

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
 Data File : BF082496.D
 Acq On : 24 Oct 2015 6:45
 Operator : UM/IZ
 Sample : G4116-03
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB3-02(0-2)

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-BF101015.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	4.926	240	244	252	rBV	831636	1453010	59.46%	6.201%
2	5.360	279	282	284	rBV	1950865	2285171	93.52%	9.752%
3	5.749	314	316	322	rVB	30243	29893	1.22%	0.128%
4	6.412	371	374	376	rBV	1729004	2307151	94.41%	9.846%
5	6.526	381	384	386	rBV	2467995	2443638	100.00%	10.429%
6	6.754	402	404	406	rBV	505598	499191	20.43%	2.130%
7	6.903	415	417	420	rBV	1532577	1810195	74.08%	7.725%
8	7.326	451	454	457	rBV	1362043	1389318	56.85%	5.929%
9	8.046	514	517	519	rBV	460841	633848	25.94%	2.705%
10	9.120	608	611	614	rBV	2397512	2435334	99.66%	10.393%
11	9.520	644	646	649	rVB	532512	442589	18.11%	1.889%
12	9.795	668	670	673	rBV	765857	767013	31.39%	3.273%
13	10.229	707	708	710	rVB	40733	29006	1.19%	0.124%
14	10.595	737	740	742	rBV	1475181	1530117	62.62%	6.530%
15	10.698	748	749	754	rVB	45014	67821	2.78%	0.289%
16	11.155	787	789	790	rBV	31444	39506	1.62%	0.169%
17	11.281	798	800	803	rBV	588543	703821	28.80%	3.004%
18	11.578	824	826	828	rVB	29084	25387	1.04%	0.108%
19	11.818	845	847	853	rVB2	90504	91891	3.76%	0.392%
20	12.504	903	907	908	rBV	27785	35683	1.46%	0.152%
21	12.732	925	927	929	rVB	24288	31124	1.27%	0.133%
22	12.881	937	940	942	rBV	2165374	2266629	92.76%	9.673%
23	13.829	1018	1023	1030	rBV2	46819	154413	6.32%	0.659%
24	13.967	1032	1035	1039	rVV	447454	559675	22.90%	2.389%
25	14.481	1077	1080	1082	rBV	40617	45183	1.85%	0.193%
26	14.538	1082	1085	1090	rVV5	21513	56992	2.33%	0.243%
