

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071116\
 Data File : BF088915.D
 Acq On : 11 Jul 2016 22:49
 Operator : UM/SJ
 Sample : H3921-11
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 N8-B3(0-5)C

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-BF063016.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	1.678	6	8	13	rVV	70530	93110	5.45%	0.536%
2	1.747	13	14	17	rVV	15620	24219	1.42%	0.139%
3	1.792	17	18	27	rVV	485555	952393	55.79%	5.483%
4	1.918	27	29	58	rVB2	33737	157204	9.21%	0.905%
5	4.878	285	288	293	rBV	58537	96683	5.66%	0.557%
6	5.313	323	326	328	rBV	1385643	1707141	100.00%	9.829%
7	6.353	414	417	420	rBV	1206662	1628093	95.37%	9.374%
8	6.479	426	428	431	rBV	1592534	1558828	91.31%	8.975%
9	6.707	446	448	450	rBB	357675	375698	22.01%	2.163%
10	6.867	459	462	465	rBV	1439706	1258608	73.73%	7.246%
11	7.279	495	498	500	rBV	1134426	1087428	63.70%	6.261%
12	7.999	558	561	563	rBV	543479	506810	29.69%	2.918%
13	9.073	652	655	657	rBV	1933297	1697280	99.42%	9.772%
14	9.473	687	690	692	rBV	125636	172422	10.10%	0.993%
15	9.748	711	714	716	rBV	461497	470052	27.53%	2.706%
16	10.193	751	753	754	rVB	22592	22724	1.33%	0.131%
17	10.525	780	782	785	rBV	825266	870519	50.99%	5.012%
18	10.662	791	794	799	rVB	31510	37175	2.18%	0.214%
19	11.108	831	833	834	rBV	24011	21241	1.24%	0.122%
20	11.222	841	843	844	rBV	412658	407205	23.85%	2.344%
21	11.245	844	845	846	rVB	48906	33550	1.97%	0.193%
22	11.462	861	864	868	rVB	17984	23904	1.40%	0.138%
23	11.828	894	896	901	rVB2	14489	18724	1.10%	0.108%
24	12.422	946	948	950	rBV	135273	110688	6.48%	0.637%
25	12.651	965	968	969	rBV	106413	120962	7.09%	0.696%
26	12.685	969	971	977	rVV	161294	213275	12.49%	1.228%
27	12.799	979	981	984	rVV	1041325	1236958	72.46%	7.122%
28	12.845	984	985	991	rVB3	10725	20355	1.19%	0.117%
