

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
 Data File : BF098901.D
 Acq On : 28 Sep 2017 11:51
 Operator : SJ/JU
 Sample : I5418-02
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2P-ENV-119-2(5-10)

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-BF092317.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	2.234	21	25	44	rVB2	138077	272894	6.48%	0.726%
2	2.363	45	47	61	rVB3	26422	60537	1.44%	0.161%
3	5.151	517	521	532	rBV	577502	777036	18.44%	2.068%
4	5.539	582	587	590	rBV	3371287	3725486	88.40%	9.914%
5	6.545	752	758	761	rVV	3367203	3772834	89.53%	10.039%
6	6.686	777	782	785	rBV	3794898	3782371	89.75%	10.065%
7	6.916	817	821	824	rBV	1103366	861407	20.44%	2.292%
8	7.075	843	848	851	rBV	3080986	2842658	67.46%	7.564%
9	7.481	911	917	920	rBV	2296140	2429819	57.66%	6.466%
10	7.545	925	928	932	rVB	55381	53453	1.27%	0.142%
11	8.198	1034	1039	1042	rBV	1333708	1175491	27.89%	3.128%
12	9.275	1216	1222	1225	rBV	4239145	4214127	100.00%	11.214%
13	9.663	1283	1288	1291	rBV	642515	560785	13.31%	1.492%
14	9.951	1333	1337	1341	rBV2	1459183	1296887	30.77%	3.451%
15	10.374	1406	1409	1412	rVB	80153	61600	1.46%	0.164%
16	10.745	1464	1472	1475	rBV	2409316	2427092	57.59%	6.458%
17	10.845	1485	1489	1500	rBV	92904	90426	2.15%	0.241%
18	11.292	1559	1565	1568	rBV	52639	46209	1.10%	0.123%
19	11.439	1586	1590	1593	rBV	1554123	1288430	30.57%	3.429%
20	11.957	1673	1678	1682	rBV	578516	544441	12.92%	1.449%
21	12.651	1792	1796	1804	rBV3	53081	110332	2.62%	0.294%
22	12.739	1807	1811	1818	rBV	294996	287403	6.82%	0.765%