27	14.881	1113	1115	1118	rBV	21975	34411	1.41%	0.147%
28	15.064	1129	1131	1135	rBV	18200	42157	1.73%	0.180%
29	15.144	1136	1138	1142	rVB	49895	54662	2.24%	0.233%
30	15.224	1142	1145	1151	rBV3	26625	71400	2.92%	0.305%
31	15.475	1164	1167	1173	rVB	394164	518130	21.20%	2.211%
32	15.692	1184	1186	1190	rVB	23911	36081	1.48%	0.154%
33	15.910	1203	1205	1208	rVB	39419	61340	2.51%	0.262%
34	16.035	1212	1216	1221	rBV3	29620	86166	3.53%	0.368%

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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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35	16.664	1268	1271	1274	rVB2	21951	40935	1.68%	0.175%
36	16.938	1291	1295	1298	rVB2	21452	44522	1.82%	0.190%
37	17.133	1307	1312	1318	rVB4	21596	75376	3.08%	0.322%
38	17.430	1334	1338	1344	rBV7	11551	49871	2.04%	0.213%
39	17.567	1347	1350	1355	rVB2	29483	65504	2.68%	0.280%
40	18.333	1412	1417	1422	rVB6	19867	70352	2.88%	0.300%
41	18.744	1449	1453	1457	rVB3	17595	47454	1.94%	0.203%

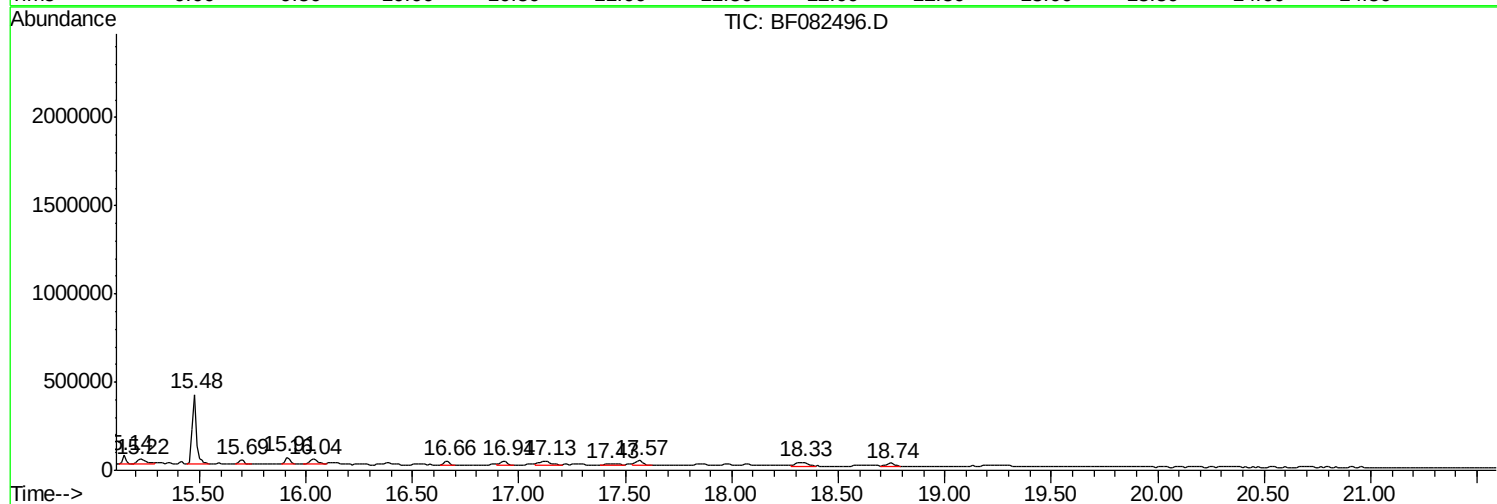
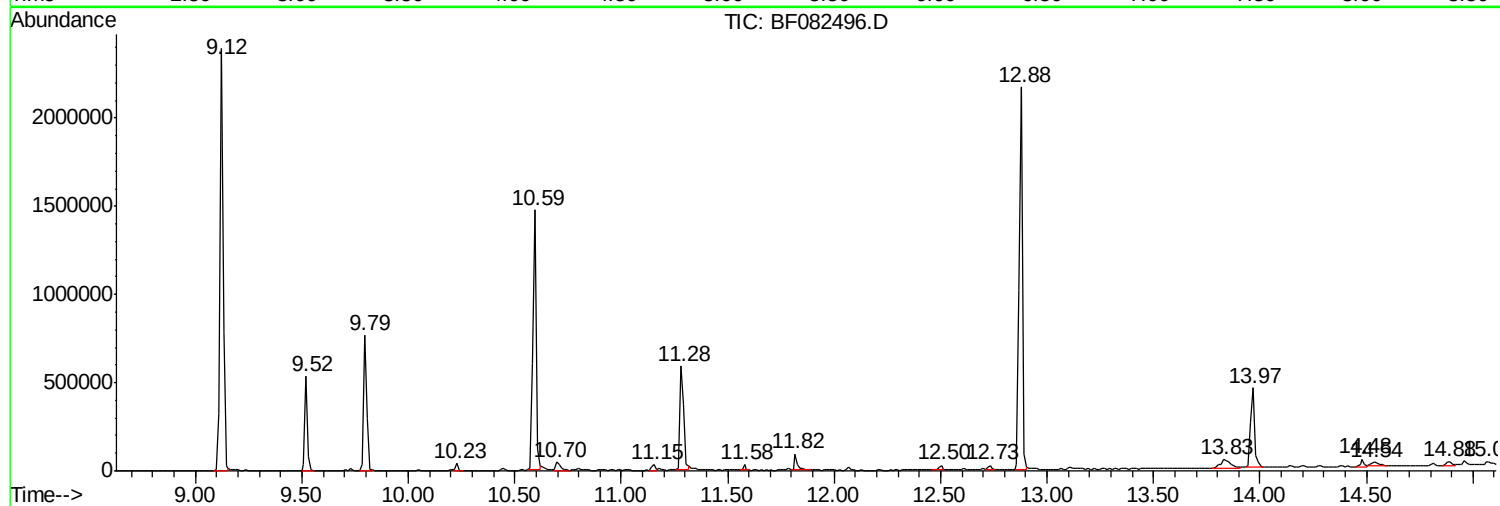
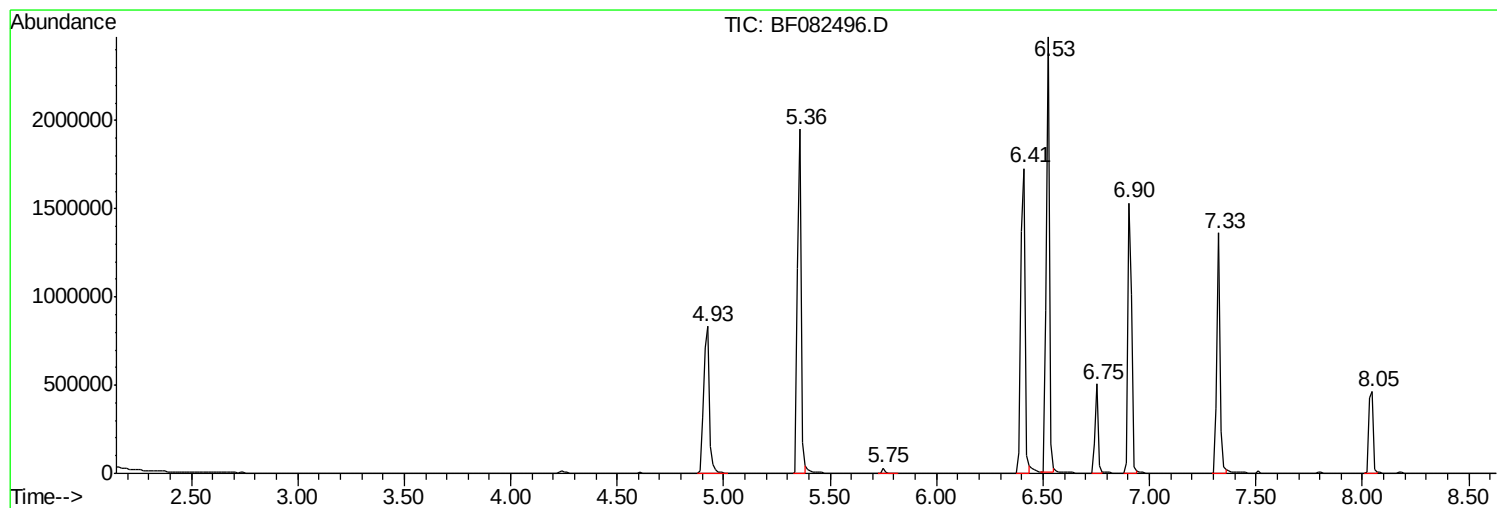
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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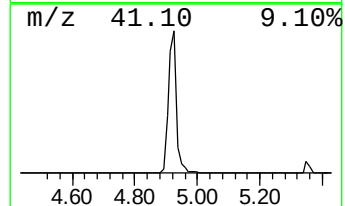
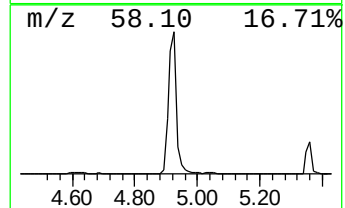
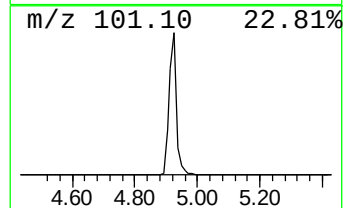
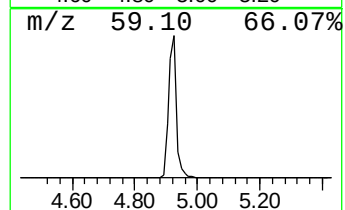
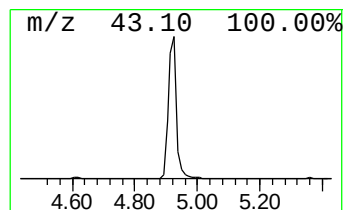
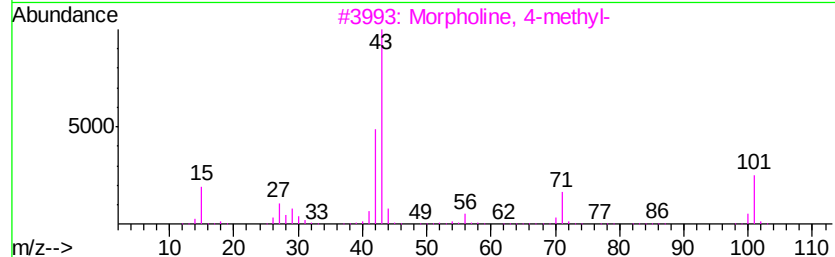
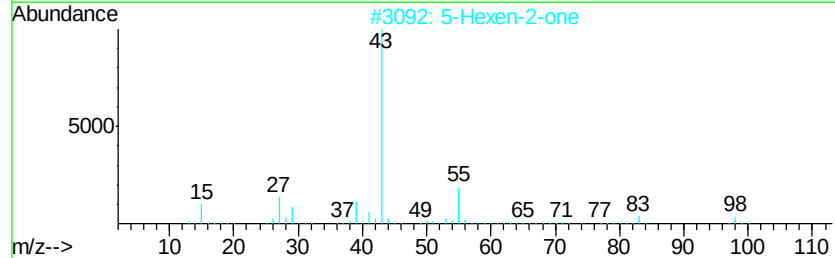
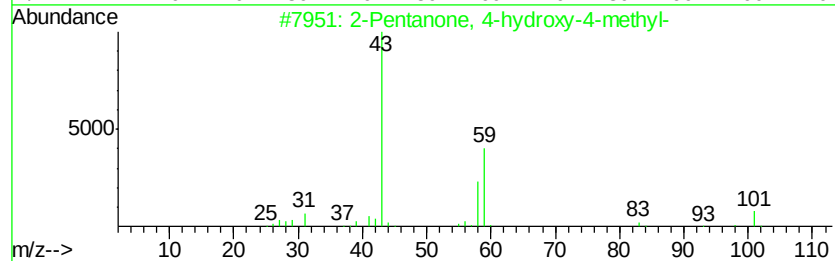
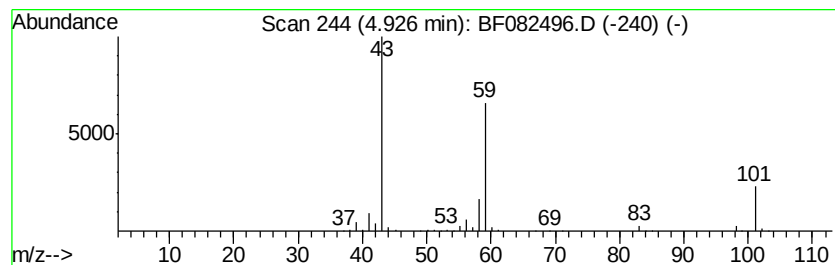
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
4.93	58.21 ng	1453010	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		5-Hexen-2-one	98	C6H10O	000109-49-9	9