29	12.982	993	997	998	rBV	13013	19755	1.16%	0.114%
30	13.051	998	1003	1004	rBV2	9591	20664	1.21%	0.119%
31	13.165	1010	1013	1015	rBV3	22007	25103	1.47%	0.145%
32	13.702	1057	1060	1064	rBV2	85981	143369	8.40%	0.825%
33	13.839	1069	1072	1077	rVV2	482906	569733	33.37%	3.280%
34	14.034	1087	1089	1094	rBV4	14518	31918	1.87%	0.184%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.354	1113	1117	1122	rBV2	70379	145252	8.51%	0.836%
36	14.491	1127	1129	1131	rVB	232508	242995	14.23%	1.399%
37	14.651	1139	1143	1145	rBV2	32945	46794	2.74%	0.269%
38	14.754	1150	1152	1154	rVB	55000	51078	2.99%	0.294%
39	14.834	1157	1159	1164	rBV	69602	124604	7.30%	0.717%
40	14.948	1166	1169	1172	rBV2	89707	178041	10.43%	1.025%
41	15.097	1180	1182	1185	rVB	32723	48887	2.86%	0.281%
42	15.154	1185	1187	1190	rBV	44074	53499	3.13%	0.308%
43	15.211	1190	1192	1195	rBV	251425	327312	19.17%	1.884%
44	15.440	1210	1212	1216	rVB	20762	27959	1.64%	0.161%
45	15.645	1228	1230	1232	rBV	37870	60659	3.55%	0.349%
46	15.691	1232	1234	1238	rVB4	26755	48127	2.82%	0.277%
47	16.343	1288	1291	1295	rVB3	21472	46772	2.74%	0.269%
48	16.491	1302	1304	1307	rBV2	18619	37270	2.18%	0.215%
49	16.605	1312	1314	1317	rVV2	14763	28883	1.69%	0.166%
50	16.697	1317	1322	1325	rVV7	12287	47325	2.77%	0.272%
51	16.788	1326	1330	1335	rVB6	15696	54341	3.18%	0.313%
52	16.880	1335	1338	1343	rVB	14165	34648	2.03%	0.199%
53	17.017	1347	1350	1353	rBV4	14311	30783	1.80%	0.177%

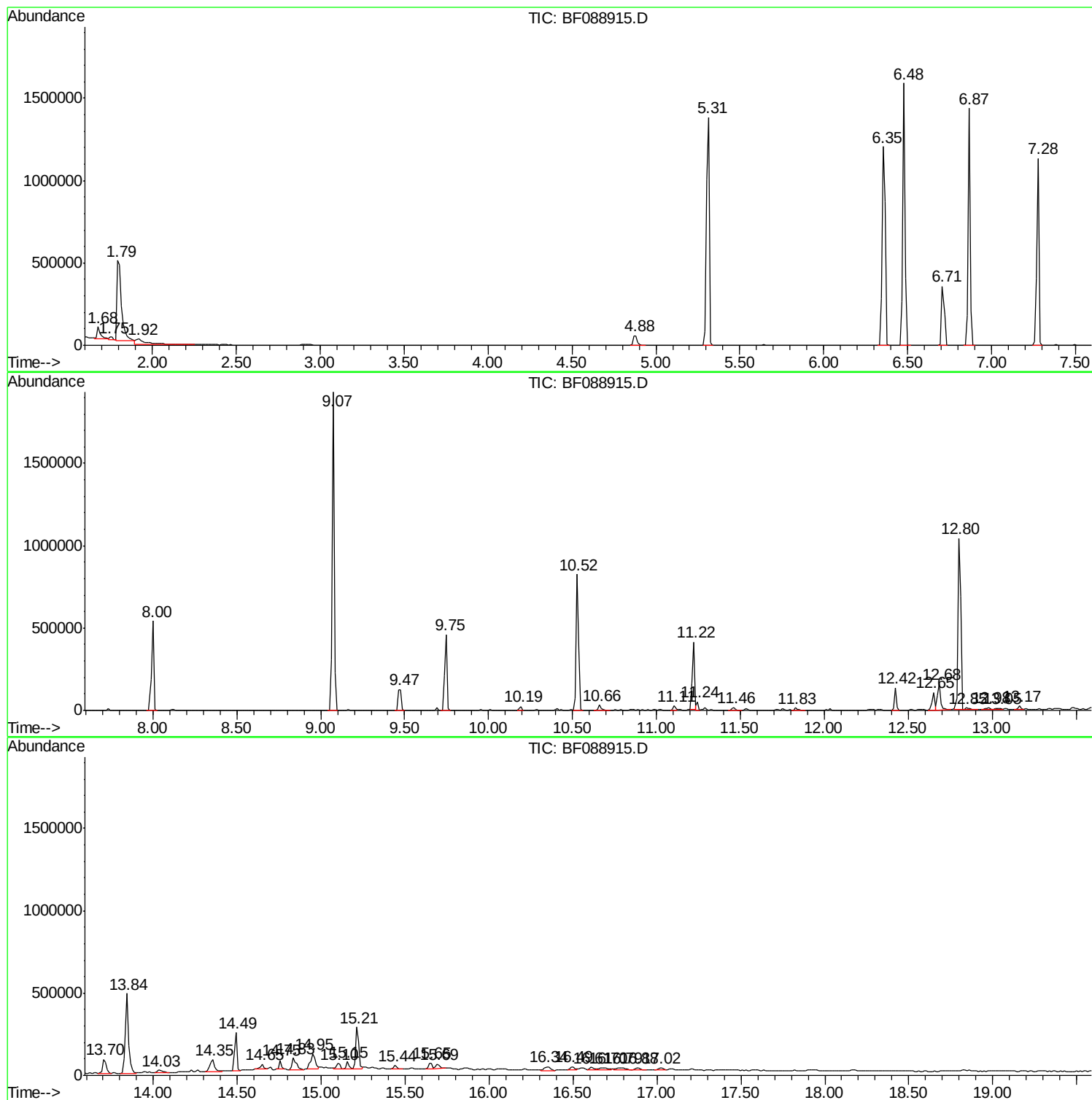
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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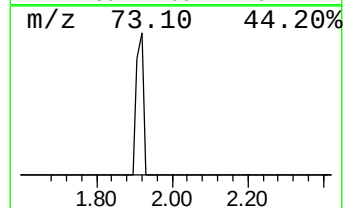
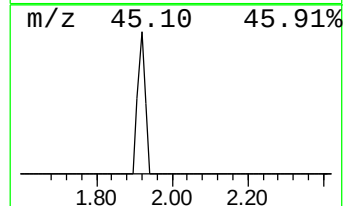
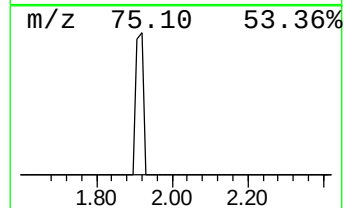
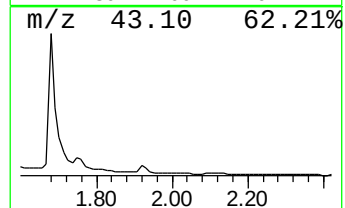
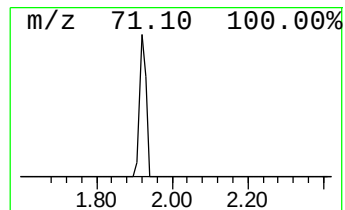