23	13.027	1855	1860	1863	rBV2	3721398	3821594	90.69%	10.169%
24	13.551	1946	1949	1951	rBV	46345	42921	1.02%	0.114%
25	13.904	2006	2009	2013	rBV	251939	253179	6.01%	0.674%
26	14.045	2031	2033	2035	rBV	80133	67618	1.60%	0.180%
27	14.080	2035	2039	2042	rVV	988396	869873	20.64%	2.315%
28	14.462	2101	2104	2108	rVB3	49901	43645	1.04%	0.116%
29	14.533	2113	2116	2120	rBV2	43900	49494	1.17%	0.132%
30	14.698	2140	2144	2147	rBV	327876	294825	7.00%	0.785%
31	14.845	2164	2169	2171	rBV3	31491	44197	1.05%	0.118%
32	14.927	2180	2183	2189	rVB	120661	122673	2.91%	0.326%
33	15.192	2225	2228	2231	rBV	49569	51047	1.21%	0.136%
34	15.568	2287	2292	2300	rVB	581041	793168	18.82%	2.111%

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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	16.033	2366	2371	2375	rBV	65734	100454	2.38%	0.267%
36	16.551	2454	2459	2467	rVB2	72366	133452	3.17%	0.355%
37	17.162	2559	2563	2570	rVB2	48682	88684	2.10%	0.236%
38	17.886	2681	2686	2696	rVB4	49985	121367	2.88%	0.323%

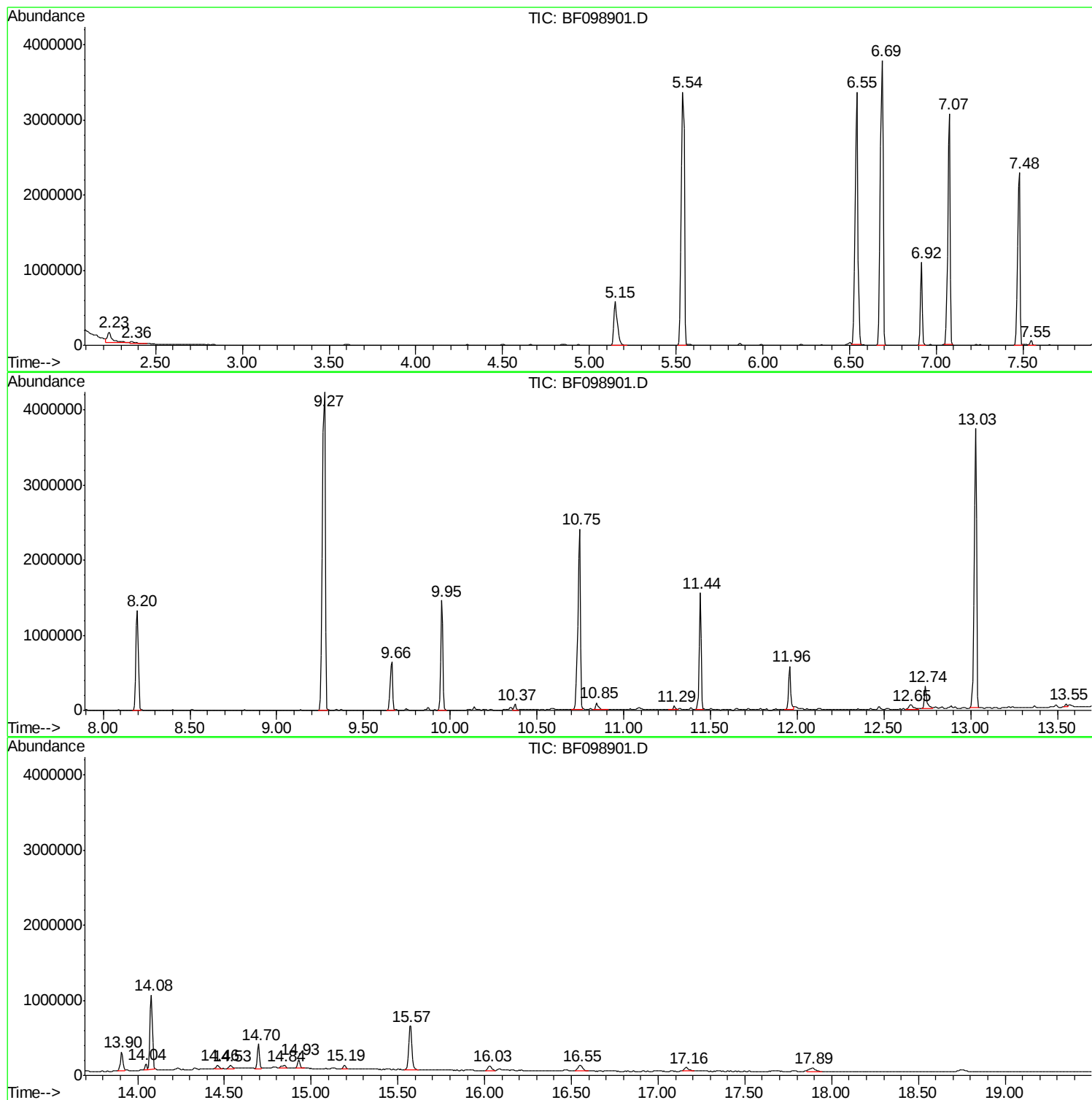
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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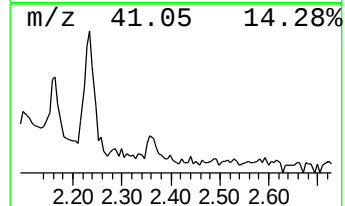
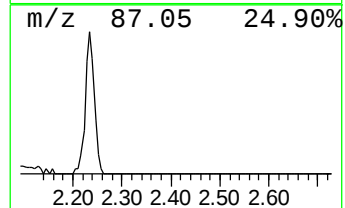
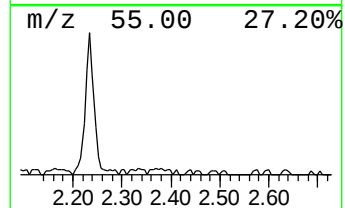
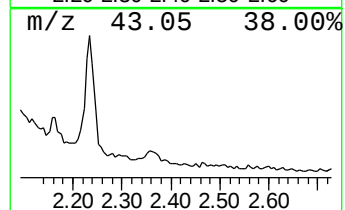
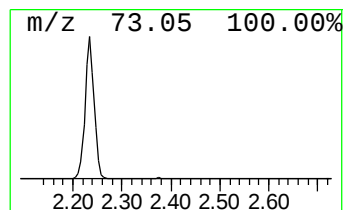
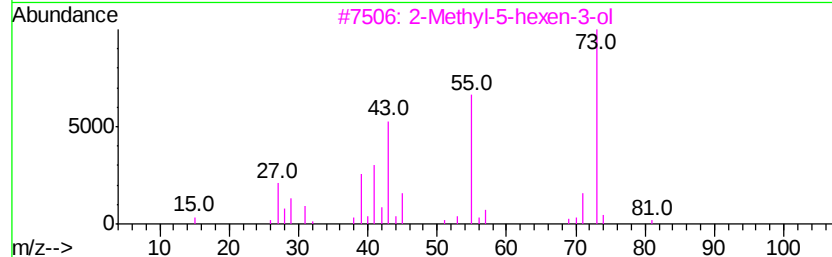
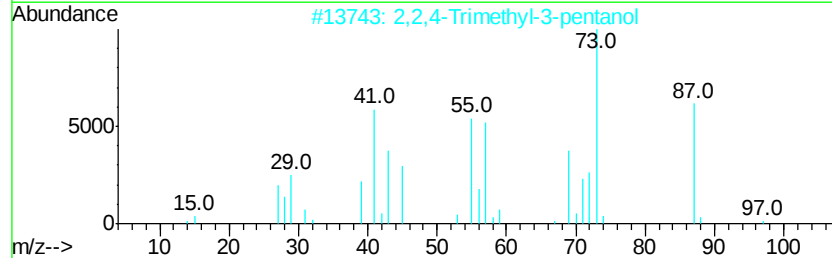
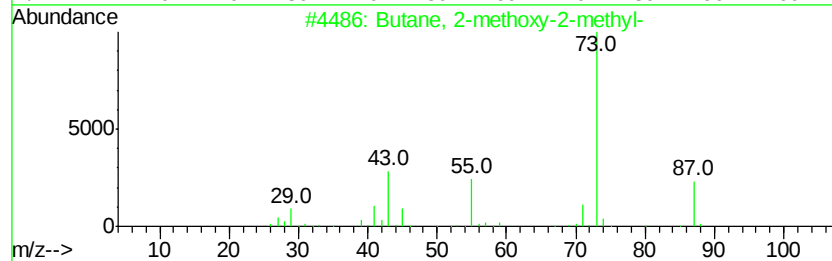