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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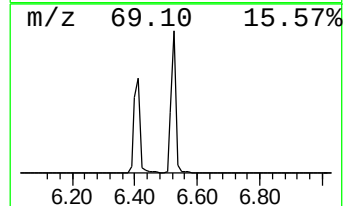
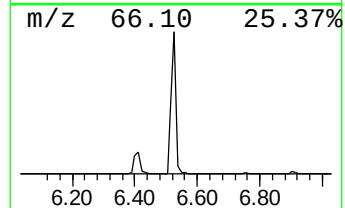
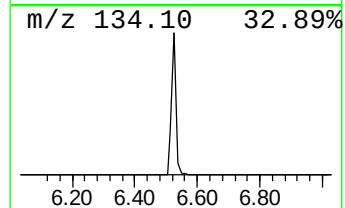
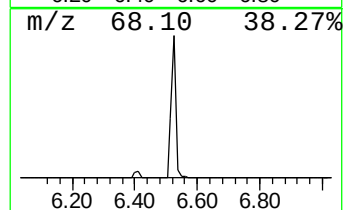
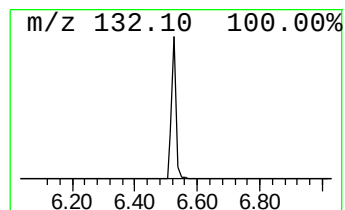
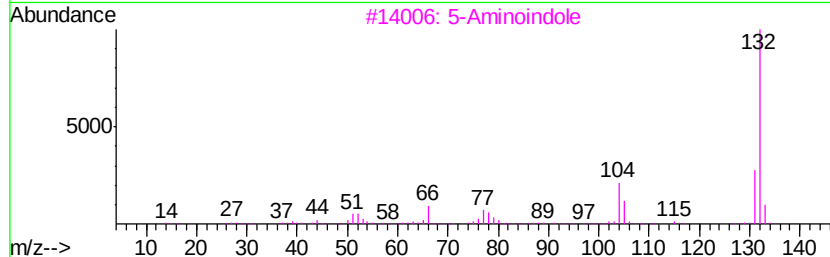
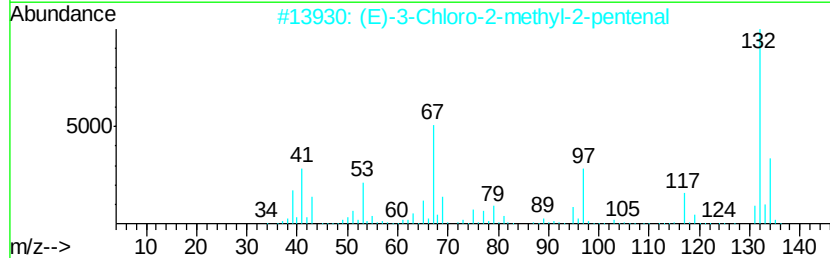
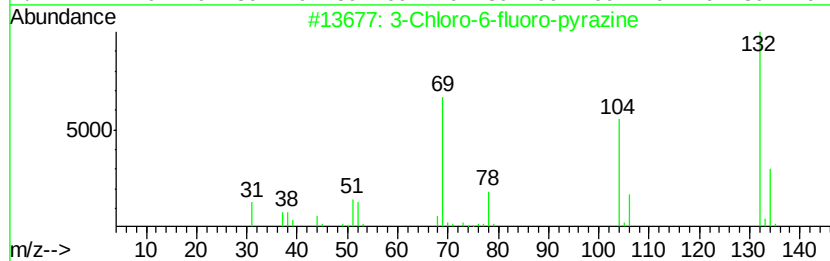
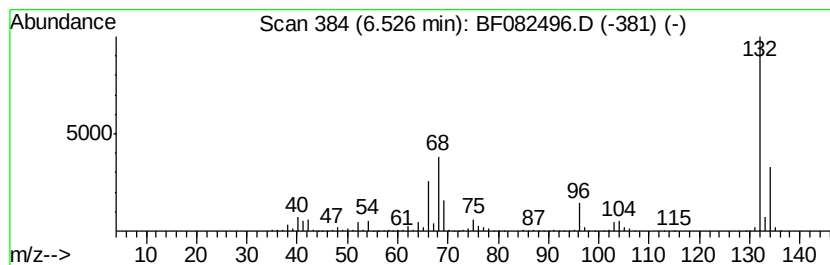
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	97.90 ng	2443640	1,4-Dichlorobenzene-d4	6.75

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	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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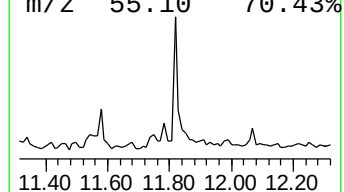
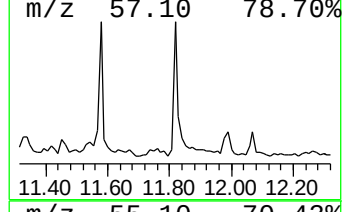
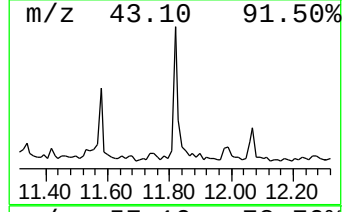
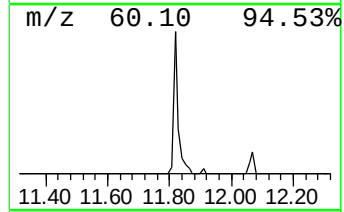
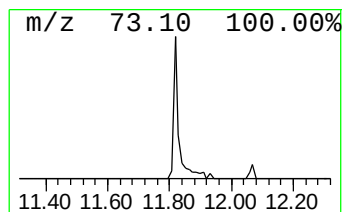
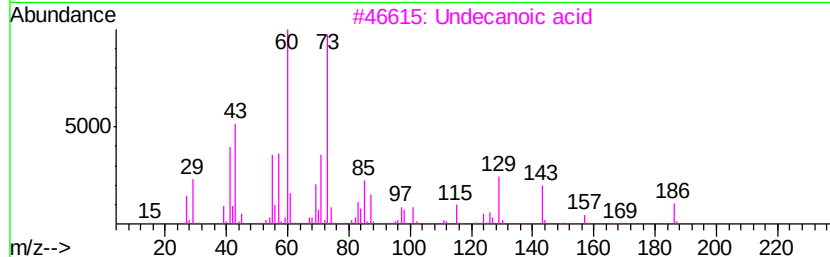
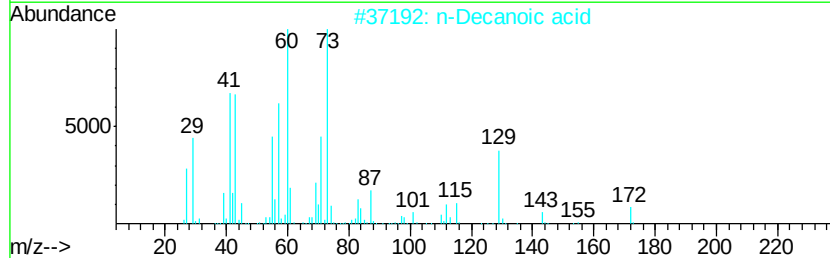
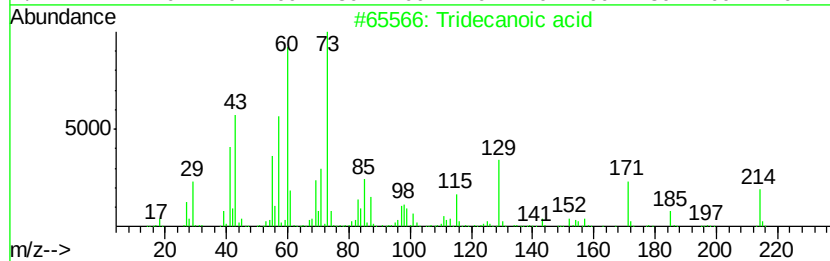
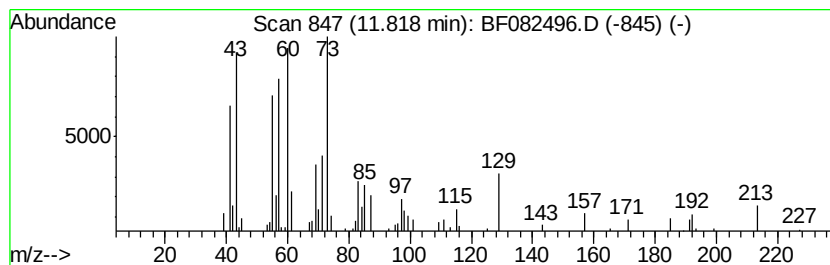
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	2.61 ng	91891	Phenanthrene-d10	11.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	86
2		n-Decanoic acid	172	C10H20O2	000334-48-5	64
3		Undecanoic acid	186	C11H22O2	000112-37-8	64
4		Sedoheptulosan	192	C7H12O6	000469-90-9	27
5		Vitamin d3	384	C27H44O	001406-16-2	27



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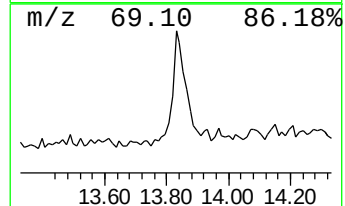
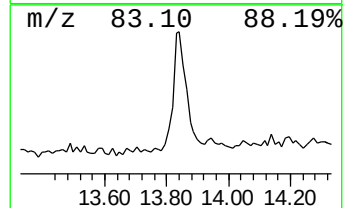
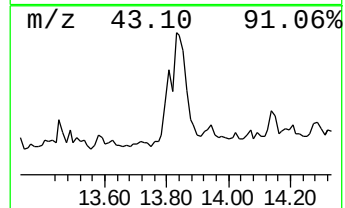
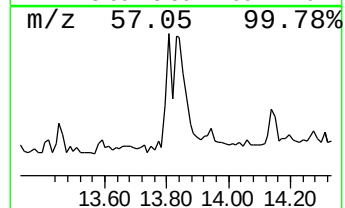
