

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
 Data File : BF093517.D
 Acq On : 10 Mar 2017 11:25
 Operator : SJ/MA
 Sample : I2176-06
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EW-05

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-BF030717.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	4.927	263	266	268	rBV	659787	1130945	1.29%	0.281%
2	5.201	288	290	292	rVB	1694892	2320561	2.65%	0.577%
3	5.361	302	304	308	rBV	1778390	3245010	3.70%	0.807%
4	5.624	310	327	328	rBV3	725290	5283513	6.03%	1.313%
5	6.081	347	367	369	rBV	4773630	21808461	24.87%	5.421%
6	6.196	375	377	379	rVB	2995767	3954554	4.51%	0.983%
7	6.447	397	399	404	rVB2	1503985	2981385	3.40%	0.741%
8	6.539	404	407	409	rBV	3110639	3538603	4.04%	0.880%
9	6.756	409	426	428	rBV3	2842323	15084271	17.20%	3.749%
10	6.813	428	431	432	rVB	2653794	5171498	5.90%	1.285%
11	6.904	437	439	444	rVB2	2586961	4053836	4.62%	1.008%
12	7.133	458	459	463	rBV4	556458	891065	1.02%	0.221%
13	7.213	463	466	469	rBV	1625806	2699693	3.08%	0.671%
14	7.327	469	476	479	rVB	3269800	5616347	6.41%	1.396%
15	7.384	479	481	484	rVB3	1262233	2339009	2.67%	0.581%
16	7.464	484	488	490	rBV4	1168253	3686297	4.20%	0.916%
17	7.510	490	492	493	rVB	995221	1278550	1.46%	0.318%
18	7.556	493	496	497	rVB3	995808	1765946	2.01%	0.439%
19	7.602	497	500	502	rBV	1069326	1822208	2.08%	0.453%
20	7.670	505	506	509	rVB3	907836	1193593	1.36%	0.297%
21	7.716	509	510	514	rVB4	522798	893204	1.02%	0.222%
22	7.784	514	516	518	rBV3	741560	1593052	1.82%	0.396%
23	7.842	518	521	525	rBV4	773796	2447338	2.79%	0.608%
24	7.922	525	528	529	rBV3	588321	1315213	1.50%	0.327%
25	8.036	531	538	541	rBV4	1536896	5425238	6.19%	1.348%
26	8.104	541	544	545	rBV	2254041	2614239	2.98%	0.650%
27	8.413	545	571	573	rBV3	7828431	87680747	100.00%	21.794%
28	8.642	589	591	593	rBV2	1132159	1554868	1.77%	0.386%
29	8.710	594	597	598	rBV	2032100	2713798	3.10%	0.675%
30	8.870	609	611	614	rVB2	848048	1229997	1.40%	0.306%
31	8.950	617	618	620	rVB	1382634	1116492	1.27%	0.278%
32	9.076	626	629	630	rBV	2962458	4462402	5.09%	1.109%
33	9.133	632	634	635	rBV	2712110	3784820	4.32%	0.941%
34	9.522	665	668	672	rVB2	3792934	7591421	8.66%	1.887%

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35	9.659	678	680	682	rBV3	822547	1628690	1.86%	0.405%
36	9.705	682	684	685	rVB	2005416	2053047	2.34%	0.510%
37	9.727	685	686	688	rBV2	788455	976455	1.11%	0.243%
38	9.773	688	690	691	rBV	1061377	1841260	2.10%	0.458%
39	9.956	703	706	707	rBV3	815505	1379044	1.57%	0.343%
40	9.990	707	709	713	rVV3	1377424	2045776	2.33%	0.508%
41	10.048	713	714	715	rVV	1836229	2240371	2.56%	0.557%
42	10.116	718	720	726	rVB5	3335545	7276677	8.30%	1.809%
43	10.333	737	739	743	rBV2	736912	1408594	1.61%	0.350%
44	10.448	747	749	750	rVB	2932050	3342896	3.81%	0.831%
45	10.528	755	756	759	rBV2	645846	948953	1.08%	0.236%
46	10.608	761	763	766	rVB3	1237135	1982443	2.26%	0.493%
47	10.710	769	772	775	rVB2	5008913	7057951	8.05%	1.754%
48	10.768	775	777	779	rBV2	1188454	2007641	2.29%	0.499%
49	10.802	779	780	782	rVB2	1532147	1634676	1.86%	0.406%
50	10.836	782	783	784	rBV	1409756	1215355	1.39%	0.302%
51	10.916	787	790	791	rVV2	608018	1018953	1.16%	0.253%
52	10.950	791	793	794	rVB2	1155906	1109139	1.26%	0.276%
53	10.985	794	796	797	rBV	2208540	2867547	3.27%	0.713%
54	11.030	797	800	804	rVB3	3896346	7605745	8.67%	1.890%
55	11.133	808	809	811	rBV	808183	1046799	1.19%	0.260%
56	11.168	811	812	813	rVV	1419042	1172525	1.34%	0.291%
57	11.271	813	821	823	rVV	5014128	20823770	23.75%	5.176%
58	11.362	826	829	832	rVB	3567018	6113913	6.97%	1.520%
59	11.488	838	840	844	rVB2	571512	1288052	1.47%	0.320%
60	11.911	866	877	879	rBV5	6108943	29977028	34.19%	7.451%
61	11.945	879	880	883	rVV3	2257294	4779867	5.45%	1.188%
62	12.002	883	885	886	rVV	1720717	2704724	3.08%	0.672%
63	12.025	886	887	890	rVV2	2092275	2958561	3.37%	0.735%
64	12.082	890	892	894	rVV2	2384607	3914188	4.46%	0.973%
65	12.116	894	895	898	rVV2	1385120	2048932	2.34%	0.509%
66	12.551	929	933	938	rBV2	1626912	5133120	5.85%	1.276%
67	12.631	938	940	944	rVB2	1695196	3054589	3.48%	0.759%
68	12.859	958	960	962	rVB	2464913	2218687	2.53%	0.551%
69	12.905	962	964	967	rBV	1340815	1761826	2.01%	0.438%
70	12.974	967	970	972	rBV2	4069747	9879670	11.27%	2.456%
71	13.019	972	974	975	rVV2	3810365	6665916	7.60%	1.657%

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72	13.099	978	981	984	rVV4	2909686	7972762	9.09%	1.982%
73	13.156	984	986	988	rVV	4132355	6571791	7.50%	1.633%
74	13.202	988	990	992	rVV	2160676	3130427	3.57%	0.778%
75	13.282	994	997	1001	rBV	817545	1540644	1.76%	0.383%
76	13.922	1048	1053	1054	rVV2	2020336	3011071	3.43%	0.748%
77	13.956	1054	1056	1057	rVV	1308789	1723633	1.97%	0.428%
78	14.036	1060	1063	1065	rVV3	941404	2186018	2.49%	0.543%
79	14.082	1065	1067	1069	rVV	1254443	1499866	1.71%	0.373%
80	14.882	1135	1137	1139	rVV2	511923	1033865	1.18%	0.257%
81	15.328	1174	1176	1182	rVB	752582	1130109	1.29%	0.281%
82	17.465	1359	1363	1368	rVB2	402534	1044996	1.19%	0.260%

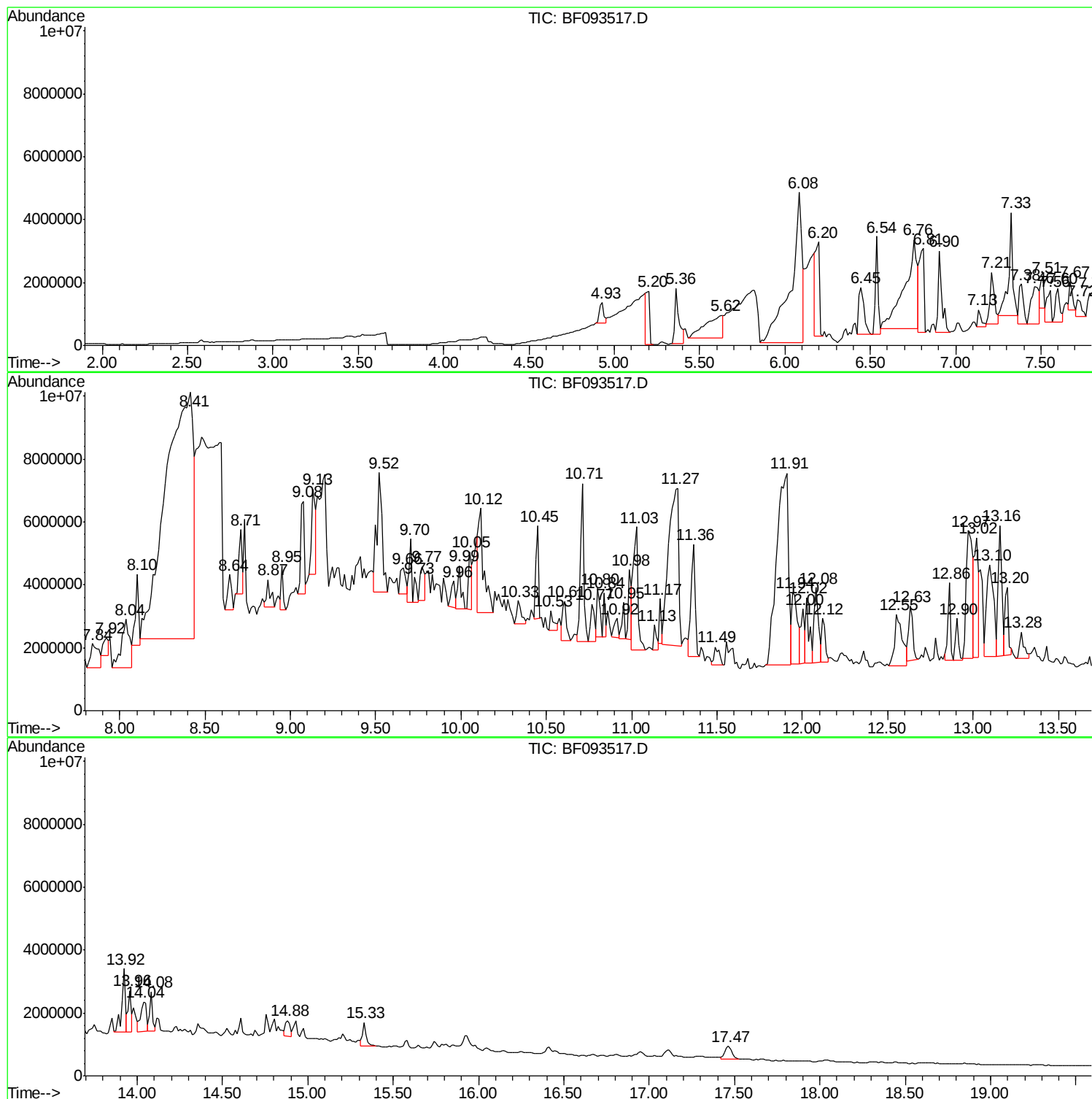
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EW-05

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030917\
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Sample : I2176-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EW-05

