

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
 Data File : BF102262.D
 Acq On : 20 Jan 2018 13:37
 Operator : SJ/JU
 Sample : J1115-09
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-34-2.5-3.0

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_F\METHODS\8270-BF010918.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	4.922	477	482	492	rVB	161003	233048	7.14%	0.809%
2	5.334	547	552	555	rBV	3212478	3221636	98.66%	11.189%
3	6.363	721	727	731	rBV	3000492	3265340	100.00%	11.340%
4	6.492	744	749	752	rBV	3436402	3244161	99.35%	11.267%
5	6.722	784	788	791	rBV	969974	882717	27.03%	3.066%
6	6.875	810	814	817	rBV	2883080	2486979	76.16%	8.637%
7	7.286	879	884	887	rBV	2125789	2021608	61.91%	7.021%
8	8.004	1001	1006	1009	rBV	1254395	1166458	35.72%	4.051%
9	9.080	1184	1189	1192	rBV	3476423	3168165	97.02%	11.003%
10	9.475	1252	1256	1259	rBV	538208	481830	14.76%	1.673%
11	9.686	1288	1292	1295	rBV	114322	91172	2.79%	0.317%
12	9.751	1299	1303	1307	rVB	1244397	1140755	34.94%	3.962%
13	10.180	1373	1376	1380	rVB	114708	103383	3.17%	0.359%
14	10.404	1408	1414	1416	rBV2	30394	40871	1.25%	0.142%
