

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
 Data File : BF092287.D
 Acq On : 16 Jan 2017 16:14
 Operator : UM/SJ
 Sample : I1219-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC011217-LIQUID-TODT-HILL

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-BF122116.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	2.038	20	22	38	rVB	264856	514837	7.80%	0.638%
2	2.255	38	41	50	rVB	27793	75857	1.15%	0.094%
3	2.564	65	68	73	rVB	59475	102767	1.56%	0.127%
4	3.936	185	188	193	rBV	44166	89767	1.36%	0.111%
5	4.667	250	252	263	rBV	762982	1147769	17.40%	1.422%
6	5.124	290	292	293	rBV	49989	71118	1.08%	0.088%
7	5.147	293	294	303	rVB	2137922	3165368	47.98%	3.921%
8	5.353	308	312	314	rBV2	38330	74586	1.13%	0.092%
9	5.387	314	315	319	rVB	94595	93326	1.41%	0.116%
10	5.490	321	324	333	rVB2	89395	229455	3.48%	0.284%
11	6.176	380	384	387	rBV	33231	83432	1.26%	0.103%
12	6.233	387	389	396	rVV	1498300	2265919	34.35%	2.807%
13	6.336	396	398	400	rVV	5418045	5236778	79.38%	6.487%
14	6.427	404	406	412	rVB	202568	267035	4.05%	0.331%
15	6.564	416	418	420	rBV	1062381	1305702	19.79%	1.617%
16	6.656	424	426	429	rBV	236837	462877	7.02%	0.573%
17	6.713	429	431	434	rVB	3737276	4911437	74.45%	6.084%
18	6.987	450	455	456	rBV2	77696	144116	2.18%	0.179%
19	7.136	465	468	471	rBV	3712313	4229114	64.11%	5.239%
20	7.262	477	479	480	rBV	67394	97208	1.47%	0.120%
21	7.296	480	482	485	rVV	149757	192179	2.91%	0.238%
22	7.422	489	493	498	rVB2	191230	523769	7.94%	0.649%
23	7.524	498	502	505	rBV3	80658	176411	2.67%	0.219%
24	7.616	508	510	512	rBV	836659	731314	11.09%	0.906%
25	7.787	523	525	528	rBV	95909	155109	2.35%	0.192%
26	7.844	528	530	532	rVV	1579562	1861051	28.21%	2.305%
27	7.890	532	534	538	rVB	289050	331046	5.02%	0.410%
28	8.005	541	544	546	rBV2	38541	83231	1.26%	0.103%
29	8.130	553	555	556	rBV	675276	610786	9.26%	0.757%
30	8.153	556	557	559	rVB	774194	611730	9.27%	0.758%
31	8.245	559	565	568	rBV2	313783	484373	7.34%	0.600%
32	8.450	579	583	584	rBV2	60805	150973	2.29%	0.187%
33	8.496	585	587	588	rVV	1036953	907942	13.76%	1.125%
34	8.530	588	590	592	rVV2	1745589	1990271	30.17%	2.465%

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35	8.610	595	597	599 rBV	87280	109291	1.66%	0.135%
36	8.656	599	601	605 rVB3	56850	93370	1.42%	0.116%
37	8.736	605	608	610 rBV2	77324	135646	2.06%	0.168%
38	8.839	613	617	622 rVV4	110080	375879	5.70%	0.466%
39	8.930	622	625	627 rVB	6570395	6596994	100.00%	8.172%
40	9.022	627	633	635 rBV4	86127	79537	1.21%	0.099%
41	9.182	643	647	648 rBV4	42138	112102	1.70%	0.139%
42	9.273	652	655	657 rBV	500983	544398	8.25%	0.674%
43	9.330	657	660	661 rVV3	196634	309847	4.70%	0.384%
44	9.365	661	663	666 rVV	934573	986040	14.95%	1.221%
45	9.433	666	669	670 rVB	702317	796081	12.07%	0.986%
46	9.479	670	673	677 rVB5	44981	83096	1.26%	0.103%
47	9.548	677	679	681 rBV2	125438	163641	2.48%	0.203%
48	9.593	681	683	687 rVB2	2212467	2337367	35.43%	2.895%
49	9.719	689	694	697 rBV3	154971	296229	4.49%	0.367%
50	9.788	697	700	701 rBV2	36442	69345	1.05%	0.086%
51	9.833	701	704	706 rBV	811480	1043535	15.82%	1.293%
52	9.936	711	713	714 rVV	74449	77175	1.17%	0.096%
53	9.993	714	718	719 rVV2	78733	90722	1.38%	0.112%
54	10.039	719	722	725 rVB3	218115	410344	6.22%	0.508%
55	10.222	735	738	740 rVB2	60087	67773	1.03%	0.084%
56	10.290	740	744	745 rBV2	335981	552949	8.38%	0.685%
57	10.382	747	752	754 rVV3	2764794	4155107	62.98%	5.147%
58	10.416	754	755	758 rVV2	206183	233008	3.53%	0.289%
59	10.473	758	760	762 rVV	132718	157216	2.38%	0.195%
60	10.519	762	764	769 rVB	429717	522729	7.92%	0.647%
61	10.770	784	786	790 rVB	111823	126852	1.92%	0.157%
62	10.851	790	793	798 rVB3	117667	262453	3.98%	0.325%
63	10.953	799	802	806 rBV3	102823	272717	4.13%	0.338%
64	11.068	810	812	815 rVV	1928542	1747882	26.50%	2.165%
65	11.273	827	830	832 rVB	6318729	6472211	98.11%	8.017%
66	11.319	832	834	838 rVB3	59689	111095	1.68%	0.138%
67	11.388	838	840	843 rBV	256386	301125	4.56%	0.373%
68	11.445	843	845	849 rVB3	110301	197937	3.00%	0.245%
69	11.628	857	861	863 rBV	560430	1001952	15.19%	1.241%
70	11.662	863	864	871 rVV	217121	316670	4.80%	0.392%
71	11.788	874	875	877 rVV	109304	110623	1.68%	0.137%

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72	11.856	880	881	884	rVB3	60078	75212	1.14%	0.093%
73	12.039	895	897	899	rBV	356576	331001	5.02%	0.410%
74	12.131	903	905	907	rBV	73569	83455	1.27%	0.103%
75	12.176	907	909	911	rBV	107812	110414	1.67%	0.137%
76	12.325	920	922	923	rBV	71545	106495	1.61%	0.132%
77	12.359	923	925	927	rVV	267182	249506	3.78%	0.309%
78	12.405	927	929	932	rVV2	719555	1121347	17.00%	1.389%
79	12.485	935	936	938	rVV2	124408	146080	2.21%	0.181%
80	12.554	940	942	944	rVV2	93026	162367	2.46%	0.201%
81	12.656	948	951	954	rVV	4954416	6515927	98.77%	8.071%
82	12.702	954	955	958	rVB	136969	170855	2.59%	0.212%
83	12.896	969	972	974	rBV	118383	234625	3.56%	0.291%
84	13.022	981	983	985	rBV	130739	193925	2.94%	0.240%
85	13.125	988	992	993	rBV4	92710	231412	3.51%	0.287%
86	13.205	996	999	1000	rBV	200593	328847	4.98%	0.407%
87	13.239	1000	1002	1006	rVB2	156396	253409	3.84%	0.314%
88	13.365	1010	1013	1018	rVB2	134728	337279	5.11%	0.418%
89	13.445	1018	1020	1022	rBV2	108096	221587	3.36%	0.274%
90	13.548	1027	1029	1030	rBV2	182553	327175	4.96%	0.405%
91	13.697	1038	1042	1046	rBV	2067092	2420152	36.69%	2.998%
92	13.982	1065	1067	1070	rBV	271992	464757	7.04%	0.576%
93	14.291	1091	1094	1097	rBV	262735	489212	7.42%	0.606%
94	14.577	1117	1119	1123	rVB	192169	323370	4.90%	0.401%
95	15.045	1158	1160	1163	rBV	867205	1133020	17.17%	1.403%

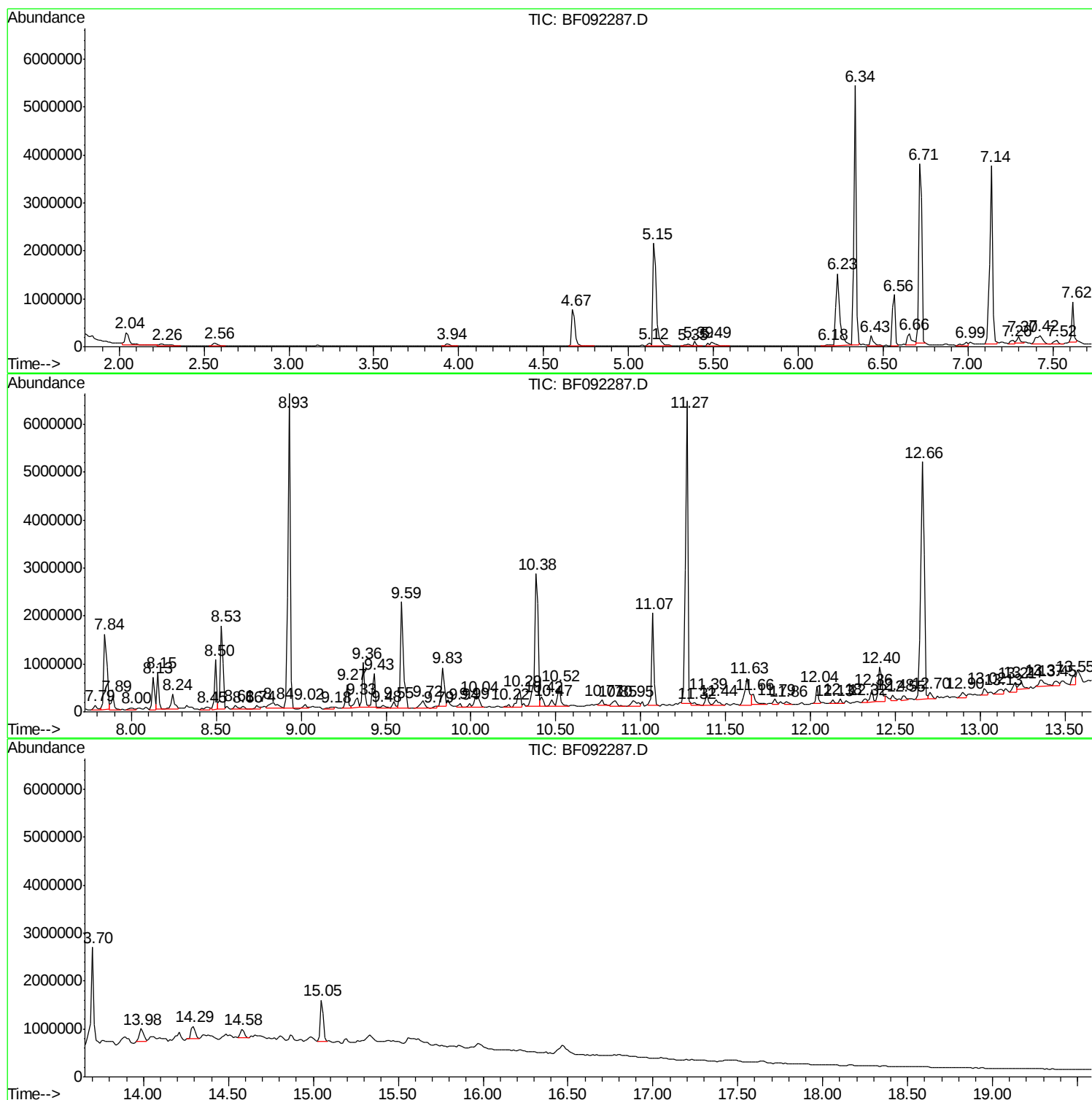
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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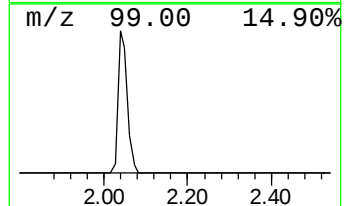
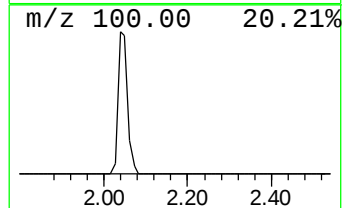
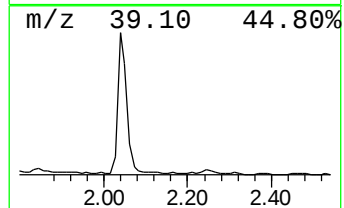
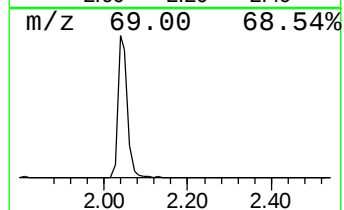
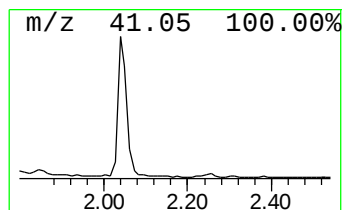
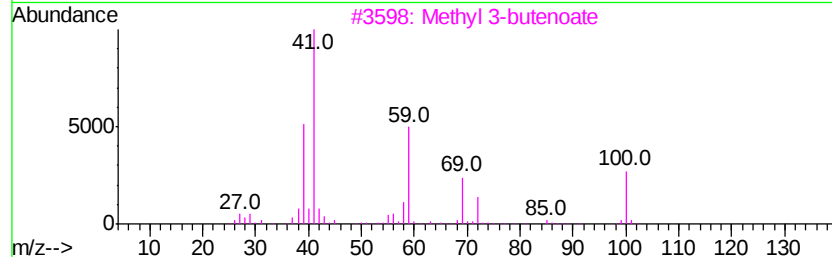
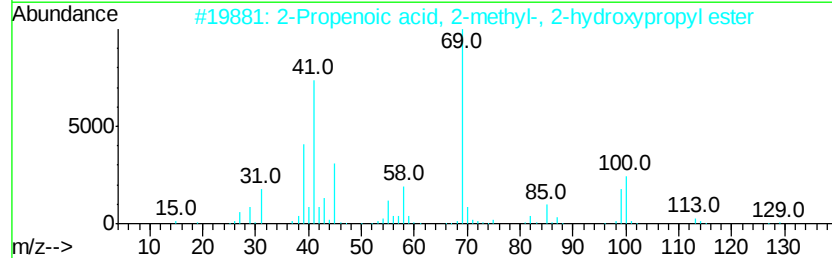
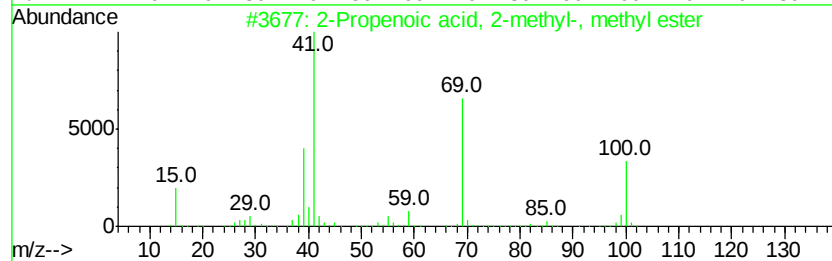
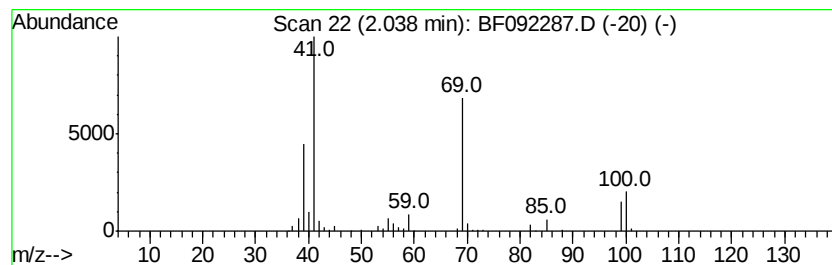
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Propenoic acid, 2-methyl-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.04	7.89 ng	514837	1,4-Dichlorobenzene-d4	6.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propenoic acid, 2-methyl-, met...	100	C5H8O2	000080-62-6	72
2			2-Propenoic acid, 2-methyl-, 2-h...	144	C7H12O3	000923-26-2	64
3			Methyl 3-butenote	100	C5H8O2	003724-55-8	45
4			2-Butenoic acid, methyl ester, (E)-	100	C5H8O2	000623-43-8	42
5			Cyclopropanecarboxylic acid, met...	100	C5H8O2	002868-37-3	36



