

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121318\
 Data File : BF111365.D
 Acq On : 13 Dec 2018 12:39
 Operator : JU/SJ
 Sample : J6334-07
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B3-121018

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.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	2.875	116	134	141	rVB2	103124	302116	3.92%	0.519%
2	3.804	284	292	300	rVB3	90954	196240	2.54%	0.337%
3	3.946	310	316	322	rVB2	55244	94738	1.23%	0.163%
4	4.057	330	335	338	rBV2	52175	86062	1.12%	0.148%
5	4.093	338	341	346	rVB	116315	152677	1.98%	0.263%
6	4.246	360	367	370	rBV3	43935	79890	1.04%	0.137%
7	4.304	370	377	380	rVV4	42059	78691	1.02%	0.135%
8	4.428	393	398	405	rVB3	178945	281320	3.65%	0.484%
9	4.540	411	417	426	rBV3	100949	138973	1.80%	0.239%
10	4.904	475	479	482	rBV5	44261	78577	1.02%	0.135%
11	4.946	482	486	490	rVB2	177241	223904	2.90%	0.385%
12	4.987	490	493	495	rBV	191419	234167	3.03%	0.403%
13	5.210	526	531	534	rBV	100615	117266	1.52%	0.202%
14	5.269	534	541	544	rVV	275577	265716	3.44%	0.457%
15	5.410	556	565	573	rBV	2529979	2709218	35.11%	4.658%
16	5.569	588	592	597	rBV3	77622	105281	1.36%	0.181%
17	5.822	630	635	639	rVB3	89658	112365	1.46%	0.193%
18	5.963	653	659	662	rVB2	192502	224700	2.91%	0.386%
19	6.051	671	674	676	rBV	155945	133833	1.73%	0.230%
20	6.257	700	709	711	rBV	168549	230054	2.98%	0.396%
21	6.328	718	721	723	rBV3	85752	102532	1.33%	0.176%
22	6.351	723	725	730	rVB	136495	118576	1.54%	0.204%
23	6.393	730	732	734	rBV2	82311	77821	1.01%	0.134%
24	6.422	734	737	744	rVV	2011285	1648148	21.36%	2.834%
25	6.563	753	761	764	rBV	5272205	4765502	61.76%	8.194%
26	6.622	768	771	775	rVB	322280	280261	3.63%	0.482%
27	6.793	797	800	803	rBV	1521899	1199807	15.55%	2.063%
28	6.851	808	810	812	rBV	101034	87321	1.13%	0.150%
29	6.951	823	827	830	rBV	5486969	4761339	61.71%	8.187%
30	6.975	830	831	836	rVB	365859	212759	2.76%	0.366%
31	7.045	838	843	845	rBV	194006	159693	2.07%	0.275%
32	7.075	845	848	851	rVB2	78309	77214	1.00%	0.133%
33	7.116	851	855	857	rBV	318747	253476	3.29%	0.436%
34	7.192	864	868	872	rBV	141987	116869	1.51%	0.201%

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35	7.357	889	896	902	rBV2	4075741	4827670	62.57%	8.301%
36	7.445	907	911	914	rVB2	106040	120334	1.56%	0.207%
37	7.569	926	932	934	rBV	258699	254142	3.29%	0.437%
38	7.592	934	936	942	rVB2	142913	164010	2.13%	0.282%
39	7.687	947	952	954	rBV2	84138	119603	1.55%	0.206%
40	7.734	957	960	961	rVV2	106407	123199	1.60%	0.212%
41	7.751	961	963	969	rVB	237857	233149	3.02%	0.401%
42	7.816	969	974	977	rBV2	524689	518970	6.73%	0.892%
43	7.851	977	980	984	rVV3	104171	131362	1.70%	0.226%
44	7.898	984	988	990	rVV2	80339	111766	1.45%	0.192%
45	8.075	1013	1018	1020	rBV	2063339	1771851	22.96%	3.047%
46	8.092	1020	1021	1025	rVB	374287	301115	3.90%	0.518%
47	8.787	1134	1139	1145	rVB2	203005	208972	2.71%	0.359%
48	8.886	1151	1156	1160	rBV	98698	98180	1.27%	0.169%
49	9.157	1197	1202	1205	rBV	7194940	7007696	90.82%	12.049%
50	9.828	1312	1316	1320	rBV	2251350	1935612	25.09%	3.328%
51	10.616	1445	1450	1454	rBV	4117357	4406544	57.11%	7.577%
52	11.310	1564	1568	1572	rBV	2277450	2096786	27.18%	3.605%
53	11.845	1655	1659	1676	rBV	592837	612195	7.93%	1.053%
54	12.627	1789	1792	1801	rBV	288413	346554	4.49%	0.596%
55	12.904	1834	1839	1842	rBV	7138314	7715664	100.00%	13.267%
56	13.804	1988	1992	2001	rVB2	417588	511442	6.63%	0.879%
57	13.951	2012	2017	2023	rBV	1873471	1900293	24.63%	3.267%
58	14.127	2043	2047	2054	rBV	199472	199811	2.59%	0.344%
59	14.433	2096	2099	2105	rBV	269549	237351	3.08%	0.408%
60	14.733	2146	2150	2153	rBV	292483	279332	3.62%	0.480%
61	15.063	2202	2206	2213	rBV	255953	283215	3.67%	0.487%
62	15.386	2256	2261	2265	rBV	1164921	1358103	17.60%	2.335%
63	15.433	2265	2269	2274	rVB	206508	273827	3.55%	0.471%
64	15.857	2337	2341	2345	rVB	135904	193610	2.51%	0.333%
65	16.345	2420	2424	2430	rVB3	68595	108755	1.41%	0.187%