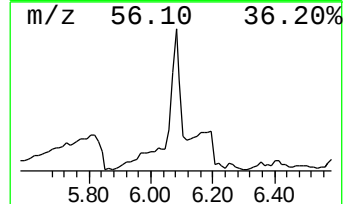
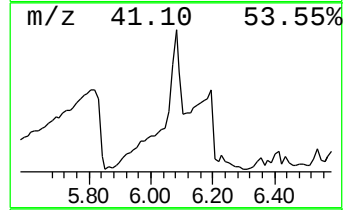
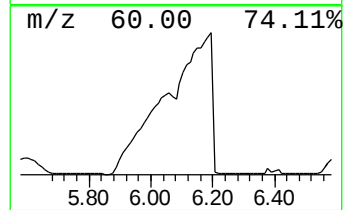
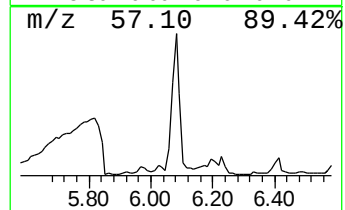
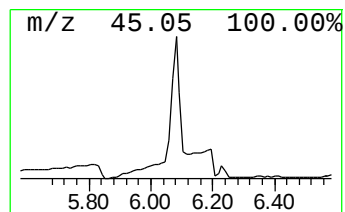
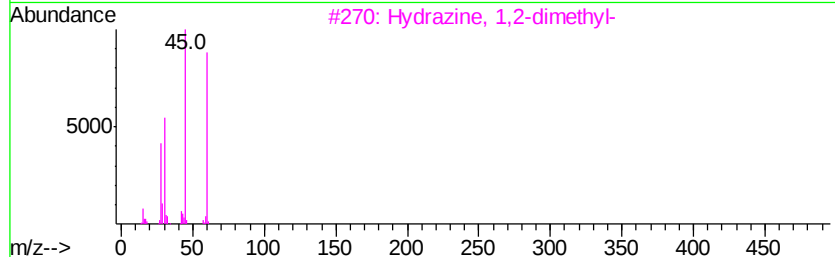
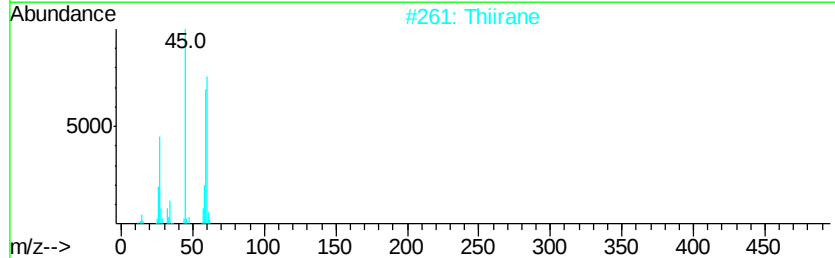
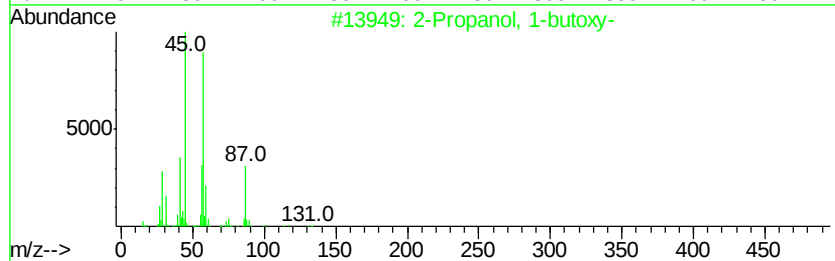
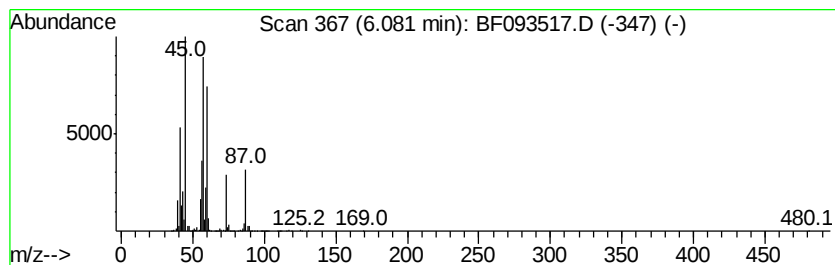
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.08 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.08	28.92 ng	21808500	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	47
2		Thiirane	60	C2H4S	000420-12-2	38
3		Hvdrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	38
4		3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	35
5		Butanoic acid	88	C4H8O2	000107-92-6	27



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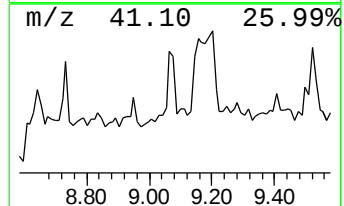
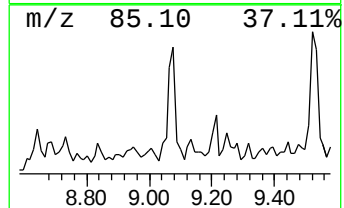
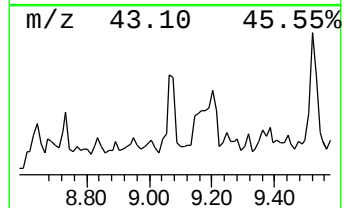
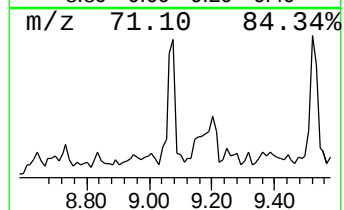
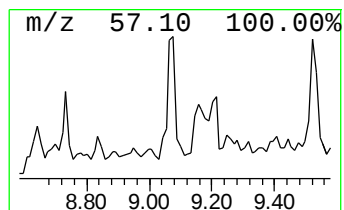
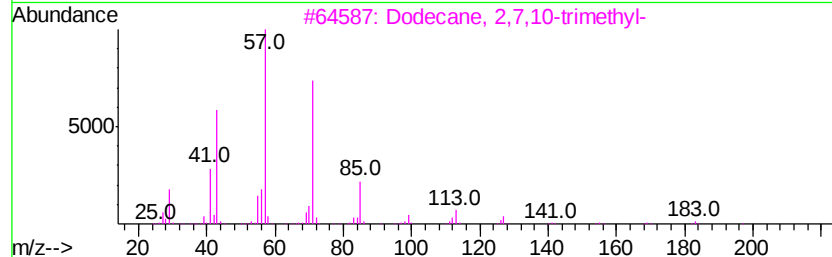
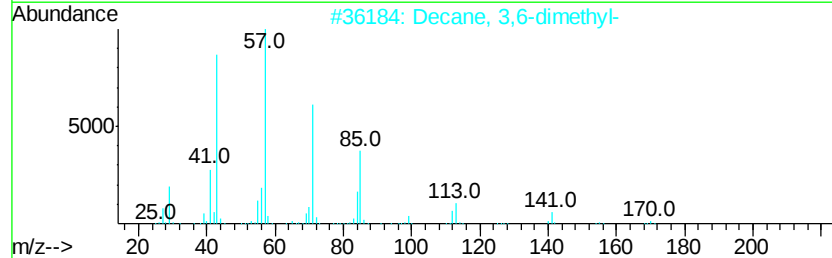
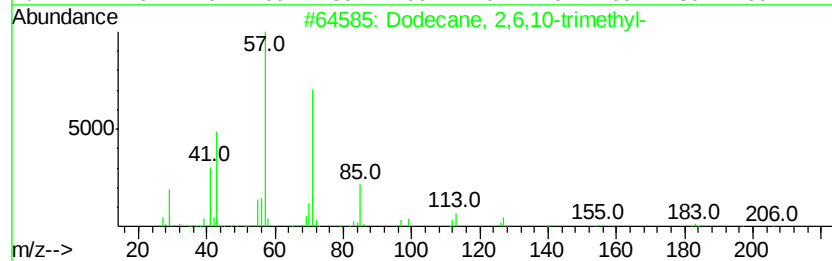
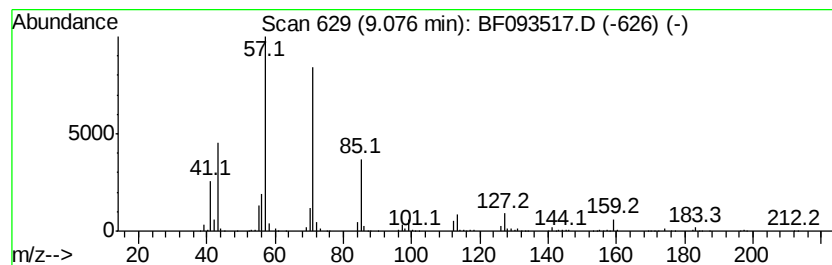
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Dodecane, 2,6,10-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.08	48.47 ng	4462400	Acenaphthene-d10	9.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	90
2		Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	87
3		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
4		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	78
5		Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	72



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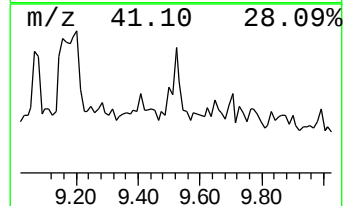
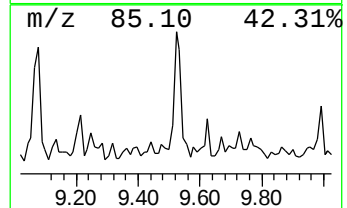
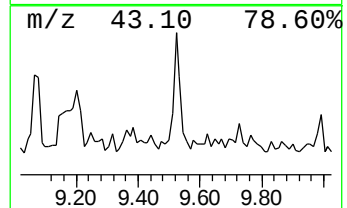
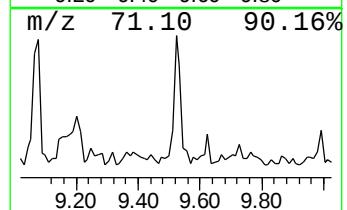
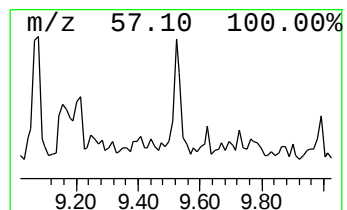
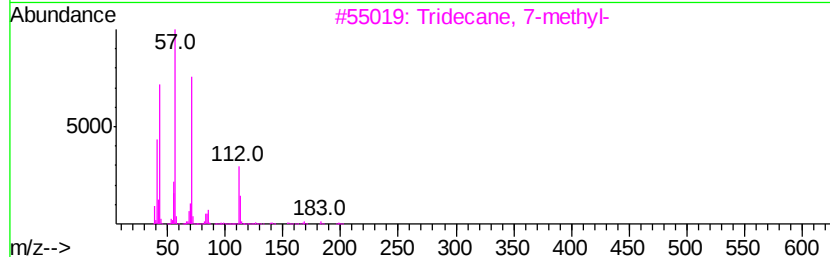
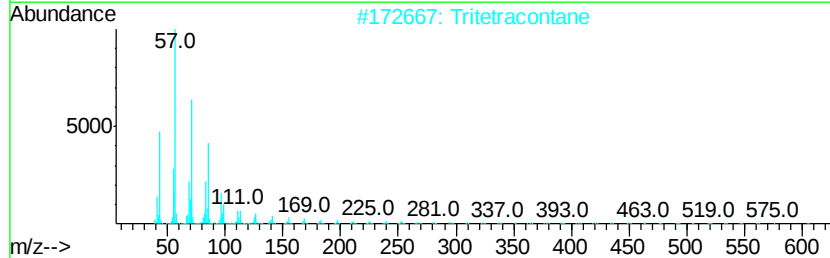
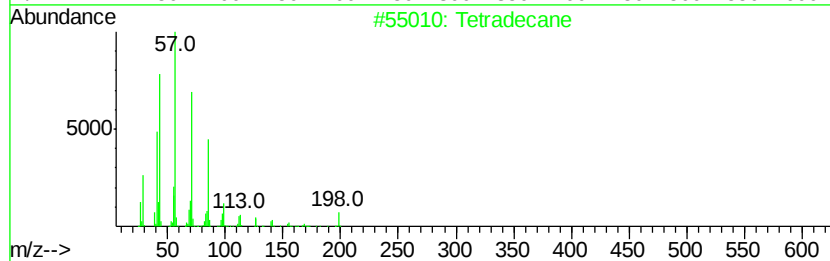
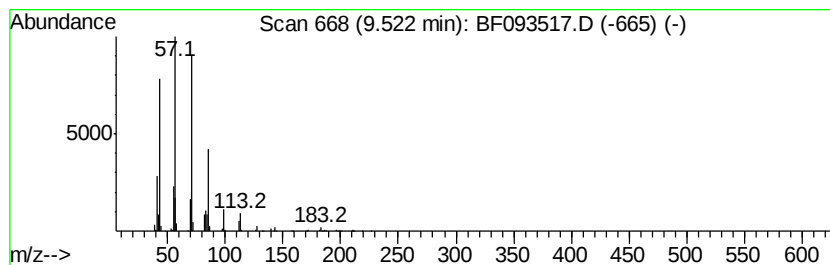
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetradecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.52	82.46 ng	7591420	Acenaphthene-d10	9.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	83
2		Tritetracontane	605	C43H88	007098-21-7	83
3		Tridecane, 7-methyl-	198	C14H30	026730-14-3	76
4		Nonane, 4-methyl-5-propyl-	184	C13H28	062185-55-1	70
5		Hexadecane	226	C16H34	000544-76-3	64