15	10.545	1431	1438	1441	rBV	1663888	1613314	49.41%	5.603%
16	10.657	1454	1457	1466	rVB	91759	93639	2.87%	0.325%
17	11.239	1552	1556	1559	rBV	1020881	933371	28.58%	3.242%
18	12.821	1821	1825	1828	rBV	2273833	1978425	60.59%	6.871%
19	13.715	1973	1977	1981	rBV	349398	349934	10.72%	1.215%
20	13.868	1999	2003	2007	rBV	827997	791705	24.25%	2.750%
21	14.351	2080	2085	2089	rBV2	44654	61361	1.88%	0.213%
22	14.962	2185	2189	2191	rBV	30649	34542	1.06%	0.120%
23	15.292	2240	2245	2249	rBV	606214	777162	23.80%	2.699%
24	15.727	2315	2319	2323	rBV2	64266	97046	2.97%	0.337%
25	15.774	2323	2327	2334	rVB4	49049	80826	2.48%	0.281%
26	16.204	2394	2400	2405	rBV2	69617	124581	3.82%	0.433%
27	16.756	2489	2494	2500	rVB3	54348	102750	3.15%	0.357%
28	17.409	2600	2605	2614	rVB3	51473	116337	3.56%	0.404%
29	18.180	2732	2736	2745	rVB6	35651	90535	2.77%	0.314%

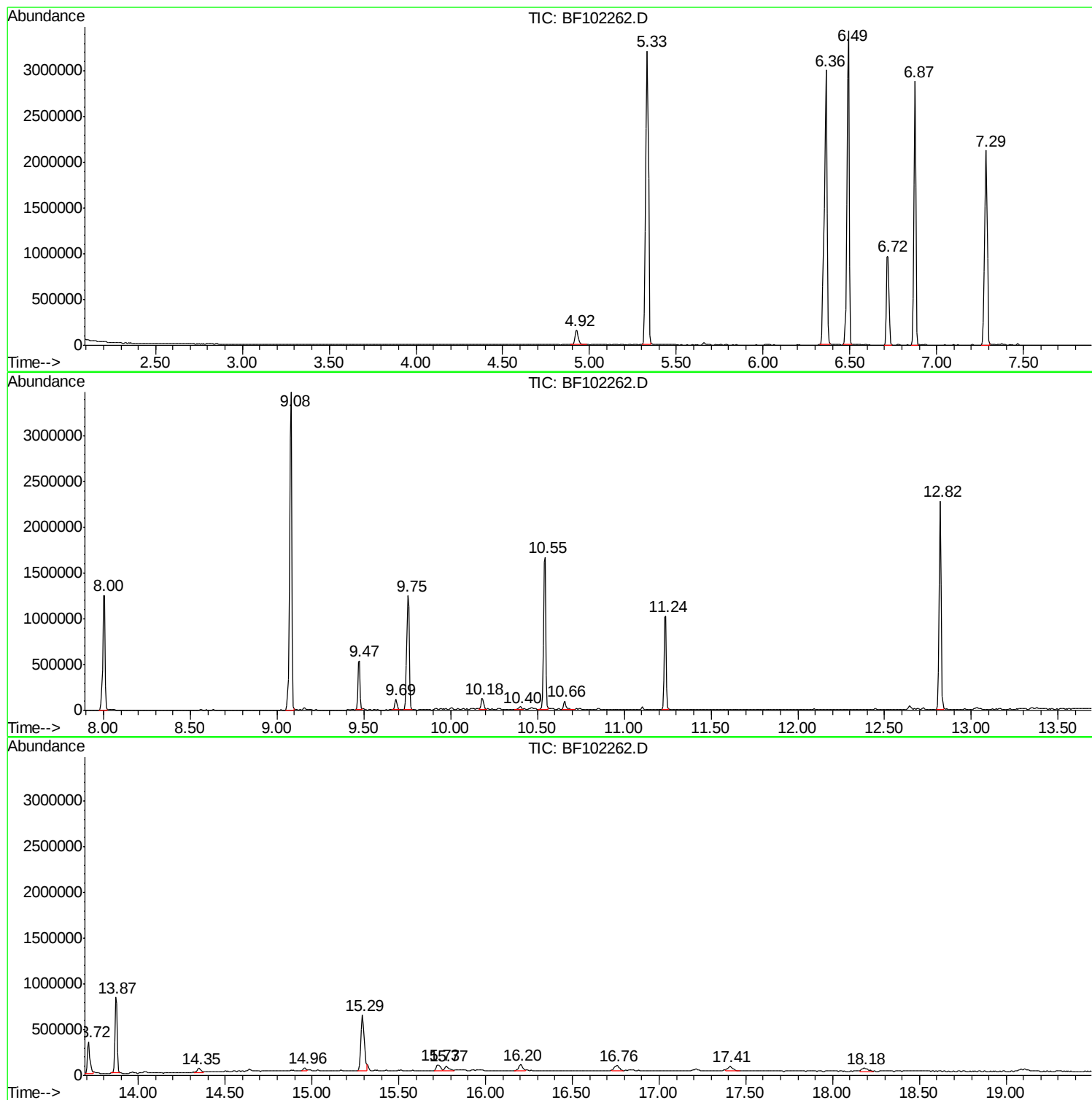
Sum of corrected areas: 28793651

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102262.D
Acq On : 20 Jan 2018 13:37
Operator : SJ/JU