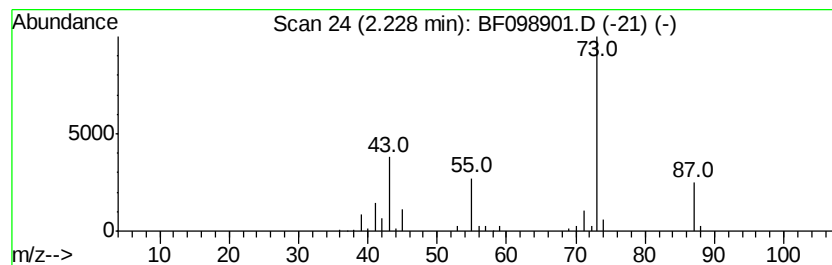
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	6.34 ng	272894	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	12
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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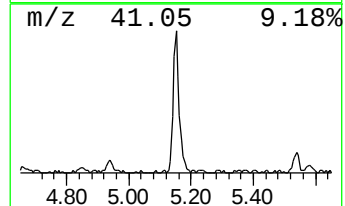
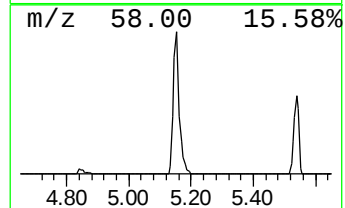
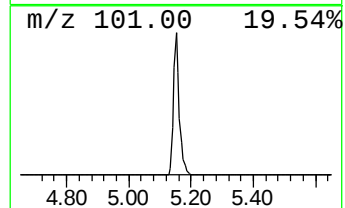
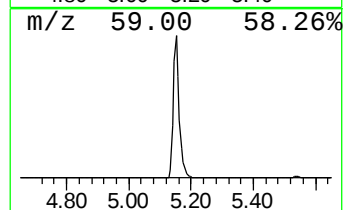
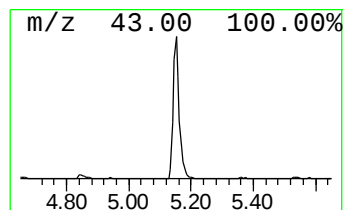
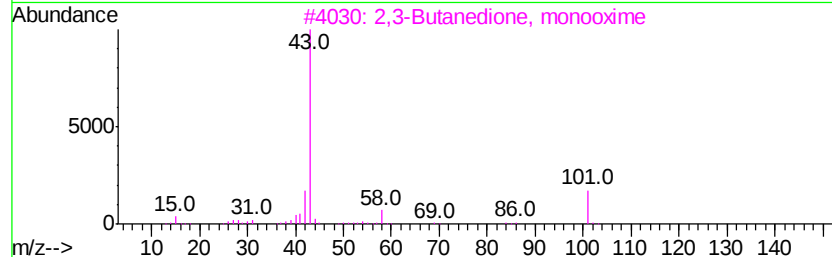
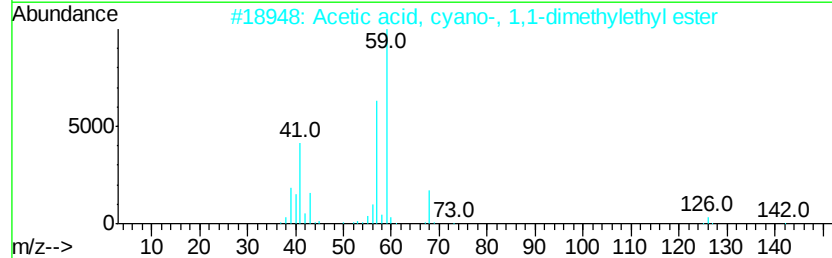
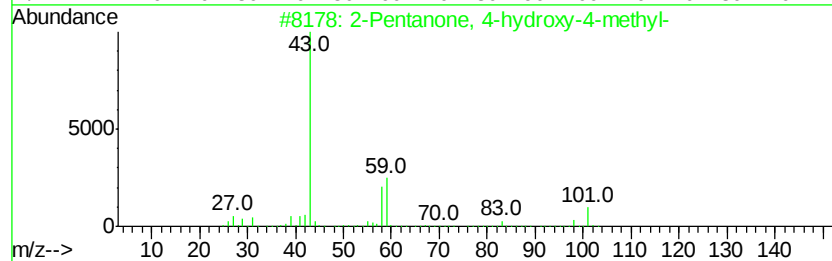
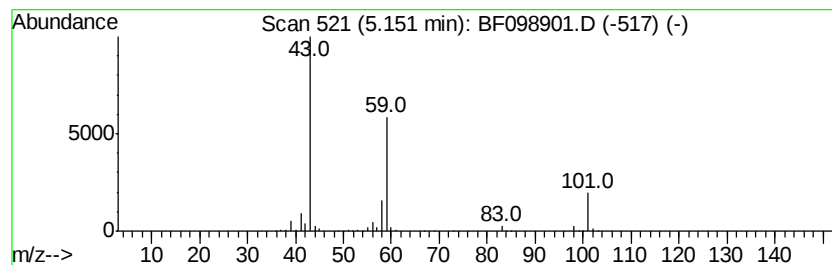
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	18.04 ng	777036	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9



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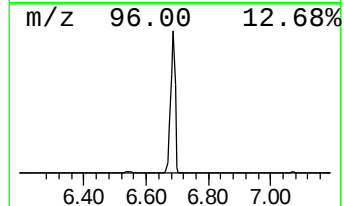
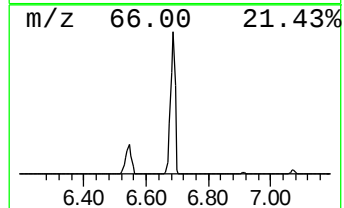
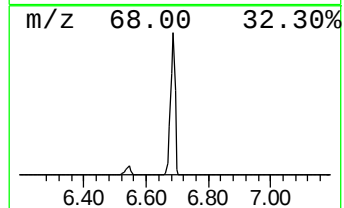
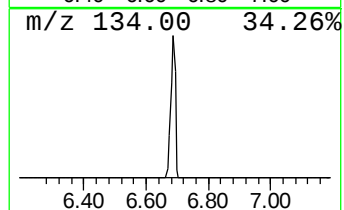
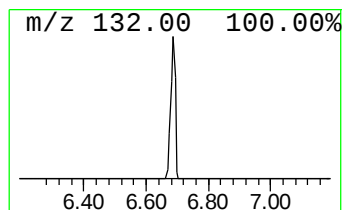
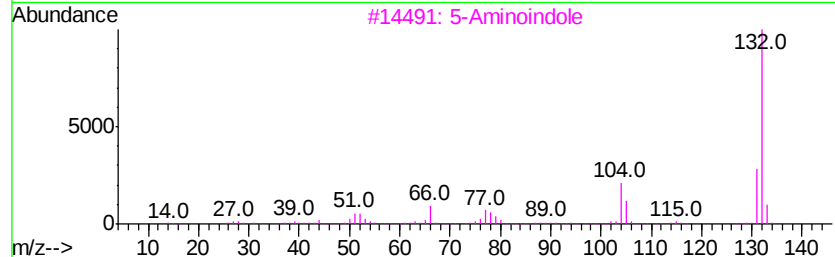
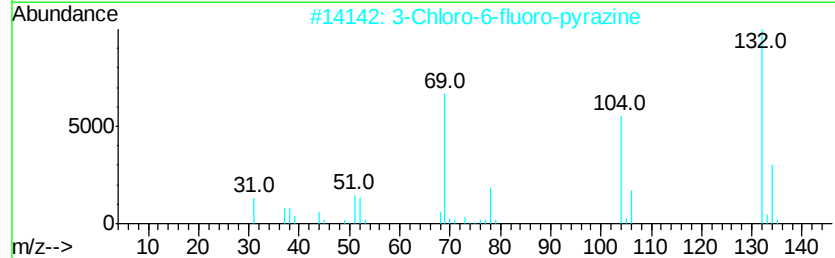
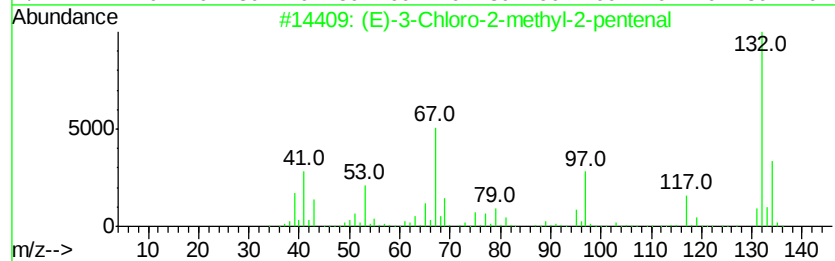
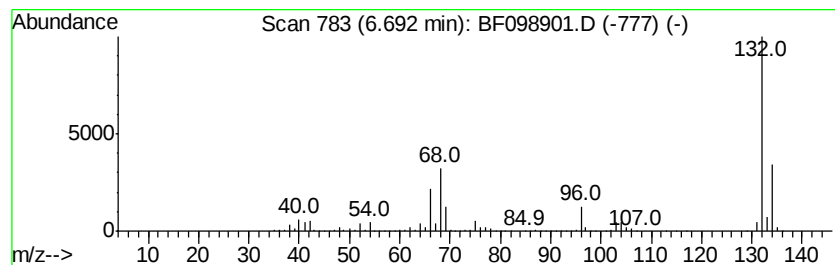
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	87.82 ng	3782370	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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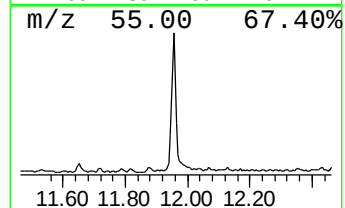
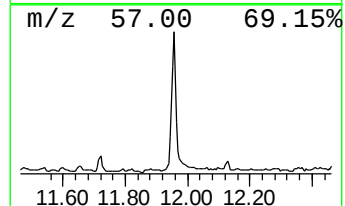
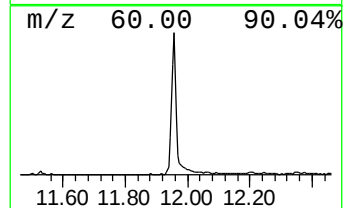
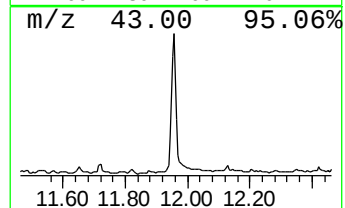