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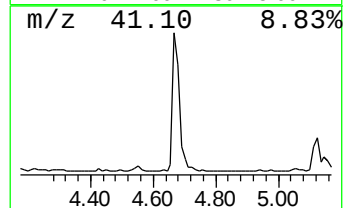
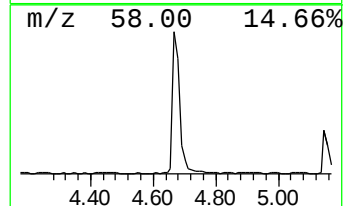
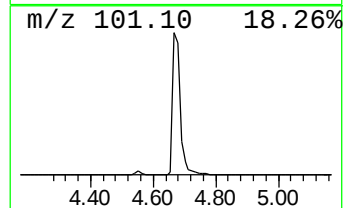
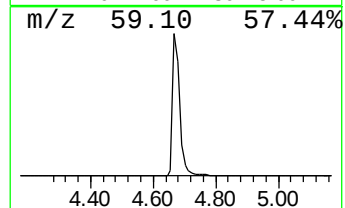
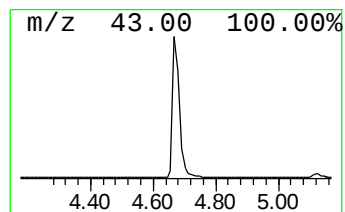
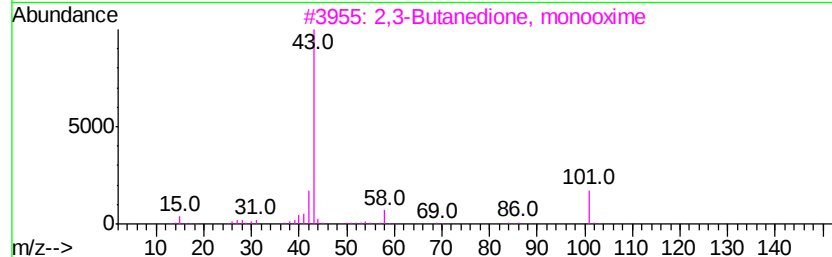
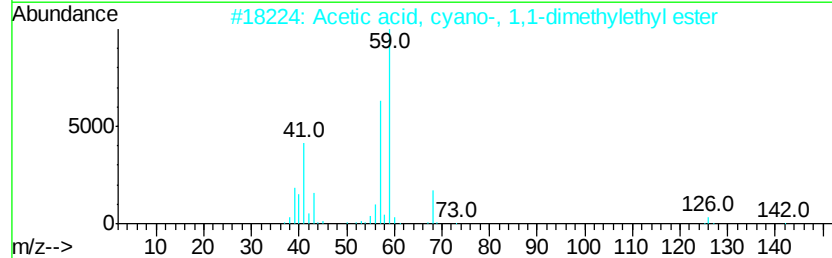
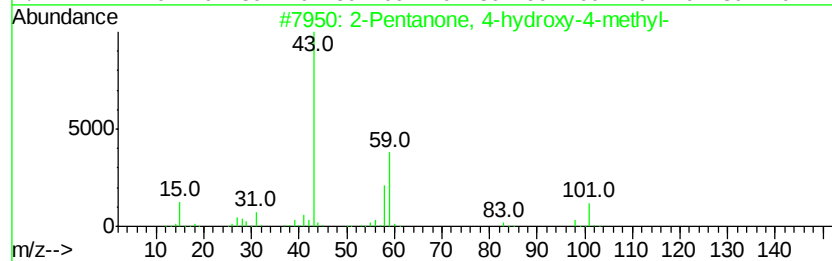
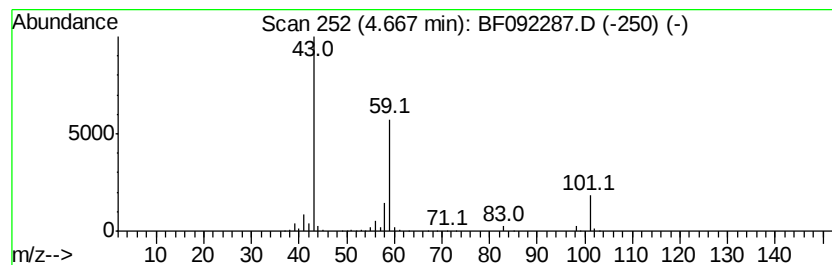
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.67	17.58 ng	1147770	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethyl ester	141	C7H11NO2	001116-98-9	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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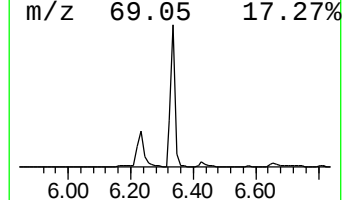
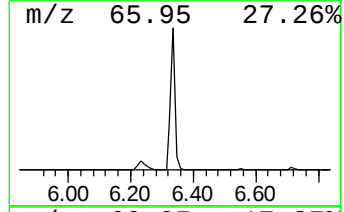
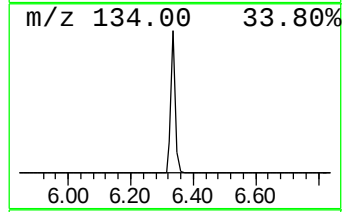
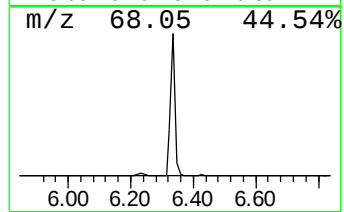
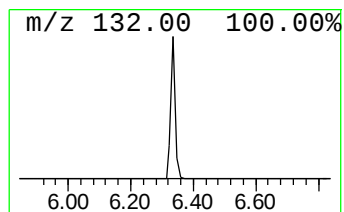
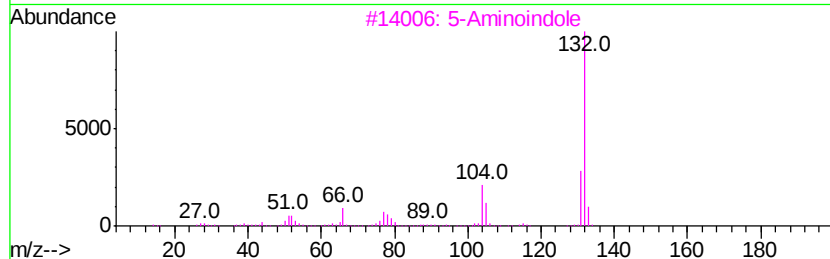
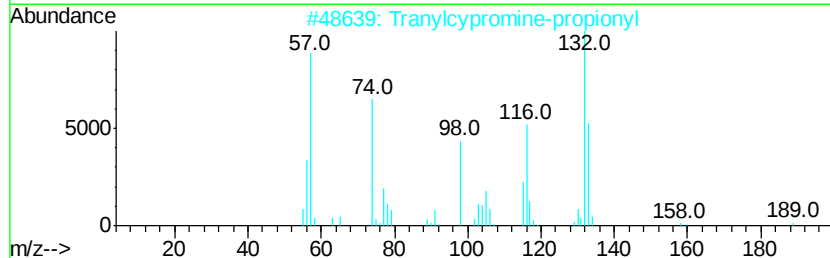
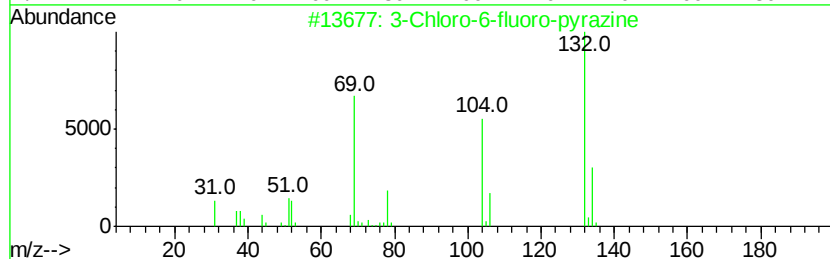
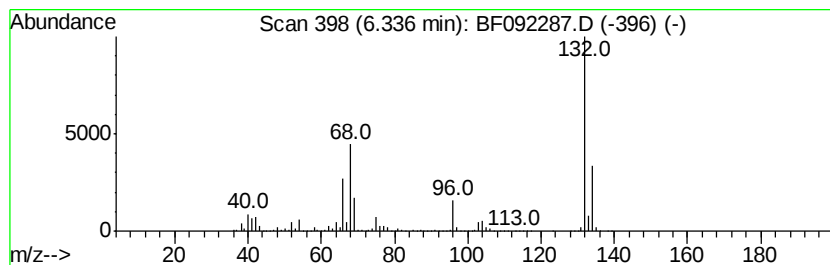
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.34 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	80.21 ng	5236780	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Aminoindole	132	C8H8N2	005192-03-0	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9