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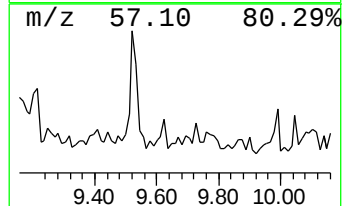
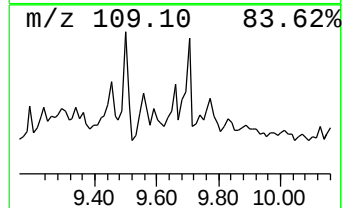
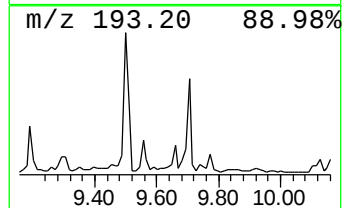
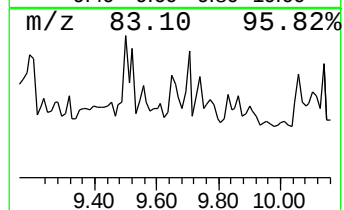
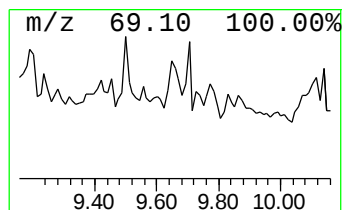
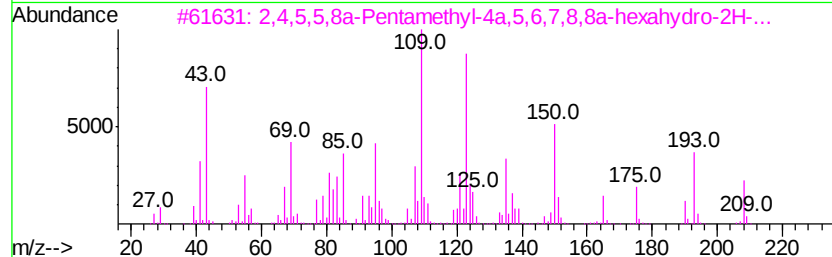
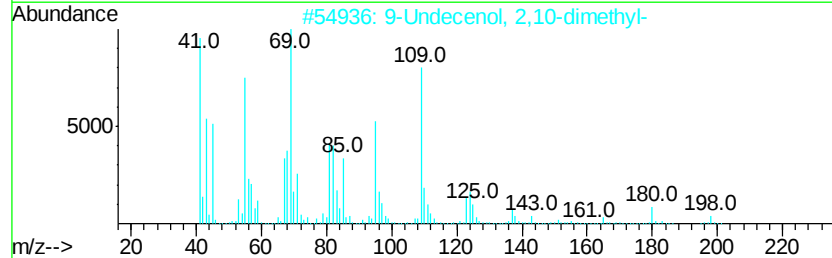
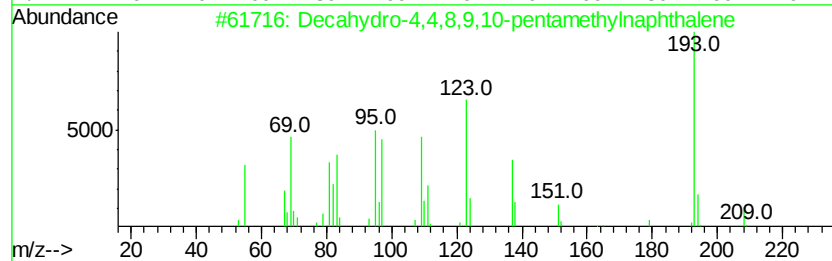
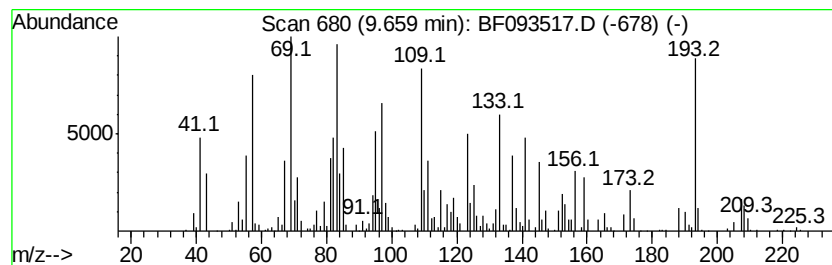
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown9.66 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.66	17.69 ng	1628690	Acenaphthene-d10	9.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	42
2		9-Undecenol, 2,10-dimethyl-	198	C13H26O	1000131-86-0	30
3		2,4,5,5,8a-Pentamethyl-4a,5,6,7,...	208	C14H24O	1000195-30-1	30
4		Methyl tetrahydroionol	212	C14H28O	060241-53-4	16
5		Imidazole, 2-[1,1-dimethoxy-2,2,...	210	C7H9F3N2O2	111838-35-8	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030917\
Data File : BF093517.D
Acq On : 10 Mar 2017 11:25
Operator : SJ/MA
Sample : I2176-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EW-05

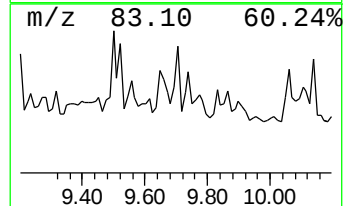
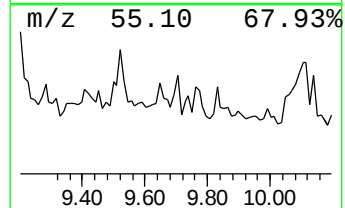
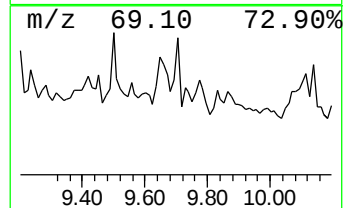
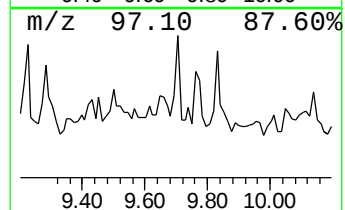
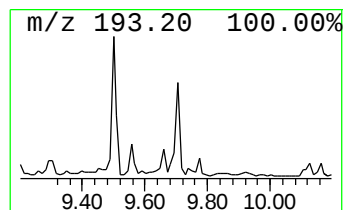
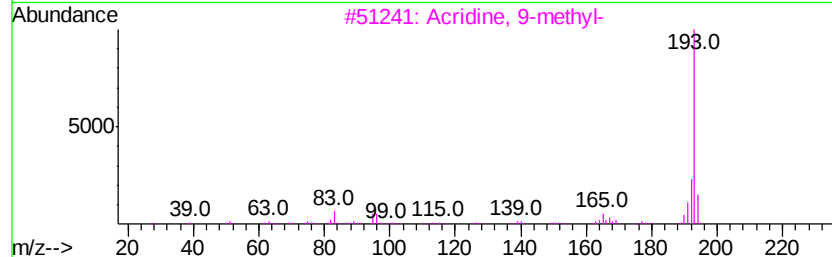
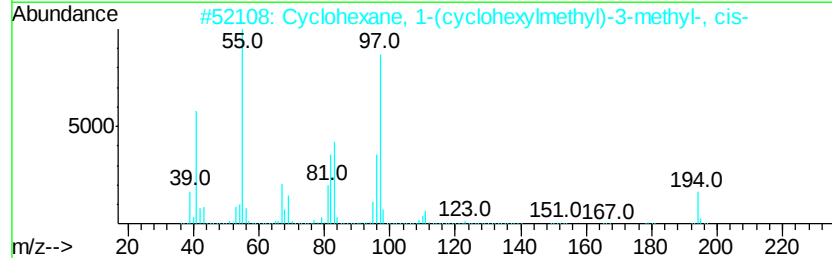
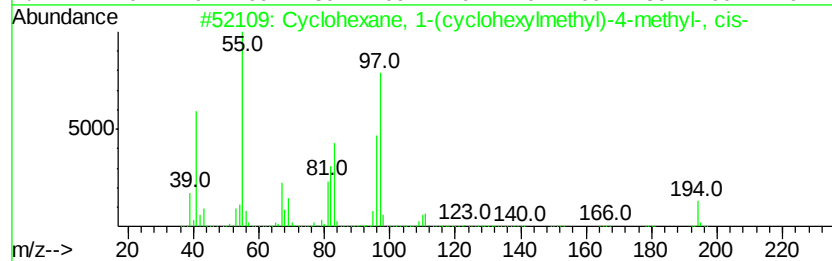
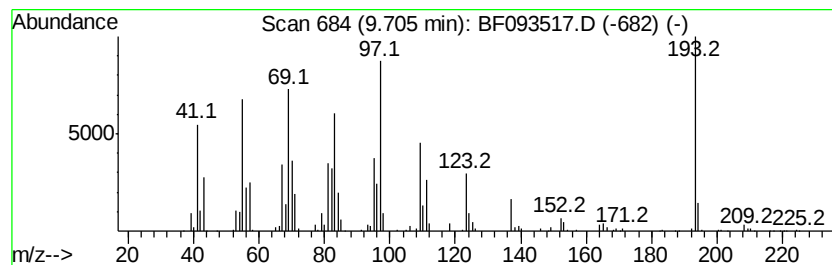
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown9.70 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.70	22.30 ng	2053050	Acenaphthene-d10	9.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-(cyclohexylmethyl)...	194	C14H26	054823-97-1	38
2		Cyclohexane, 1-(cyclohexylmethyl)...	194	C14H26	054823-96-0	30
3		Acridine, 9-methyl-	193	C14H11N	000611-64-3	25
4		Cyclohexane, 1-(cyclohexylmethyl)...	194	C14H26	054824-04-3	22
5		2-Bromopropionic acid, 1-(cyclop...	248	C10H17BrO2	1000293-39-1	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
Data File : BF093517.D
Acq On : 10 Mar 2017 11:25
Operator : SJ/MA
Sample : I2176-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EW-05

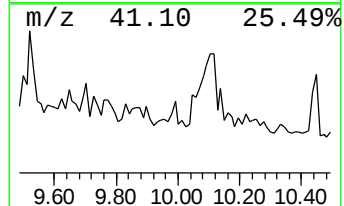
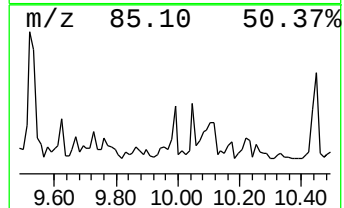
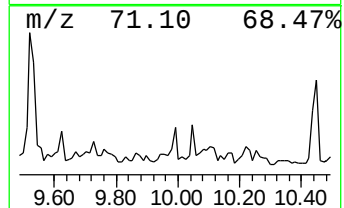
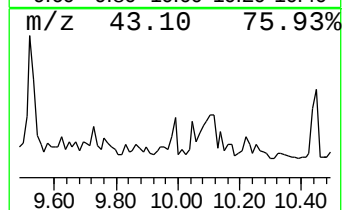
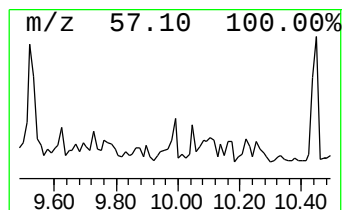
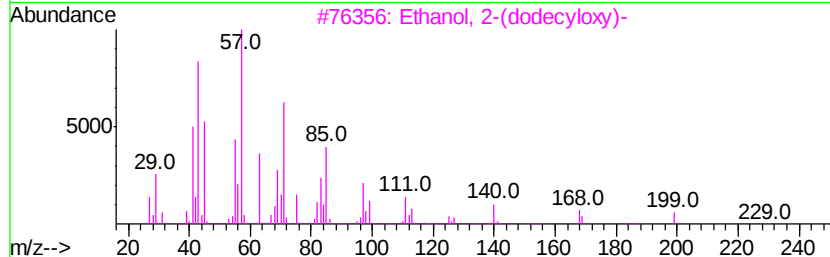
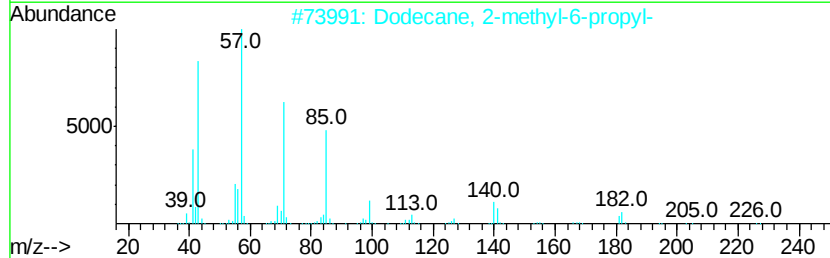
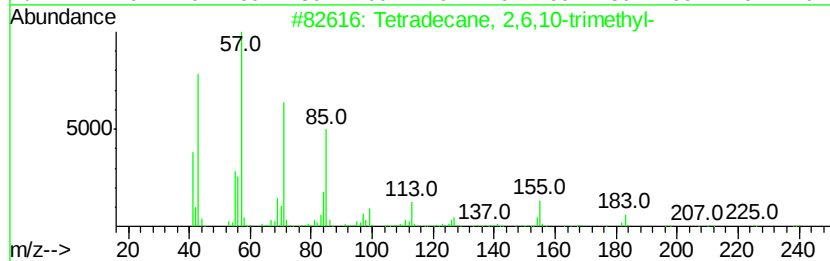
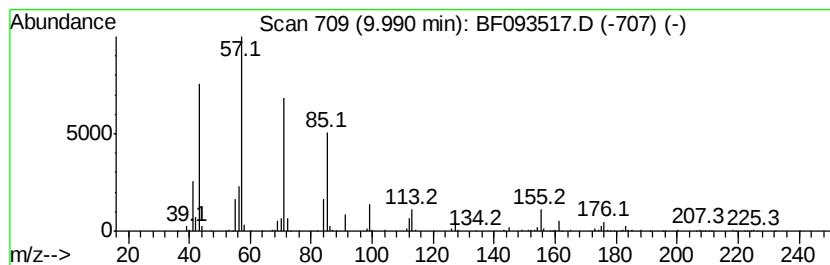
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetradecane, 2,6,10-trimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.99	22.22 ng	2045780	Acenaphthene-d10	9.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	83
2		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	74
3		Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	72
4		Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	64
5		Undecane, 2-methyl-	170	C12H26	007045-71-8	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
Data File : BF093517.D
Acq On : 10 Mar 2017 11:25
Operator : SJ/MA
Sample : I2176-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