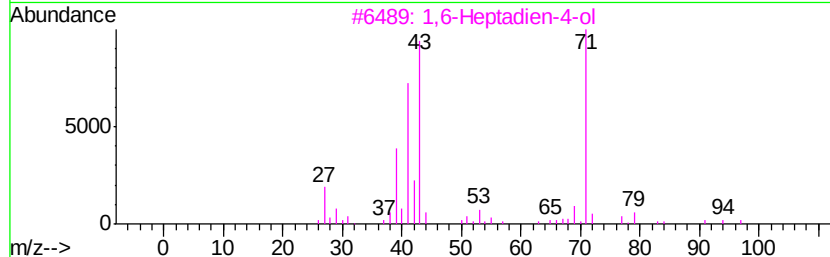
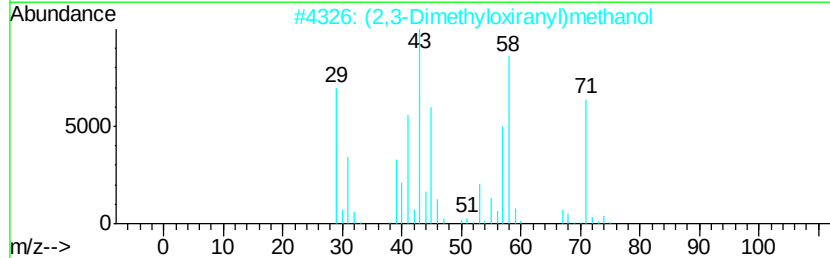
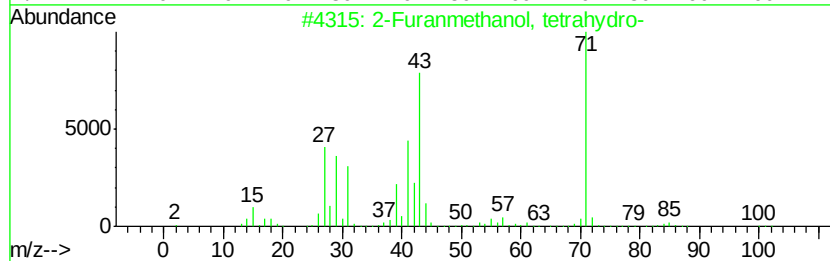
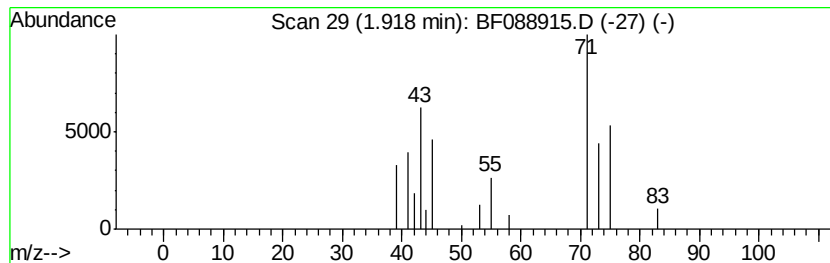
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown1.92 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.92	8.37 ng	157204	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Furanmethanol, tetrahydro-	102	C5H10O2	000097-99-4	9
2			(2,3-Dimethyloxiranyl)methanol	102	C5H10O2	1000306-71-8	9
3			1,6-Heptadien-4-ol	112	C7H12O	002883-45-6	9
4			Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	9
5			Pantolactone	130	C6H10O3	000599-04-2	9



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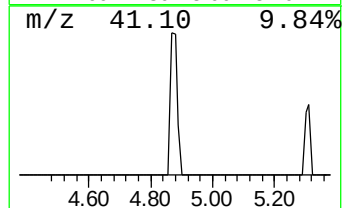
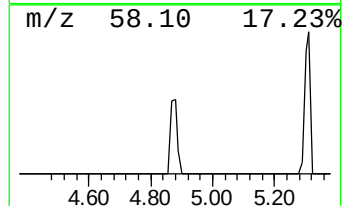
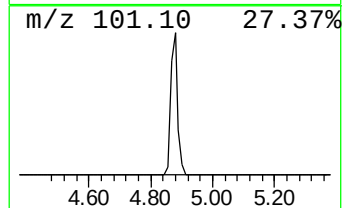
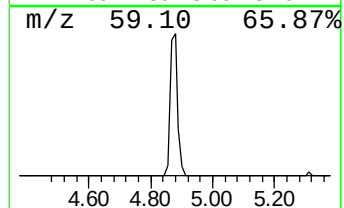
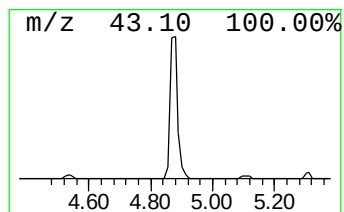
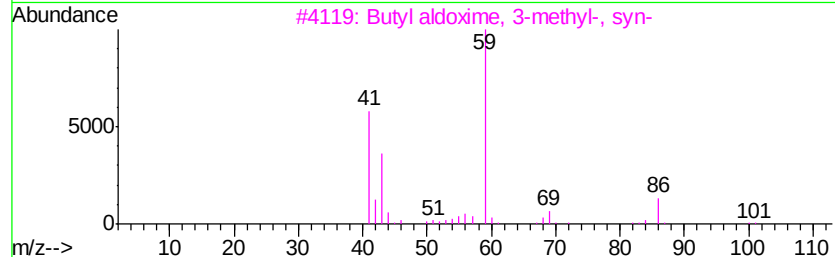
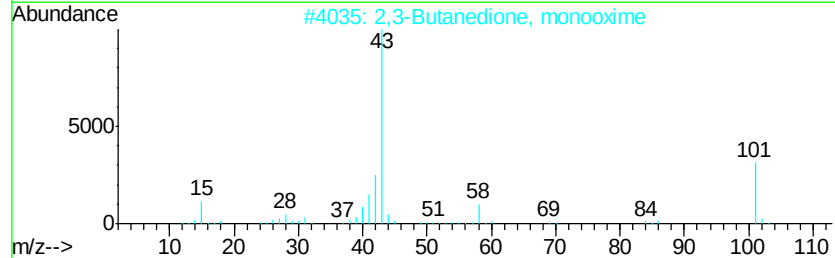
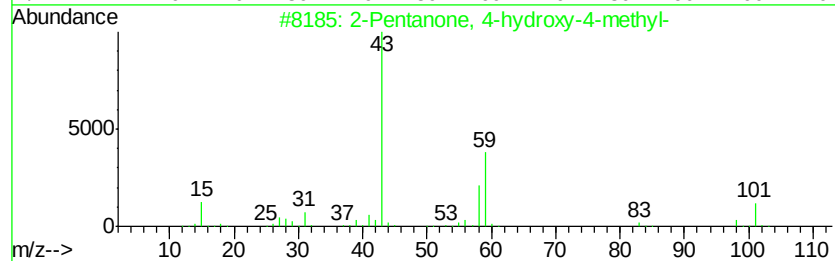
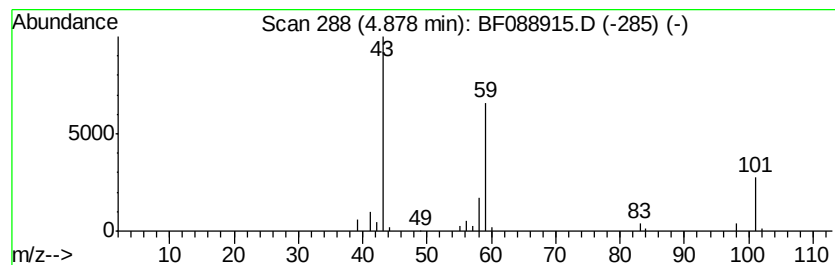
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	5.15 ng	96683	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	16
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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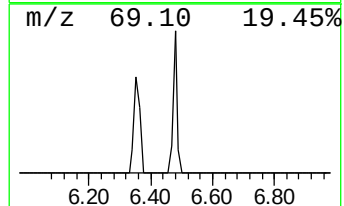
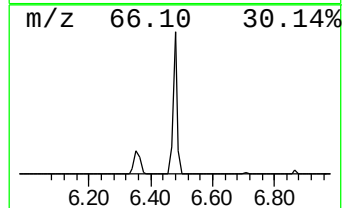
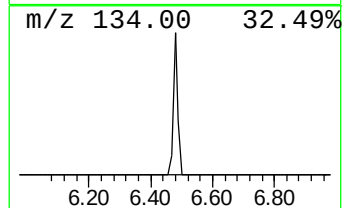
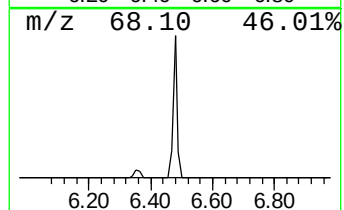
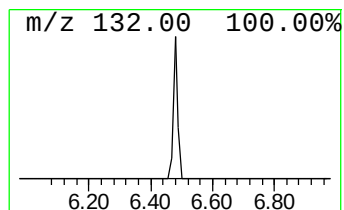
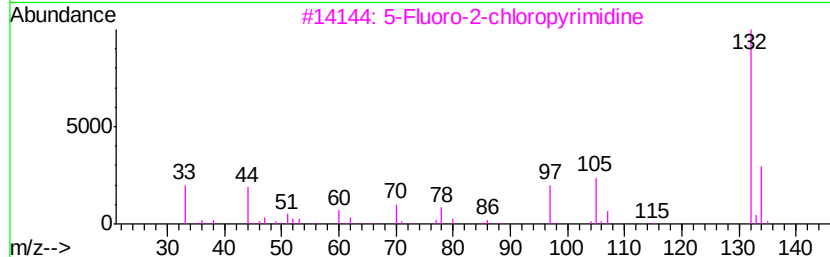
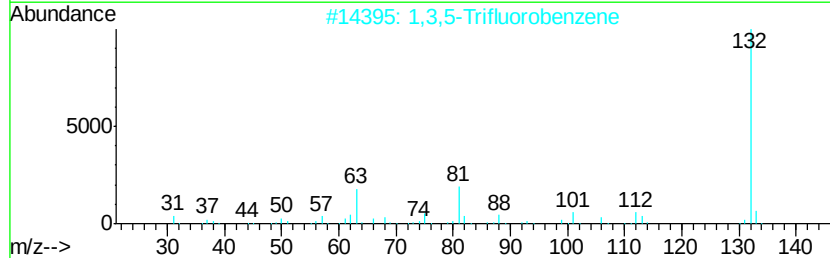
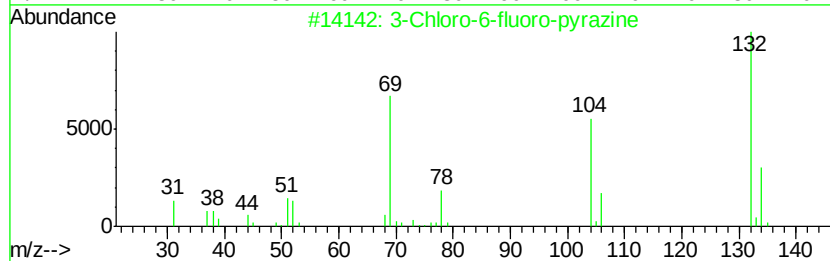
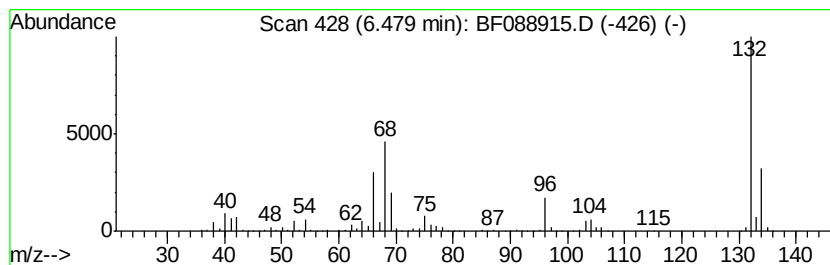
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	82.98 ng	1558830	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	14	