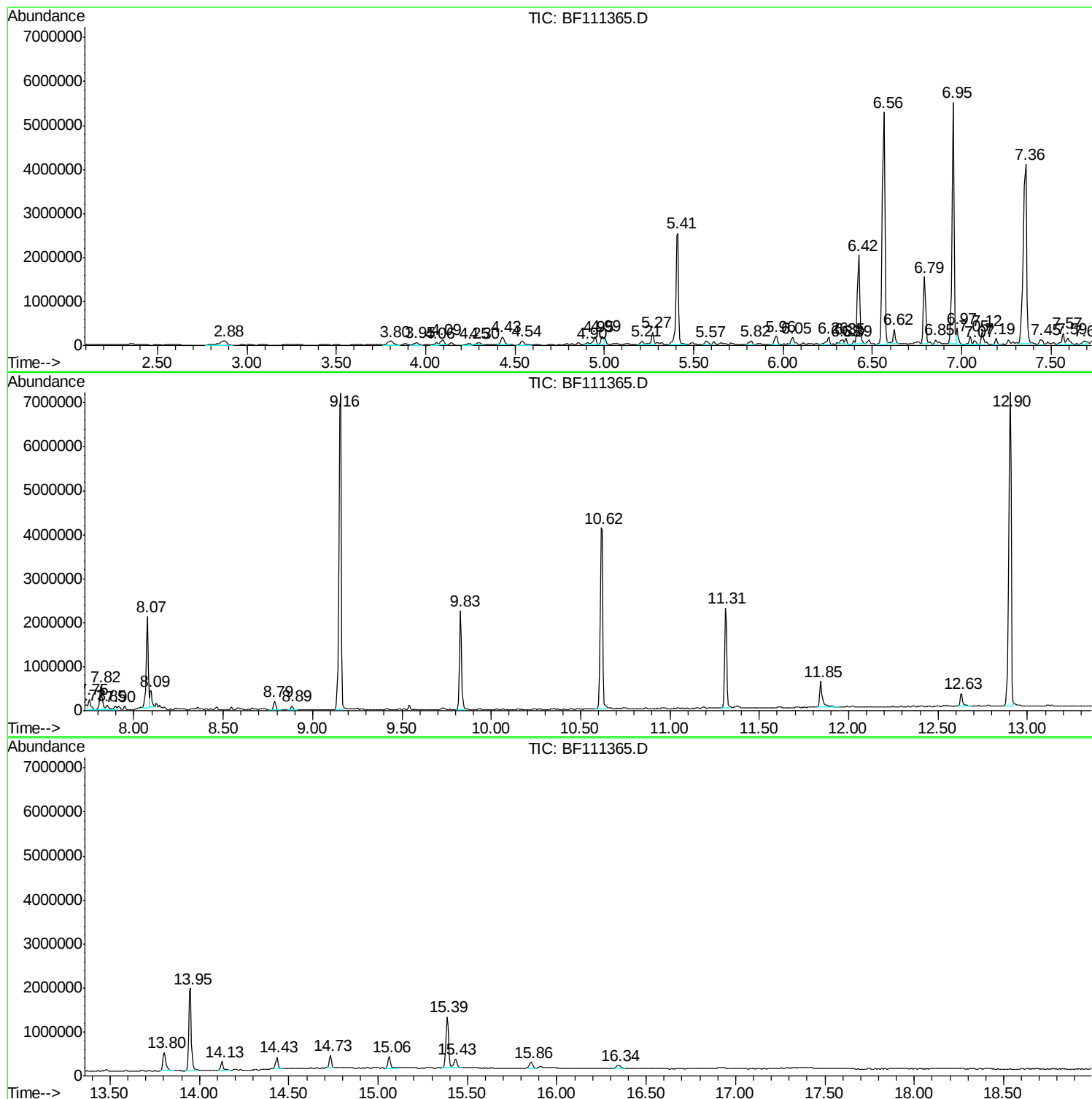
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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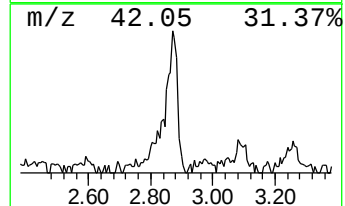
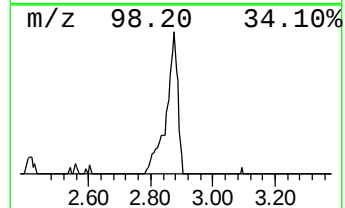
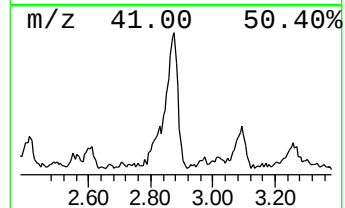
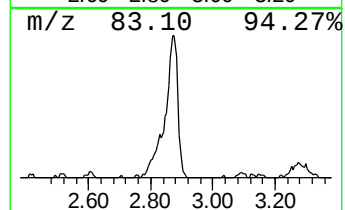
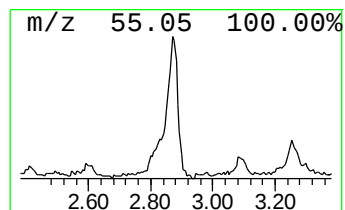
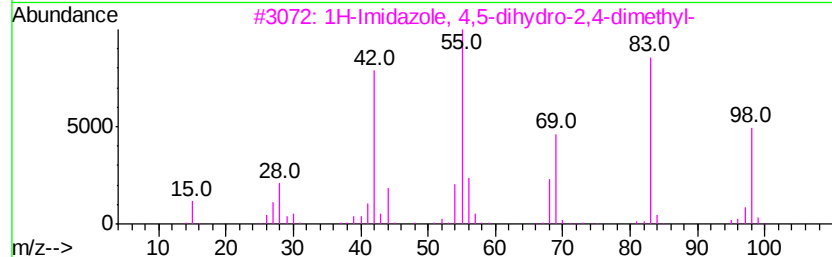
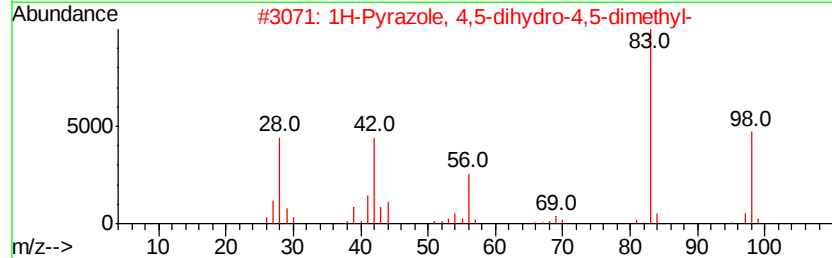
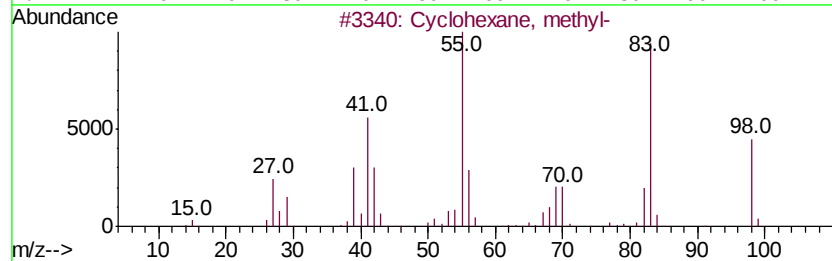
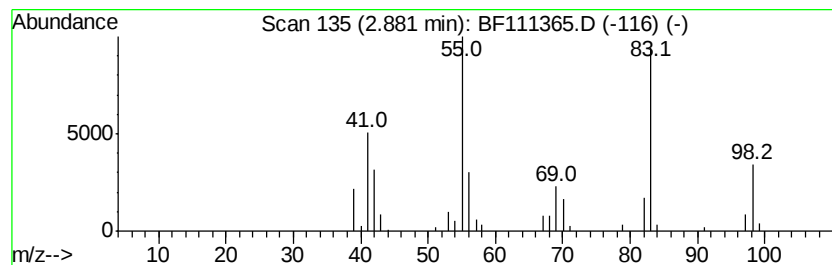