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BNA_F
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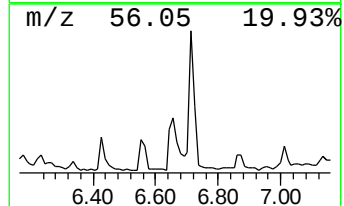
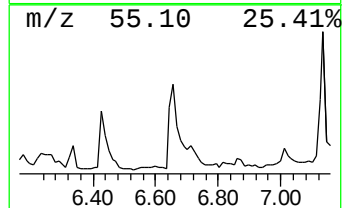
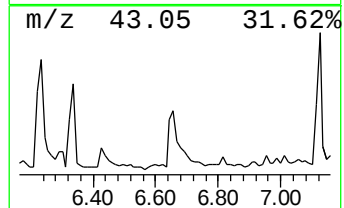
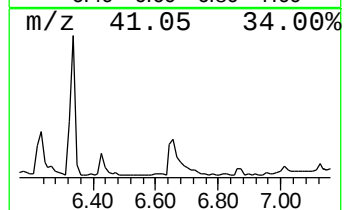
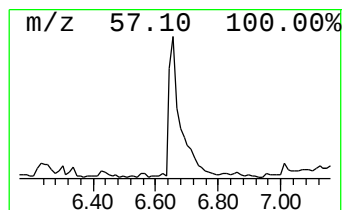
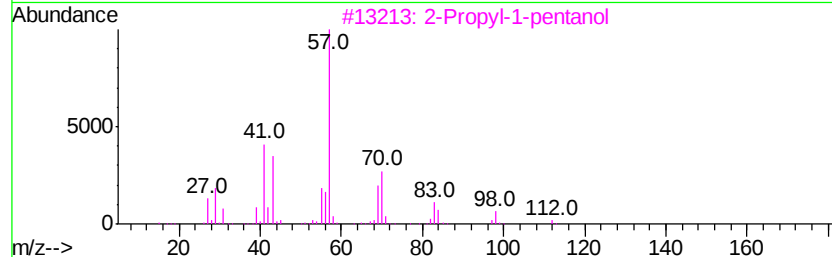
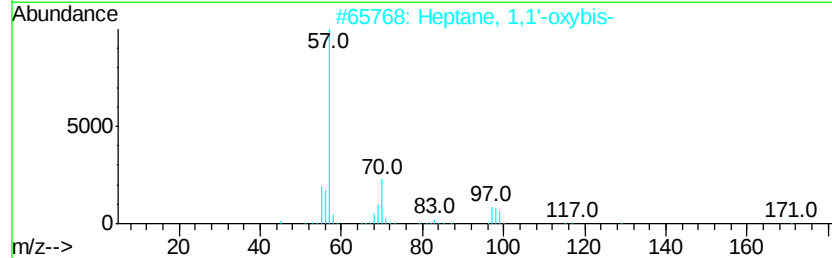
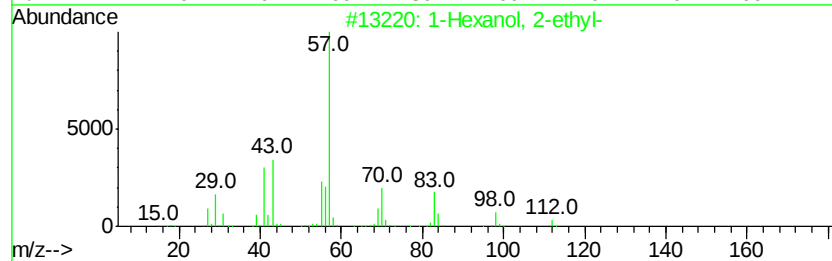
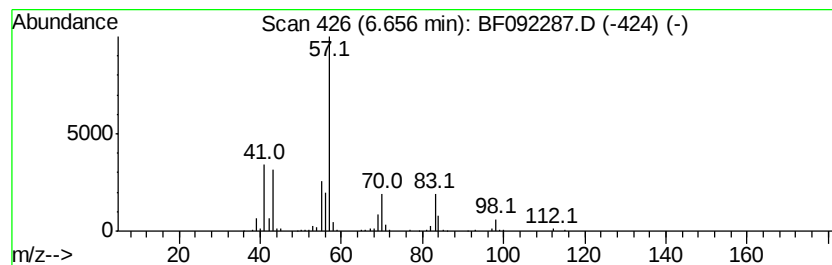
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	7.09 ng	462877	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
3		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
4		dl-2-Ethylhexyl chloroformate	192	C9H17ClO2	024468-13-1	42
5		1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011617\
Data File : BF092287.D
Acq On : 16 Jan 2017 16:14
Operator : UM/SJ
Sample : I1219-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
WC011217-LIQUID-TODT-HILL

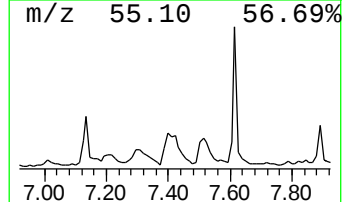
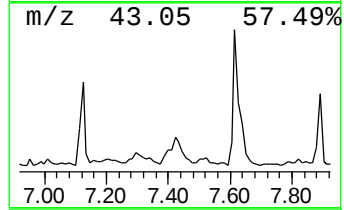
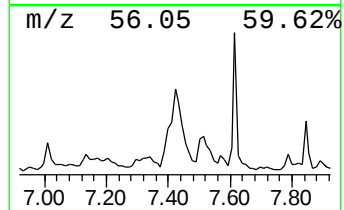
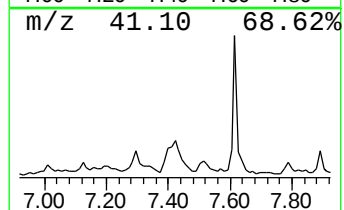
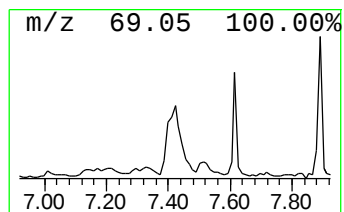
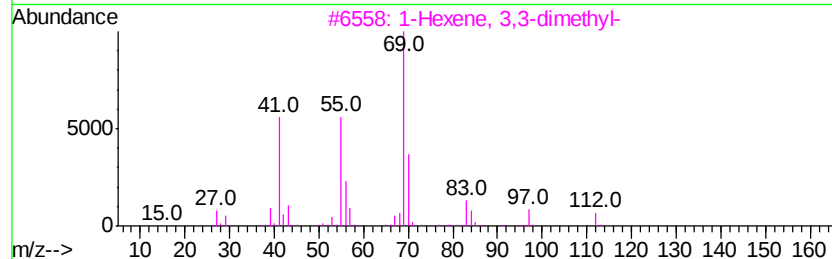
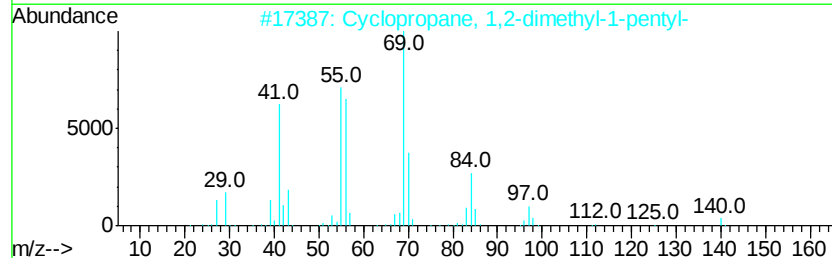
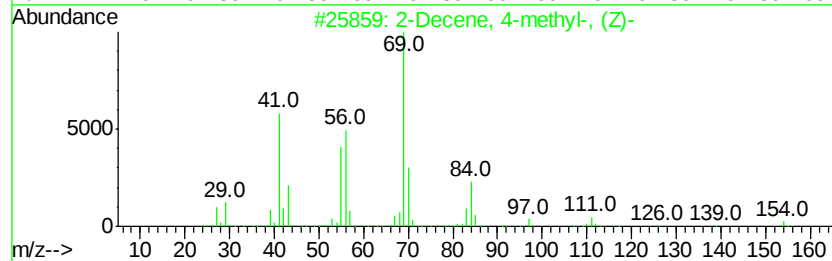
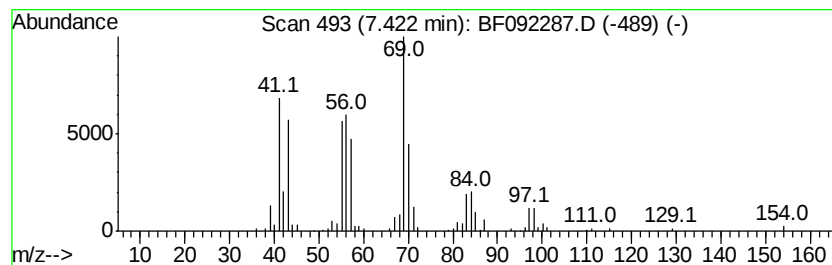
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Decene, 4-methyl-, (Z)- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	5.63 ng	523769	Naphthalene-d8	7.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Decene, 4-methyl-, (Z)-	154	C11H22	074630-30-1	59
2		Cyclopropane, 1,2-dimethyl-1-pen...	140	C10H20	062238-04-4	59
3		1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	50
4		Cyanamide, dimethyl-	70	C3H6N2	001467-79-4	47
5		1-Nonanol	144	C9H20O	000143-08-8	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011617\
Data File : BF092287.D
Acq On : 16 Jan 2017 16:14
Operator : UM/SJ
Sample : I1219-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
WC011217-LIQUID-TODT-HILL