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12	
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10	
5	N-(3,4-Methylenedioxyphenyl)isop...	267	C17H17NO2	1000378-96-6	10	



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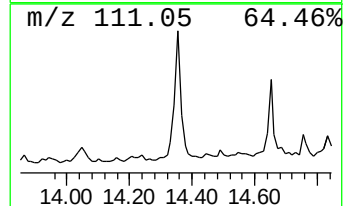
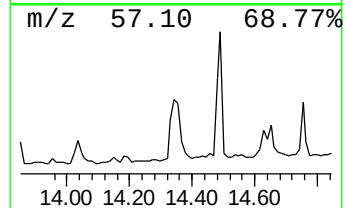
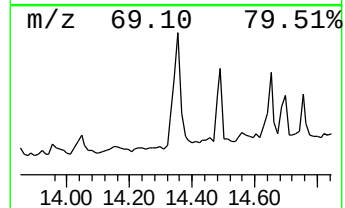
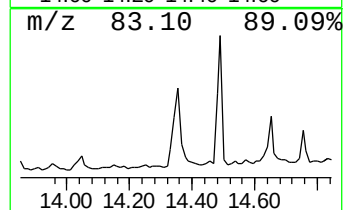
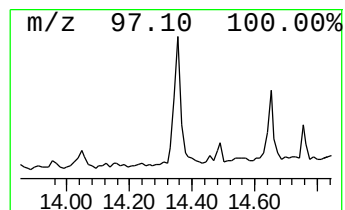
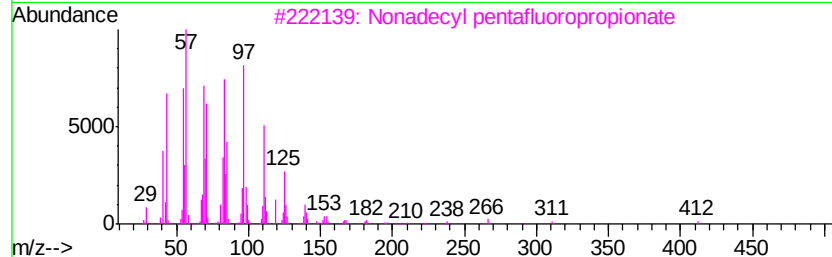
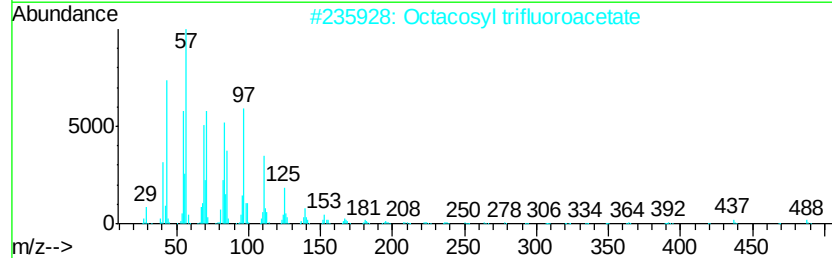
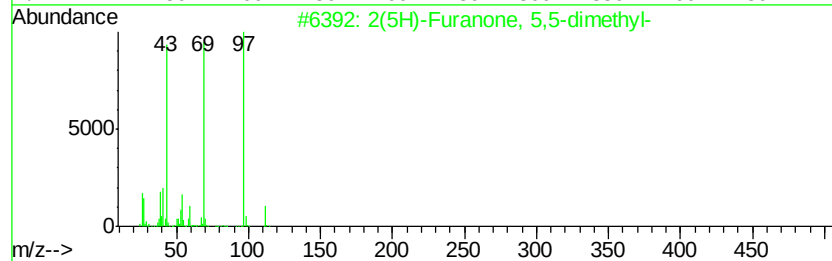
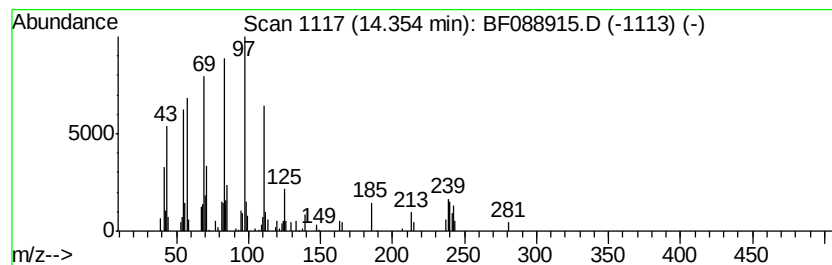
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown14.35 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.35	5.10 ng	145252	Chrysene-d12	13.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(5H)-Furanone, 5,5-dimethyl-	112	C6H8O2	020019-64-1	38
2	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	15
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	11
4	Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	11
5	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	11



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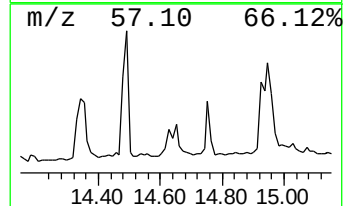
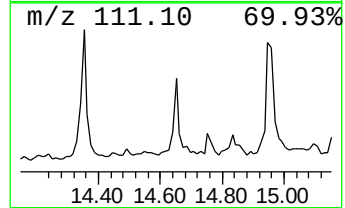
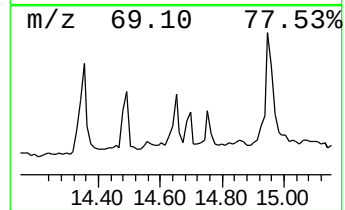
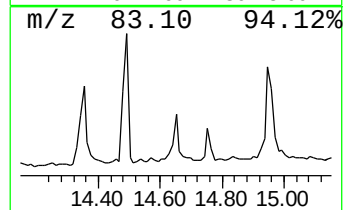
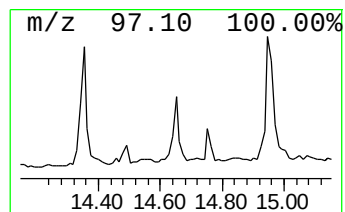
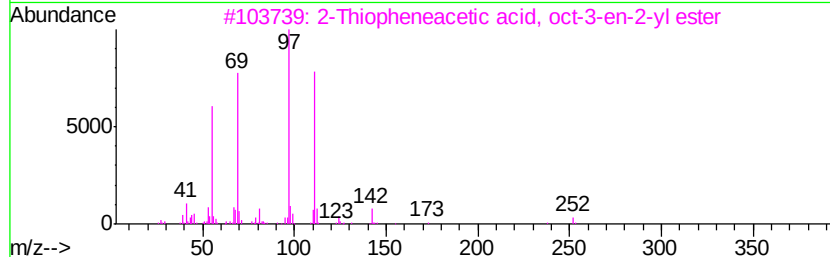
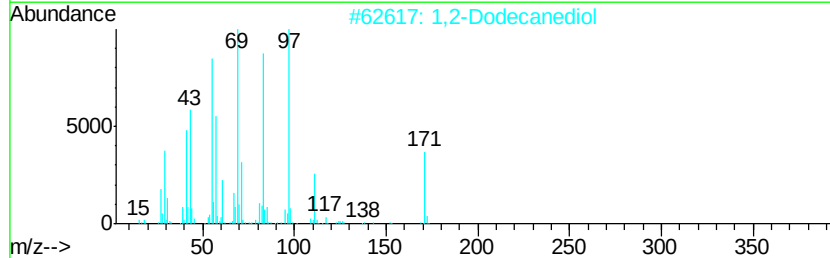
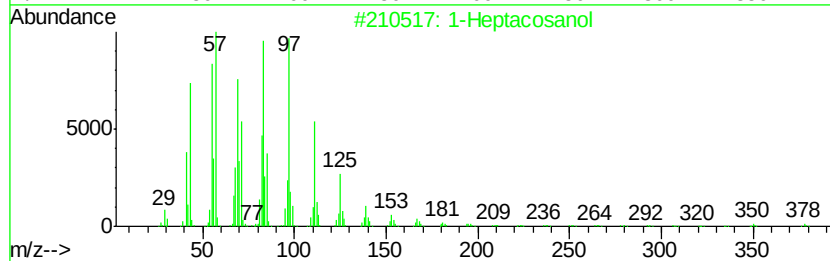
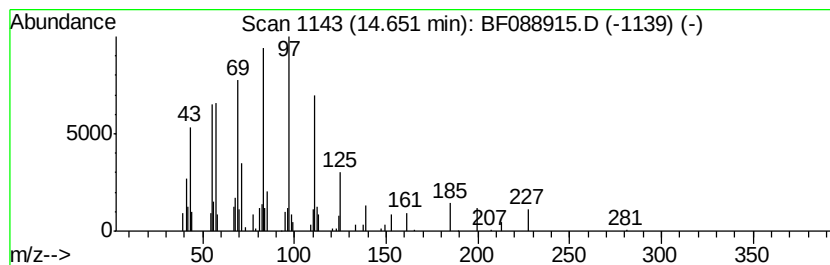
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ClientSampleId :
N8-B3(0-5)C

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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 9 1-Heptacosanol Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	2.86 ng	46794	Perylene-d12	15.21