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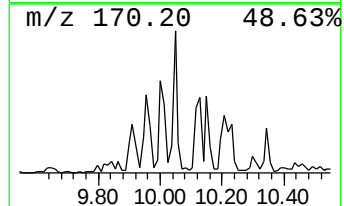
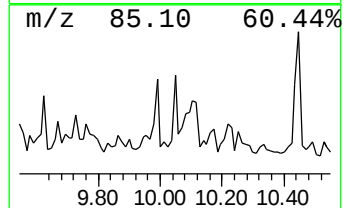
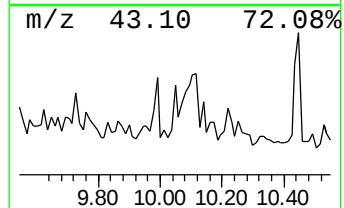
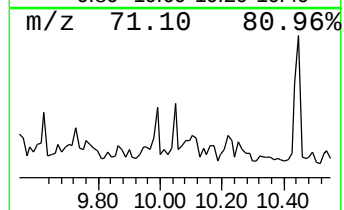
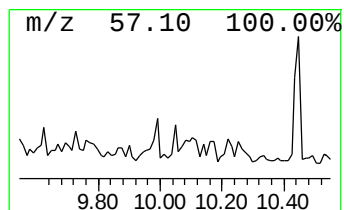
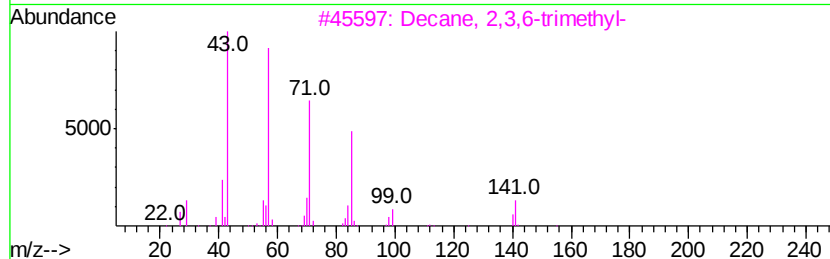
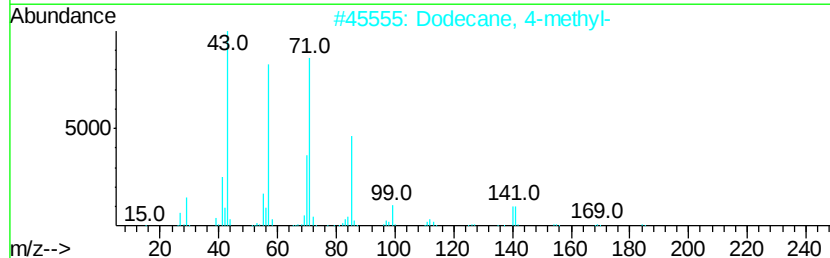
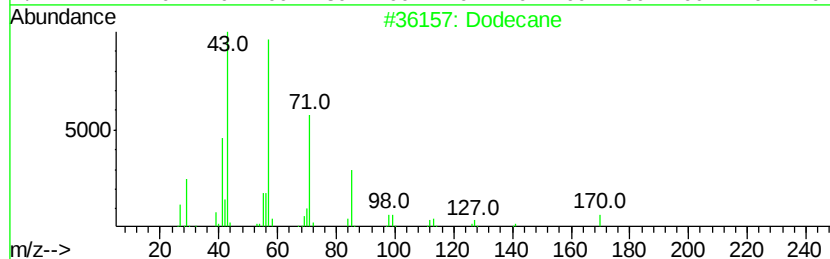
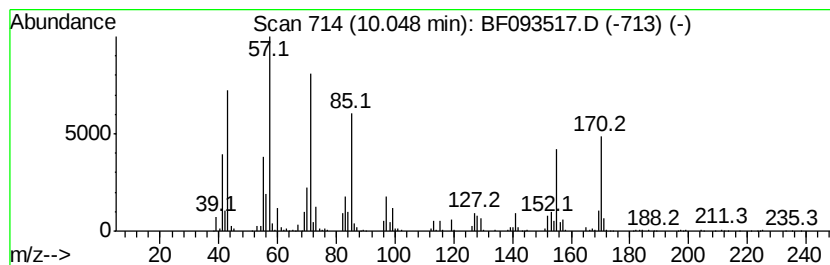
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown10.05 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.05	24.34 ng	2240370	Acenaphthene-d10	9.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane	170	C12H26	000112-40-3	49
2		Dodecane, 4-methyl-	184	C13H28	006117-97-1	49
3		Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	46
4		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	46
5		Nonadecane	268	C19H40	000629-92-5	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
Data File : BF093517.D
Acq On : 10 Mar 2017 11:25
Operator : SJ/MA
Sample : I2176-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
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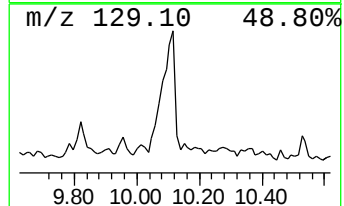
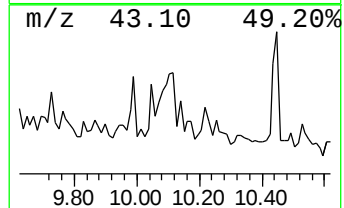
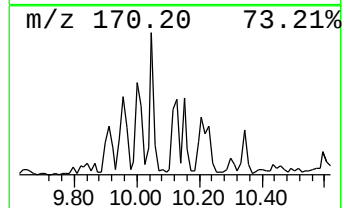
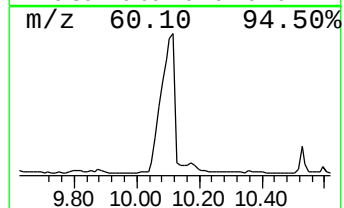
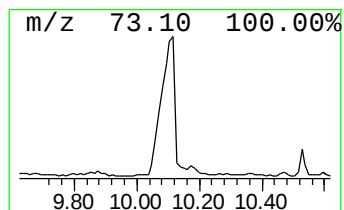
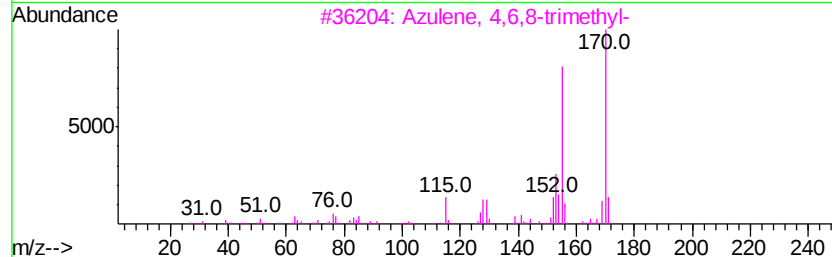
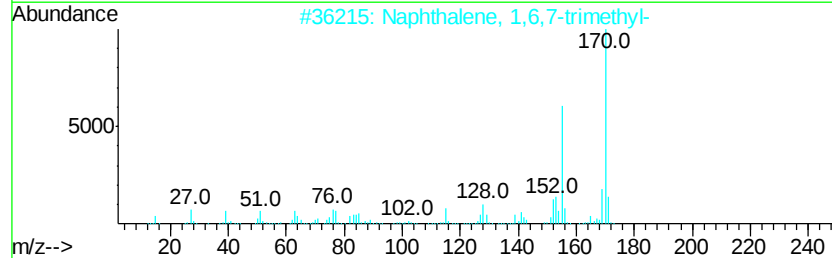
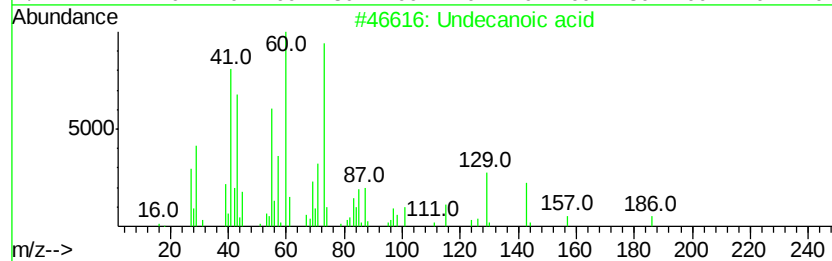
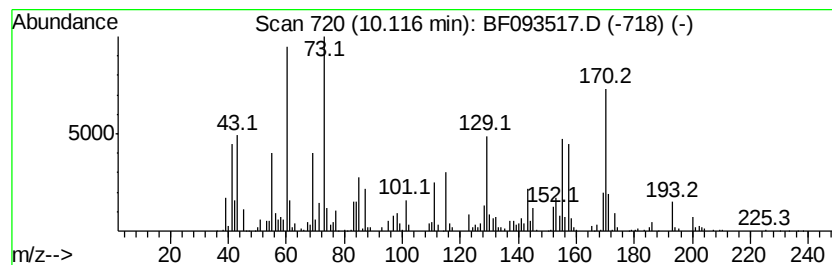
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown10.12 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.12	79.04 ng	7276680	Acenaphthene-d10	9.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecanoic acid	186	C11H22O2	000112-37-8	47
2		Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	42
3		Azulene, 4,6,8-trimethyl-	170	C13H14	000941-81-1	38
4		Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	25
5		Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030917\
Data File : BF093517.D
Acq On : 10 Mar 2017 11:25
Operator : SJ/MA
Sample : I2176-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

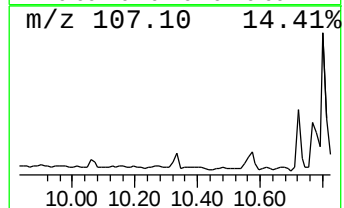
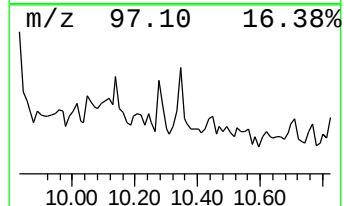
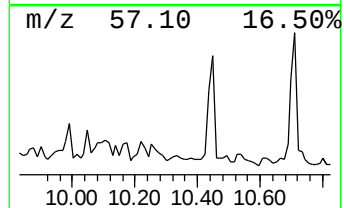
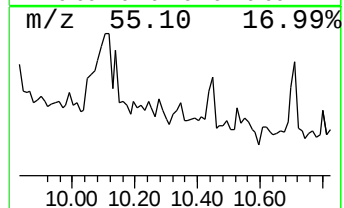
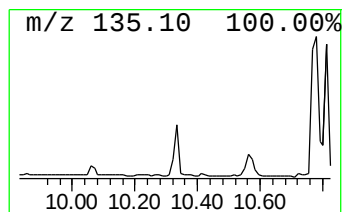
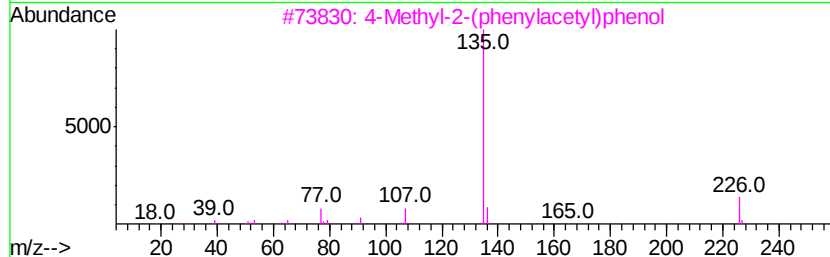
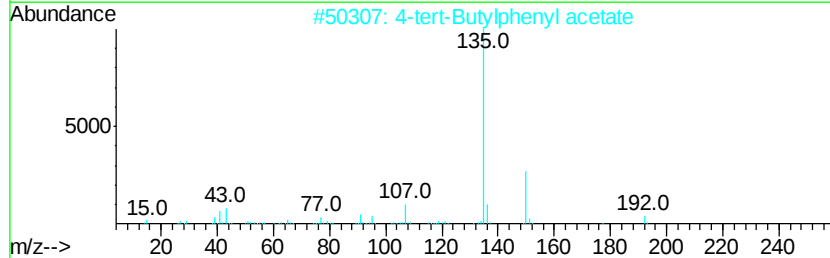
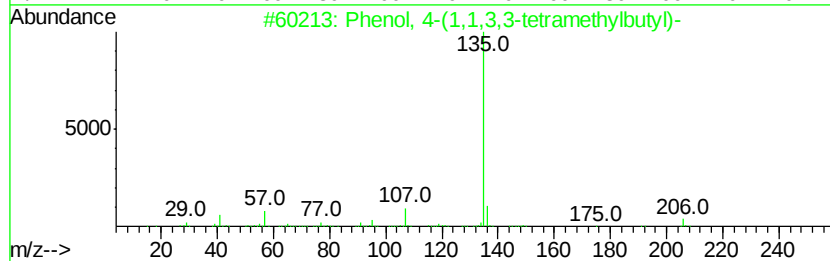
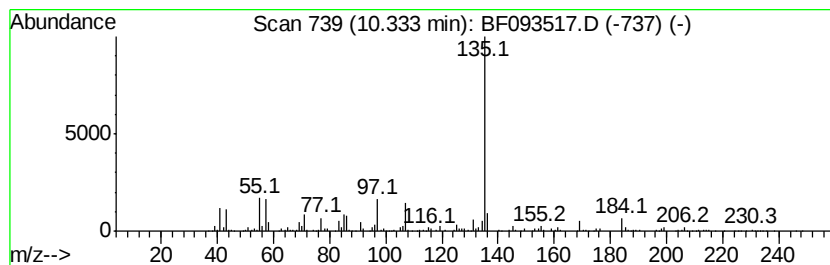
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Phenol, 4-(1,1,3,3-tetramet... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.33	15.30 ng	1408590	Acenaphthene-d10	9.81		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64	
2	4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	59	
3	4-Methyl-2-(phenylacetyl)phenol	226	C15H14O2	024258-63-7	53	
4	p-Anisic acid, cyclobutyl ester	206	C12H14O3	1000292-45-6	53	
5	1-Adamantan-1-yl-6-chloro-7-fluo...	375	C20H19ClFN03	1000210-85-1	53	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030917\
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Sample : I2176-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