Sample : J1115-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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\BF012018\
Data File : BF102262.D
Acq On : 20 Jan 2018 13:37
Operator : SJ/JU
Sample : J1115-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-2.5-3.0

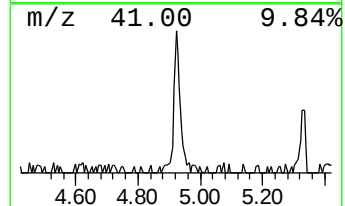
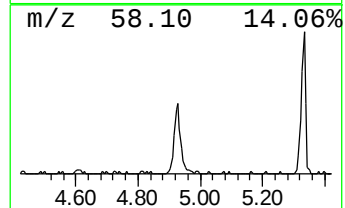
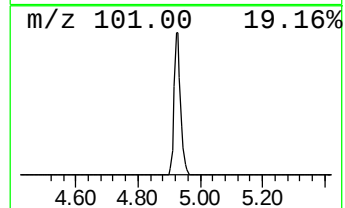
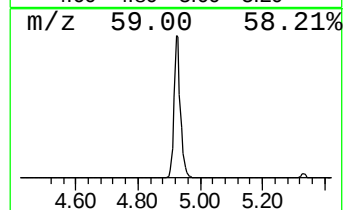
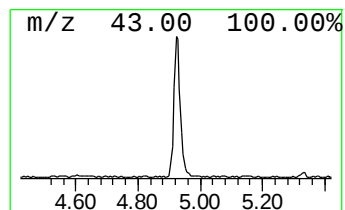
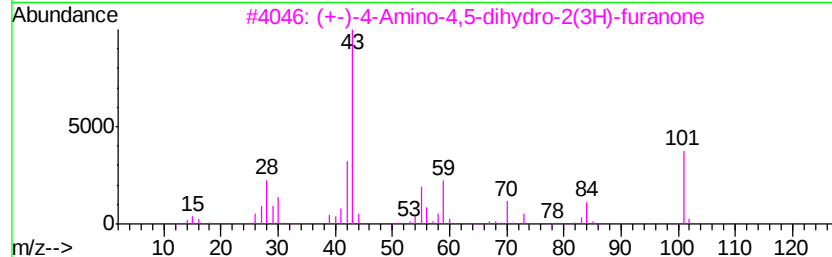
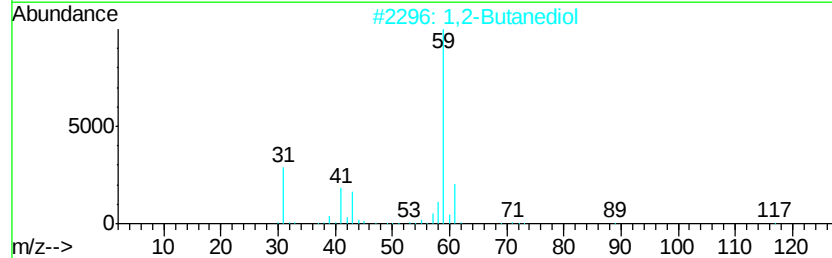
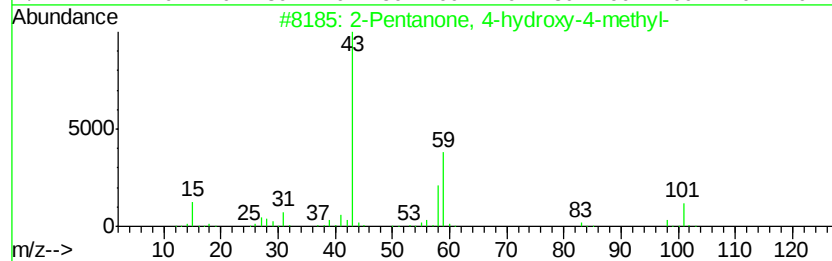
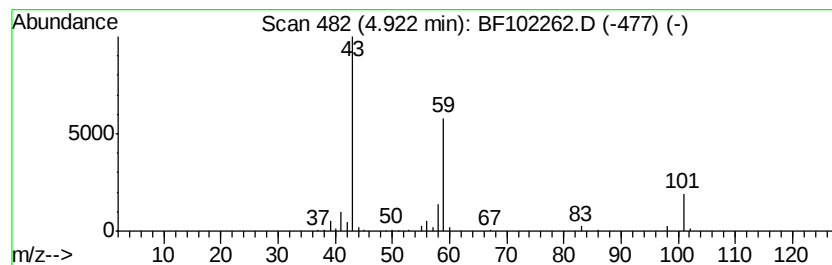
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	5.28 ng	233048	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			1,2-Butanediol	90	C4H10O2	000584-03-2	23
3			(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102262.D
Acq On : 20 Jan 2018 13:37
Operator : SJ/JU
Sample : J1115-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-2.5-3.0

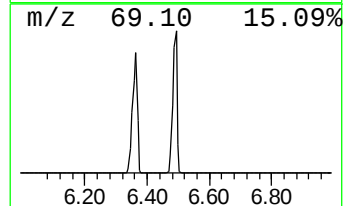
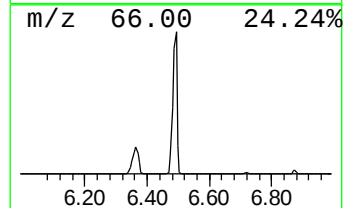
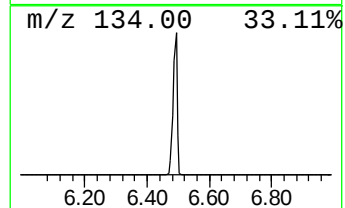