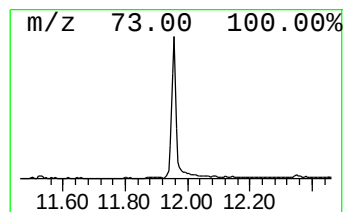
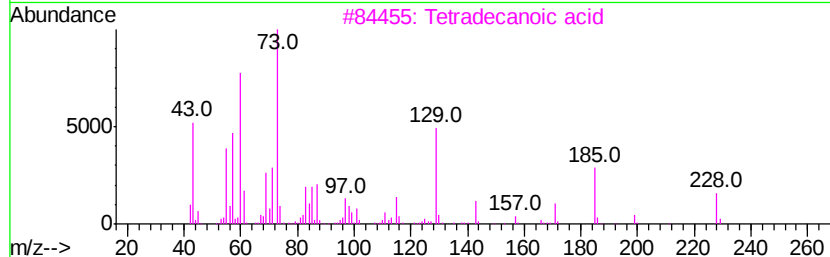
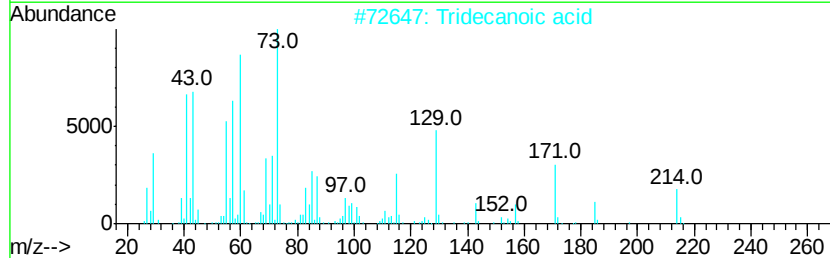
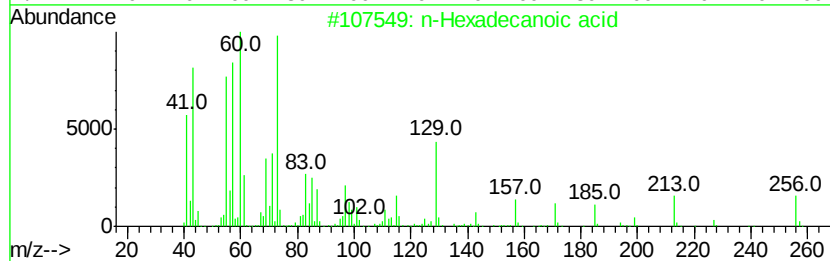
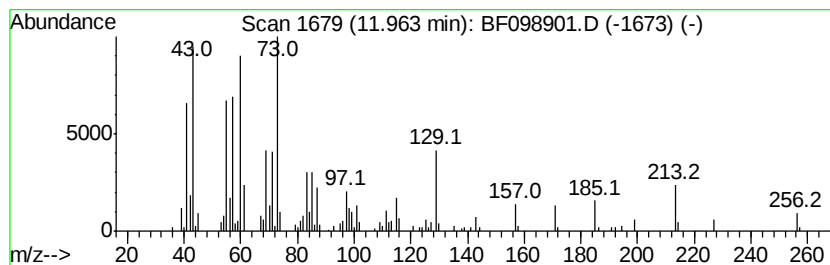
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.96	8.45 ng	544441	Phenanthrene-d10	11.44	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70



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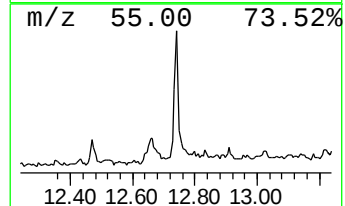
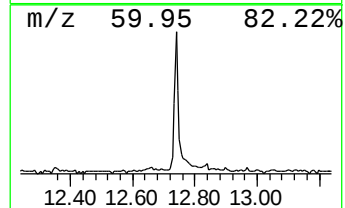
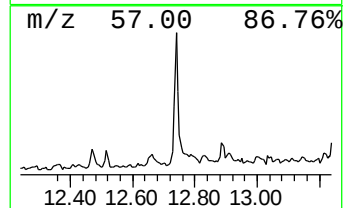
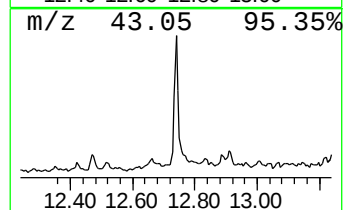
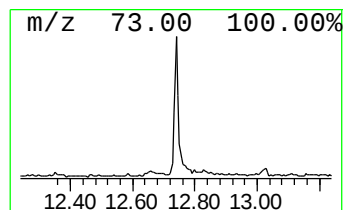
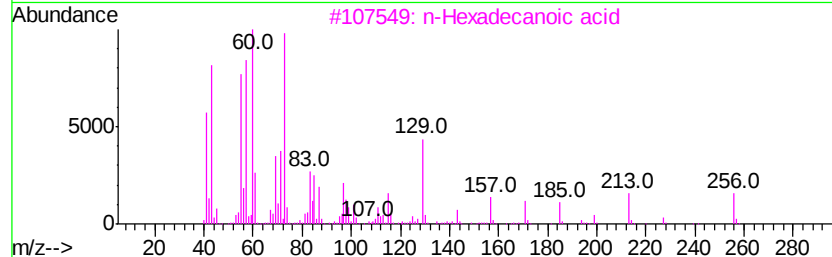
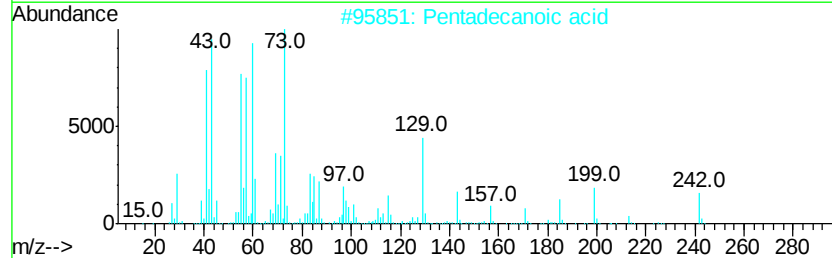
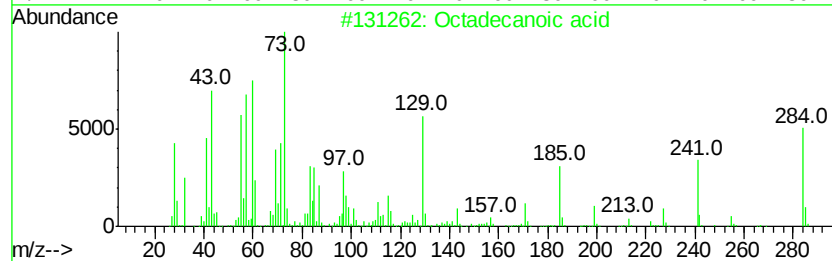
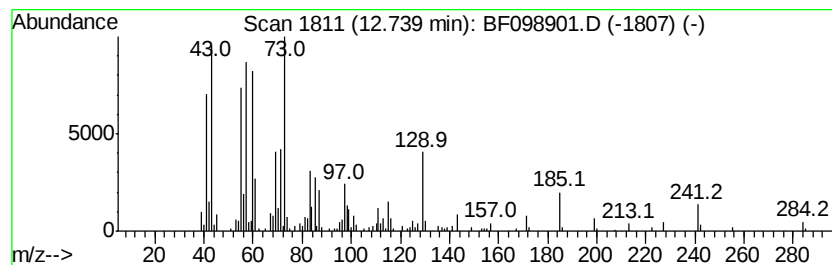
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	4.46 ng	287403	Phenanthrene-d10	11.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	86
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098901.D
Acq On : 28 Sep 2017 11:51
Operator : SJ/JU
Sample : I5418-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

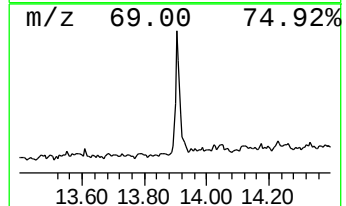
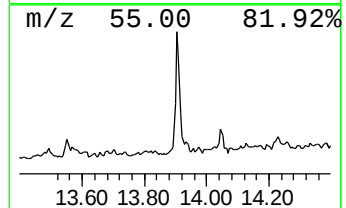
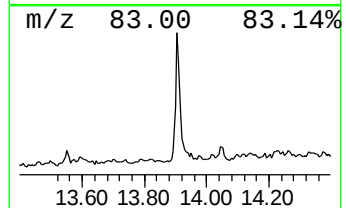
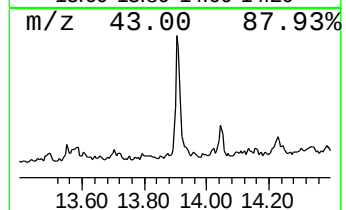
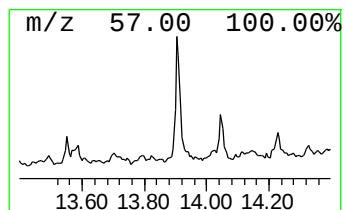
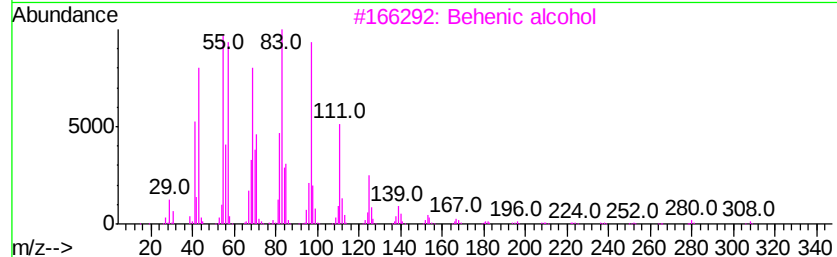
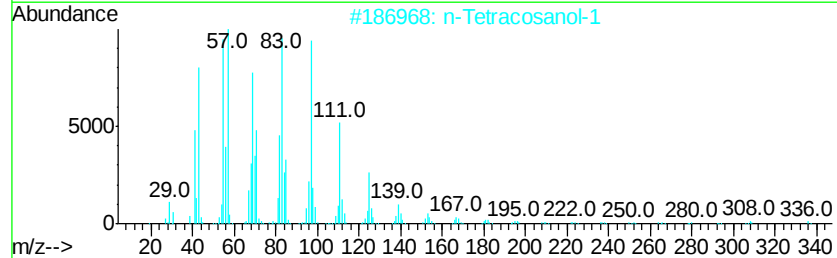
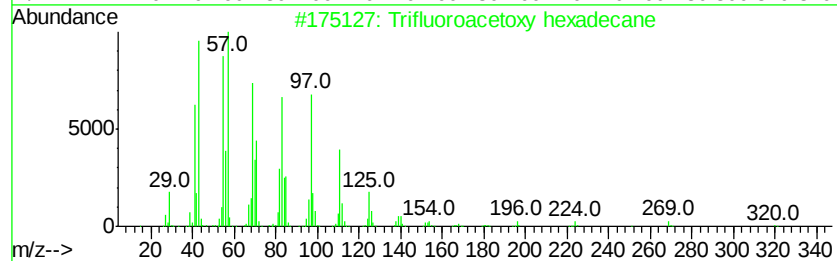
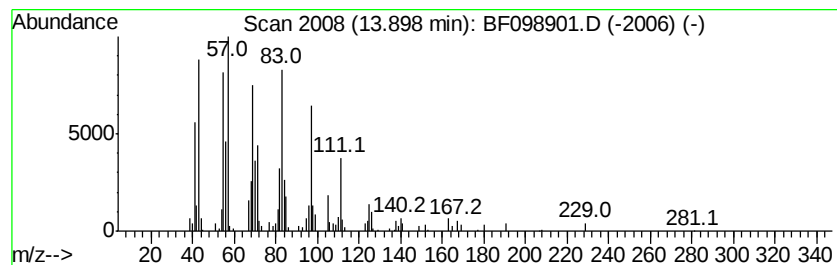