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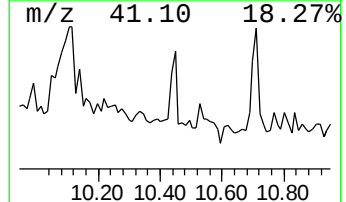
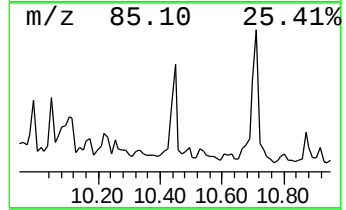
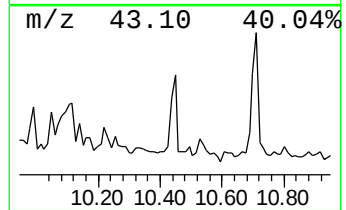
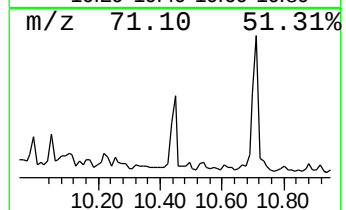
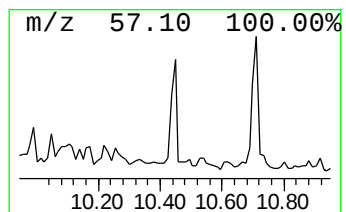
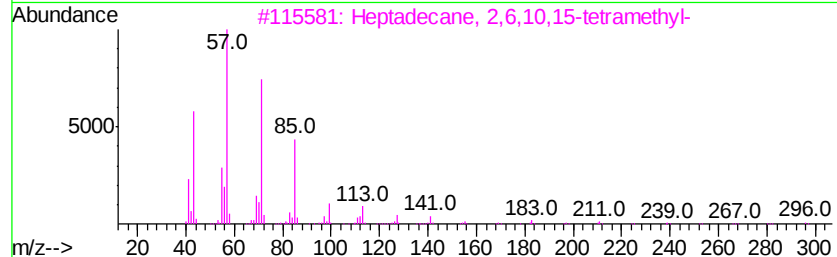
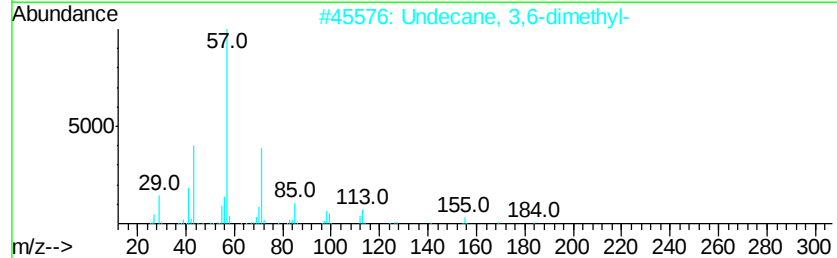
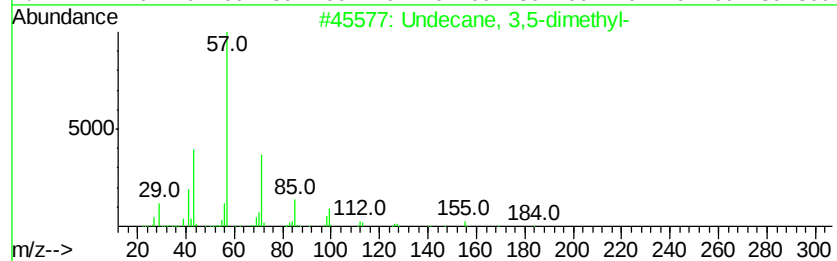
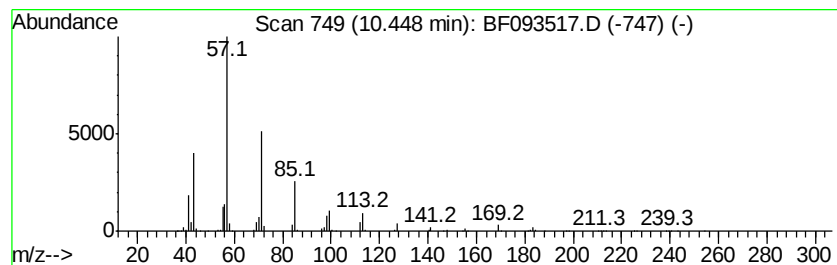
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Undecane, 3,5-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	36.31 ng	3342900	Acenaphthene-d10	9.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	87
2		Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	81
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
4		Undecane, 5-ethyl-	184	C13H28	017453-94-0	72
5		Tridecane, 6-methyl-	198	C14H30	013287-21-3	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030917\
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Operator : SJ/MA
Sample : I2176-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EW-05

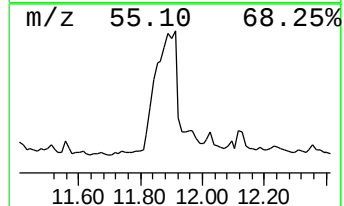
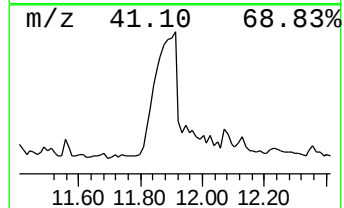
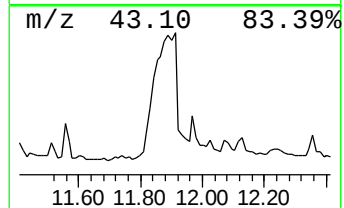
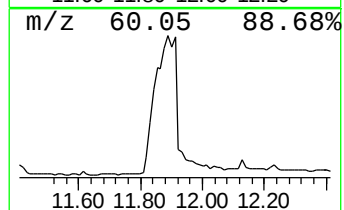
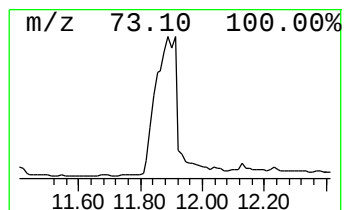
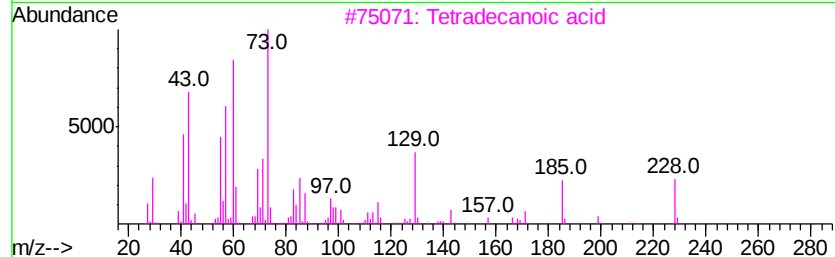
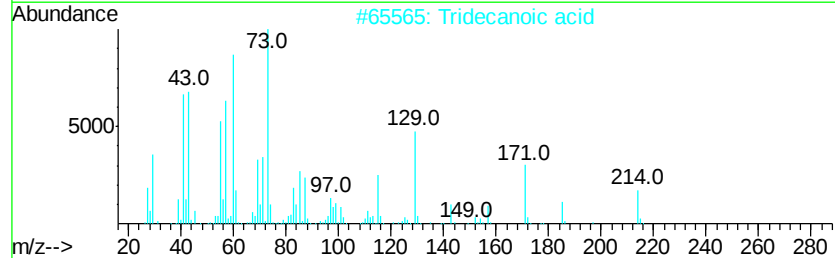
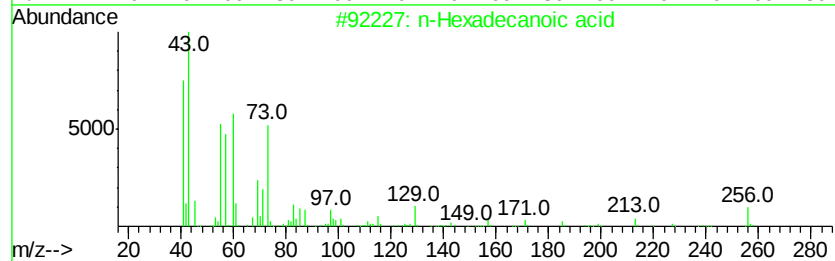
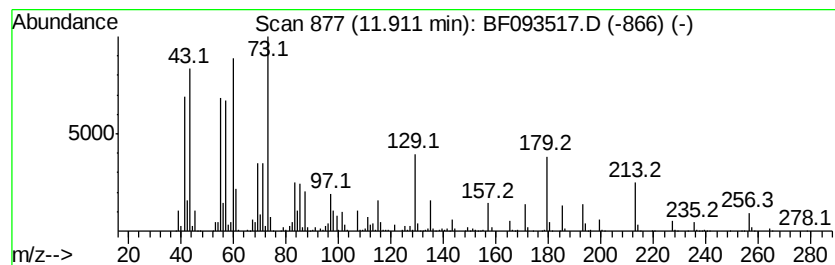
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	28.79 ng	29977000	Phenanthrene-d10	11.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	92
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4		n-Decanoic acid	172	C10H20O2	000334-48-5	60
5		Undecanoic acid	186	C11H22O2	000112-37-8	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030917\
Data File : BF093517.D
Acq On : 10 Mar 2017 11:25
Operator : SJ/MA
Sample : I2176-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