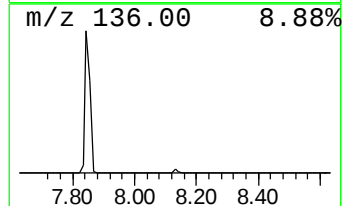
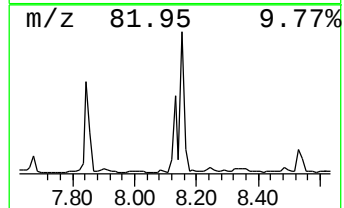
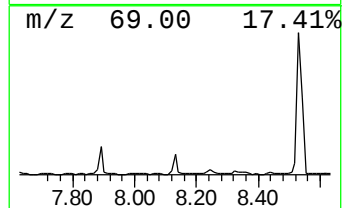
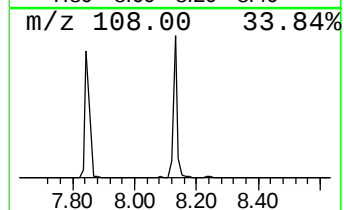
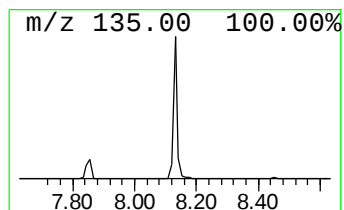
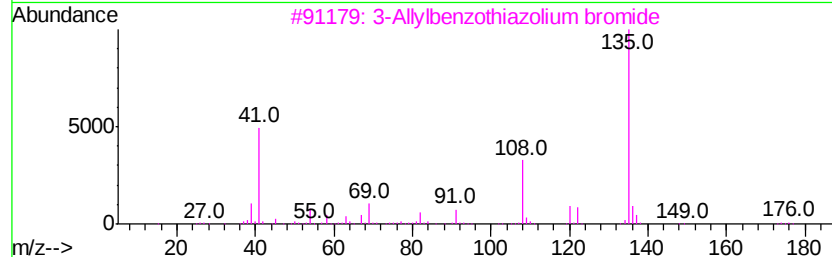
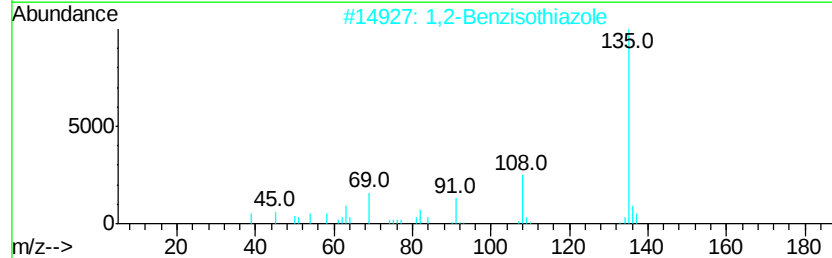
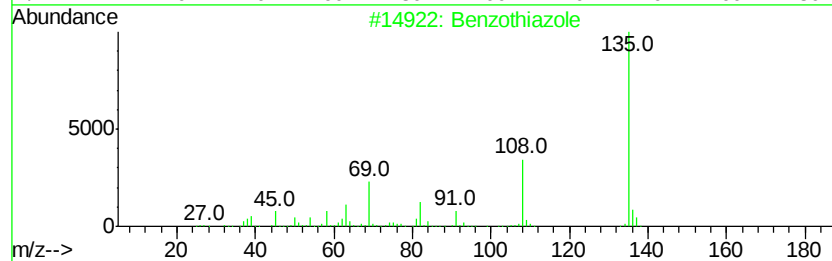
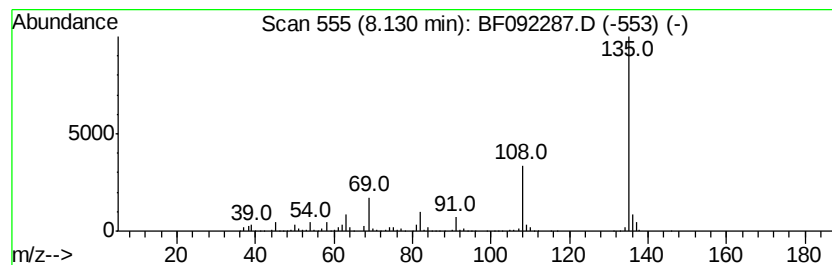
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzothiazole Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.13	6.56 ng	610786	Napthalene-d8	7.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzothiazole	135	C7H5NS	000095-16-9	97
2		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	91
3		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	90
4		Adenine	135	C5H5N5	000073-24-5	59
5		1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011617\
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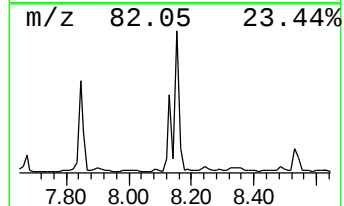
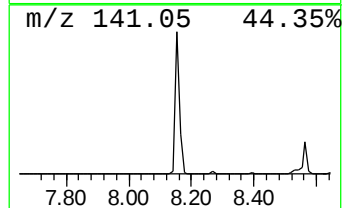
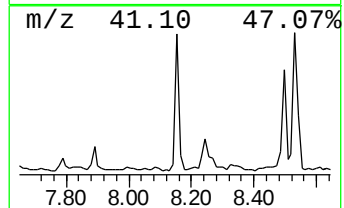
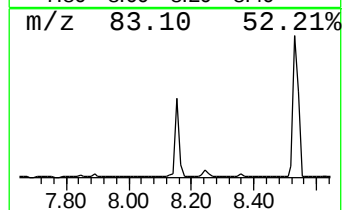
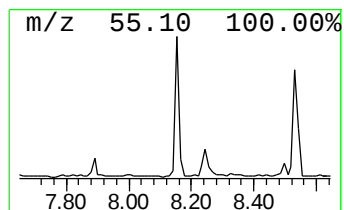
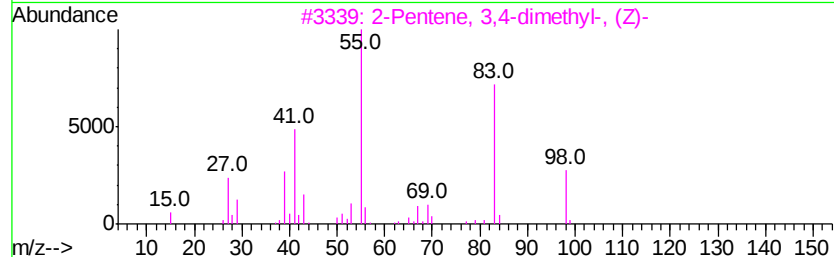
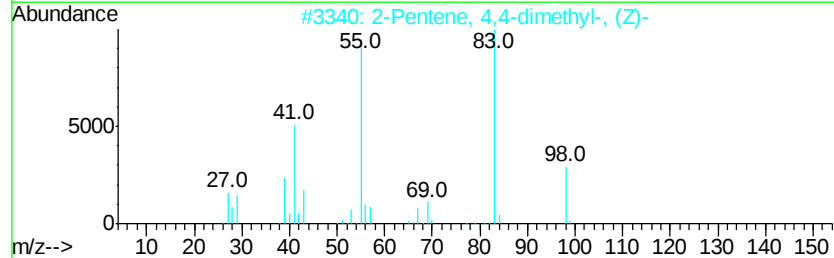
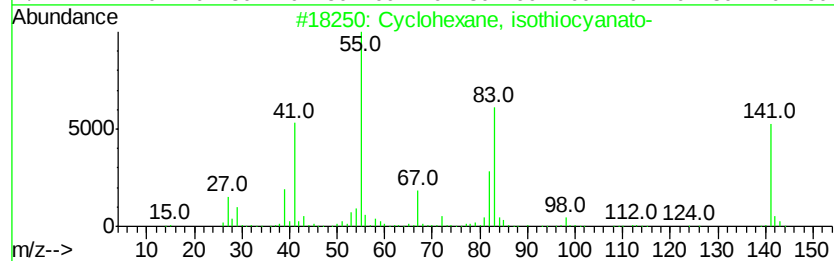
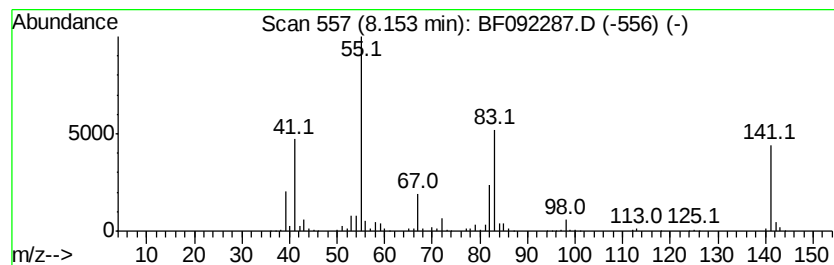
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclohexane, isothiocyanato- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	6.57 ng	611730	Naphthalene-d8	7.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, isothiocyanato-	141	C7H11NS	001122-82-3	97
2		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	35
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	35
4		1-Hexene, 6-bromo-	162	C6H11Br	002695-47-8	32
5		Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011617\
Data File : BF092287.D
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Operator : UM/SJ
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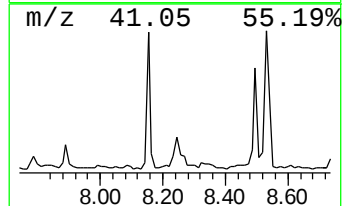
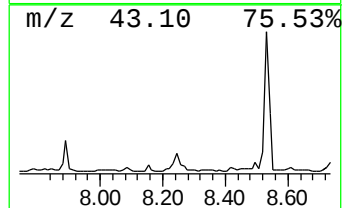
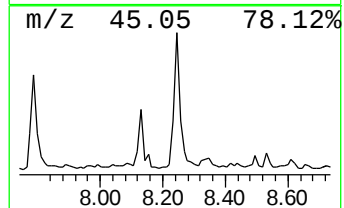
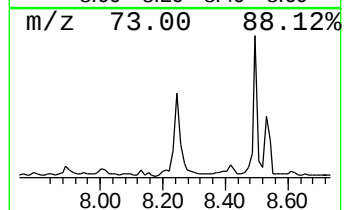
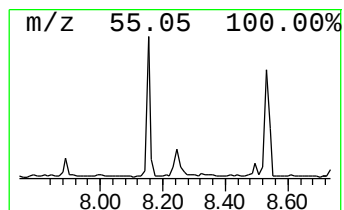
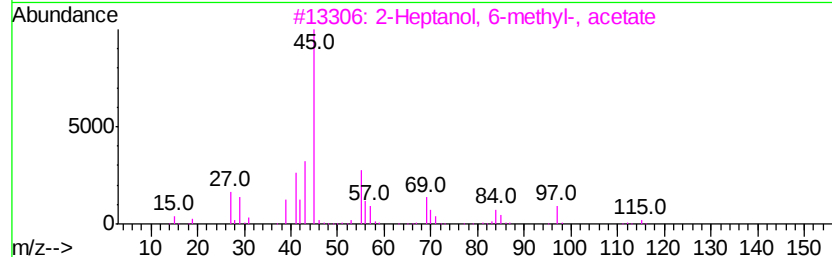
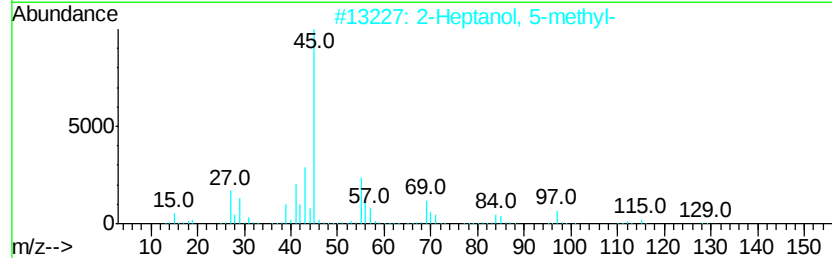
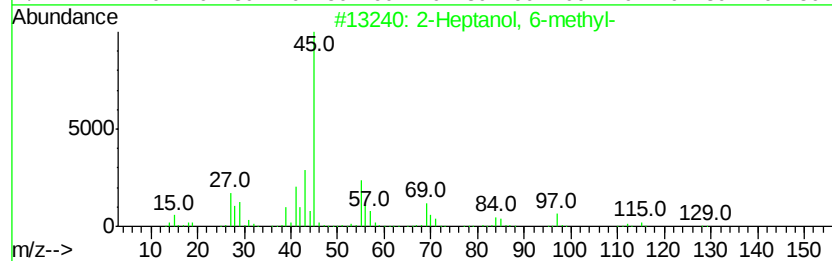
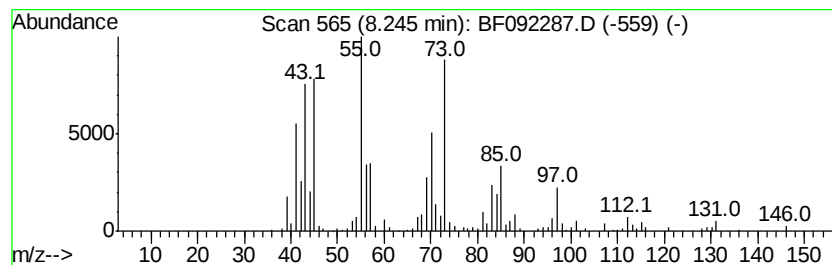
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown8.24 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.24	5.21 ng	484373	Napthalene-d8	7.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanol, 6-methyl-			130	C8H18O	004730-22-7	43
2	2-Heptanol, 5-methyl-			130	C8H18O	054630-50-1	43
3	2-Heptanol, 6-methyl-, acetate			130	C8H18O	067952-57-2	38
4	1-Octene, 6-methyl-			126	C9H18	013151-10-5	27
5	2-Propenoic acid, octyl ester			184	C11H20O2	002499-59-4	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011617\
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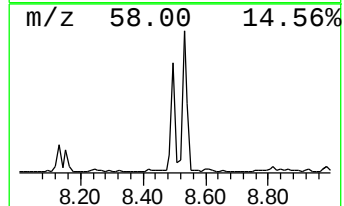
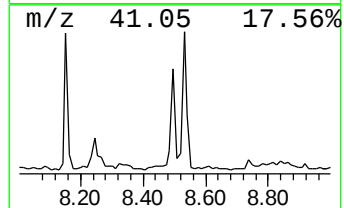
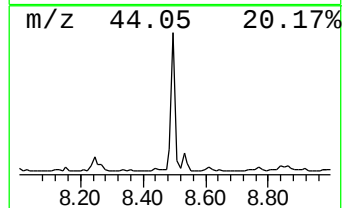
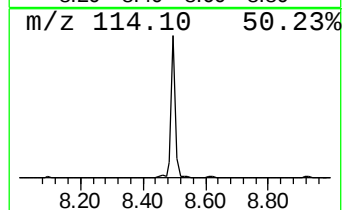
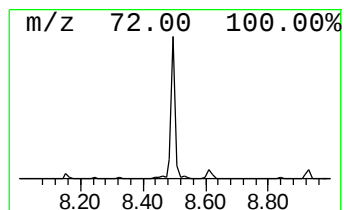
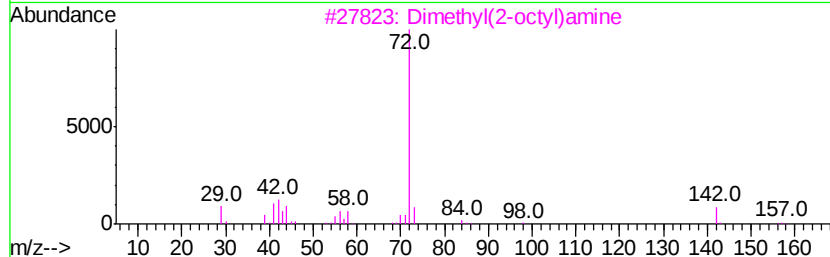
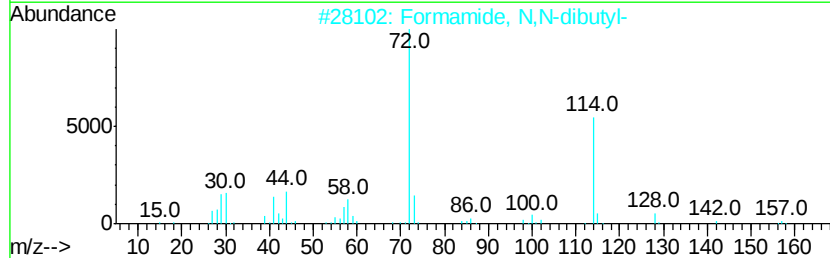
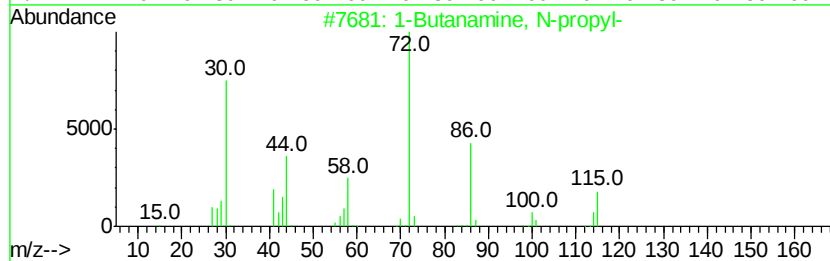
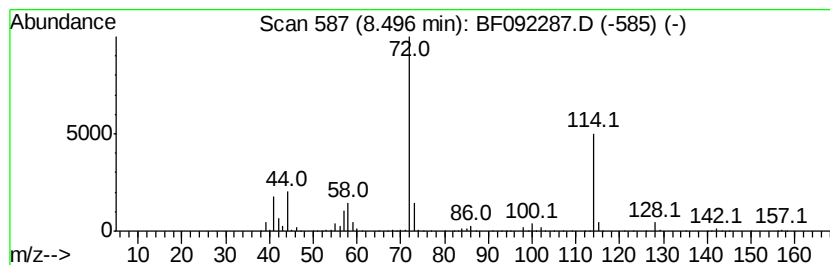
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown8.50 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.50	9.76 ng	907942	Naphthalene-d8	7.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanamine, N-propyl-	115	C7H17N	020193-21-9	49
2			Formamide, N,N-dibutyl-	157	C9H19NO	000761-65-9	49
3			Dimethyl(2-octyl)amine	157	C10H23N	007378-97-4	47
4			1-Propanamine, n-propyl-	101	C6H15N	000142-84-7	28
5			1,2-Ethanediamine, N,N'-diethyl-...	144	C8H20N2	000106-66-1	25