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ClientSampleId :
SASP2P-ENV-119-2(5-10)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.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 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	5.82 ng	253179	Chrysene-d12	14.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098901.D
Acq On : 28 Sep 2017 11:51
Operator : SJ/JU
Sample : I5418-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

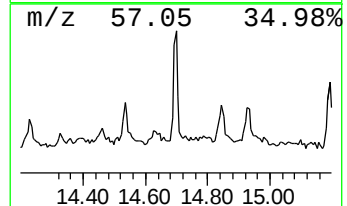
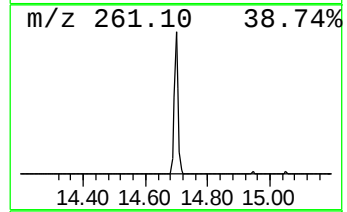
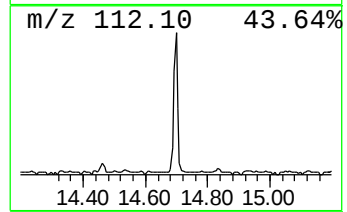
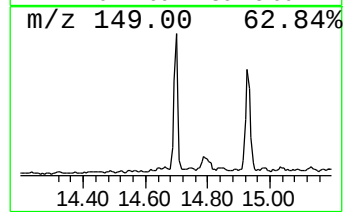
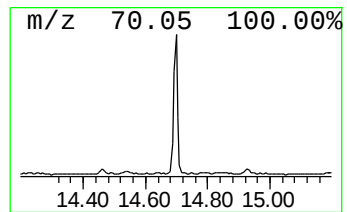
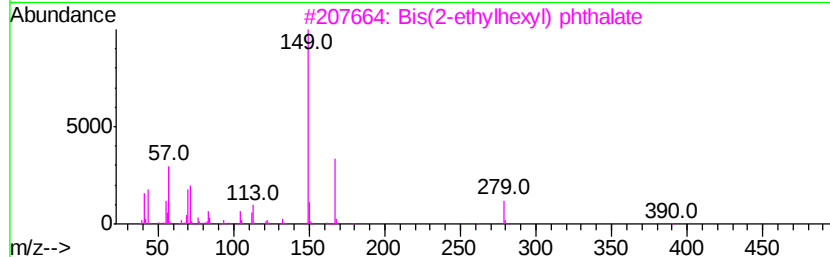
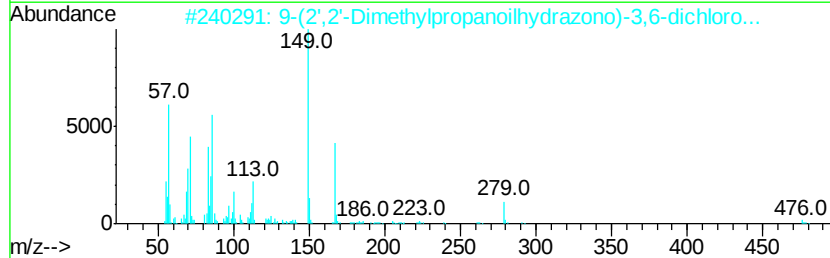
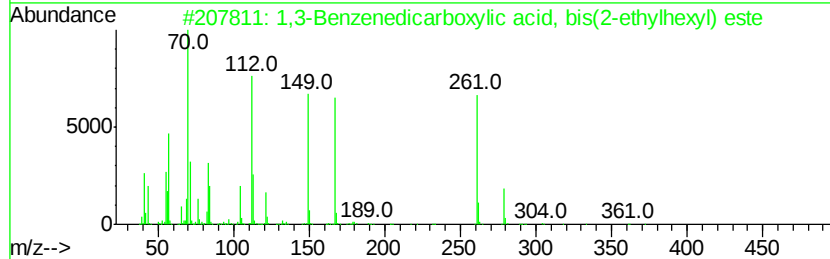
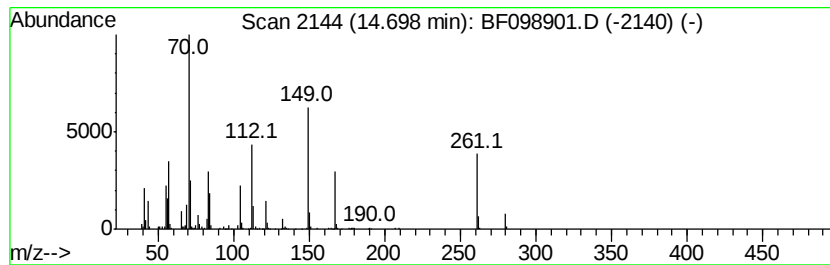
Instrument :
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ClientSampleId :
SASP2P-ENV-119-2(5-10)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,3-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.70	6.78 ng	294825	Chrysene-d12		14.08
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	58
2	9-(2',2'-Dimethylpropanoilhydraz...	576	C30H42Cl2N4O3	1000111-04-6	25
3	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	22
4	Diisooctyl phthalate	390	C24H38O4	000131-20-4	22
5	Phthalic acid, 3,5-difluoropheny...	418	C24H28F2O4	1000315-53-1	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098901.D
Acq On : 28 Sep 2017 11:51
Operator : SJ/JU
Sample : I5418-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