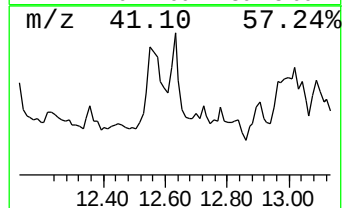
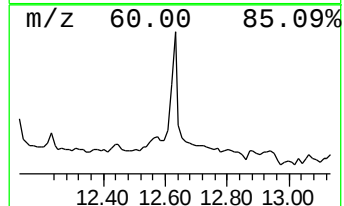
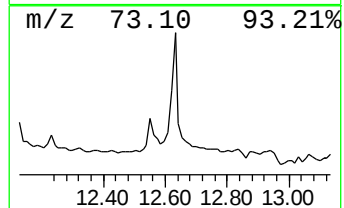
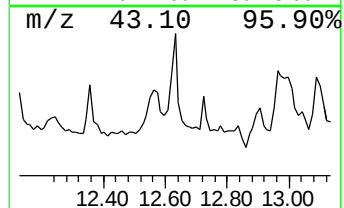
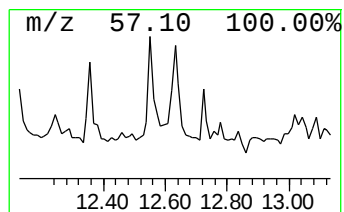
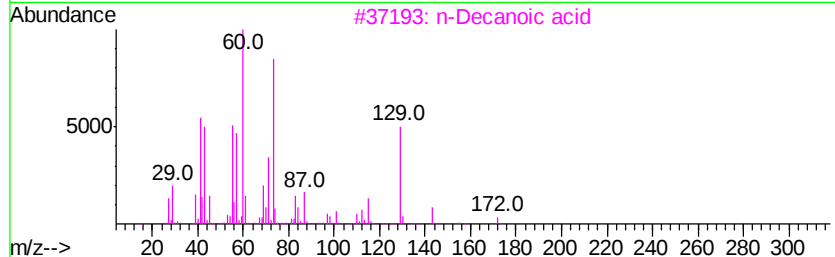
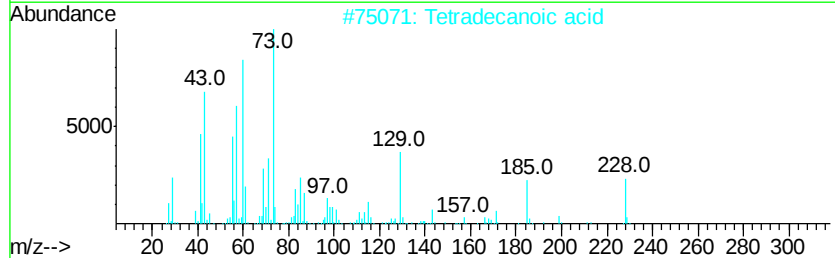
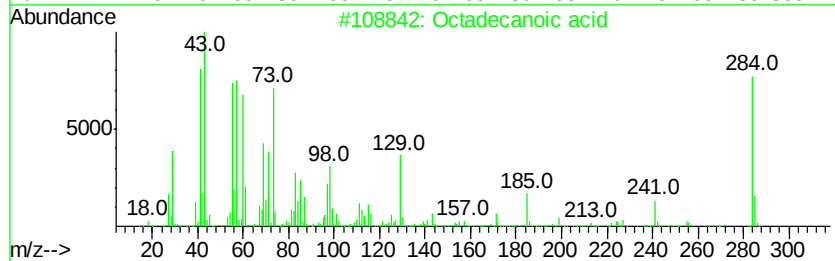
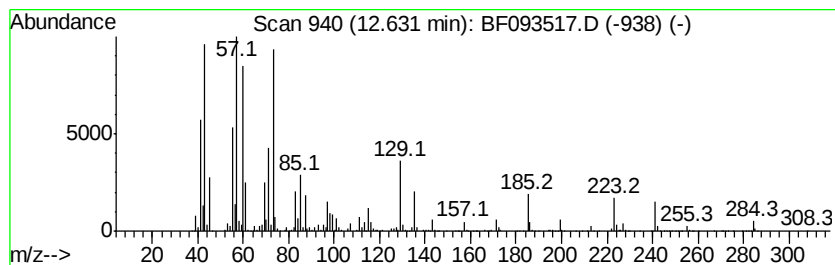
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Octadecanoic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.63	20.29 ng	3054590	Chrysene-d12	13.92		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	87
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	62
3		n-Decanoic acid	172	C10H20O2	000334-48-5	46
4		Undecanoic acid	186	C11H22O2	000112-37-8	46
5		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
Data File : BF093517.D
Acq On : 10 Mar 2017 11:25
Operator : SJ/MA
Sample : I2176-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

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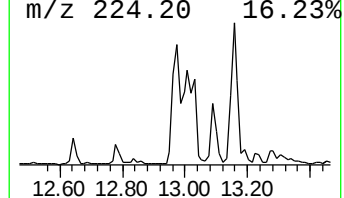
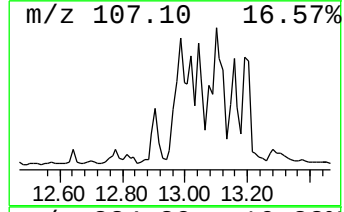
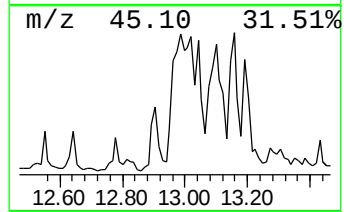
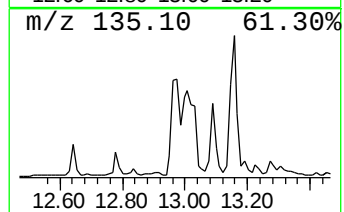
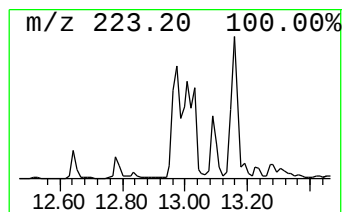
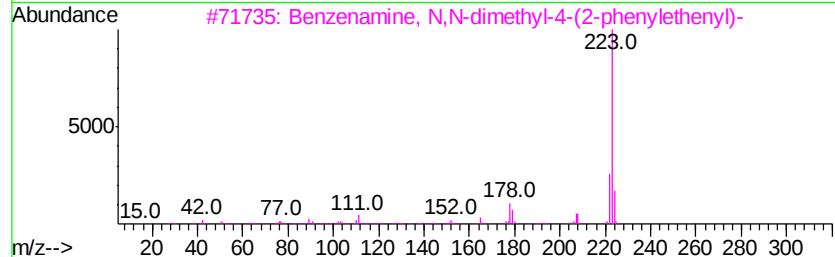
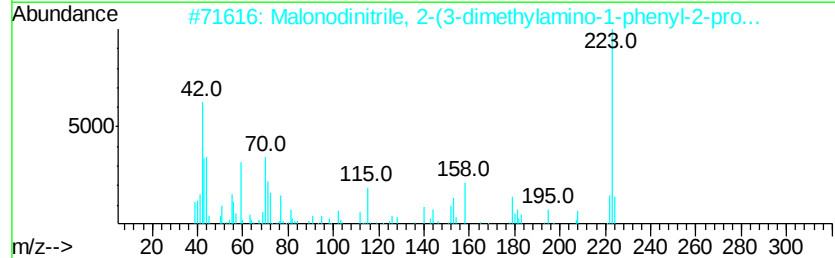
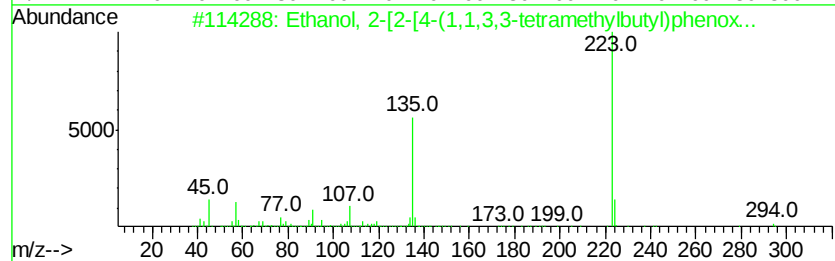
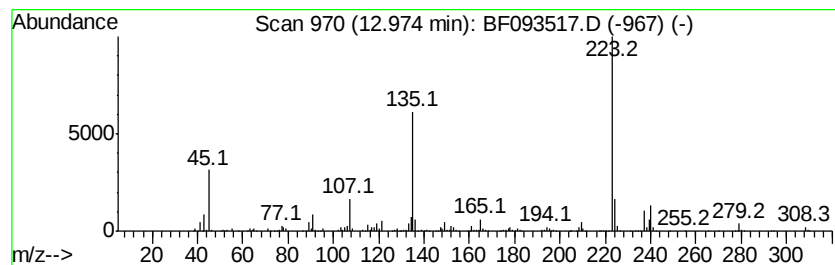
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Ethanol, 2-[2-[4-(1,1,3,3-t... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.97	65.62 ng	9879670	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	64
2		Malonodinitrile, 2-(3-dimethylam...	223	C14H13N3	065996-13-6	35
3		Benzenamine, N,N-dimethyl-4-(2-p...	223	C16H17N	001145-73-9	25
4		(4-Oxo-2-phenyl-1,2,3,4-tetrahyd...	282	C16H14N2O3	1000190-14-1	25
5		Ethyl-bis(ethythio)acetate	208	C8H16O2S2	020461-95-4	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
Data File : BF093517.D
Acq On : 10 Mar 2017 11:25
Operator : SJ/MA
Sample : I2176-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

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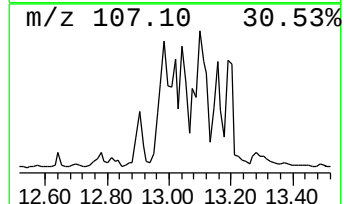
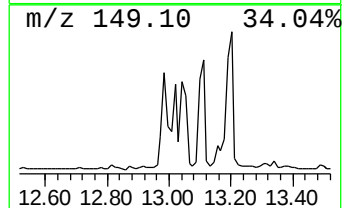
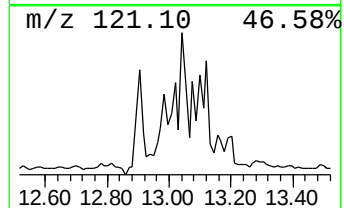
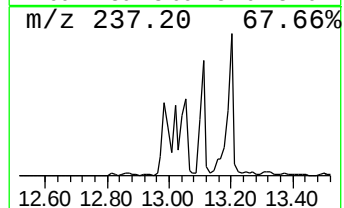
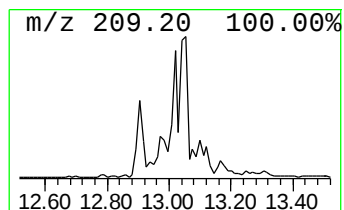
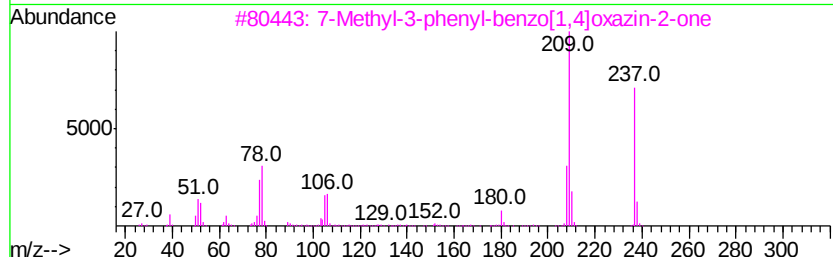
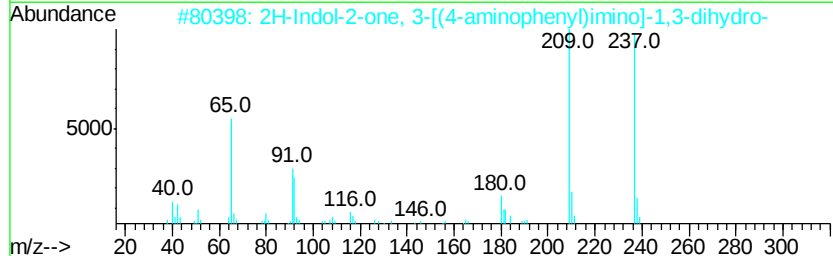
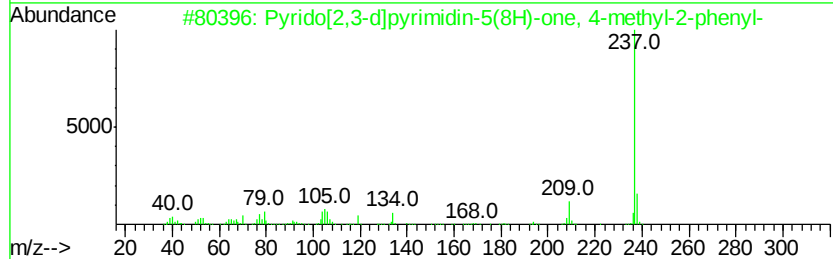
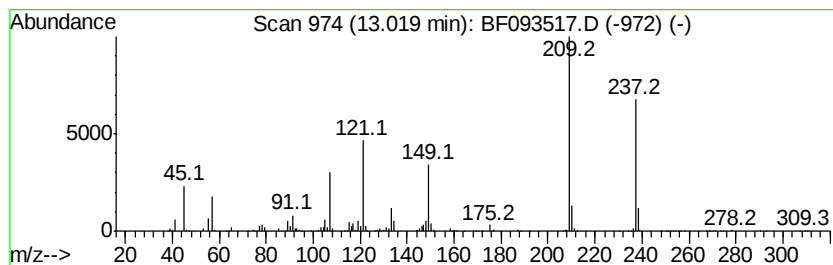
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Pyrido[2,3-d]pyrimidin-5(8H)... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.02	44.28 ng	6665920	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrido[2,3-d]pyrimidin-5(8H)-one...	237	C14H11N3O	161465-98-1	52
2		2H-Indol-2-one, 3-[4-aminopheny...	237	C14H11N3O	033829-07-1	38
3		7-Methyl-3-phenyl-benzo[1,4]oxaz...	237	C15H11N02	062103-88-2	38
4		Isobenzofuran-1(3H)-one, 3-butox...	282	C18H18O3	296877-49-1	32
5		Benzoxazole, 2-methyl-5-phenyl-	209	C14H11NO	061931-68-8	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
Data File : BF093517.D
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Misc :
ALS Vial : 40 Sample Multiplier: 1