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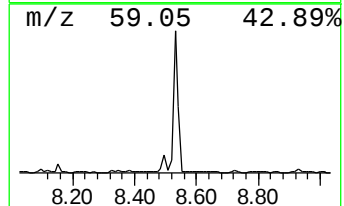
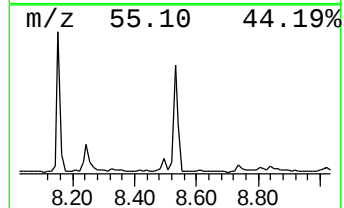
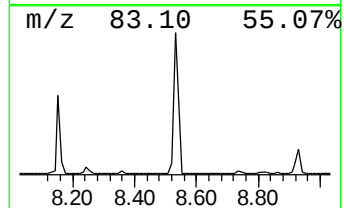
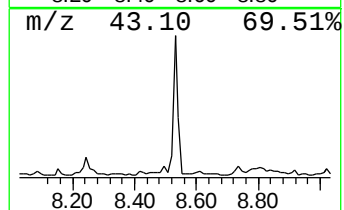
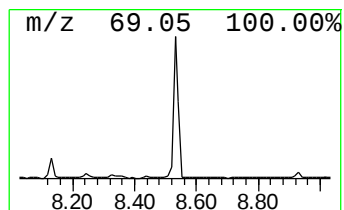
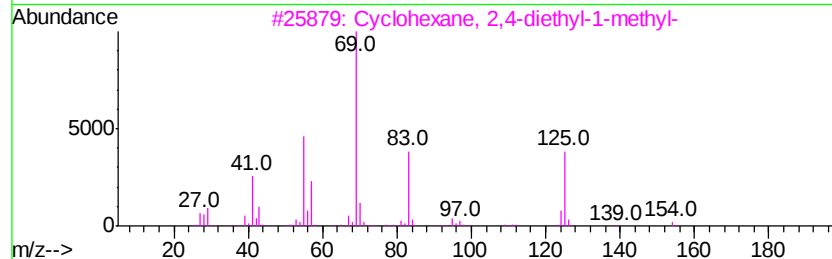
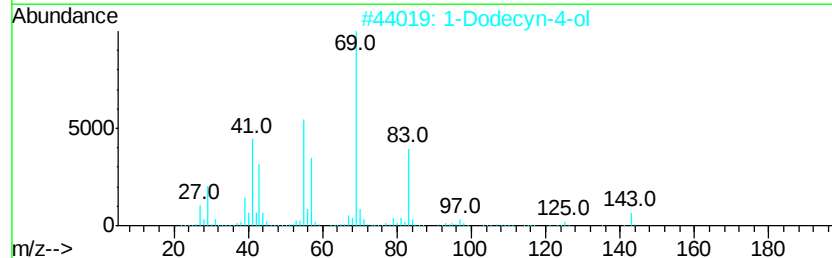
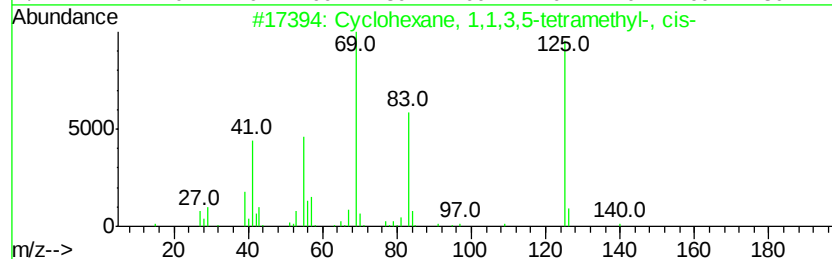
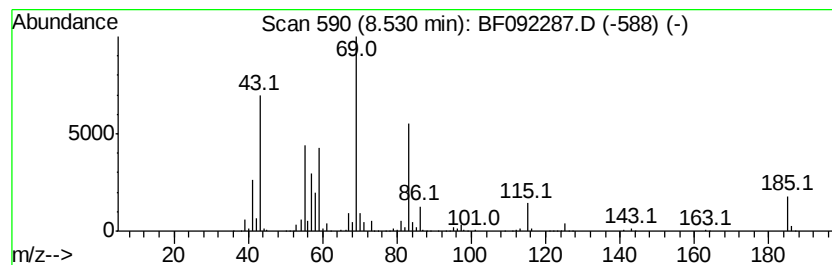
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown8.53 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.53	21.39 ng	1990270	Naphthalene-d8	7.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	43
2		1-Dodecyn-4-ol	182	C12H22O	074646-36-9	37
3		Cyclohexane, 2,4-diethyl-1-methyl-	154	C11H22	061142-70-9	37
4		Methyl 2-hydroxydecanoate	202	C11H22O3	071271-24-4	35
5		Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	32



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092287.D
Acq On : 16 Jan 2017 16:14
Operator : UM/SJ
Sample : I1219-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC011217-LIQUID-TODT-HILL

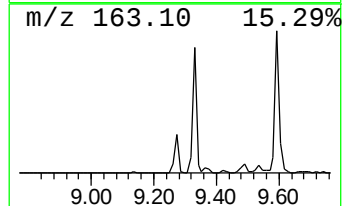
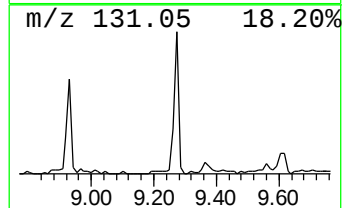
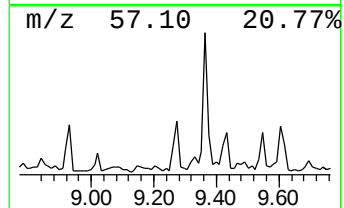
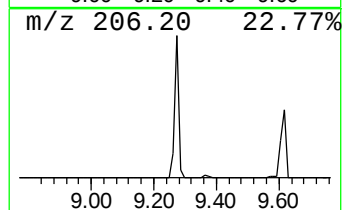
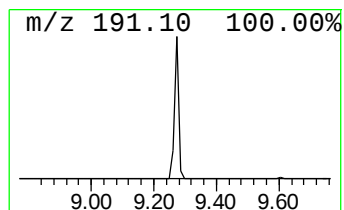
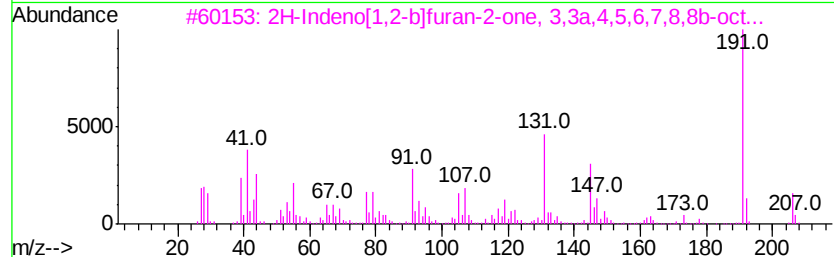
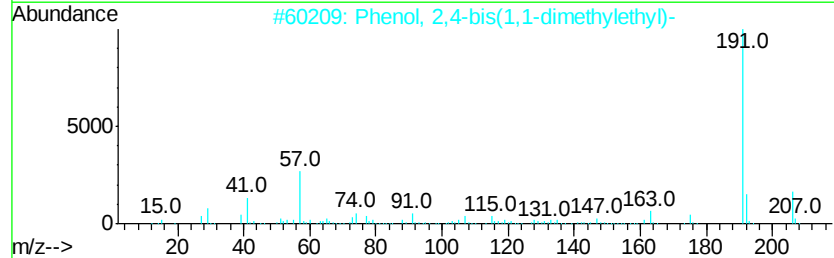
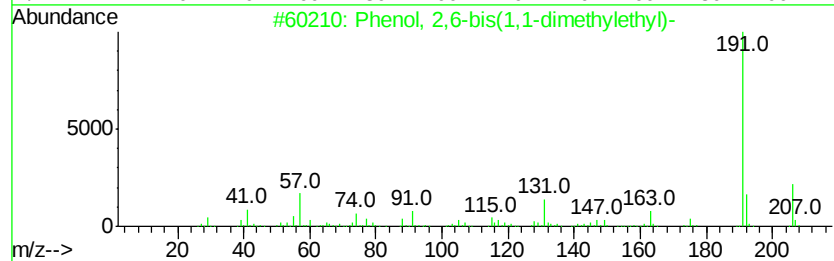
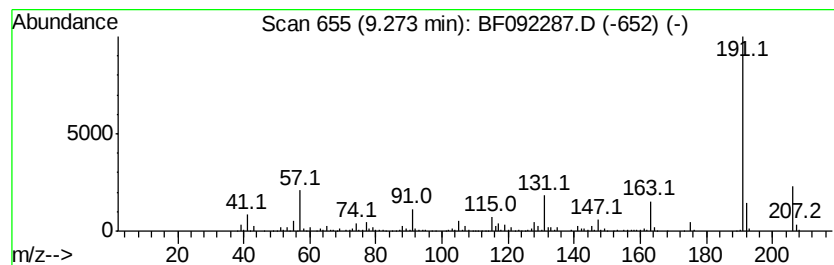
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.27	4.66 ng	544398	Acenaphthene-d10	9.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	93
2			Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	000096-76-4	87
3			2H-Indeno[1,2-b]furan-2-one, 3,3...	206	C13H18O2	1000196-74-3	80
4			Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	74
5			Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
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Operator : UM/SJ
Sample : I1219-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