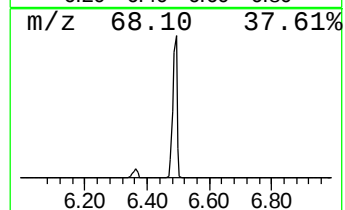
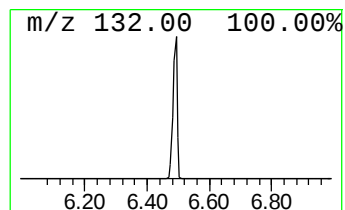
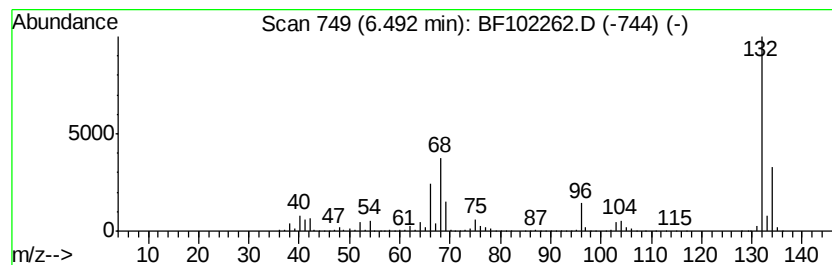
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	73.50 ng	3244160	1,4-Dichlorobenzene-d4	6.72

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		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102262.D
Acq On : 20 Jan 2018 13:37
Operator : SJ/JU
Sample : J1115-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

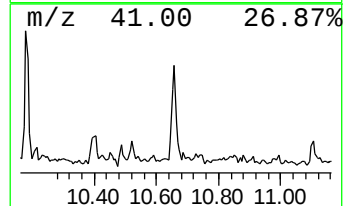
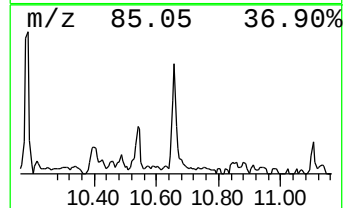
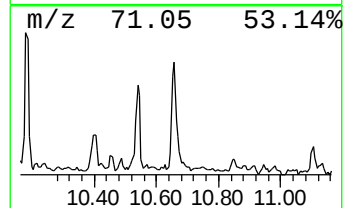
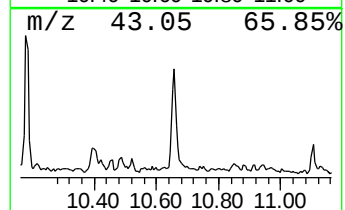
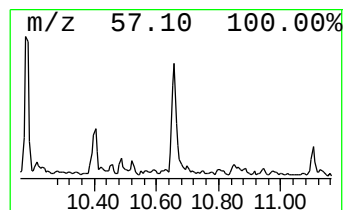
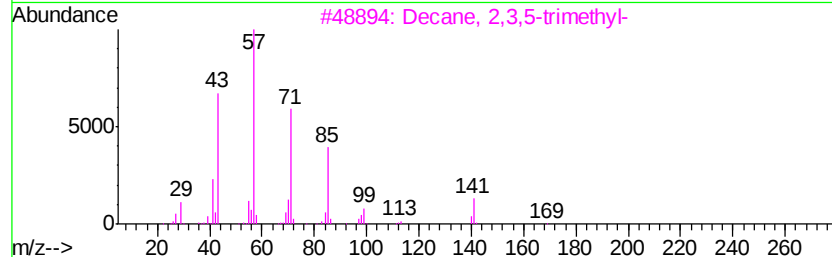
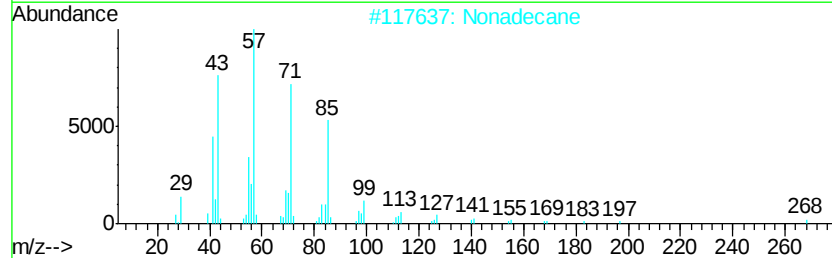
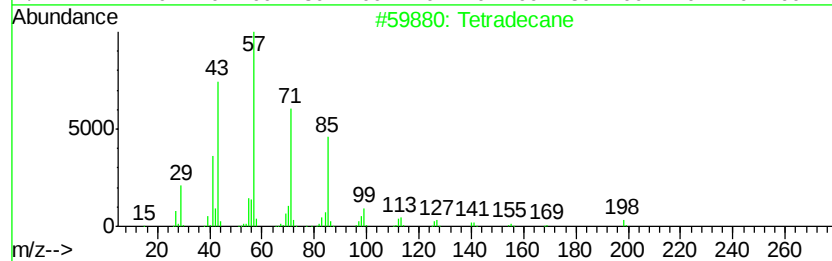
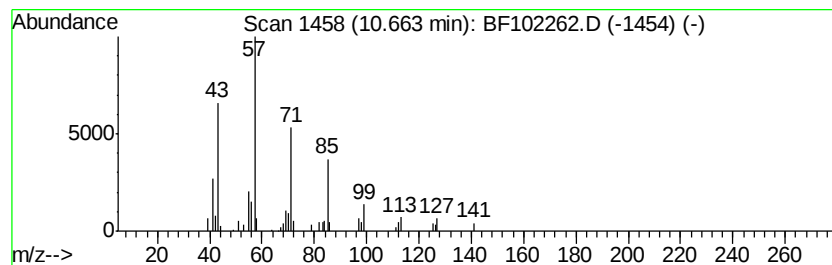
Instrument :
BNA_F
ClientSampleId :
SB-34-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.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 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.66	2.01 ng	93639	Phenanthrene-d10	11.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	87