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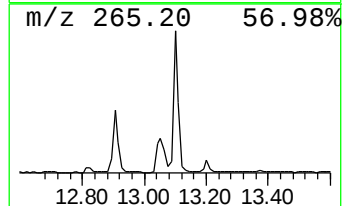
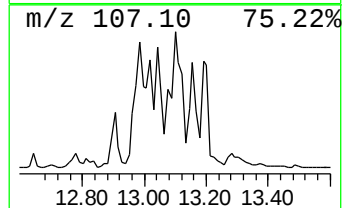
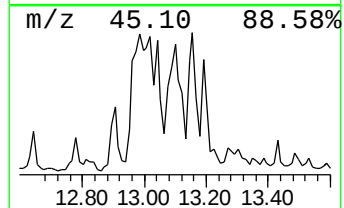
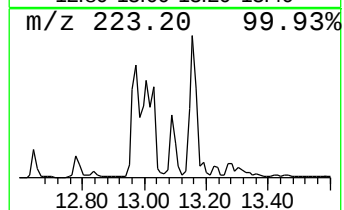
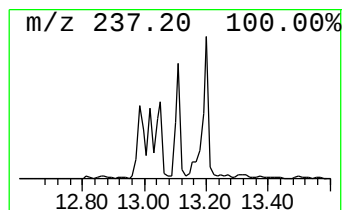
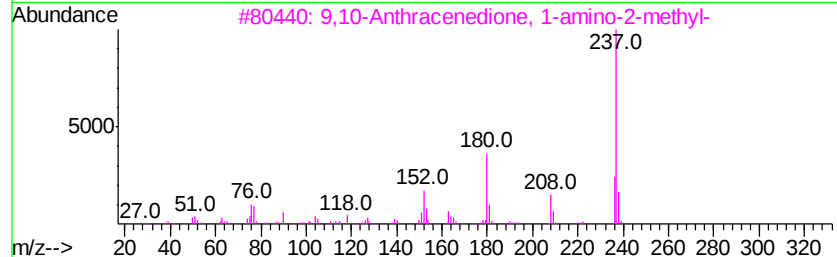
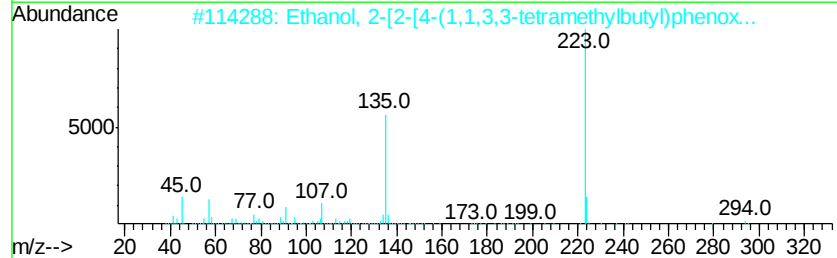
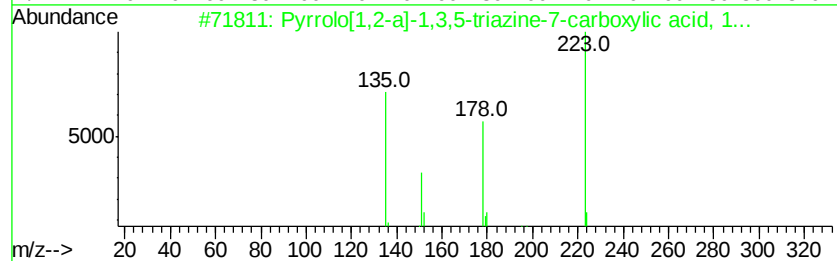
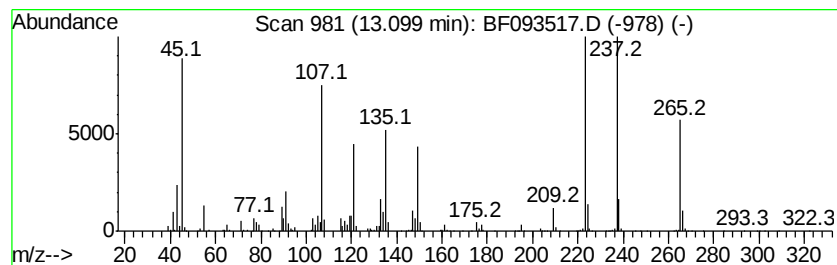
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown13.10 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.10	52.96 ng	7972760	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	30
2		Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	22
3		9,10-Anthracenedione, 1-amino-2-...	237	C15H11N02	000082-28-0	11
4		Acetamide, N-methyl-N-phenyl-	149	C9H11NO	000579-10-2	11
5		N,N'-Di-o-tolyl-formamidine	224	C15H16N2	016596-01-3	11



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
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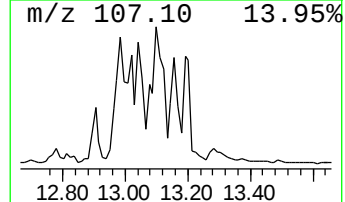
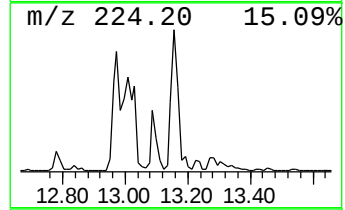
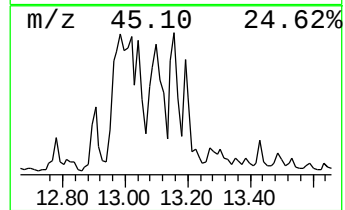
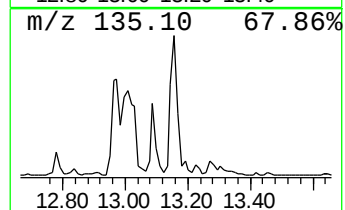
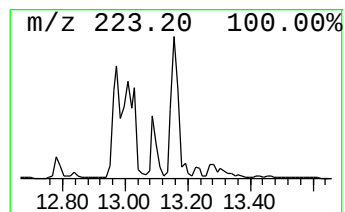
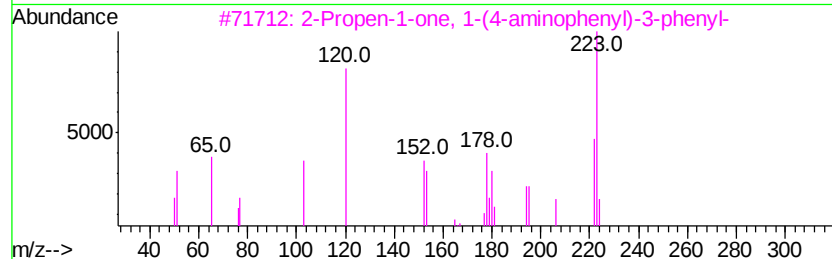
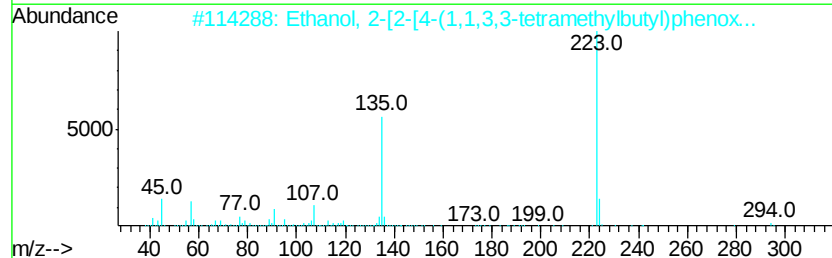
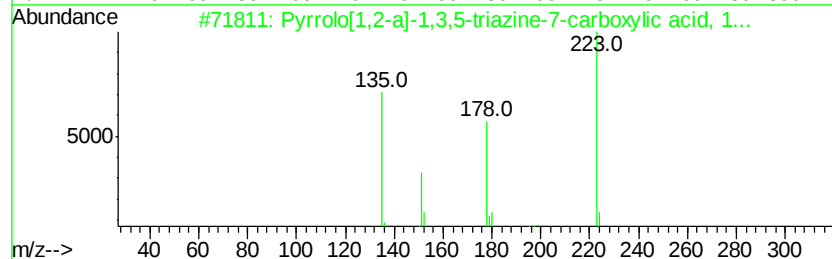
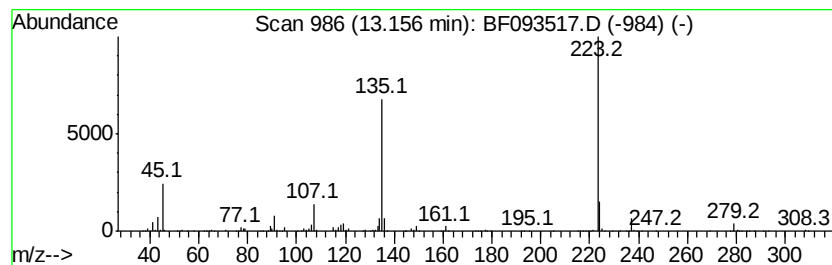
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Pyrrolo[1,2-a]-1,3,5-triazi... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.16	43.65 ng	6571790	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	86
2		Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	78
3		2-Propen-1-one, 1-(4-aminophenyl...	223	C15H13NO	002403-30-7	43
4		2,9-Dioxabicyclo[3.3.1]non-7-ene...	436	C23H32O8	1000196-04-6	38
5		1,3-Benzodioxole-5-carboxylic ac...	223	C10H9NO5	099185-29-2	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030917\
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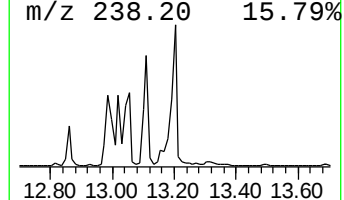
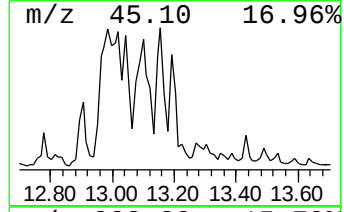
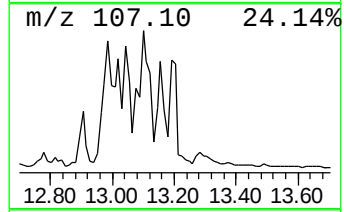
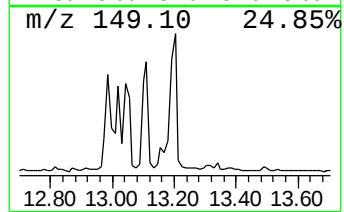
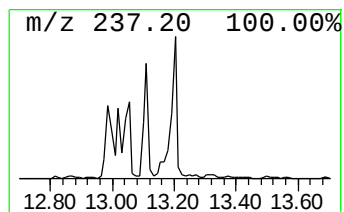
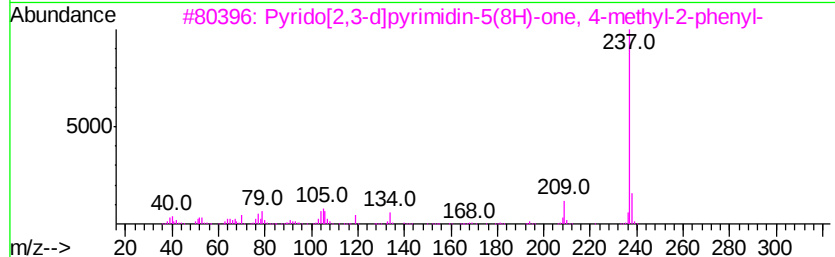
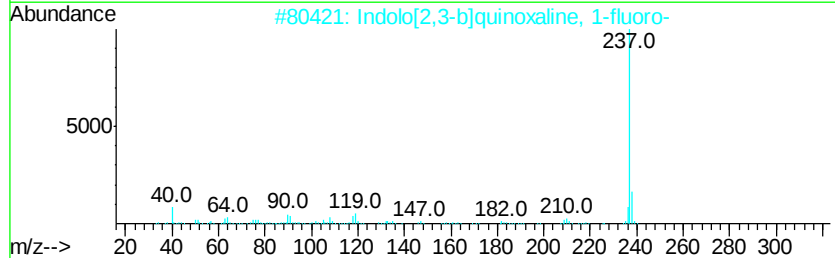
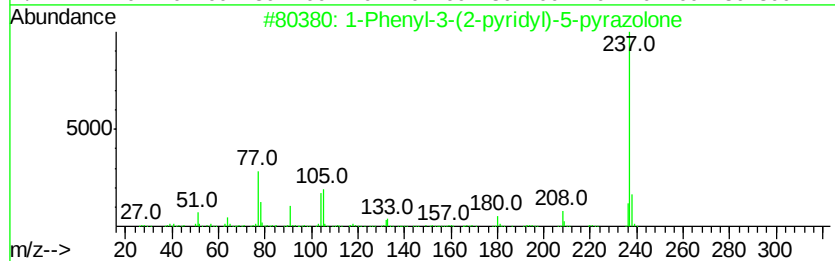
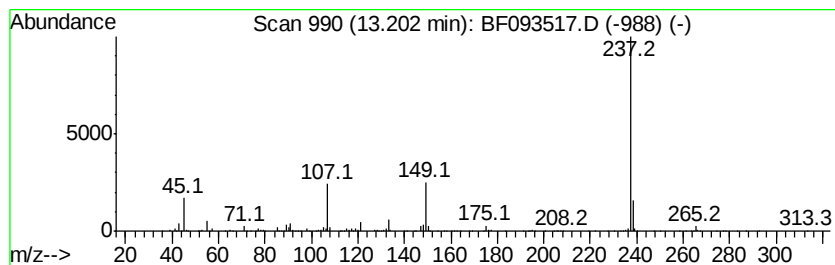
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown13.20 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.20	20.79 ng	3130430	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Phenyl-3-(2-pyridyl)-5-pyrazolone	237	C14H11N3O	021683-60-3	47
2		Indolo[2,3-b]quinoxaline, 1-fluoro-	237	C14H8FN3	296244-71-8	43
3		Pyrido[2,3-d]pyrimidin-5(8H)-one...	237	C14H11N3O	161465-98-1	38
4		1-(1-Adamantyl)-2-dichloromethyl...	320	C15H26Cl2OSi	1000283-10-6	38
5		5-Iodopyrid-2(1H)-thione	237	C5H4INS	1000251-67-5	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030917\
Data File : BF093517.D
Acq On : 10 Mar 2017 11:25
Operator : SJ/MA
Sample : I2176-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EW-05