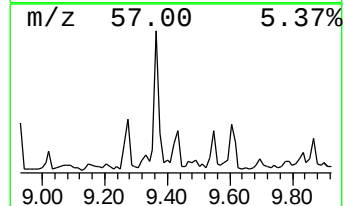
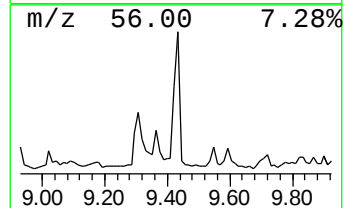
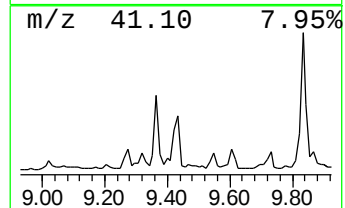
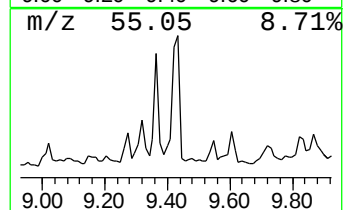
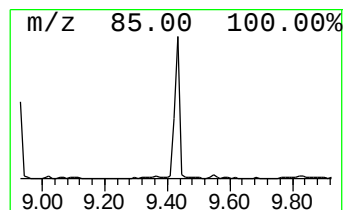
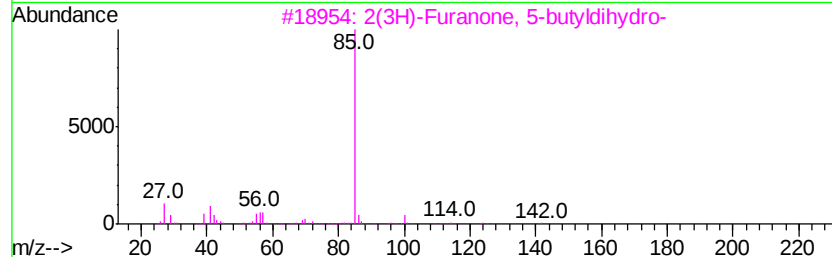
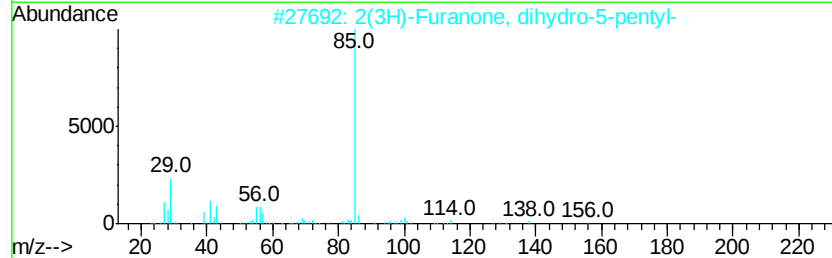
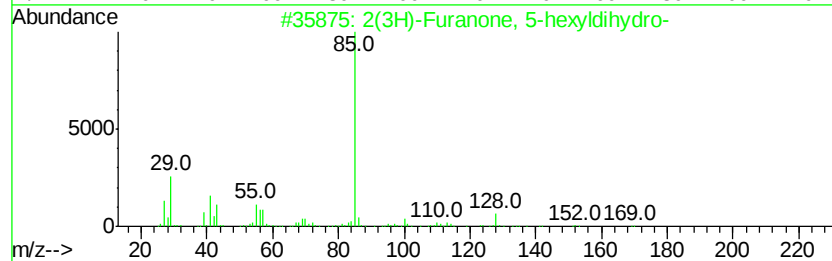
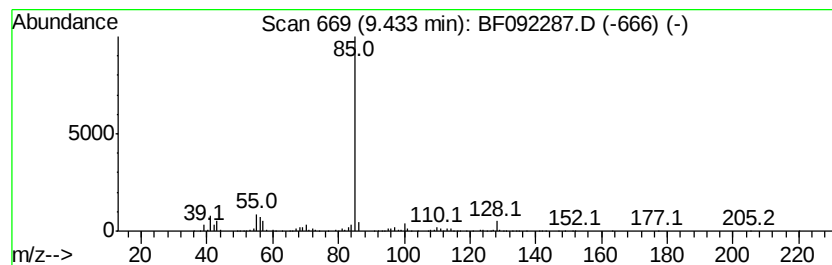
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ClientSampleId :
WC011217-LIQUID-TODT-HILL

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2(3H)-Furanone, 5-hexyldihydro... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.		
9.43	6.81 ng	796081	Acenaphthene-d10		9.59		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2(3H)-Furanone, 5-hexyldihydro-	170	C10H18O2	000706-14-9	90
2			2(3H)-Furanone, dihydro-5-pentyl-	156	C9H16O2	000104-61-0	72
3			2(3H)-Furanone, 5-butylidihydro-	142	C8H14O2	000104-50-7	72
4			2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	72
5			2(3H)-Furanone, 5-heptyldihydro-	184	C11H20O2	000104-67-6	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092287.D
Acq On : 16 Jan 2017 16:14
Operator : UM/SJ
Sample : I1219-02
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ClientSampleId :
WC011217-LIQUID-TODT-HILL

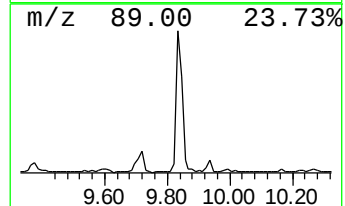
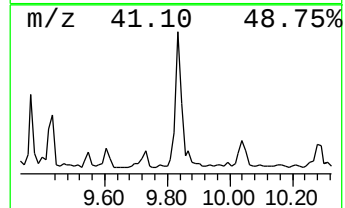
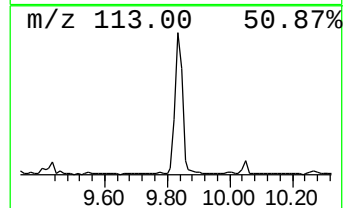
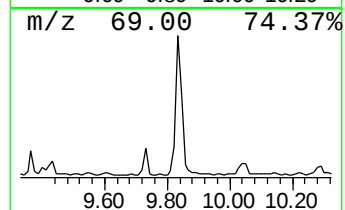
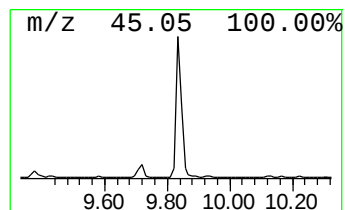
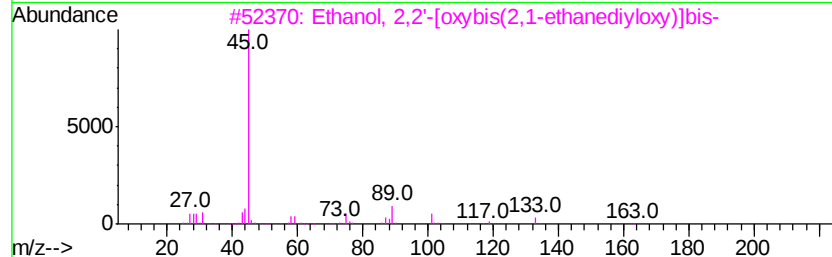
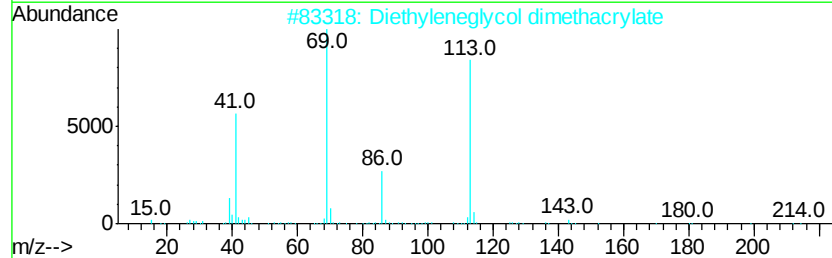
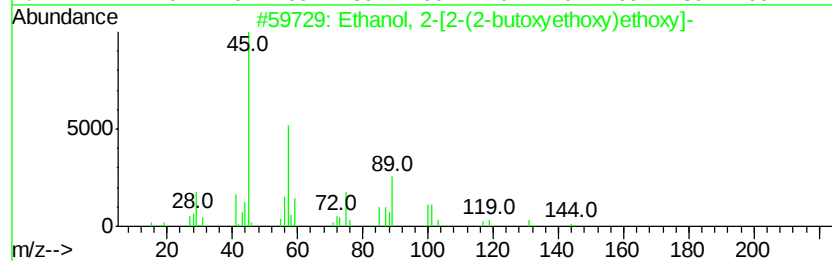
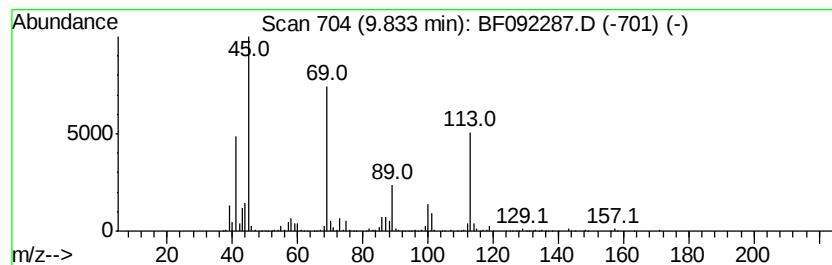
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown9.83 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	8.93 ng	1043540	Acenaphthene-d10	9.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	38
2		Diethyleneglycol dimethacrylate	242	C12H18O5	002358-84-1	32
3		Ethanol, 2,2'-[oxybis(2,1-ethane...	194	C8H18O5	000112-60-7	27
4		Ethanol, 2-[2-(ethenvloxy)ethoxy]-	132	C6H12O3	000929-37-3	27
5		Triethylene glycol	150	C6H14O4	000112-27-6	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
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Acq On : 16 Jan 2017 16:14
Operator : UM/SJ
Sample : I1219-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

