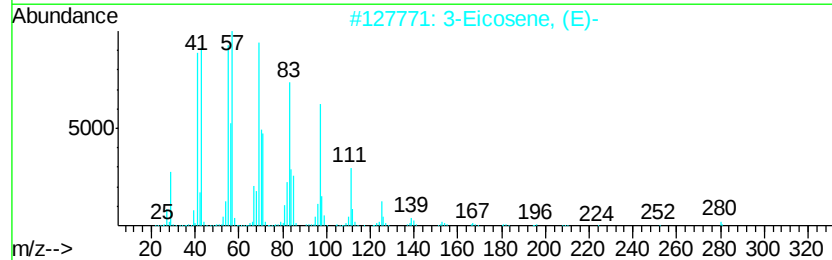
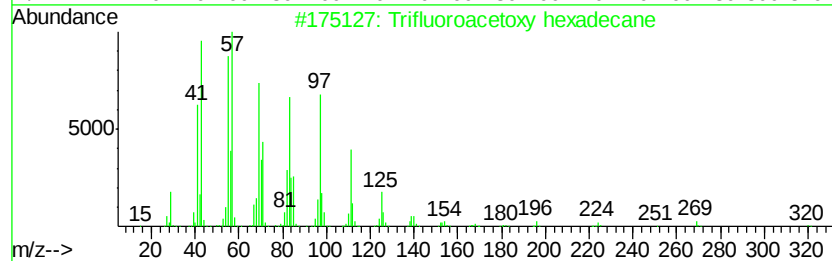
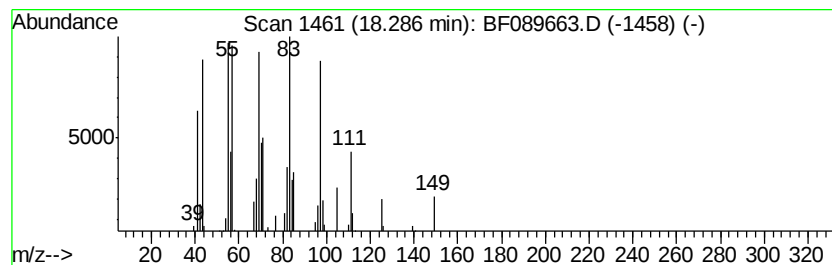
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	8.22 ng	158164	Chrysene-d12	18.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3		9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	90
5		n-Heptadecanol-1	256	C17H36O	001454-85-9	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080816\
Data File : BF089663.D
Acq On : 8 Aug 2016 16:01
Operator : UM/SJ
Sample : H4351-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CORE-E

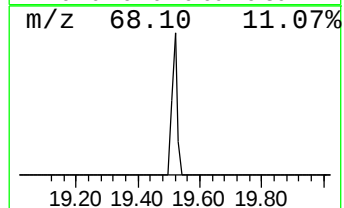
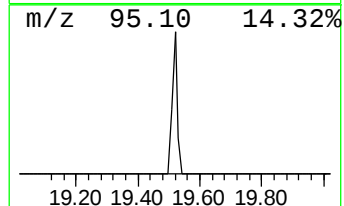
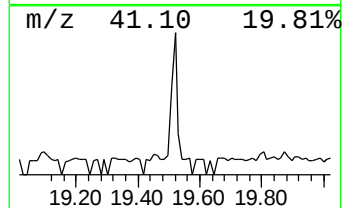
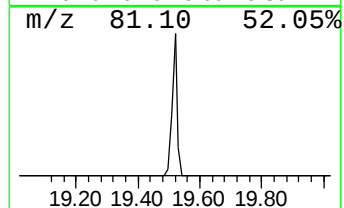
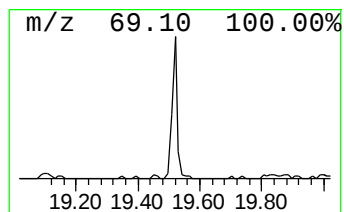
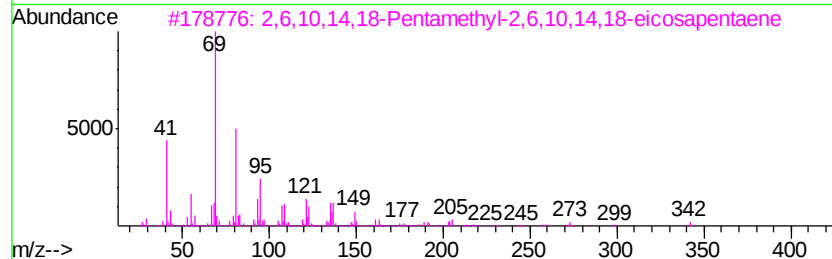
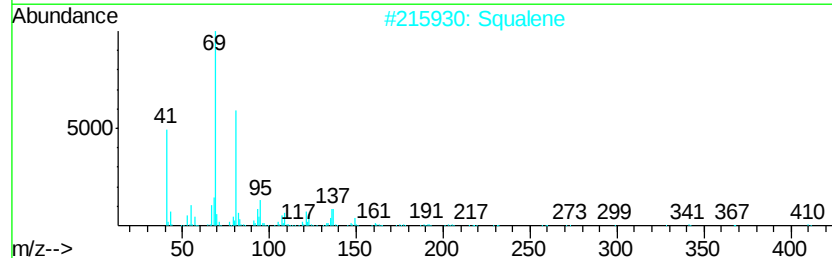
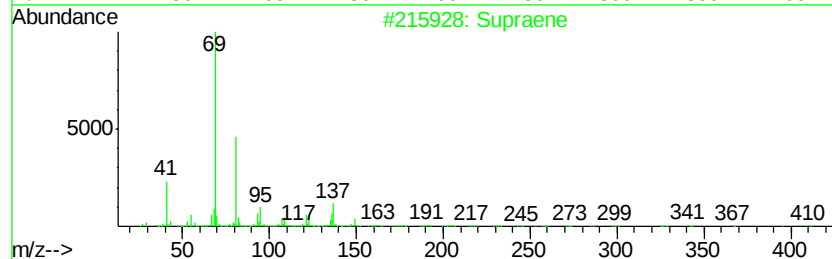
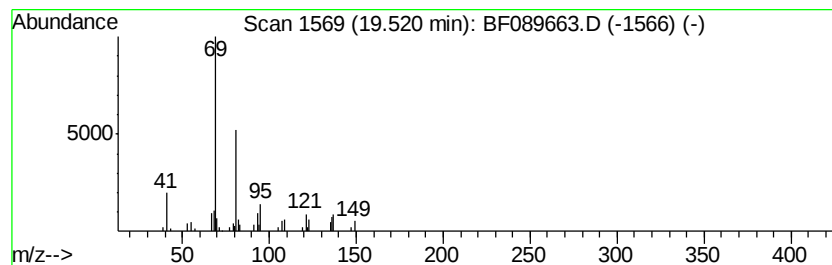
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.52	3.80 ng	53232	Perylene-d12	20.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	83
4		trans-Farnesol	222	C15H26O	000106-28-5	78
5		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	56



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080816\
Data File : BF089663.D
Acq On : 8 Aug 2016 16:01
Operator : UM/SJ
Sample : H4351-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CORE-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.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...	4.64	30.5	ng	367567	1	7.42	240995	20.0
unknown7.07	7.07	141.2	ng	1701700	1	7.42	240995	20.0
Tetradecane	13.90	2.4	ng	51035	4	14.66	429729	20.0
Undecanoic acid	15.67	2.3	ng	48933	4	14.66	429729	20.0
Octadecanoic acid	16.78	7.0	ng	134400	5	18.37	384684	20.0
Trifluoroacetoxy ...	18.29	8.2	ng	158164	5	18.37	384684	20.0
Supraene	19.52	3.8	ng	53232	6	20.02	279839	20.0