2	Nonadecane	268	C19H40	000629-92-5	86
3	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
4	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	78
5	Heptadecane	240	C17H36	000629-78-7	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102262.D
Acq On : 20 Jan 2018 13:37
Operator : SJ/JU
Sample : J1115-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-2.5-3.0

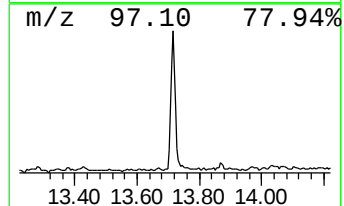
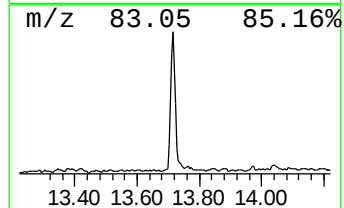
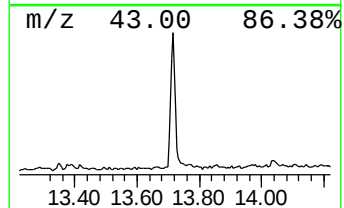
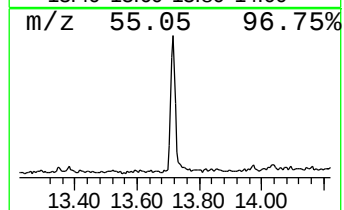
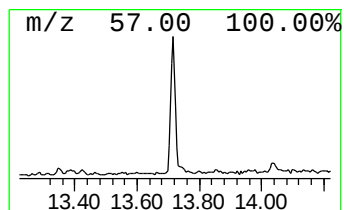
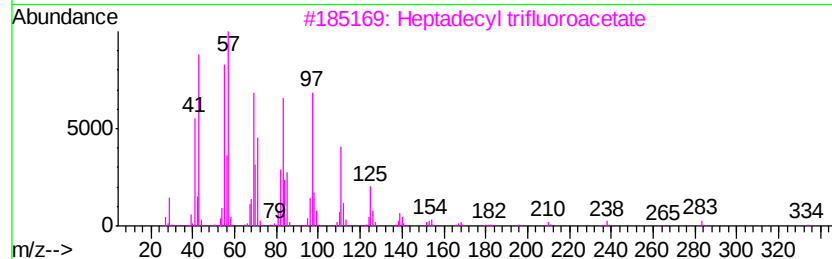
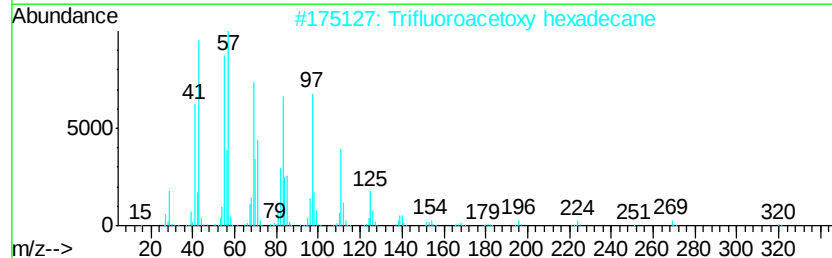
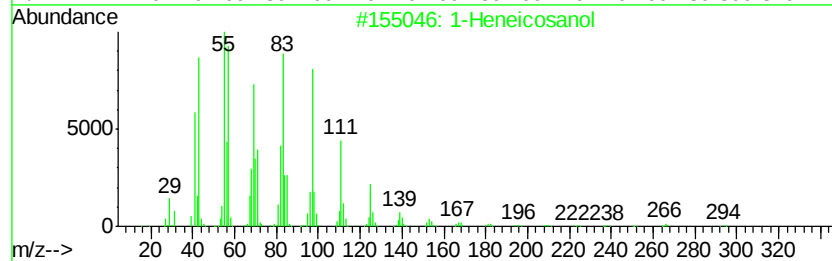
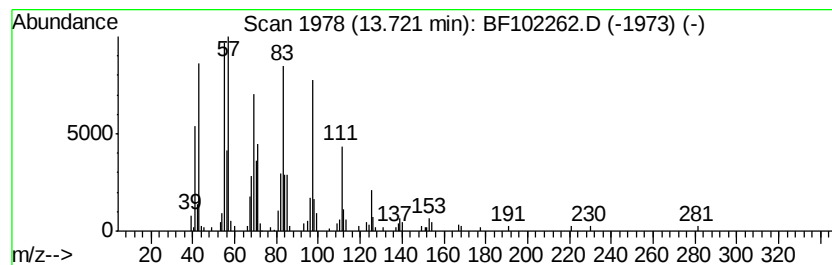
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	8.84 ng	349934	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	93
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	92



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102262.D
Acq On : 20 Jan 2018 13:37
Operator : SJ/JU