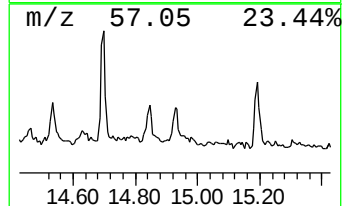
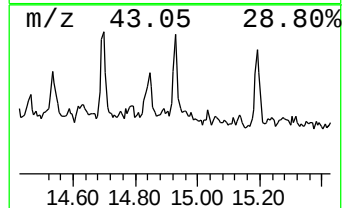
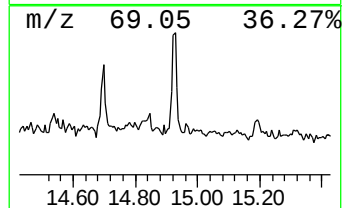
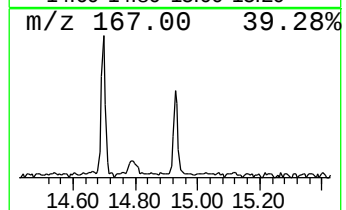
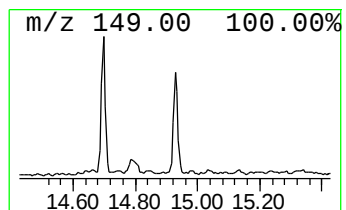
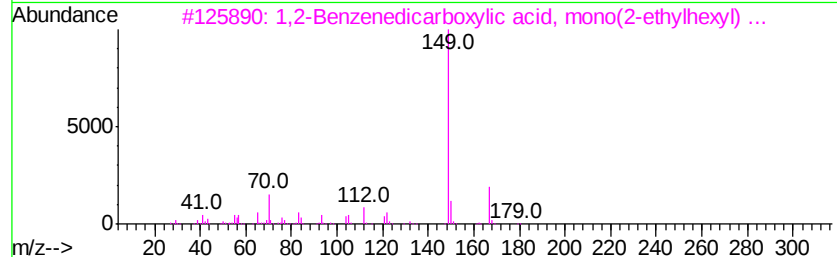
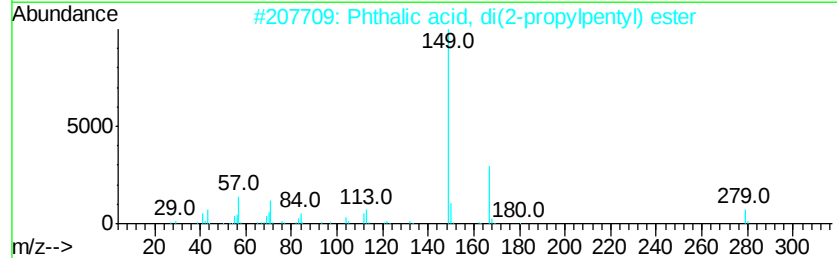
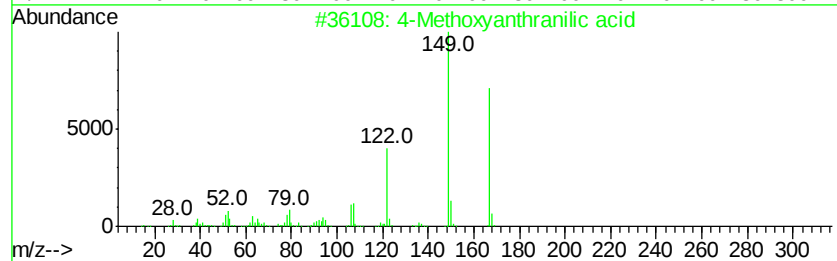
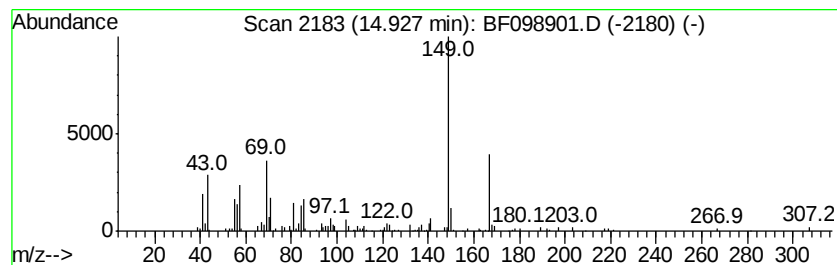
Instrument :
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ClientSampleId :
SASP2P-ENV-119-2(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 4-Methoxyanthranilic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.93	3.09 ng	122673	Perylene-d12	15.57		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methoxvanthranilic acid	167	C8H9NO3	004294-95-5	72	
2	Phthalic acid, di(2-propylpentyl...	390	C24H38O4	1000377-93-5	64	
3	1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	004376-20-9	64	
4	Dicyclohexyl phthalate	330	C20H26O4	000084-61-7	64	
5	Phthalic acid, monocyclohexyl ester	248	C14H16O4	007517-36-4	64	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098901.D
Acq On : 28 Sep 2017 11:51
Operator : SJ/JU
Sample : I5418-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-119-2(5-10)

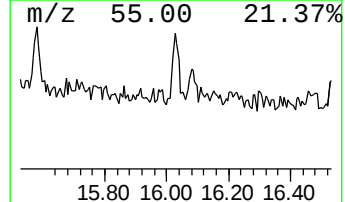
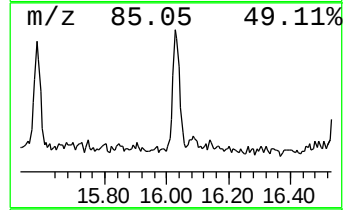
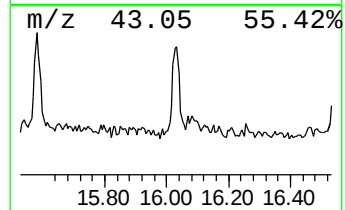
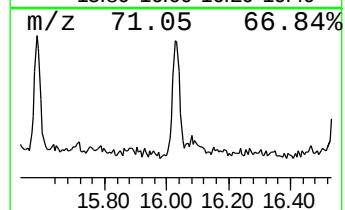
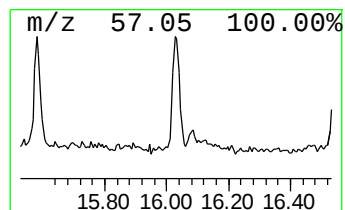
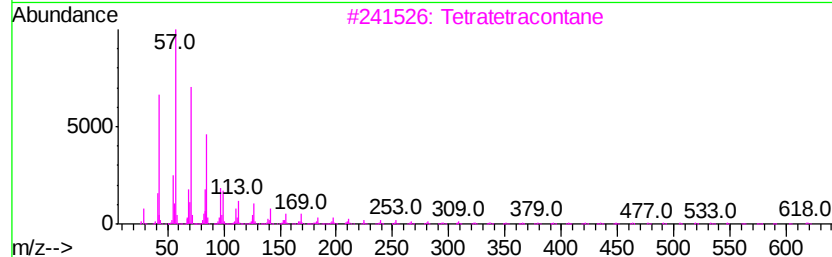
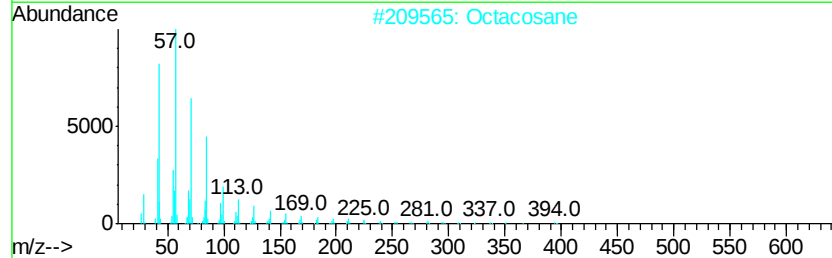