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heptacosanol	396 C27H56O	002004-39-9	72
2	1,2-Dodecanediol	202 C12H26O2	001119-87-5	58
3	2-Thiopheneacetic acid, oct-3-en...	252 C14H20O2S	1000299-38-6	46
4	Cyclohexanecarboxylic acid, 4-pe...	338 C22H42O2	1000280-60-1	25
5	Cyclohexanecarboxylic acid, 3-pe...	338 C22H42O2	1000280-60-0	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071116\
Data File : BF088915.D
Acq On : 11 Jul 2016 22:49
Operator : UM/SJ
Sample : H3921-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N8-B3(0-5)C

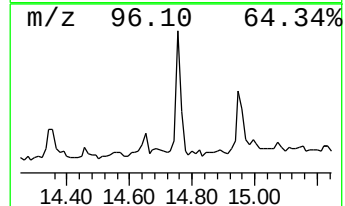
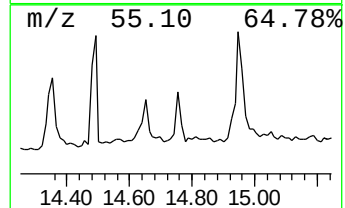
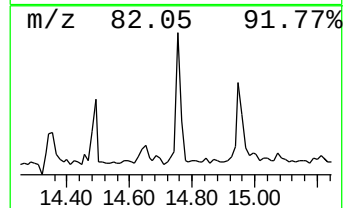
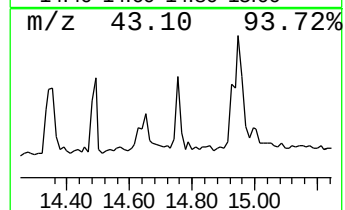
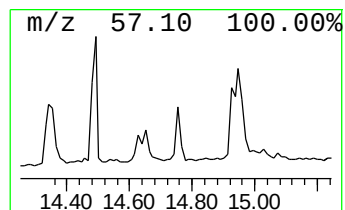
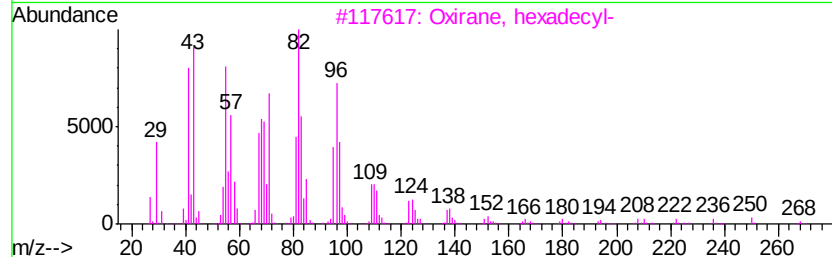
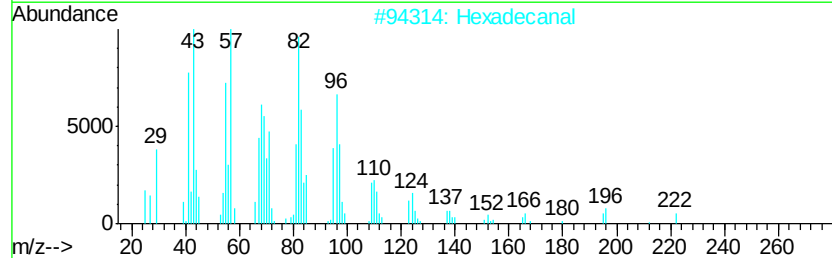
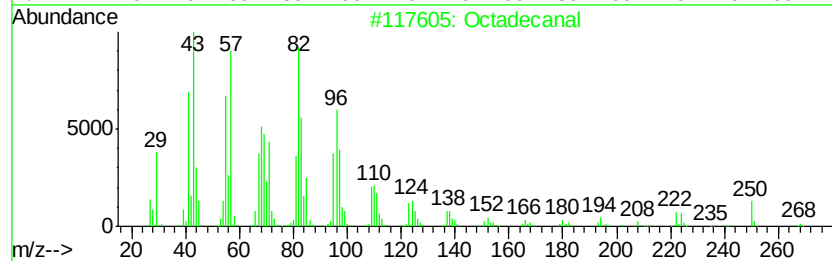
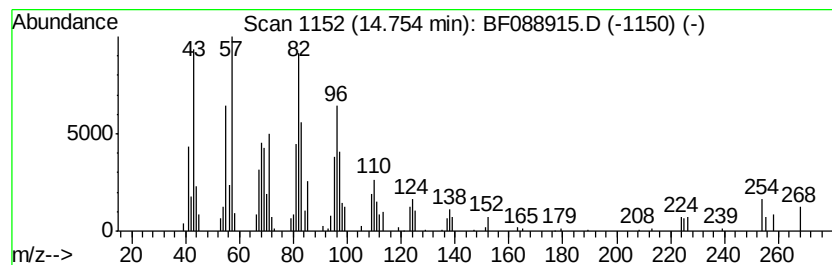
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanal Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	3.12 ng	51078	Perylene-d12	15.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	91
2			Hexadecanal	240	C16H32O	000629-80-1	91
3			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
4			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87
5			Heptadecanal	254	C17H34O	1000376-70-0	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088915.D
Acq On : 11 Jul 2016 22:49
Operator : UM/SJ
Sample : H3921-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

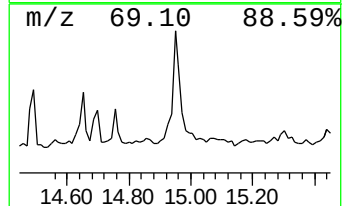
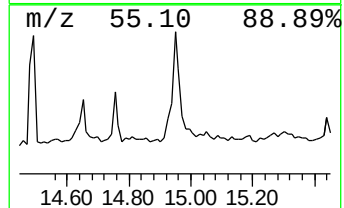
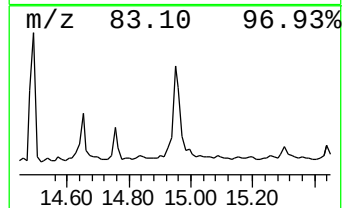
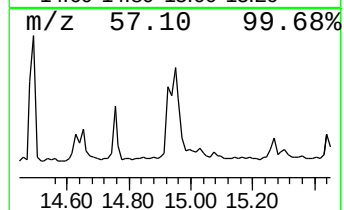
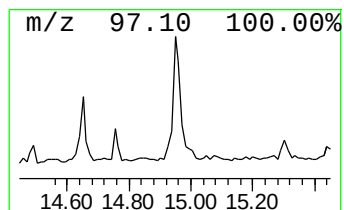
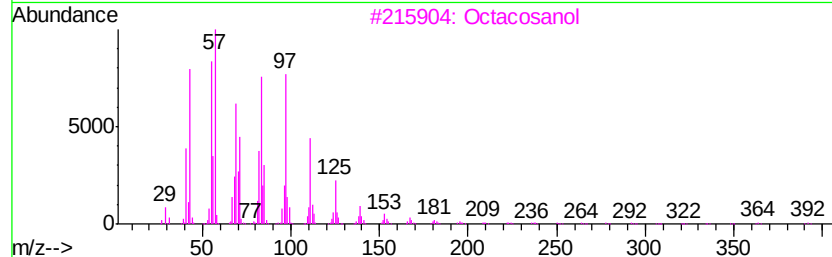