Sample : J1115-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-2.5-3.0

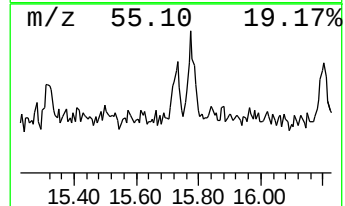
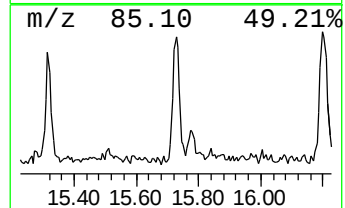
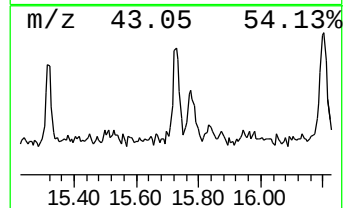
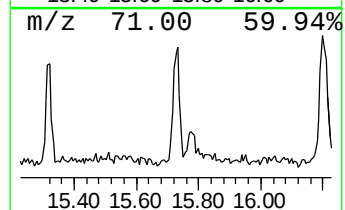
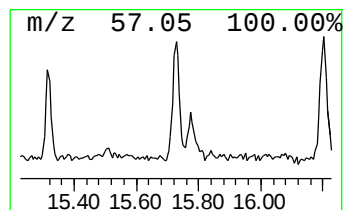
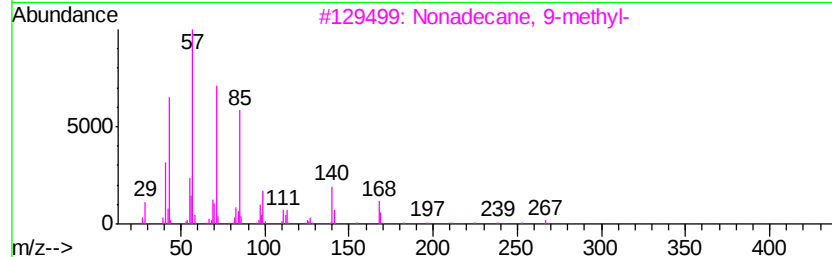
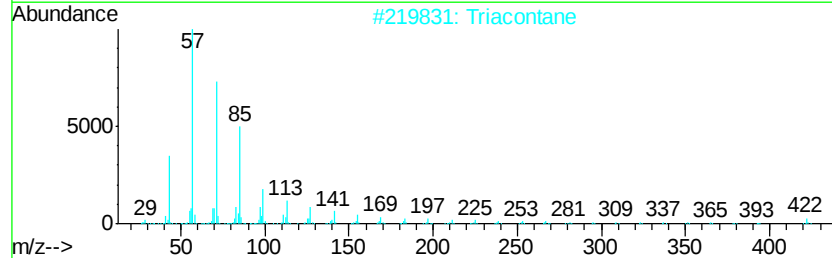
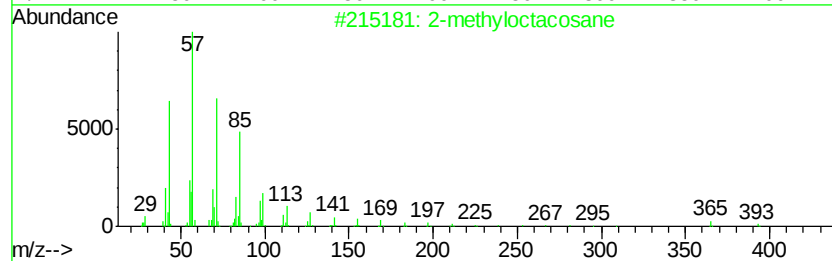
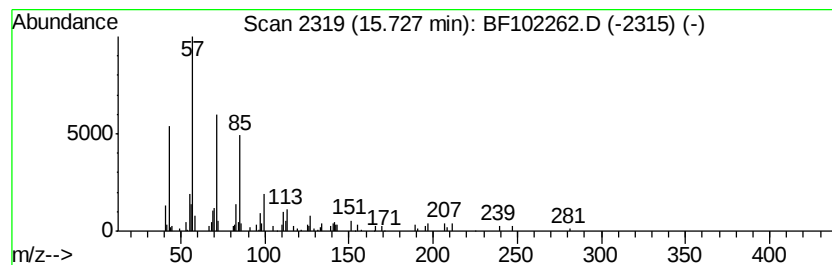
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	2.50 ng	97046	Perylene-d12	15.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane		408	C29H60	1000376-72-8	87
2	triacontane		422	C30H62	000638-68-6	86
3	Nonadecane, 9-methyl-		282	C20H42	013287-24-6	86
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	86
5	Heneicosane		296	C21H44	000629-94-7	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102262.D
Acq On : 20 Jan 2018 13:37
Operator : SJ/JU
Sample : J1115-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-2.5-3.0

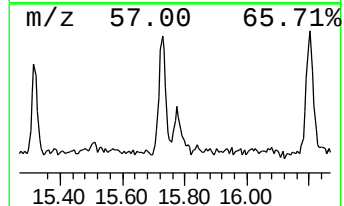
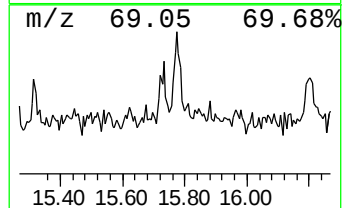
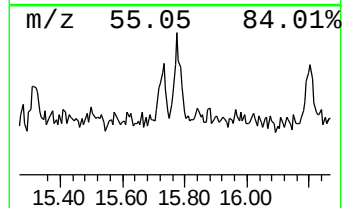