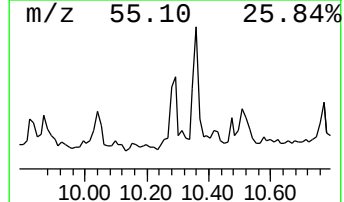
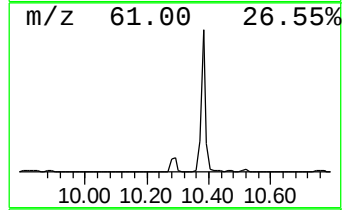
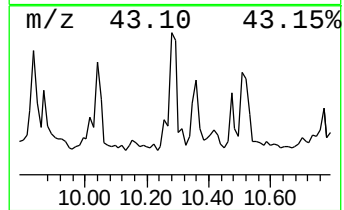
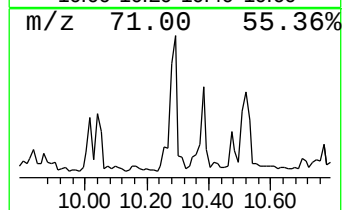
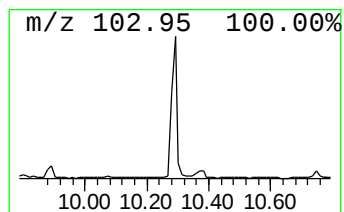
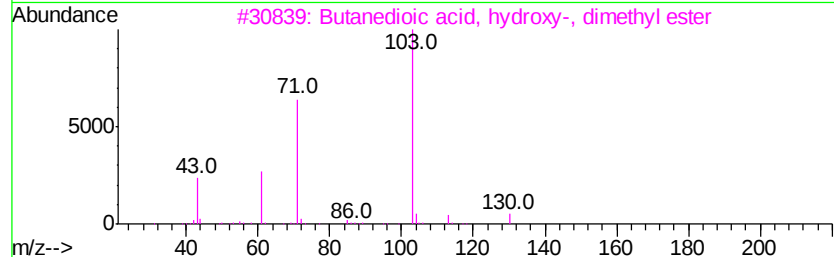
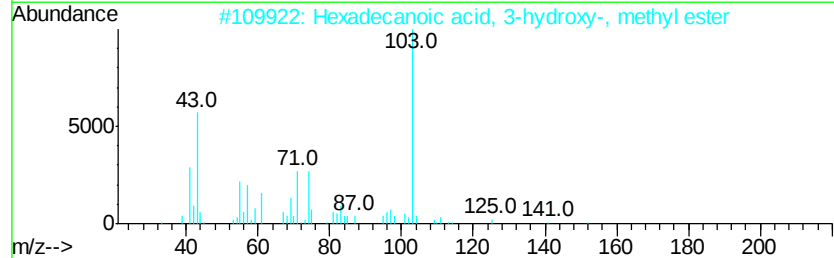
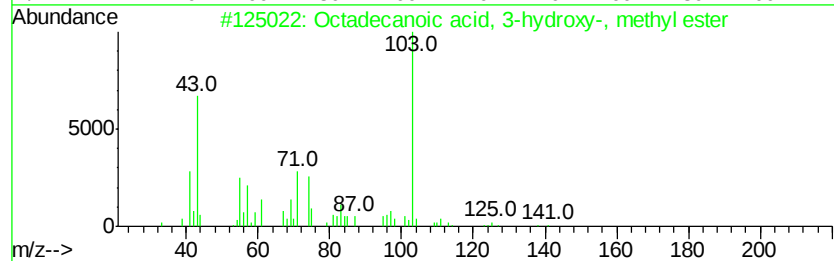
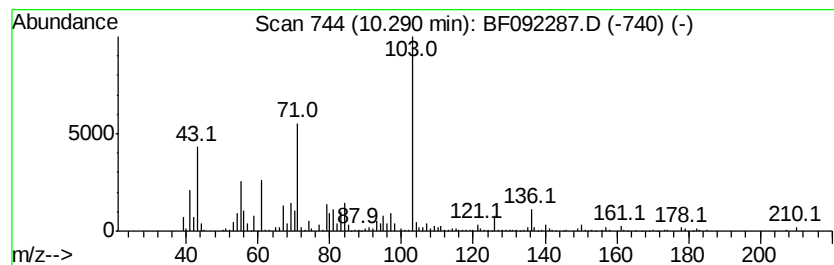
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Octadecanoic acid, 3-hydrox... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.29	4.73 ng	552949	Acenaphthene-d10		9.59	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, 3-hydroxy-, m...	314	C19H38O3	002420-36-2	52
2		Hexadecanoic acid, 3-hydroxy-, m...	286	C17H34O3	051883-36-4	50
3		Butanedioic acid, hydroxy-, dime...	162	C6H10O5	001587-15-1	45
4		Methyl 3-hydroxytetradecanoate	258	C15H30O3	055682-83-2	40
5		Decane, 1,1-diethoxy-	230	C14H30O2	034764-02-8	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011617\
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Acq On : 16 Jan 2017 16:14
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Misc :
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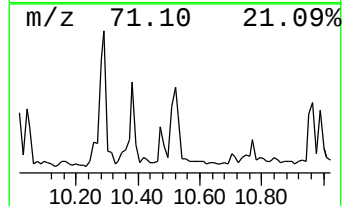
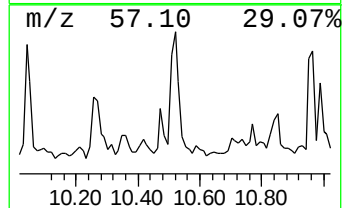
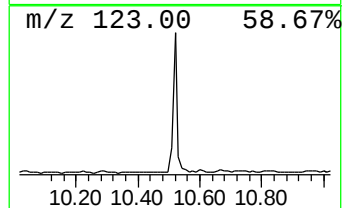
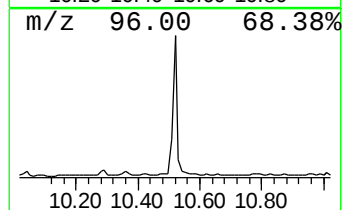
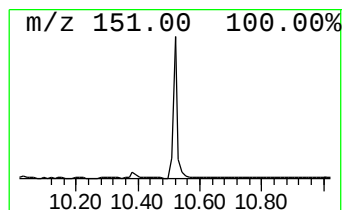
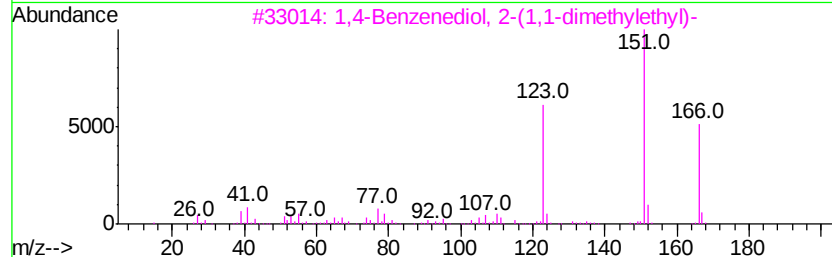
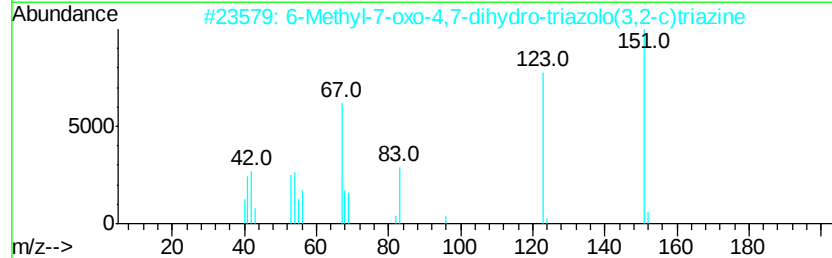
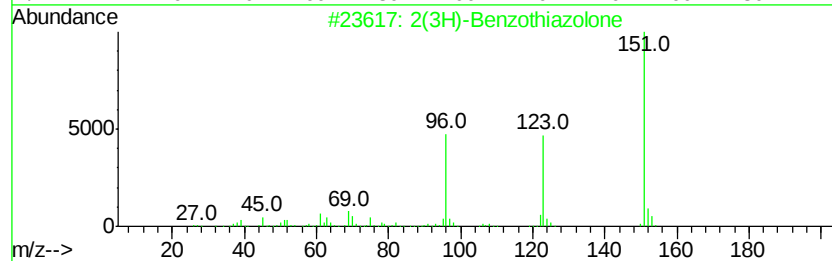
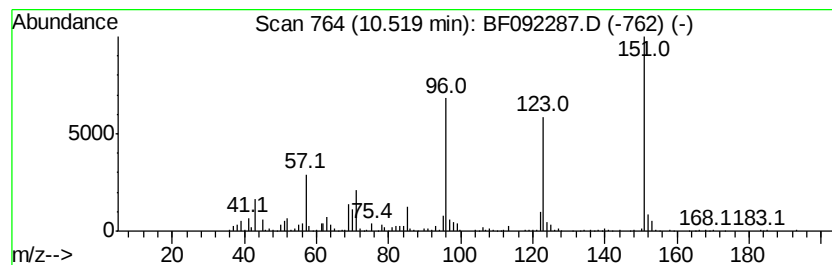
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 2(3H)-Benzothiazolone Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.52	5.98 ng	522729	Phenanthrene-d10	11.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		2(3H)-Benzothiazolone	151 C7H5NOS	000934-34-9 91
2		6-Methyl-7-oxo-4,7-dihydro-triaz...	151 C5H5N5O	057250-39-2 47
3		1,4-Benzenediol, 2-(1,1-dimethyl...	166 C10H14O2	001948-33-0 47
4		Thieno[2,3-b]pyridine-N-oxide	151 C7H5NOS	025557-50-0 38
5		1,2-Benzisothiazol-3(2H)-one	151 C7H5NOS	002634-33-5 38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092287.D
Acq On : 16 Jan 2017 16:14
Operator : UM/SJ
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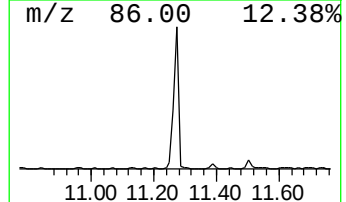
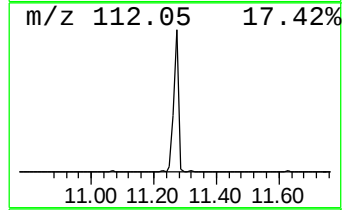
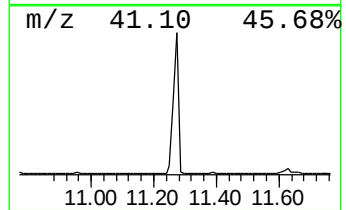
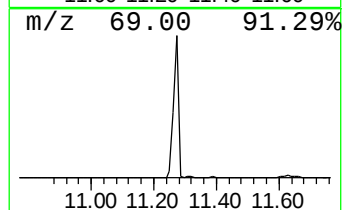
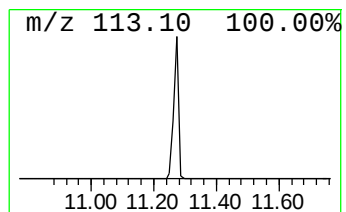
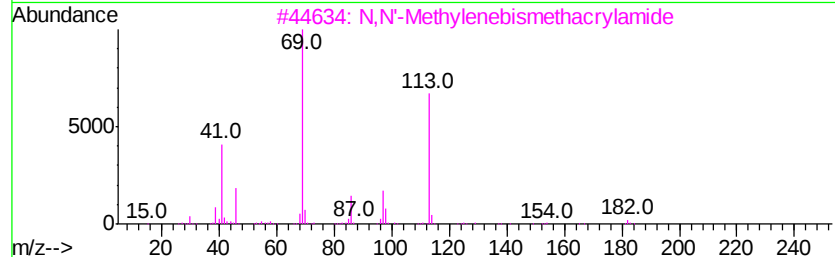
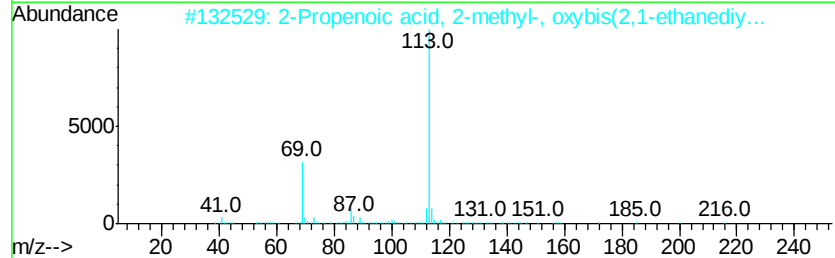
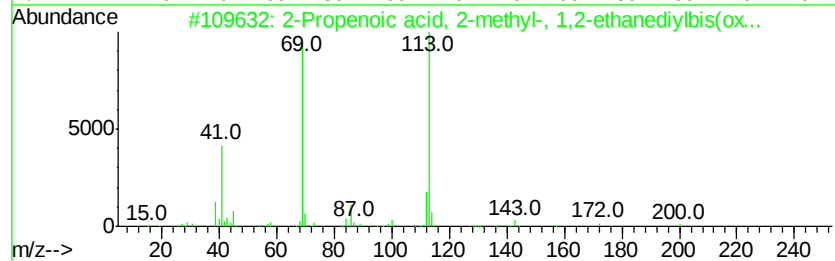
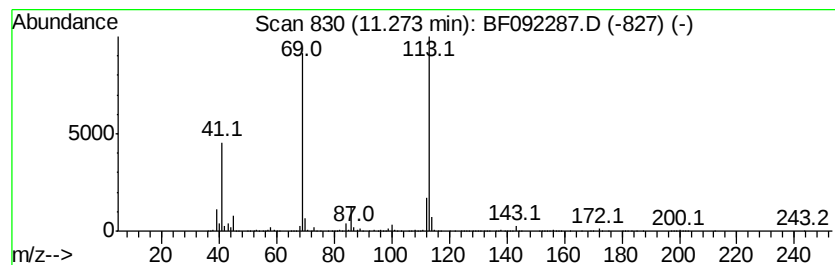
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 2-Propenoic acid, 2-methyl-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.27	74.06 ng	6472210	Phenanthrene-d10	11.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propenoic acid, 2-methyl-, 1,2...	286	C14H22O6	000109-16-0	91
2		2-Propenoic acid, 2-methyl-, oxy...	330	C16H26O7	000109-17-1	64
3		N,N'-Methylenebismethacrylamide	182	C9H14N2O2	002359-15-1	56
4		Diethylene glycol dimethacrylate	242	C12H18O5	002358-84-1	56
5		Pyrimidine-4-carboxamide, 2-chloro-	157	C5H4ClN3O	022536-66-9	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011617\
Data File : BF092287.D
Acq On : 16 Jan 2017 16:14
Operator : UM/SJ
Sample : I1219-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
WC011217-LIQUID-TODT-HILL

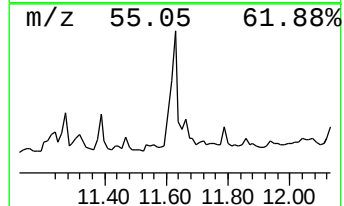
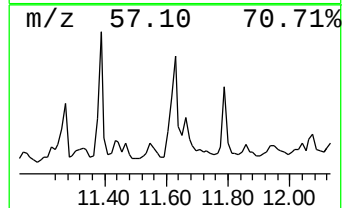
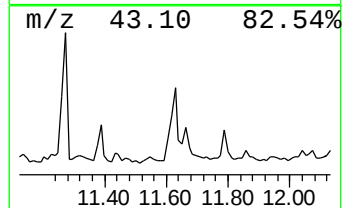
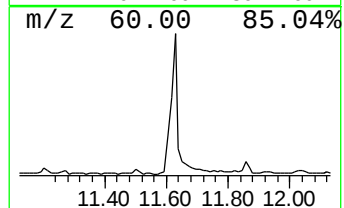
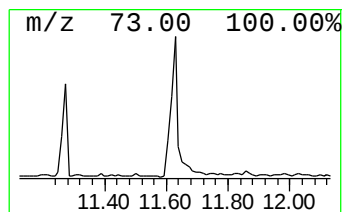
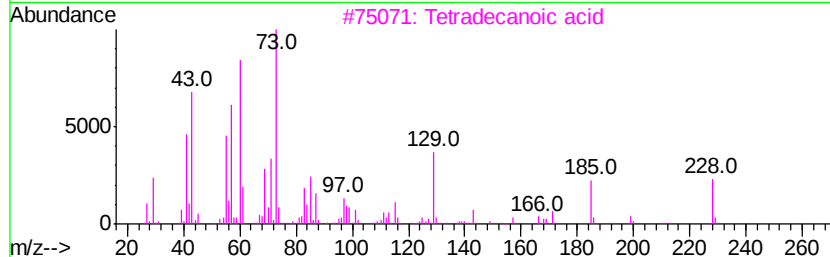
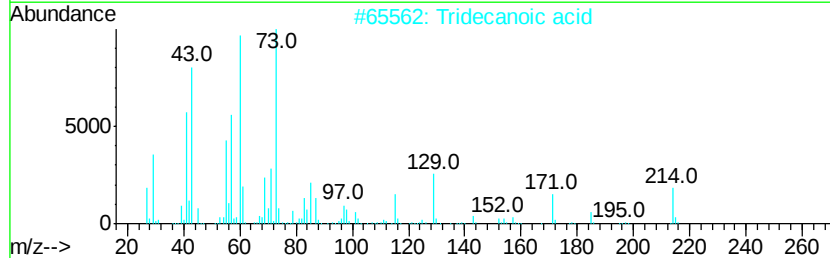
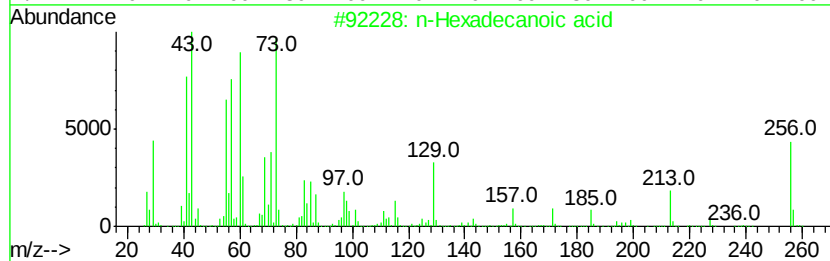
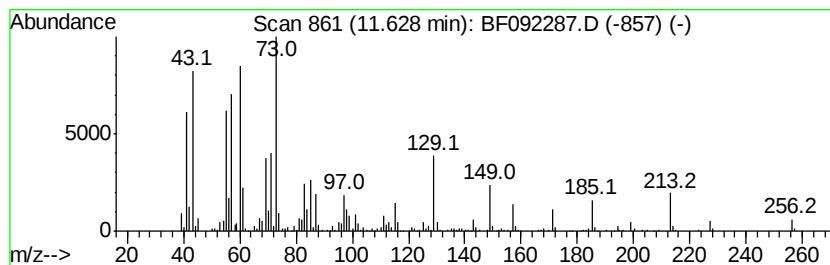
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.63	11.46 ng	1001950	Phenanthrene-d10	11.07