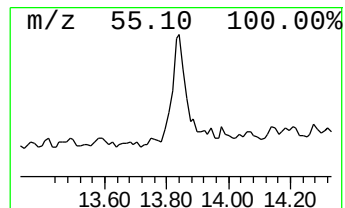
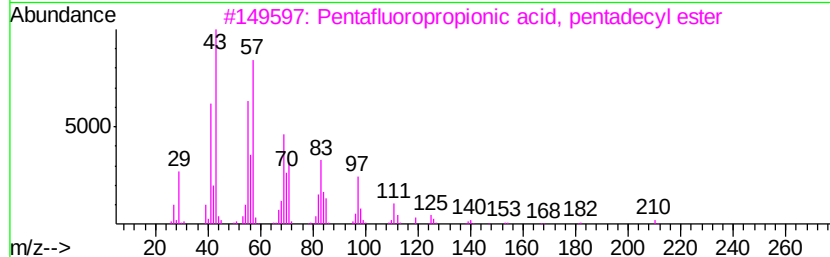
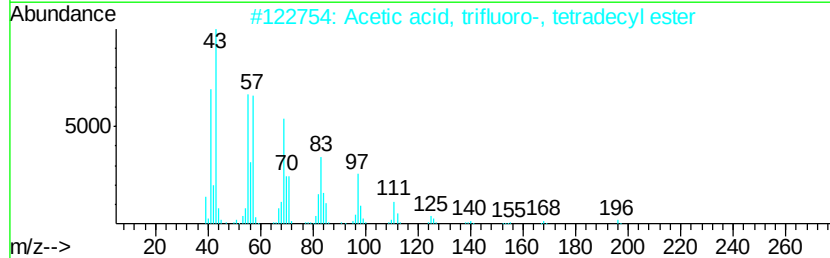
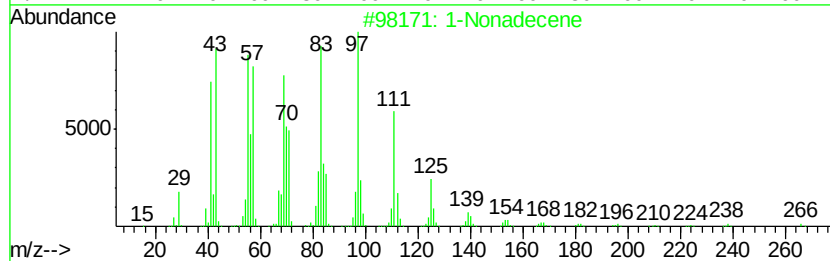
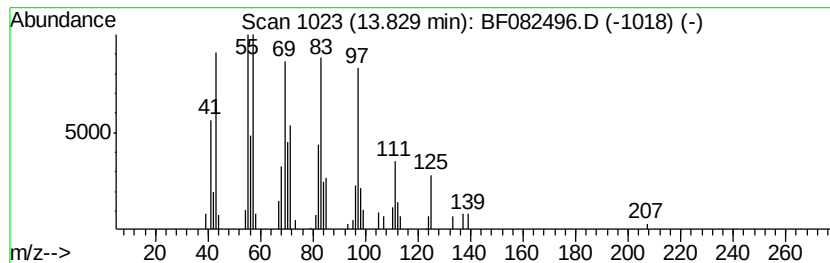
Instrument :
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ClientSampled :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	5.52 ng	154413	Chrysene-d12	13.97
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Nonadecene		266 C19H38	018435-45-5 87
2	Acetic acid, trifluoro-, tetradecyl...		310 C16H29F3O2	006222-02-2 83
3	Pentafluoropropionic acid, penta...		374 C18H31F5O2	1000280-07-5 80
4	1-Eicosanol		298 C20H42O	000629-96-9 76
5	Trichloroacetic acid, tetradecyl...		358 C16H29Cl3O2	074339-52-9 76



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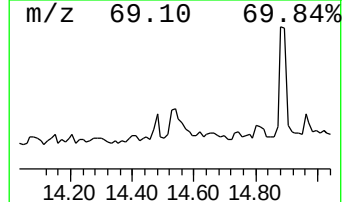
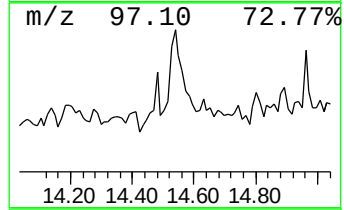
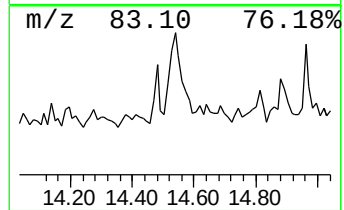
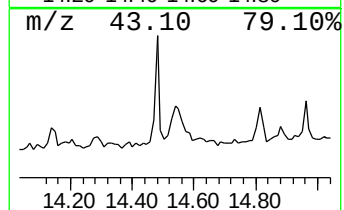
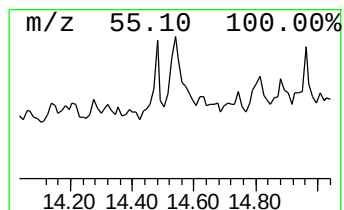
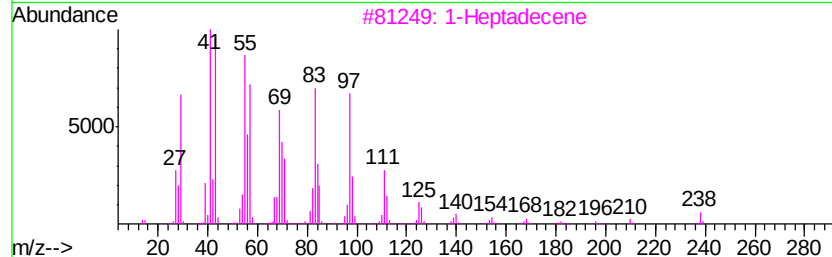
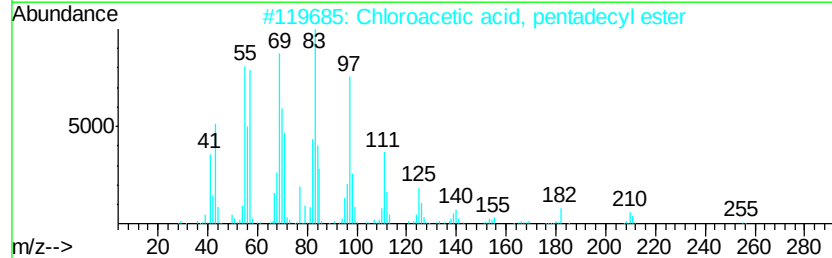
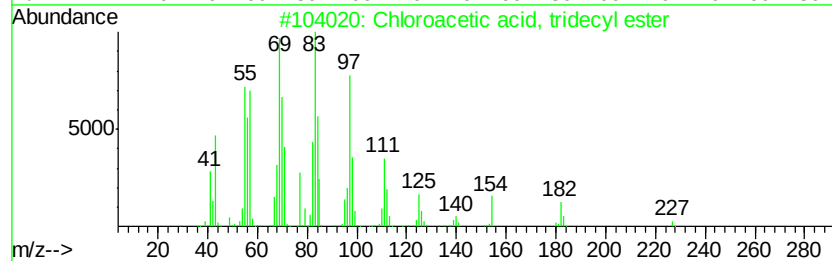
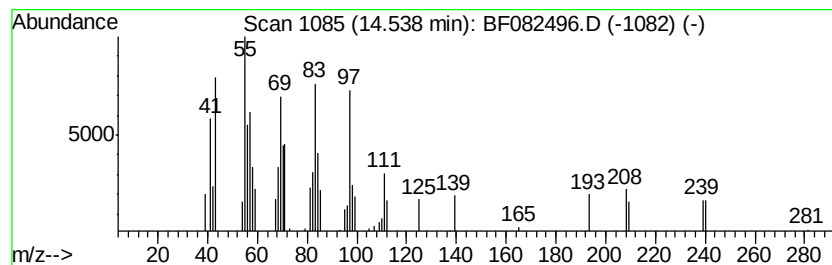
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Chloroacetic acid, tridecyl... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	2.04 ng	56992	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	76
2		Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	76
3		1-Heptadecene	238	C17H34	006765-39-5	76
4		1-Hexadecanol	242	C16H34O	036653-82-4	76
5		Chloroacetic acid, tetradecyl ester	290	C16H31ClO2	018277-86-6	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082496.D
Acq On : 24 Oct 2015 6:45
Operator : UM/IZ
Sample : G4116-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB3-02(0-2)