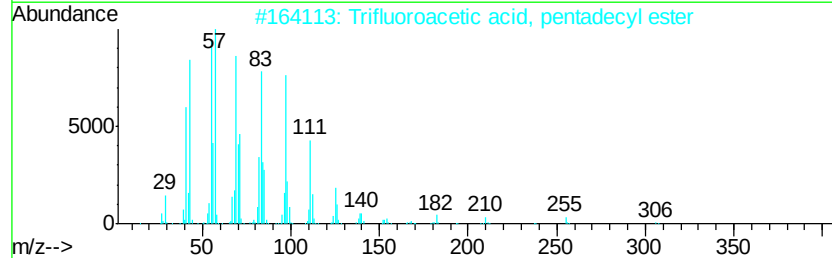
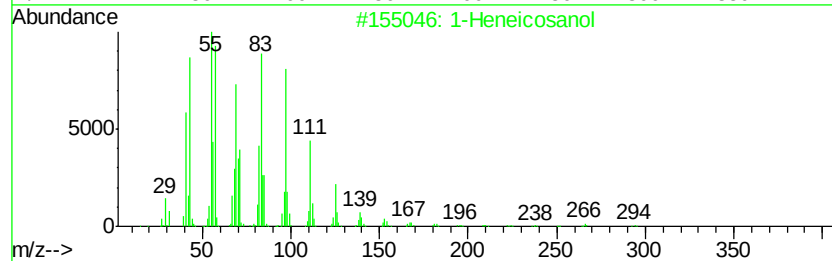
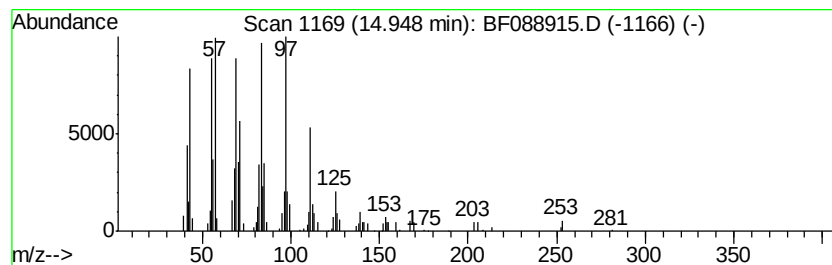
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.95	10.88 ng	178041	Perylene-d12	15.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3	Octacosanol	410	C28H58O	000557-61-9	93
4	1-Heptacosanol	396	C27H56O	002004-39-9	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071116\
Data File : BF088915.D
Acq On : 11 Jul 2016 22:49
Operator : UM/SJ
Sample : H3921-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

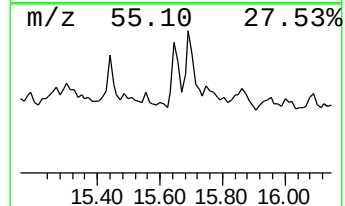
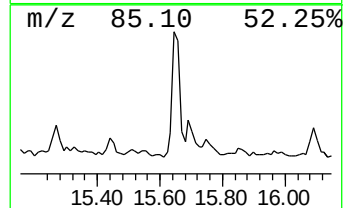
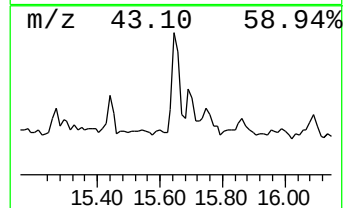
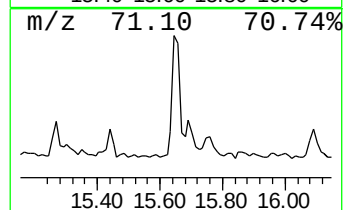
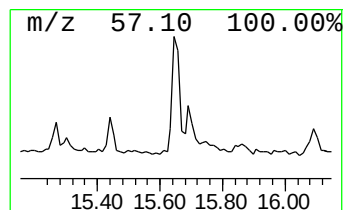
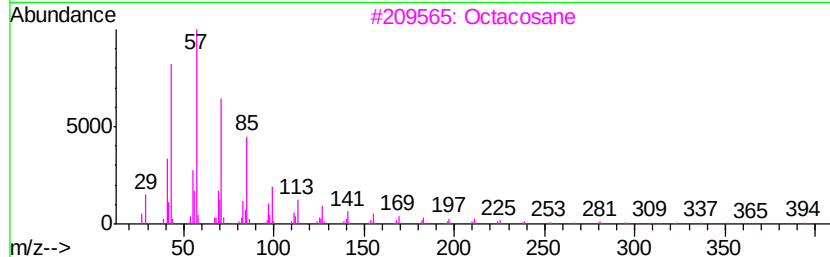
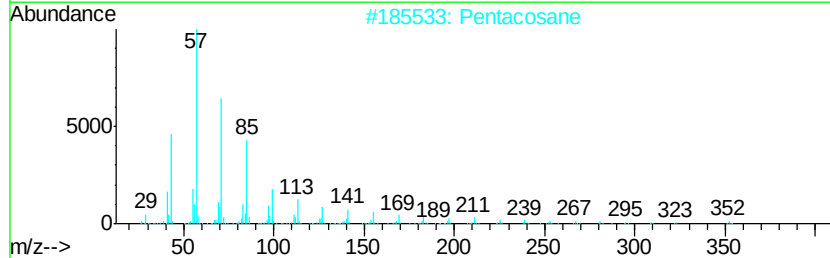
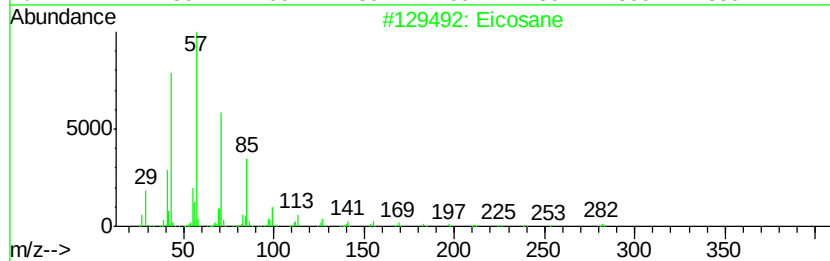
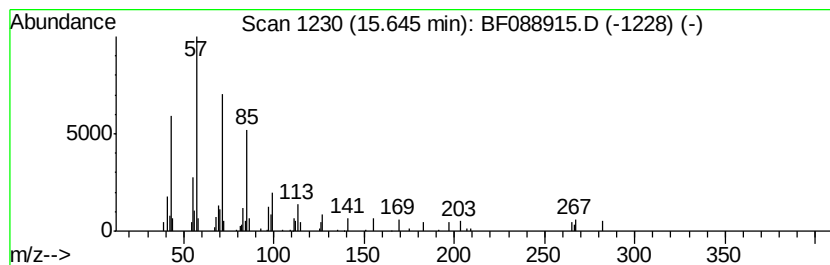
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.65	3.71 ng	60659	Perylene-d12	15.21
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	95
2	Pentacosane	352 C25H52	000629-99-2	90
3	Octacosane	394 C28H58	000630-02-4	87
4	Triacontane	422 C30H62	000638-68-6	87
5	Hexacosane	366 C26H54	000630-01-3	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088915.D
Acq On : 11 Jul 2016 22:49
Operator : UM/SJ
Sample : H3921-11
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Instrument :
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ClientSampleId :
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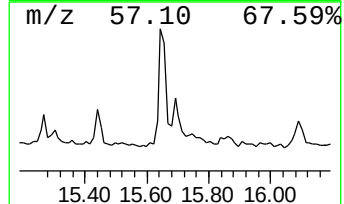
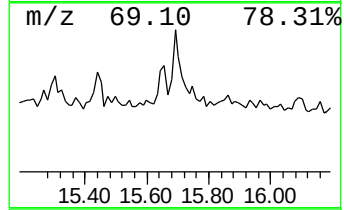
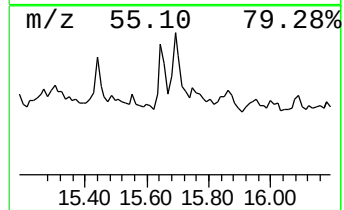
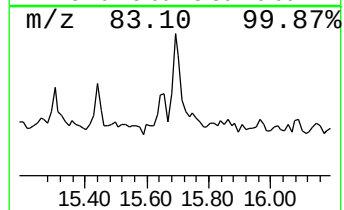
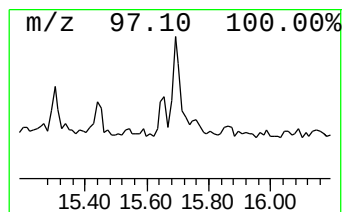
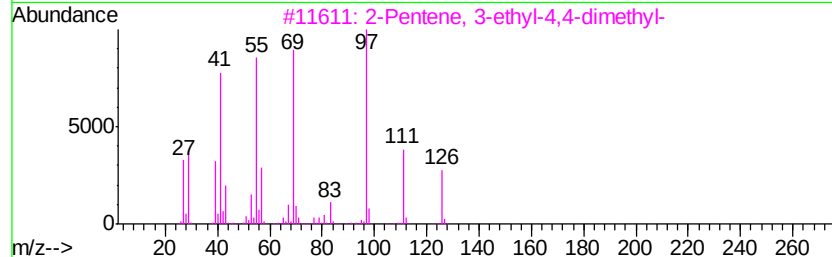