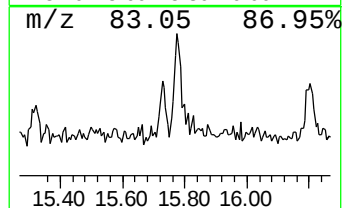
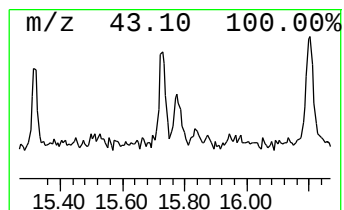
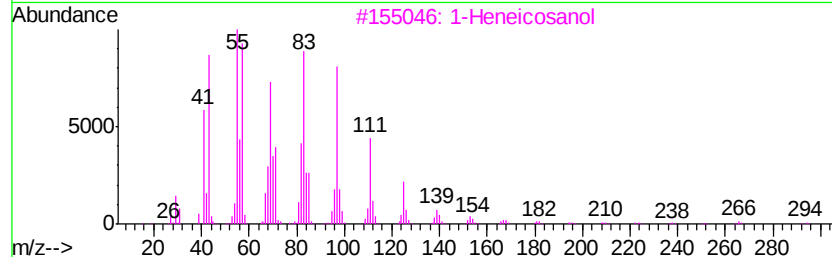
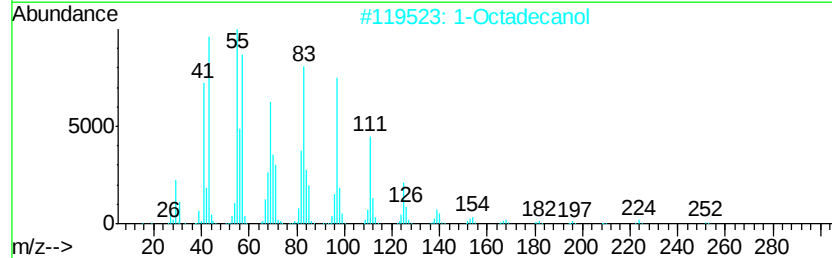
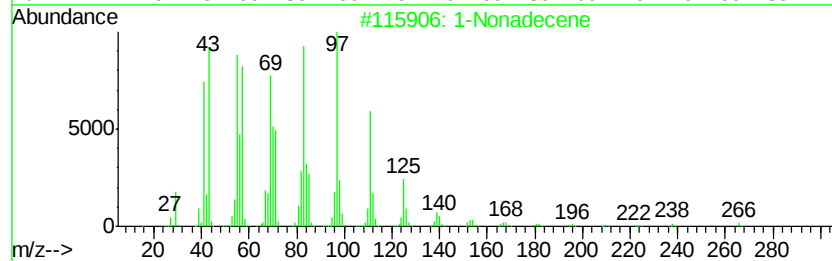
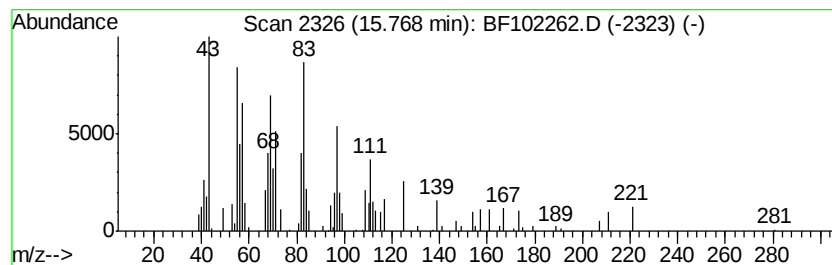
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Nonadecene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	2.08 ng	80826	Perylene-d12	15.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	87
2	1-Octadecanol		270	C18H38O	000112-92-5	81
3	1-Heneicosanol		312	C21H44O	015594-90-8	80
4	n-Heptadecanol-1		256	C17H36O	001454-85-9	76
5	Pentafluoropropionic acid, penta...		374	C18H31F5O2	959092-08-1	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102262.D
Acq On : 20 Jan 2018 13:37
Operator : SJ/JU
Sample : J1115-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

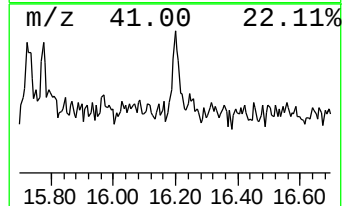
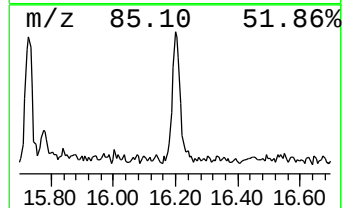
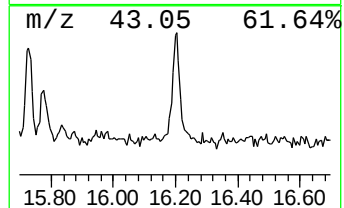
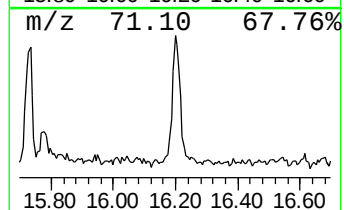
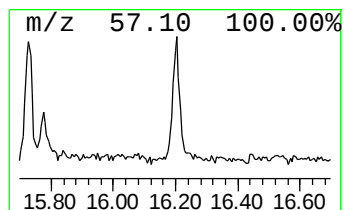
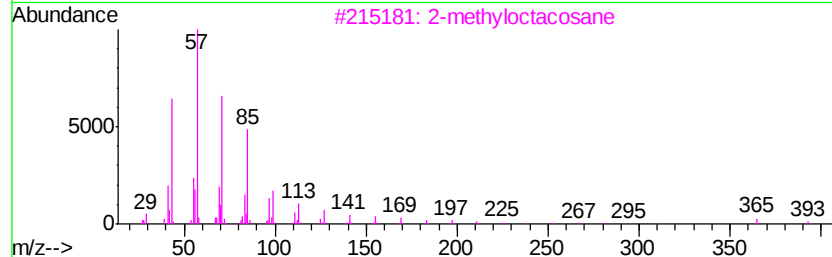