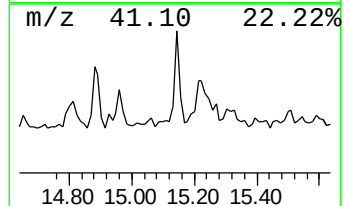
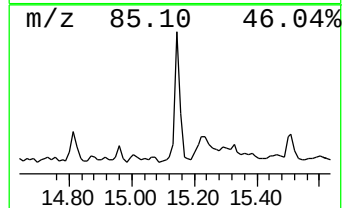
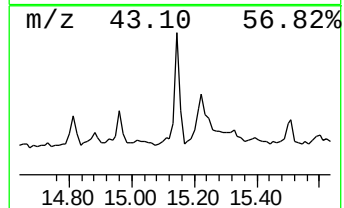
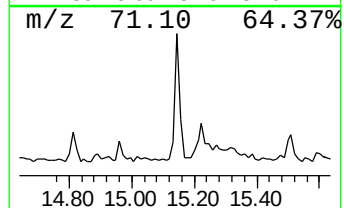
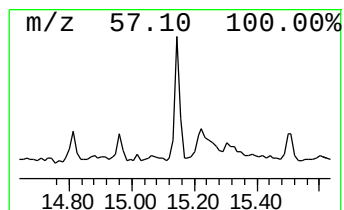
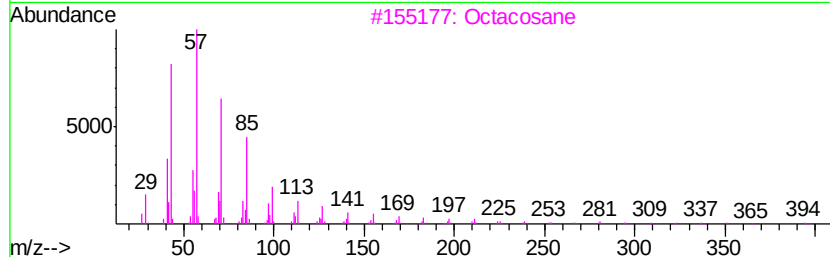
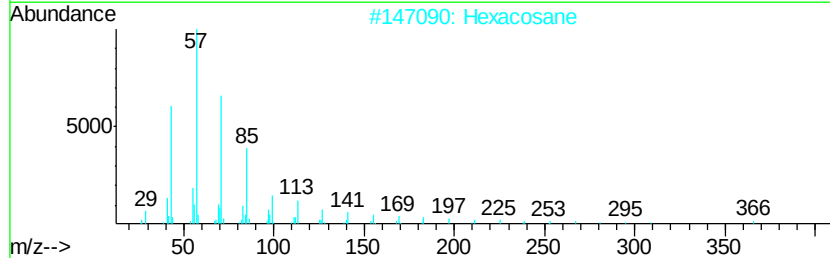
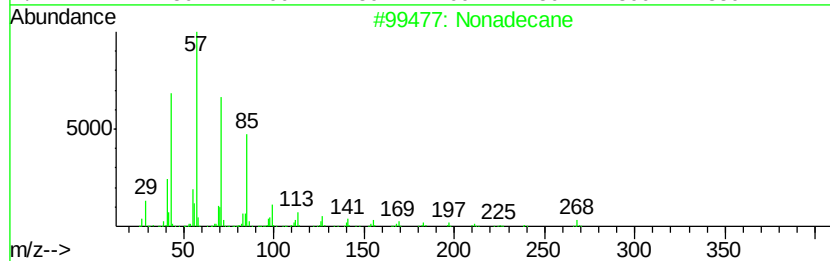
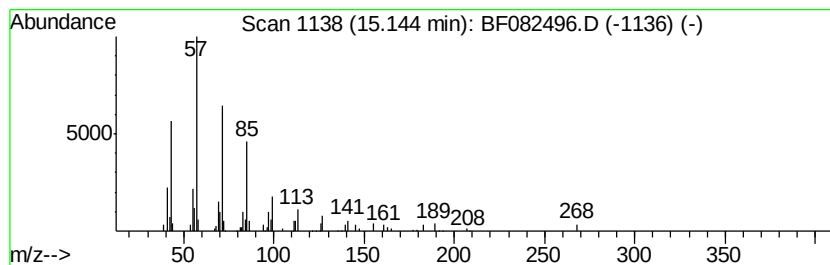
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	2.11 ng	54662	Perylene-d12	15.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	94
2	Hexacosane		366	C26H54	000630-01-3	91
3	Octacosane		394	C28H58	000630-02-4	91
4	Heneicosane		296	C21H44	000629-94-7	91
5	Hentriacontane		437	C31H64	000630-04-6	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082496.D
Acq On : 24 Oct 2015 6:45
Operator : UM/IZ
Sample : G4116-03
Misc :
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Instrument :
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ClientSampleId :
NB3-02(0-2)

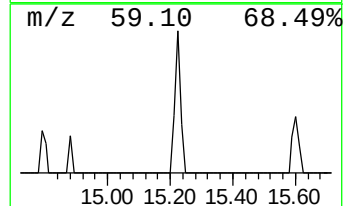
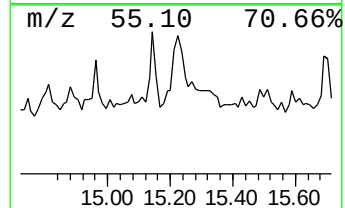
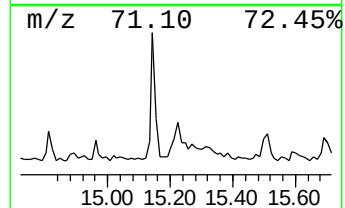
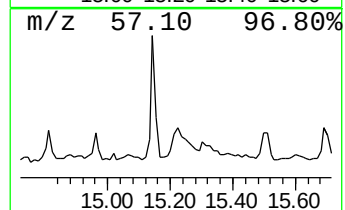
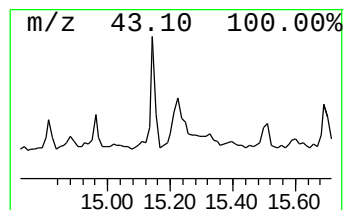
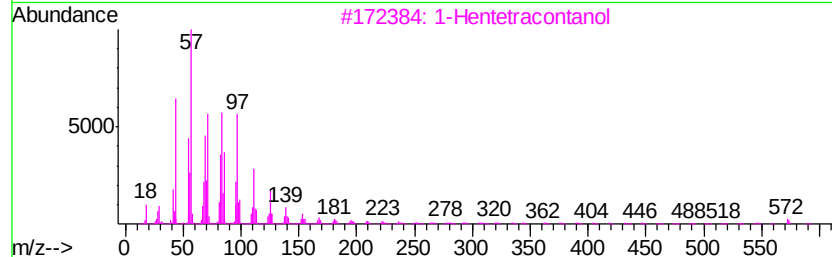
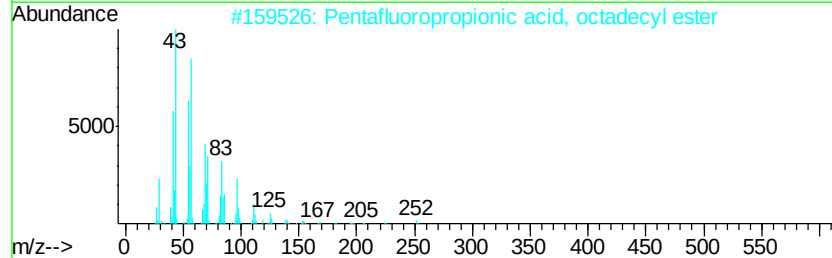
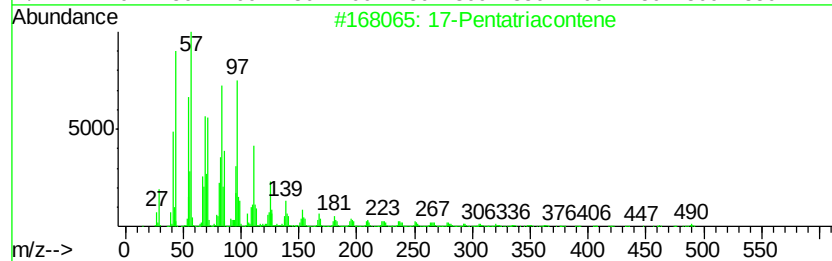
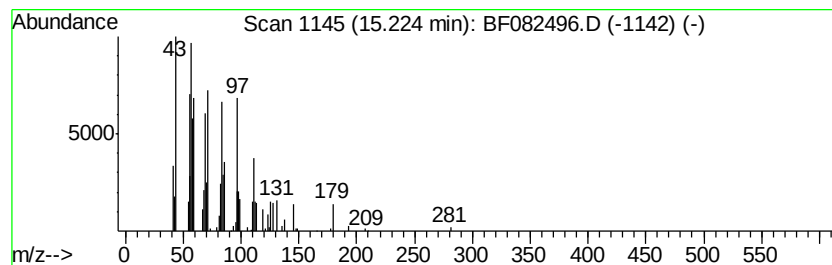
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 17-Pentatriacontene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	2.76 ng	71400	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-Pentatriacontene	491	C35H70	006971-40-0	58
2		Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	53
3		1-Hentetracontanol	593	C41H84O	040710-42-7	52