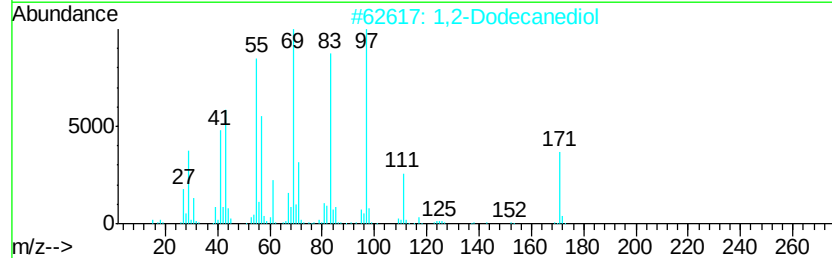
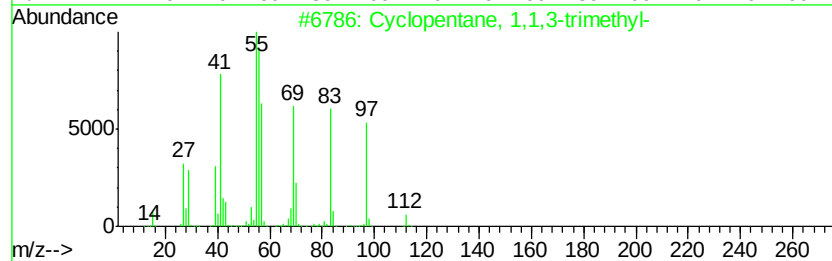
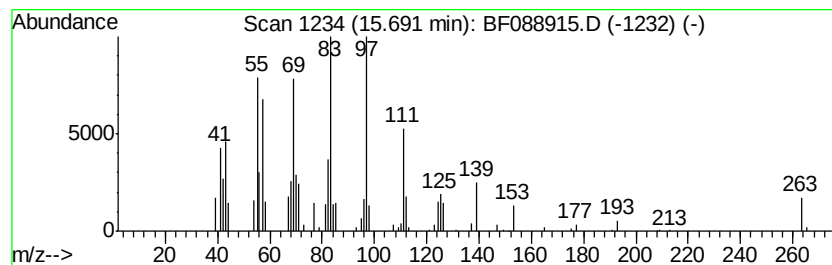
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Cyclopentane, 1,1,3-trimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	2.94 ng	48127	Perylene-d12	15.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	64
2		1,2-Dodecanediol	202	C12H26O2	001119-87-5	53
3		2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	46
4		Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	35
5		Cyclohexane, 1,2,3-trimethyl-, (...	126	C9H18	001678-81-5	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088915.D
Acq On : 11 Jul 2016 22:49
Operator : UM/SJ
Sample : H3921-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
N8-B3(0-5)C

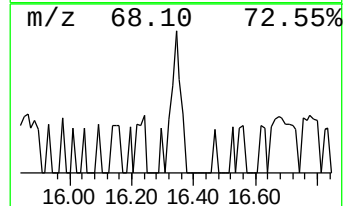
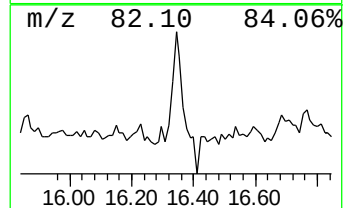
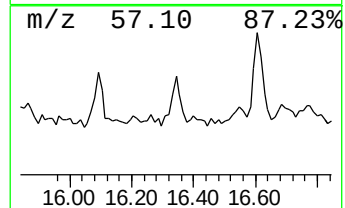
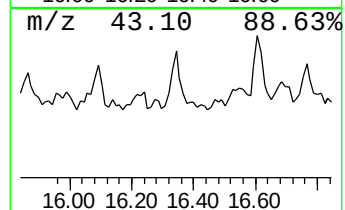
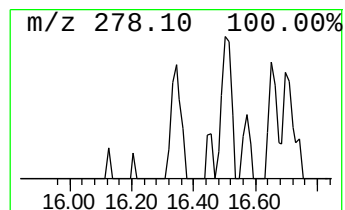
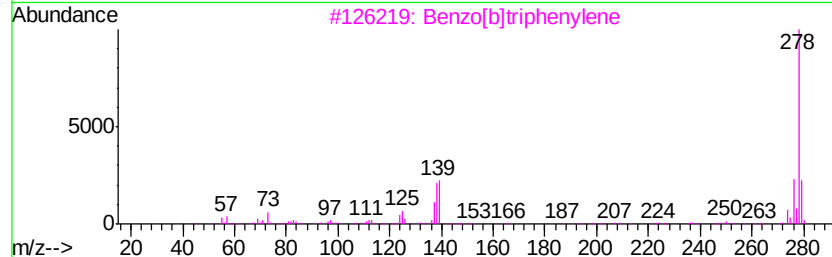
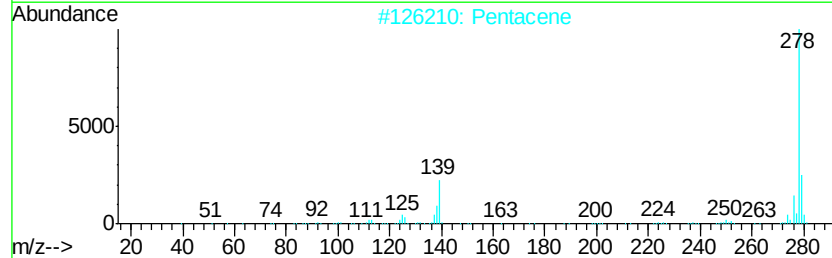
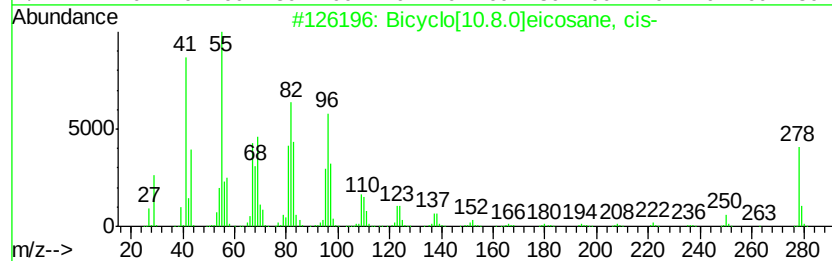
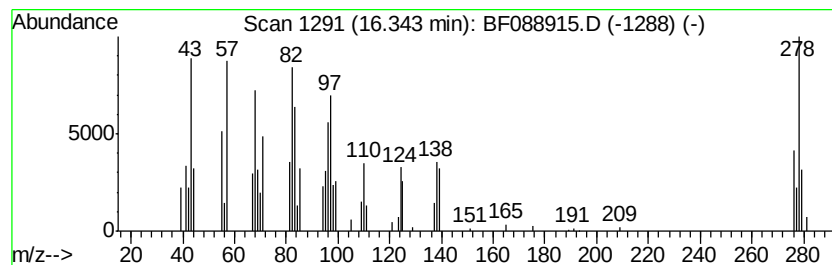
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown16.34 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.34	2.86 ng	46772	Perylene-d12	15.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	43
2			Pentacene	278	C22H14	000135-48-8	38
3			Benzo[b]triphenylene	278	C22H14	000215-58-7	27
4			Hexadecanal	240	C16H32O	000629-80-1	25
5			Pentadecanal-	226	C15H30O	002765-11-9	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071116\
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Acq On : 11 Jul 2016 22:49
Operator : UM/SJ
Sample : H3921-11
Misc :
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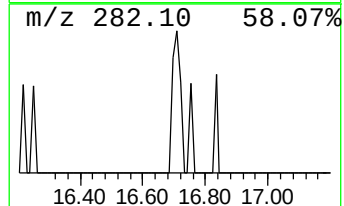