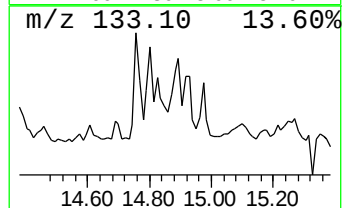
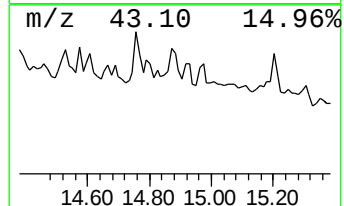
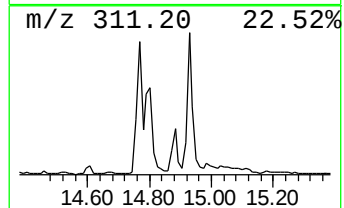
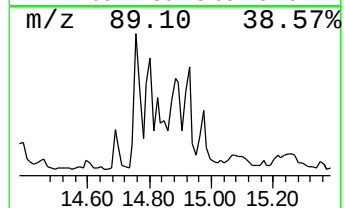
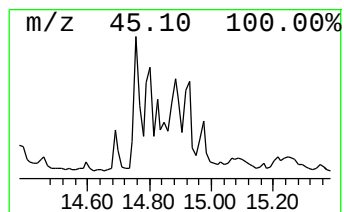
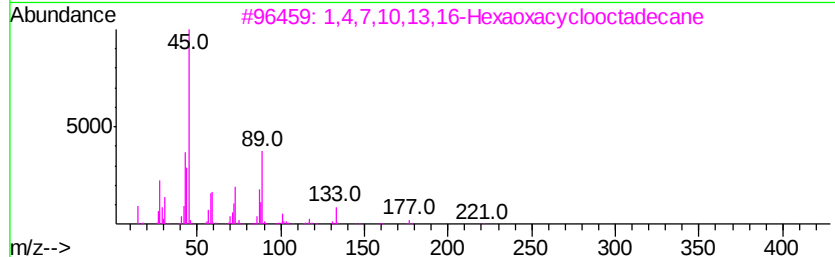
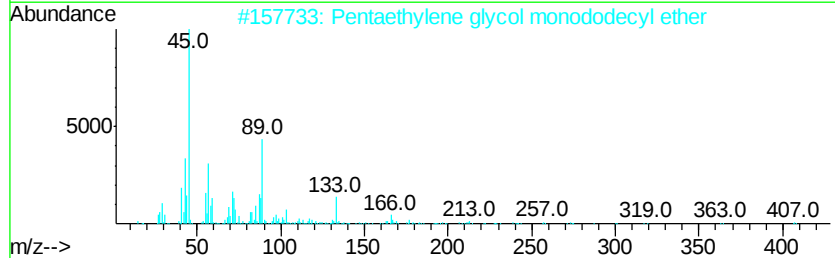
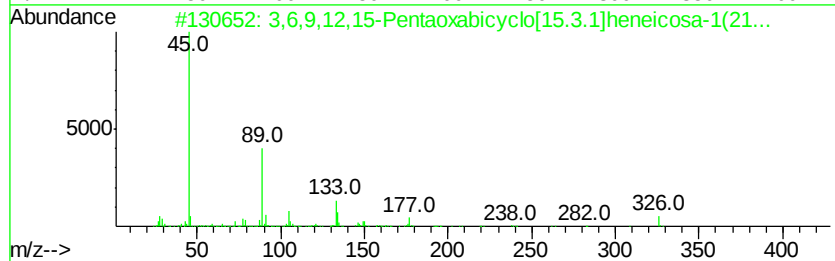
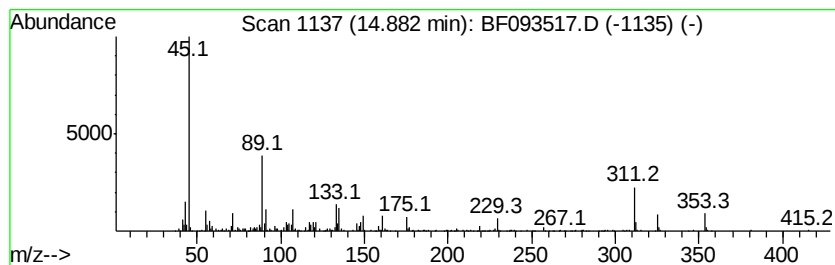
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 3,6,9,12,15-Pentaoxabicyclo... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.88	18.30 ng	1033870	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,6,9,12,15-Pentaoxabicyclo[15.3...	326	C17H26O6	071128-99-9	53
2		Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	43
3		1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	40
4		Hexadecyl	282	C12H26O7	002615-15-8	40
5		15-Crown-5	220	C10H20O5	033100-27-5	40



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030917\
Data File : BF093517.D
Acq On : 10 Mar 2017 11:25
Operator : SJ/MA
Sample : I2176-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EW-05

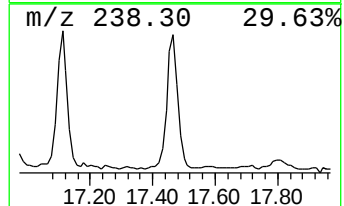
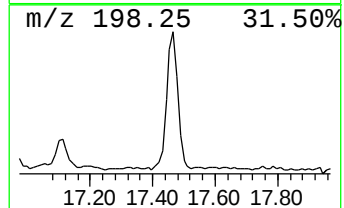
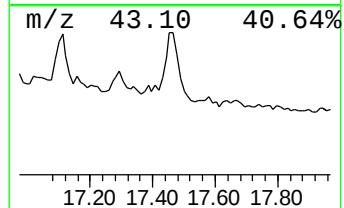
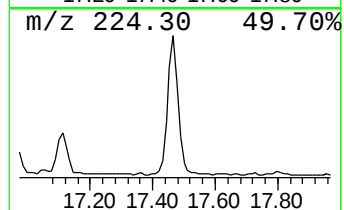
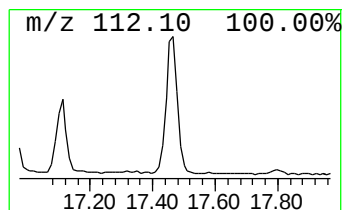
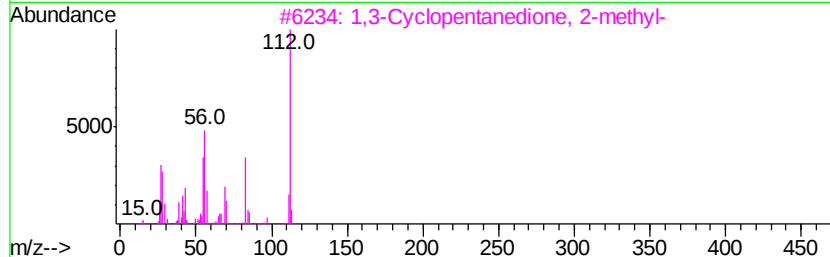
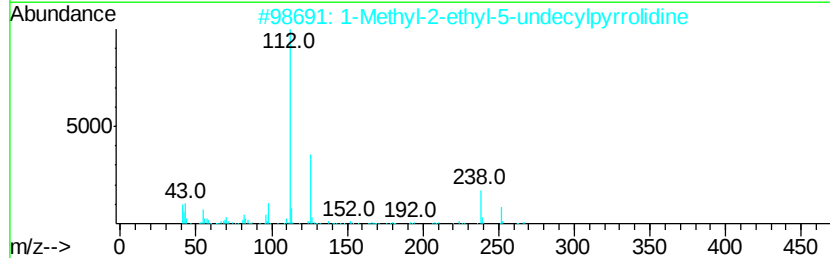
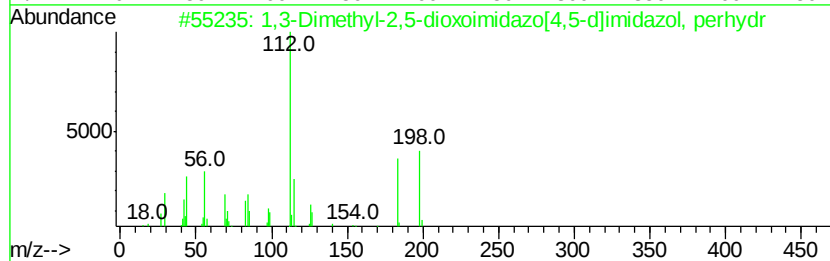
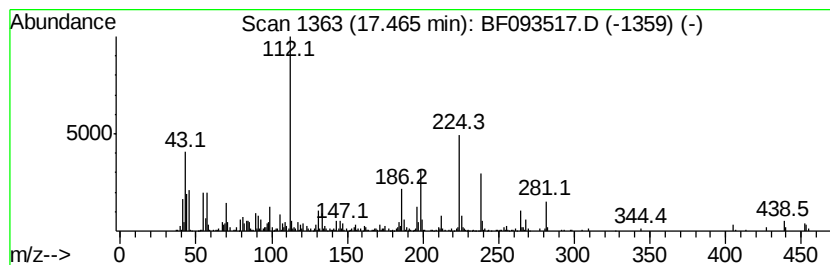
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown17.47 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.47	18.49 ng	1045000	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dimethyl-2,5-dioxoimidazo[4,...	198	C8H14N4O2	314767-27-6	38
2		1-Methyl-2-ethyl-5-undecylpyrrol...	267	C18H37N	1000111-44-6	25
3		1,3-Cyclopentanedione, 2-methyl-	112	C6H8O2	000765-69-5	22
4		Pyrazine, 1,4-dioxide	112	C4H4N2O2	002423-84-9	22
5		Acetamide, 2-cyclohexylamino)-N-...	238	C11H18N4O2	1000263-91-5	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030917\
 Data File : BF093517.D
 Acq On : 10 Mar 2017 11:25
 Operator : SJ/MA
 Sample : I2176-06
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EW-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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
unknown6.08	6.08	28.9	ng	21808500	1	6.76	15084300	20.0
Dodecane, 2,6,10-...	9.08	48.5	ng	4462400	3	9.81	1841260	20.0
Tetradecane	9.52	82.5	ng	7591420	3	9.81	1841260	20.0
unknown9.66	9.66	17.7	ng	1628690	3	9.81	1841260	20.0
unknown9.70	9.70	22.3	ng	2053050	3	9.81	1841260	20.0
Tetradecane, 2,6,...	9.99	22.2	ng	2045780	3	9.81	1841260	20.0
unknown10.05	10.05	24.3	ng	2240370	3	9.81	1841260	20.0
unknown10.12	10.12	79.0	ng	7276680	3	9.81	1841260	20.0
Phenol, 4-(1,1,3,...	10.33	15.3	ng	1408590	3	9.81	1841260	20.0
Undecane, 3,5-dim...	10.45	36.3	ng	3342900	3	9.81	1841260	20.0
n-Hexadecanoic acid	11.91	28.8	ng	29977000	4	11.28	20823800	20.0
Octadecanoic acid	12.63	20.3	ng	3054590	5	13.92	3011070	20.0
Ethanol, 2-[2-[4-...	12.97	65.6	ng	9879670	5	13.92	3011070	20.0
Pyrido[2,3-d]pyri...	13.02	44.3	ng	6665920	5	13.92	3011070	20.0
unknown13.10	13.10	53.0	ng	7972760	5	13.92	3011070	20.0
Pyrrolo[1,2-a]-1,...	13.16	43.6	ng	6571790	5	13.92	3011070	20.0
unknown13.20	13.20	20.8	ng	3130430	5	13.92	3011070	20.0
3,6,9,12,15-Penta...	14.88	18.3	ng	1033870	6	15.33	1130110	20.0
unknown17.47	17.47	18.5	ng	1045000	6	15.33	1130110	20.0