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	49
5		4-Heptafluorobutyroxytetradecane	410	C18H29F7O2	1000245-49-9	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082496.D
Acq On : 24 Oct 2015 6:45
Operator : UM/IZ
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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NB3-02(0-2)

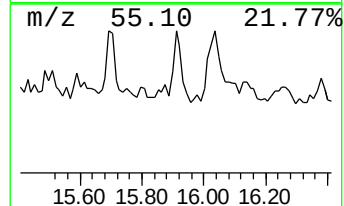
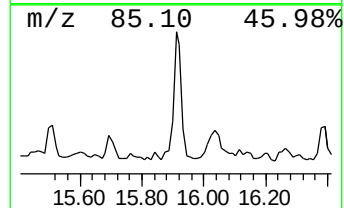
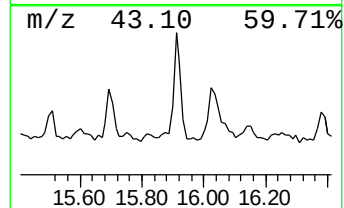
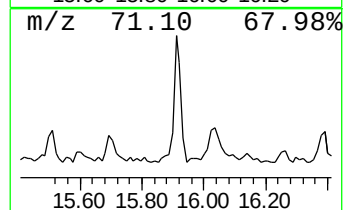
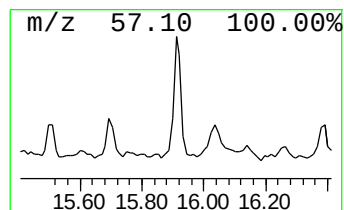
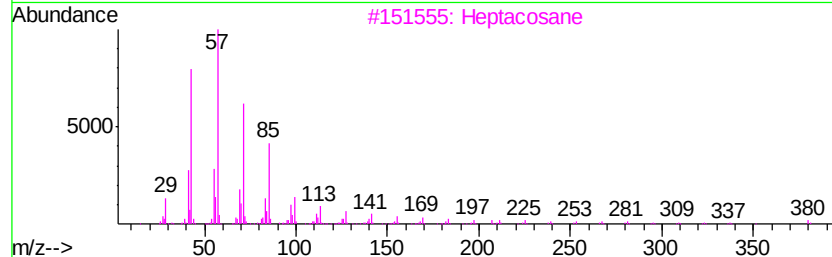
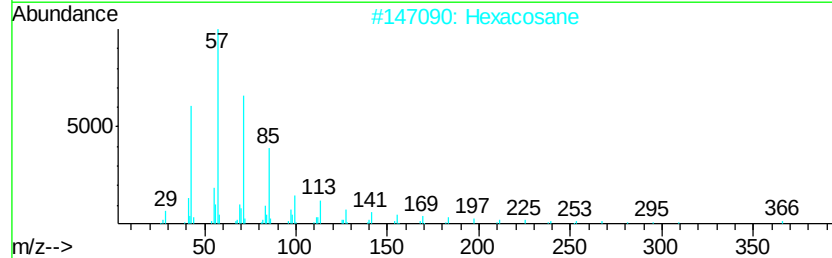
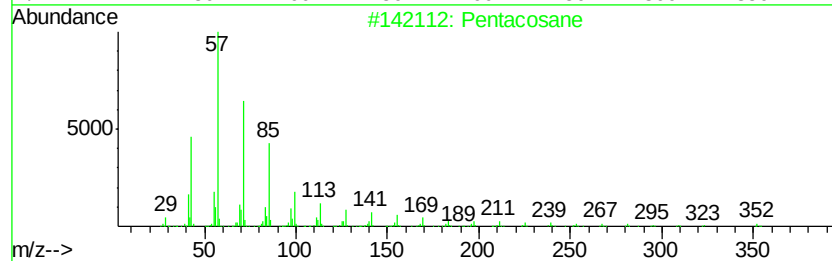
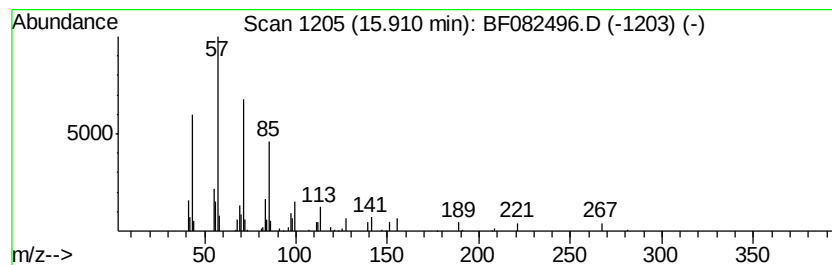
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.91	2.37 ng	61340	Perylene-d12	15.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	87
2	Hexacosane		366	C26H54	000630-01-3	87
3	Heptacosane		380	C27H56	000593-49-7	87
4	Tetratriacontane		479	C34H70	014167-59-0	83
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082496.D
Acq On : 24 Oct 2015 6:45
Operator : UM/IZ
Sample : G4116-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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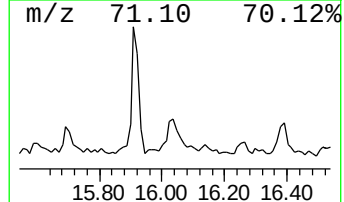
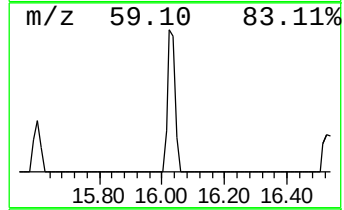
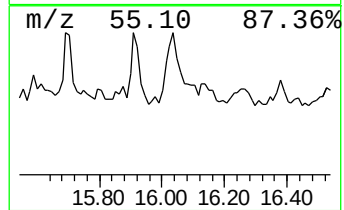
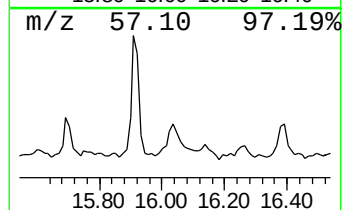
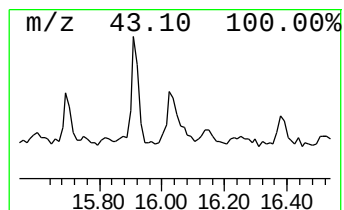
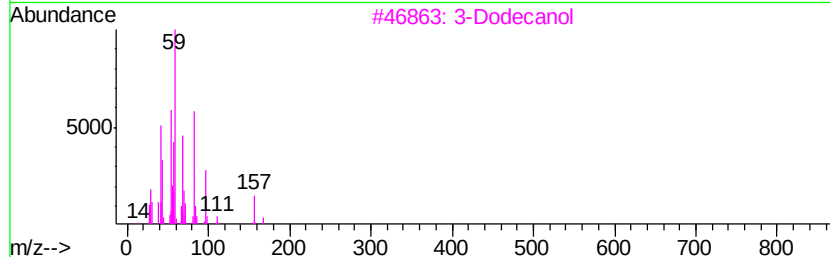
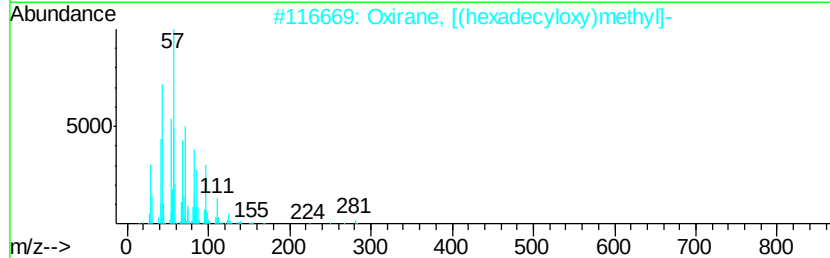
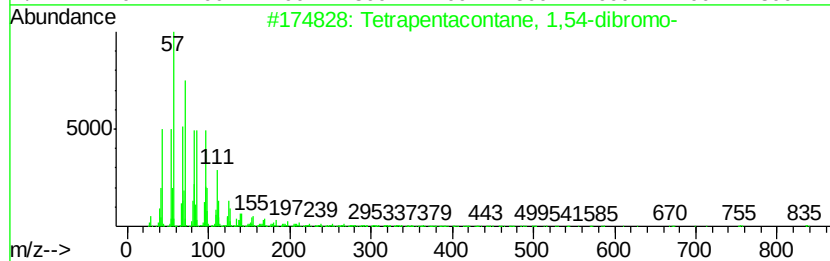
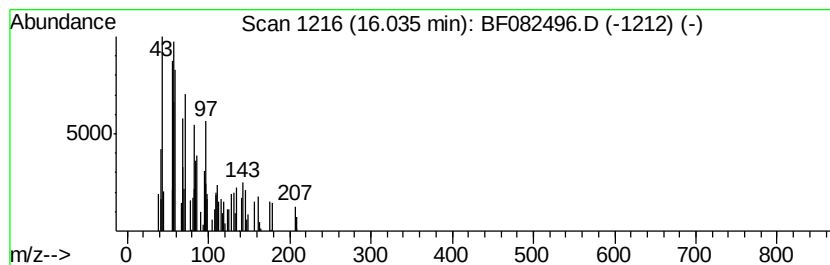
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.04 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	3.33 ng	86166	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	30