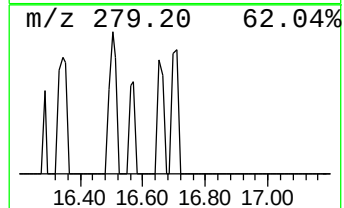
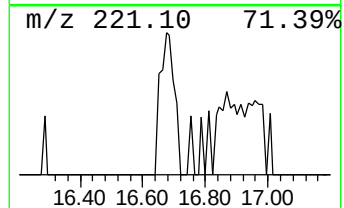
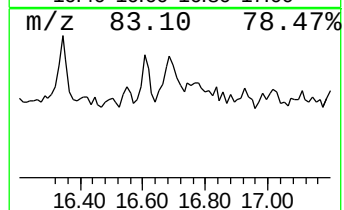
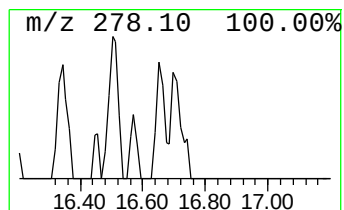
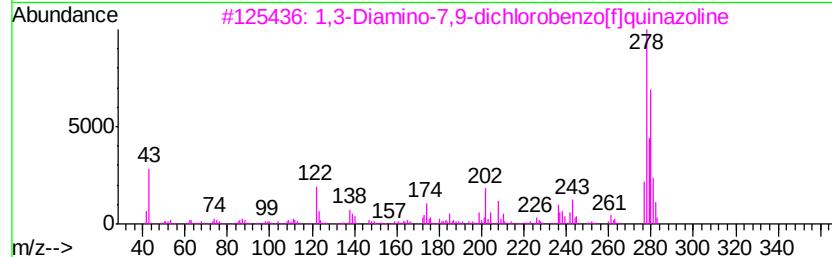
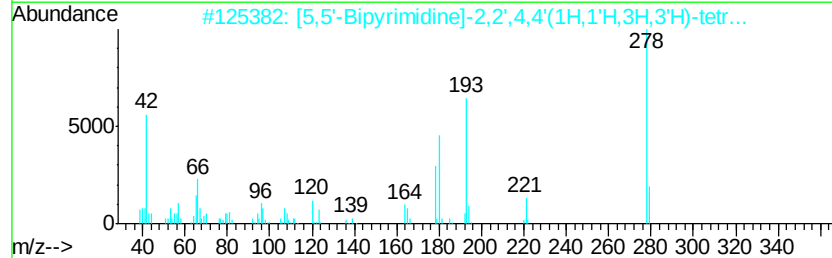
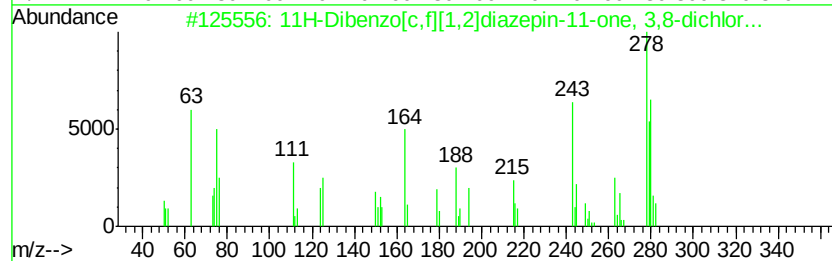
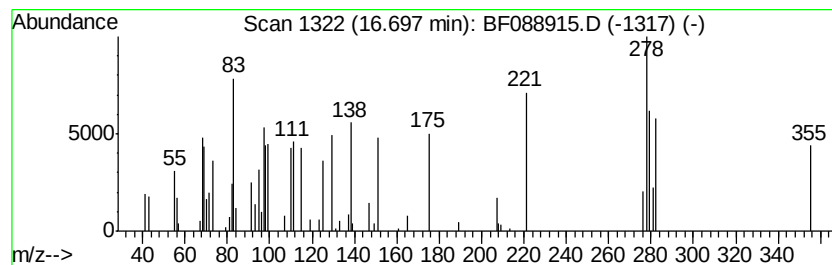
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown16.70 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.70	2.89 ng	47325	Perylene-d12	15.21		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		11H-Dibenzo[c,f][1,2]diazepin-11...	278	C13H8Cl2N2O	023469-53-6	25
2		[5,5'-Bipyrimidine]-2,2',4,4'-(1H...	278	C12H14N4O4	007033-42-3	10
3		1,3-Diamino-7,9-dichlorobenzo[f]...	278	C12H8Cl2N4	037521-58-7	10
4		10H-Phenoxaphosphine, 8-fluoro-1...	278	C14H12F03P	037041-13-7	10
5		[1,2,4]Oxadiazole-5-carboxylic a...	278	C13H14N2O5	1000316-89-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071116\
Data File : BF088915.D
Acq On : 11 Jul 2016 22:49
Operator : UM/SJ
Sample : H3921-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N8-B3(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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					#	RT	Resp	Conc
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unknown6.48	6.48	83.0	ng	1558830	1	6.71	375698	20.0
unknown14.35	14.35	5.1	ng	145252	5	13.84	569733	20.0
1-Heptacosanol	14.65	2.9	ng	46794	6	15.21	327312	20.0
Octadecanal	14.75	3.1	ng	51078	6	15.21	327312	20.0
1-Heneicosanol	14.95	10.9	ng	178041	6	15.21	327312	20.0
Eicosane	15.65	3.7	ng	60659	6	15.21	327312	20.0
Cyclopentane, 1,1...	15.69	2.9	ng	48127	6	15.21	327312	20.0
unknown16.34	16.34	2.9	ng	46772	6	15.21	327312	20.0
unknown16.70	16.70	2.9	ng	47325	6	15.21	327312	20.0
unknown16.79	16.79	3.3	ng	54341	6	15.21	327312	20.0