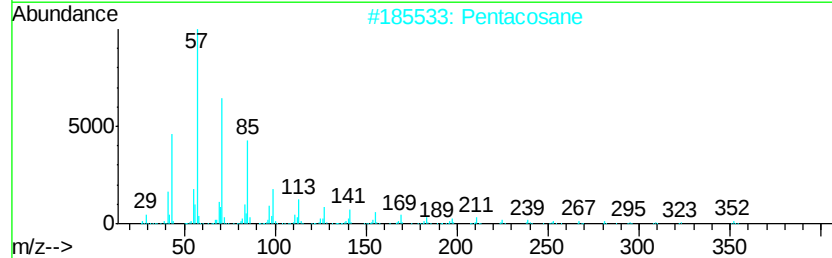
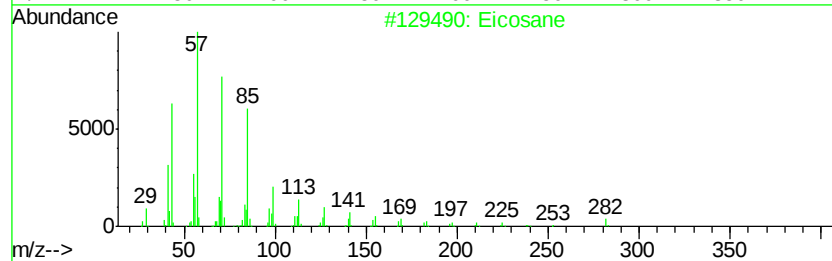
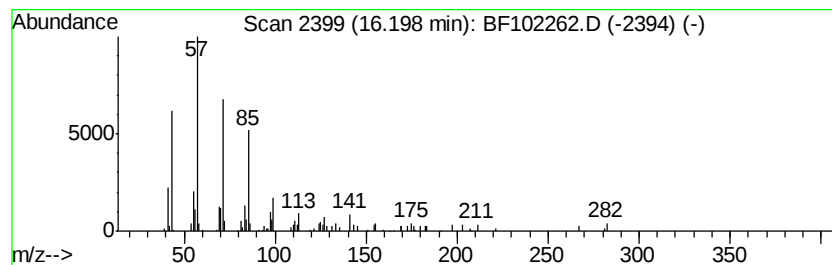
Instrument :
BNA_F
ClientSampleId :
SB-34-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	3.21 ng	124581	Perylene-d12	15.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane		282 C20H42	000112-95-8 96
2	Pentacosane		352 C25H52	000629-99-2 91
3	2-methyloctacosane		408 C29H60	1000376-72-8 91
4	triacontane		422 C30H62	000638-68-6 91
5	Heptadecane		240 C17H36	000629-78-7 91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102262.D
Acq On : 20 Jan 2018 13:37
Operator : SJ/JU
Sample : J1115-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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...	4.92	5.3	ng	233048	1	6.72	882717	20.0
unknown6.49	6.49	73.5	ng	3244160	1	6.72	882717	20.0
Tetradecane	10.66	2.0	ng	93639	4	11.24	933371	20.0
1-Heneicosanol	13.72	8.8	ng	349934	5	13.87	791705	20.0
2-methyloctacosane	15.73	2.5	ng	97046	6	15.29	777162	20.0
1-Nonadecene	15.77	2.1	ng	80826	6	15.29	777162	20.0
Eicosane	16.20	3.2	ng	124581	6	15.29	777162	20.0