2		Oxirane, [(hexadecyloxy)methyl]-	298	C19H38O2	015965-99-8	27
3		3-Dodecanol	186	C12H26O	010203-30-2	22
4		1,3-Cyclobutanedicarboxylic acid...	206	C8H11ClO4	025596-64-9	15
5		Dodecane, 6-cyclohexyl-	252	C18H36	013151-86-5	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082496.D
Acq On : 24 Oct 2015 6:45
Operator : UM/IZ
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Misc :
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Instrument :
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ClientSampleId :
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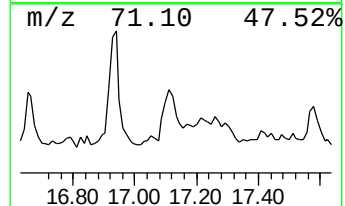
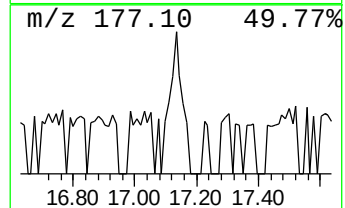
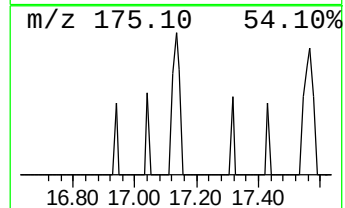
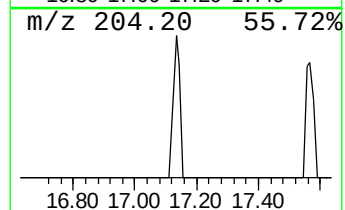
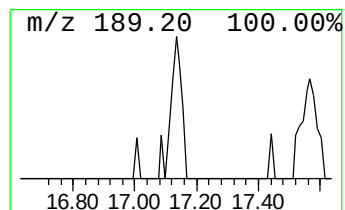
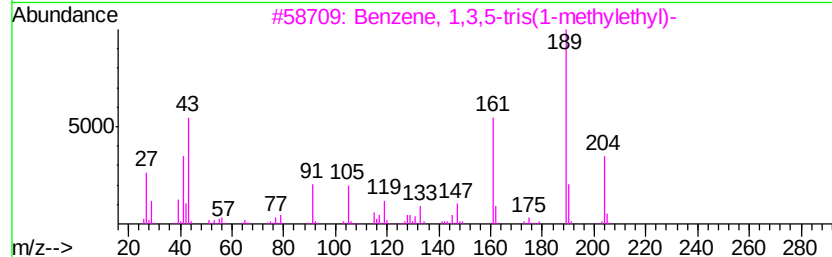
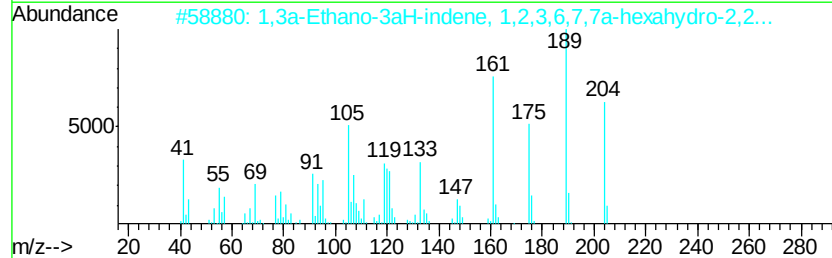
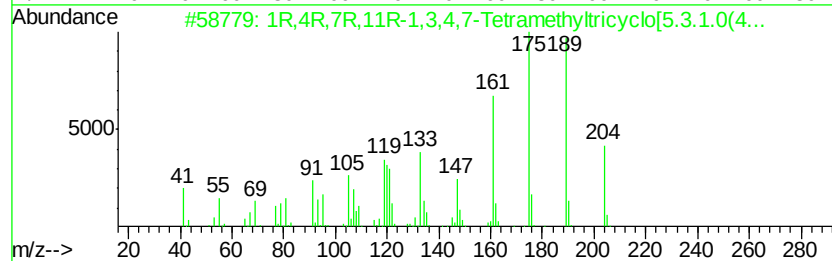
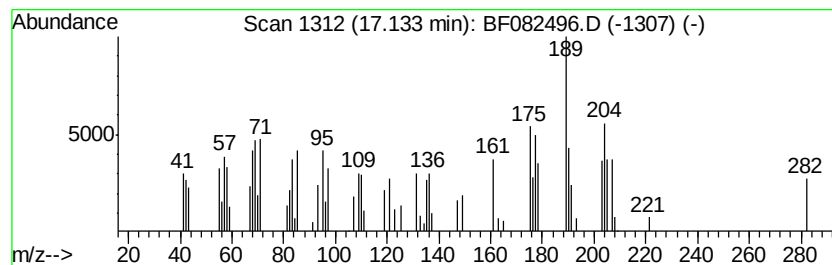
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.13 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.13	2.91 ng	75376	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1R,4R,7R,11R-1,3,4,7-Tetramethyl...	204	C15H24	137235-59-7	35
2		1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	27
3		Benzene, 1,3,5-tris(1-methylethyl)-	204	C15H24	000717-74-8	22
4		4,4,5,8-Tetramethyl-chroman-2-one	204	C13H16O2	040662-15-5	22
5		2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000192-43-5	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082496.D
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ClientSampleId :
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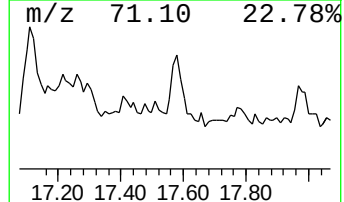