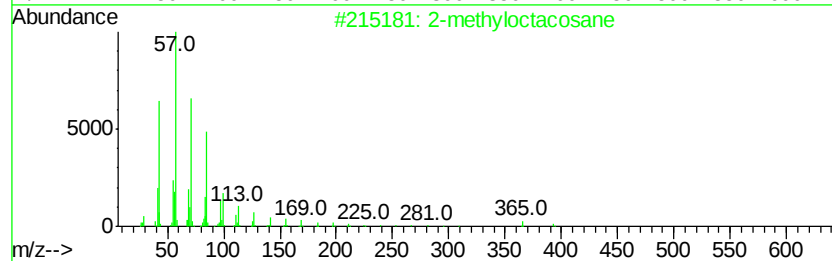
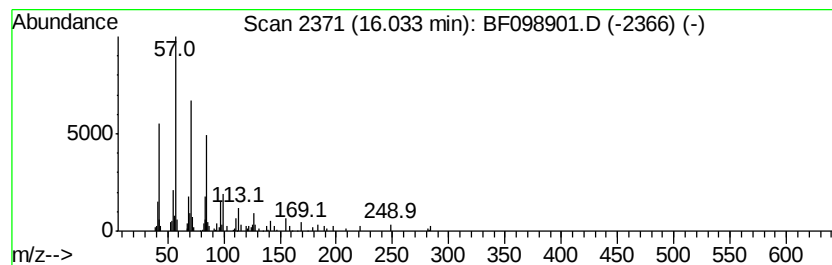
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-methyloctacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	2.53 ng	100454	Perylene-d12	15.57

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyloctacosane	408	C29H60	1000376-72-8	91
2			Octacosane	394	C28H58	000630-02-4	90
3			Tetratetracontane	619	C44H90	007098-22-8	90
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5			Eicosane	282	C20H42	000112-95-8	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098901.D
Acq On : 28 Sep 2017 11:51
Operator : SJ/JU
Sample : I5418-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-119-2(5-10)

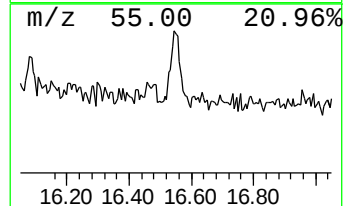
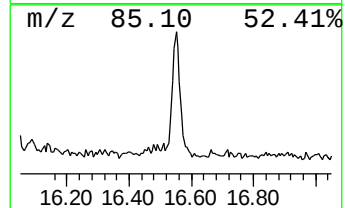
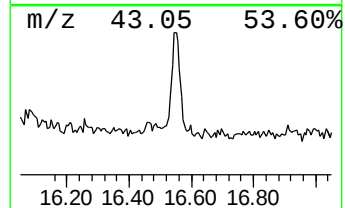
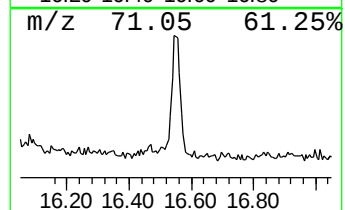
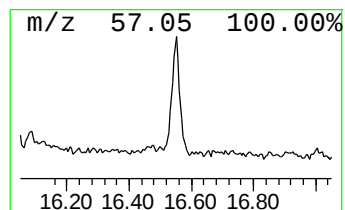
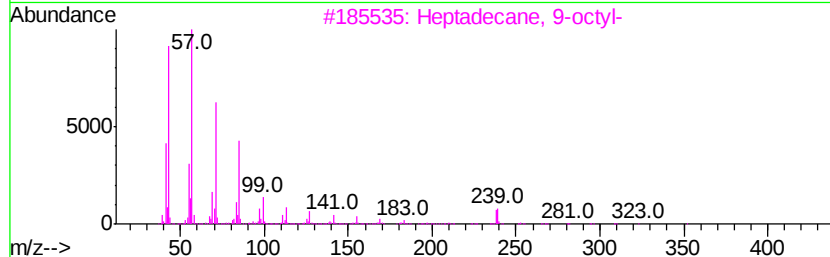
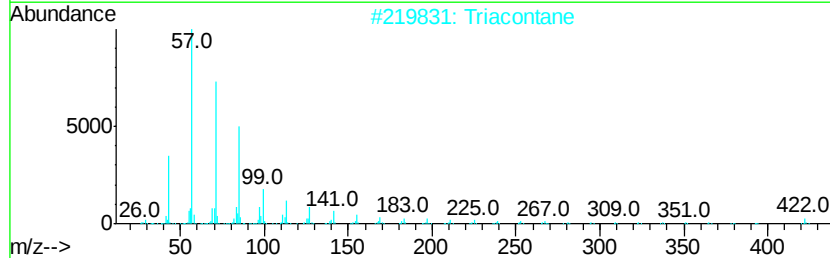
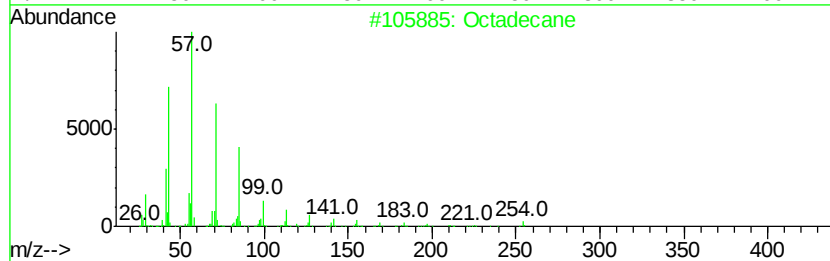
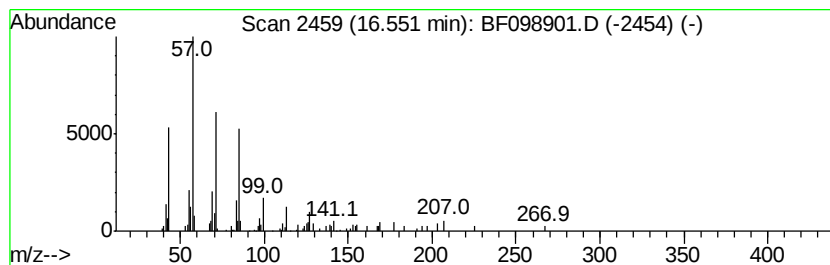
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	3.37 ng	133452	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	83
2		Triacontane	422	C30H62	000638-68-6	83
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	80
5		Tetracosane	338	C24H50	000646-31-1	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098901.D
Acq On : 28 Sep 2017 11:51
Operator : SJ/JU
Sample : I5418-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-119-2(5-10)