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	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5		n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092287.D
Acq On : 16 Jan 2017 16:14
Operator : UM/SJ
Sample : I1219-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC011217-LIQUID-TODT-HILL

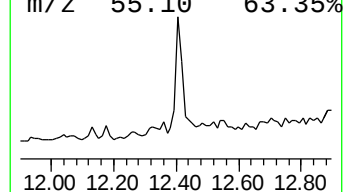
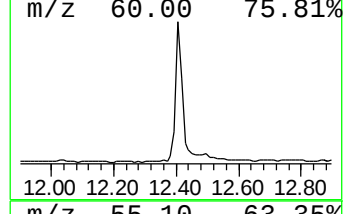
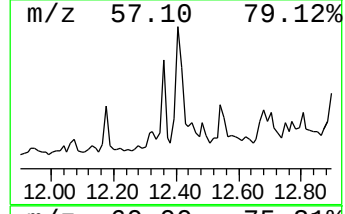
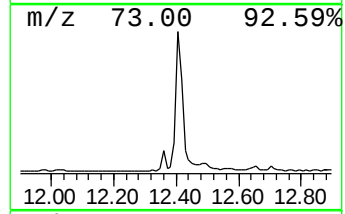
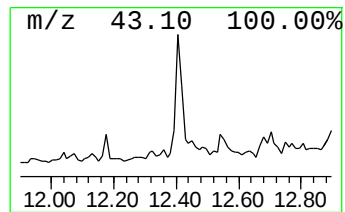
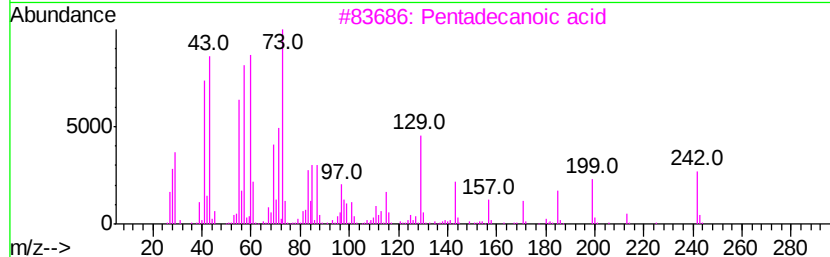
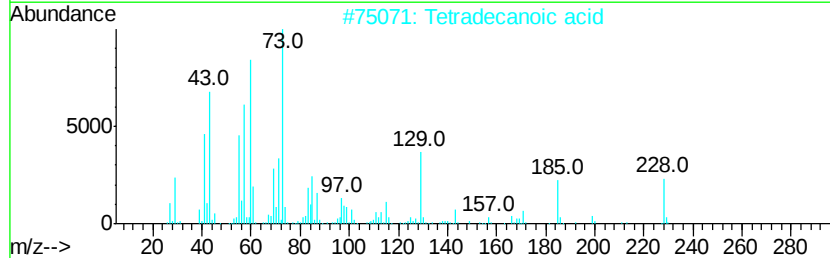
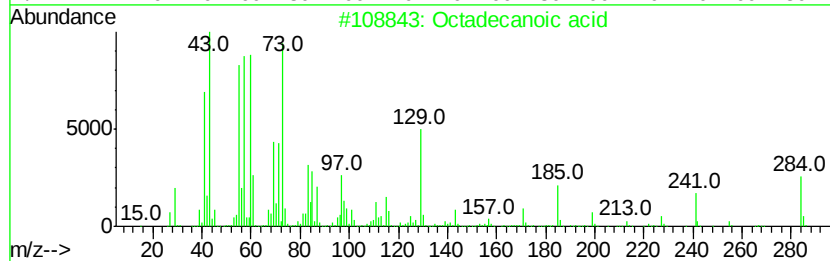
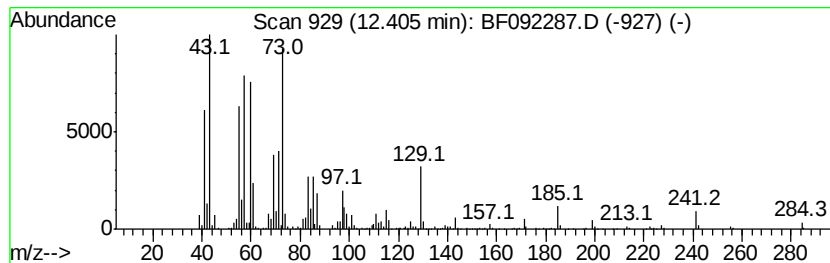
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	9.27 ng	1121350	Chrysene-d12	13.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	22
5			Butanoic acid	88	C4H8O2	000107-92-6	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011617\
Data File : BF092287.D
Acq On : 16 Jan 2017 16:14
Operator : UM/SJ
Sample : I1219-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC011217-LIQUID-TODT-HILL

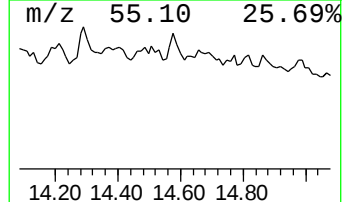
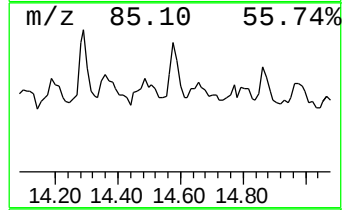
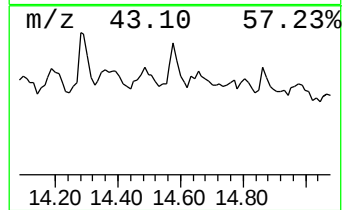
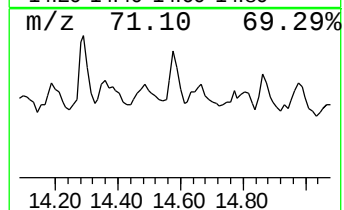
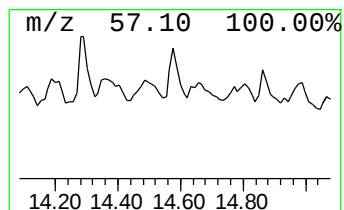
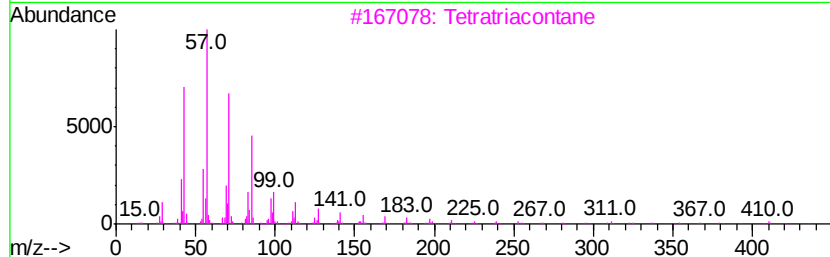
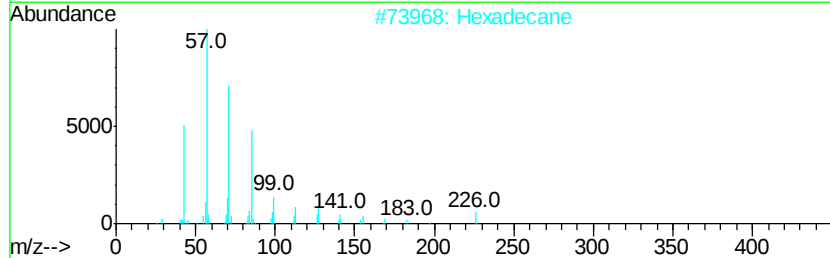
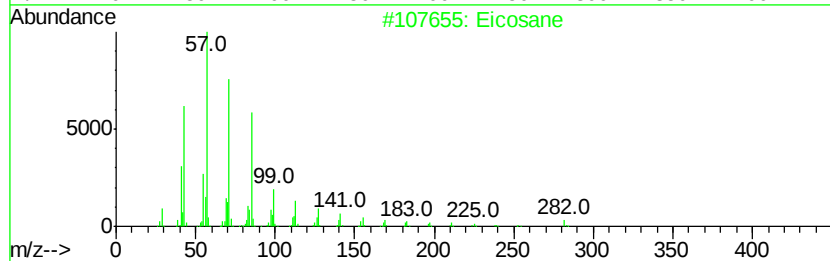
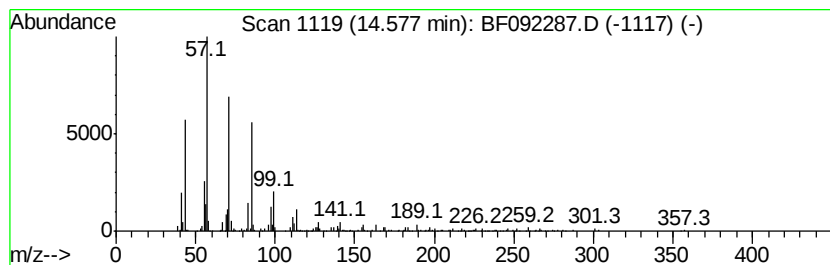
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Eicosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	5.71 ng	323370	Perylene-d12	15.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	90
2		Hexadecane	226	C16H34	000544-76-3	87
3		Tetratriacontane	479	C34H70	014167-59-0	86
4		Heptadecane	240	C17H36	000629-78-7	86
5		Octacosane	394	C28H58	000630-02-4	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011617\
 Data File : BF092287.D
 Acq On : 16 Jan 2017 16:14
 Operator : UM/SJ
 Sample : I1219-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC011217-LIQUID-TODT-HILL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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
2-Propenoic acid,...	2.04	7.9 ng		514837	1	6.56	1305700	20.0
2-Pentanone, 4-hy...	4.67	17.6 ng		1147770	1	6.56	1305700	20.0
unknown6.34	6.34	80.2 ng		5236780	1	6.56	1305700	20.0
1-Hexanol, 2-ethyl-	6.66	7.1 ng		462877	1	6.56	1305700	20.0
2-Decene, 4-methy...	7.42	5.6 ng		523769	2	7.84	1861050	20.0
Benzothiazole	8.13	6.6 ng		610786	2	7.84	1861050	20.0
Cyclohexane, isot...	8.15	6.6 ng		611730	2	7.84	1861050	20.0
unknown8.24	8.24	5.2 ng		484373	2	7.84	1861050	20.0
unknown8.50	8.50	9.8 ng		907942	2	7.84	1861050	20.0
unknown8.53	8.53	21.4 ng		1990270	2	7.84	1861050	20.0
Phenol, 2,6-bis(1...	9.27	4.7 ng		544398	3	9.59	2337370	20.0
2(3H)-Furanone, 5...	9.43	6.8 ng		796081	3	9.59	2337370	20.0
unknown9.83	9.83	8.9 ng		1043540	3	9.59	2337370	20.0
Octadecanoic acid...	10.29	4.7 ng		552949	3	9.59	2337370	20.0
2(3H)-Benzothiazo...	10.52	6.0 ng		522729	4	11.07	1747880	20.0
2-Propenoic acid,...	11.27	74.1 ng		6472210	4	11.07	1747880	20.0
n-Hexadecanoic acid	11.63	11.5 ng		1001950	4	11.07	1747880	20.0
Octadecanoic acid	12.40	9.3 ng		1121350	5	13.70	2420150	20.0
Eicosane	14.58	5.7 ng		323370	6	15.05	1133020	20.0