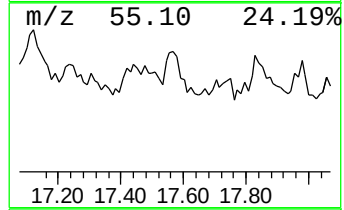
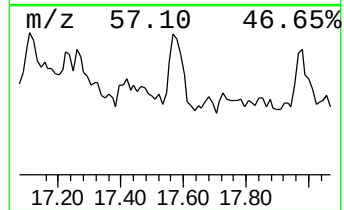
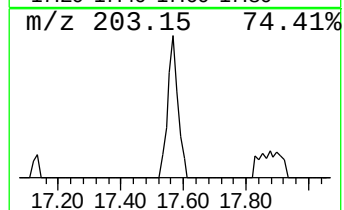
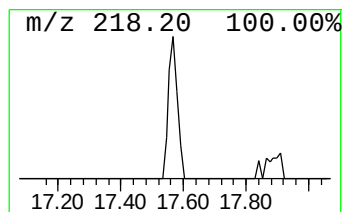
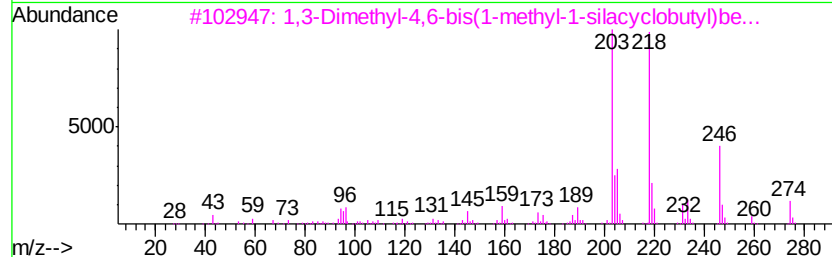
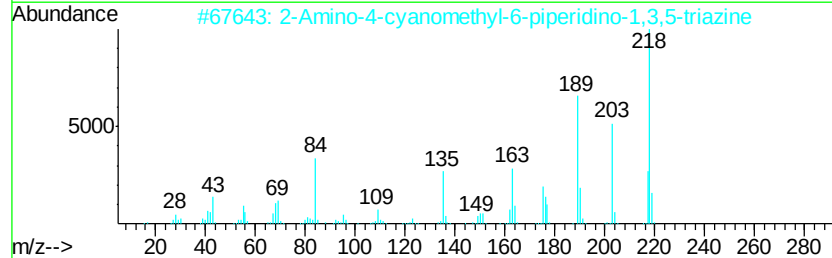
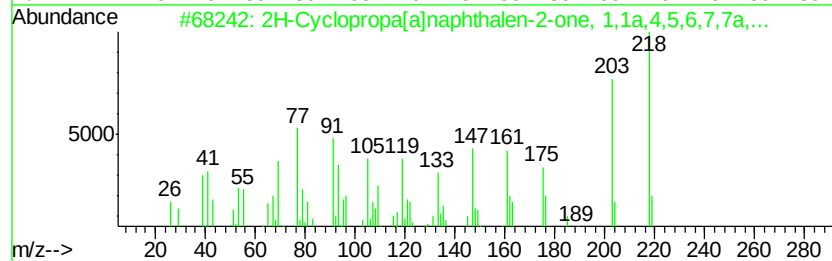
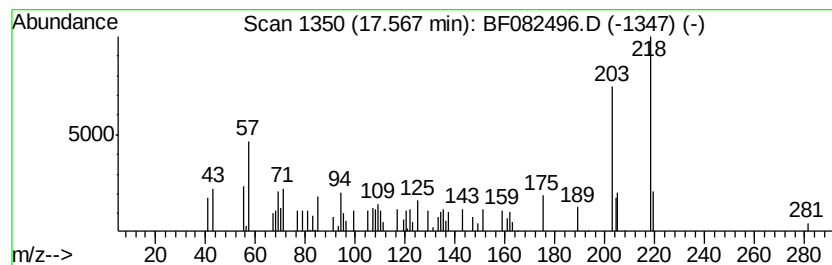
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2H-Cyclopropa[a]naphthalen-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.57	2.53 ng	65504	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	81
2		2-Amino-4-cyanomethyl-6-piperidi...	218	C10H14N6	1000241-05-9	64
3		1,3-Dimethyl-4,6-bis(1-methyl-1-...	274	C16H26Si2	1000293-75-9	59
4		2-Chloro-5,6-dimethyl-1-(2-propy...	218	C12H11ClN2	080276-20-6	59
5		6H-[1,2]Dioxeto[3',4':4,5]furo[3...	260	C14H12O5	129812-24-4	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082496.D
Acq On : 24 Oct 2015 6:45
Operator : UM/IZ
Sample : G4116-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB3-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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
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unknown6.53	6.53	97.9	ng	2443640	1	6.75	499191	20.0
Tridecanoic acid	11.82	2.6	ng	91891	4	11.28	703821	20.0
1-Nonadecene	13.83	5.5	ng	154413	5	13.97	559675	20.0
Chloroacetic acid...	14.54	2.0	ng	56992	5	13.97	559675	20.0
Nonadecane	15.14	2.1	ng	54662	6	15.48	518130	20.0
17-Pentatriacontene	15.22	2.8	ng	71400	6	15.48	518130	20.0
Pentacosane	15.91	2.4	ng	61340	6	15.48	518130	20.0
unknown16.04	16.04	3.3	ng	86166	6	15.48	518130	20.0
unknown17.13	17.13	2.9	ng	75376	6	15.48	518130	20.0
2H-Cyclopropa[a]n...	17.57	2.5	ng	65504	6	15.48	518130	20.0