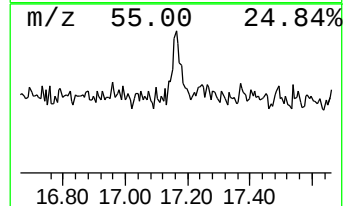
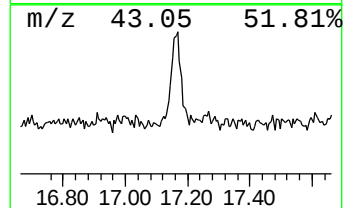
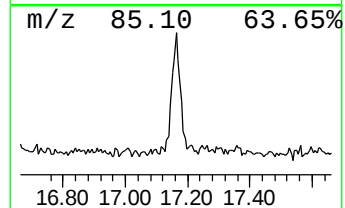
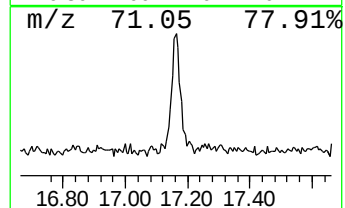
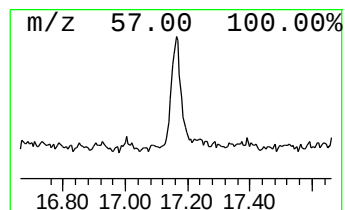
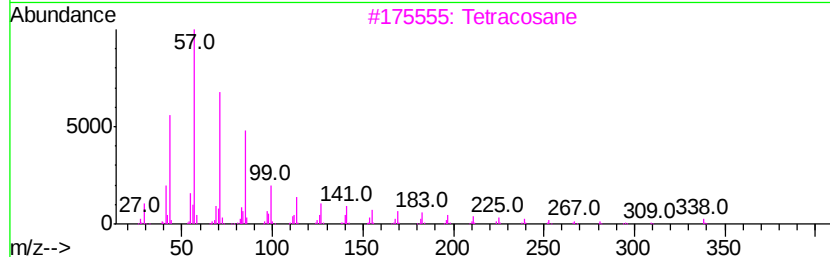
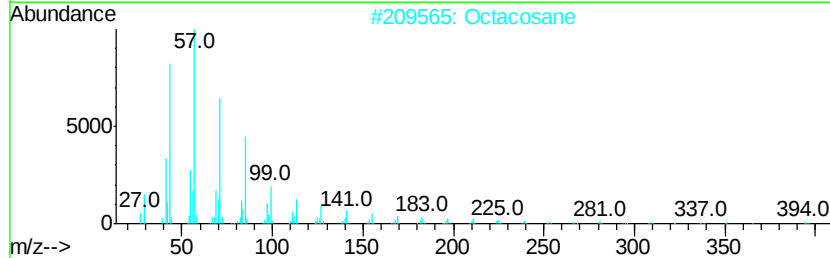
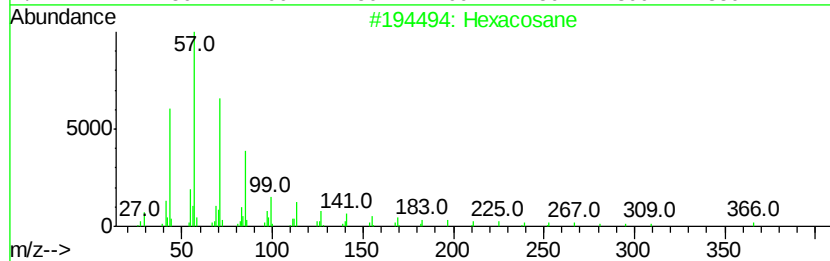
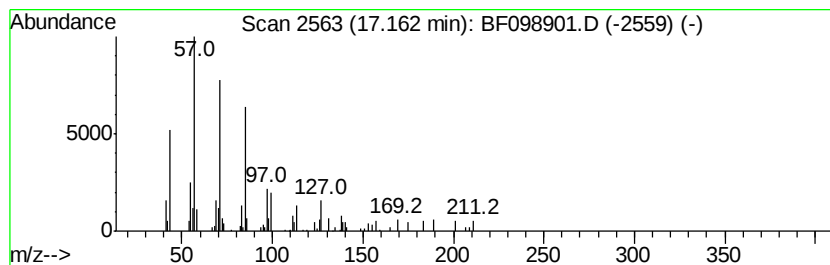
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.16	2.24 ng	88684	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	83
2		Octacosane	394	C28H58	000630-02-4	80
3		Tetracosane	338	C24H50	000646-31-1	80
4		Heneicosane	296	C21H44	000629-94-7	80
5		Pentacosane	352	C25H52	000629-99-2	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098901.D
Acq On : 28 Sep 2017 11:51
Operator : SJ/JU
Sample : I5418-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SASP2P-ENV-119-2(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
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2-Pentanone, 4-hy...	5.15	18.0	ng	777036	1	6.92	861407	20.0
unknown6.69	6.69	87.8	ng	3782370	1	6.92	861407	20.0
n-Hexadecanoic acid	11.96	8.4	ng	544441	4	11.44	1288430	20.0
Octadecanoic acid	12.74	4.5	ng	287403	4	11.44	1288430	20.0
Trifluoroacetoxy ...	13.90	5.8	ng	253179	5	14.08	869873	20.0
1,3-Benzenedicarb...	14.70	6.8	ng	294825	5	14.08	869873	20.0
4-Methoxyanthrani...	14.93	3.1	ng	122673	6	15.57	793168	20.0
2-methyloctacosane	16.03	2.5	ng	100454	6	15.57	793168	20.0
Octadecane	16.55	3.4	ng	133452	6	15.57	793168	20.0
Hexacosane	17.16	2.2	ng	88684	6	15.57	793168	20.0