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclohexane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.88	5.04 ng	302116	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, methyl-	98	C7H14	000108-87-2	94
2			1H-Pyrazole, 4,5-dihydro-4,5-dimethyl-	98	C5H10N2	028019-94-5	64
3			1H-Imidazole, 4,5-dihydro-2,4-dimethyl-	98	C5H10N2	000930-61-0	59
4			1H-Pyrazole, 4,5-dihydro-1,5-dimethyl-	98	C5H10N2	005775-96-2	59
5			4,4-Dimethyl-2-imidazoline	98	C5H10N2	002305-59-1	59



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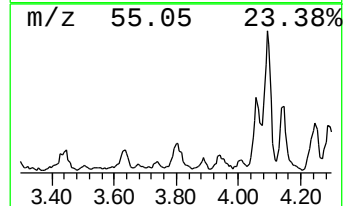
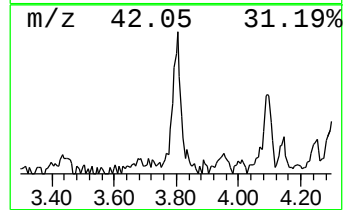
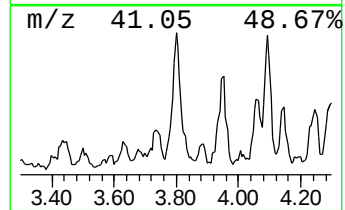
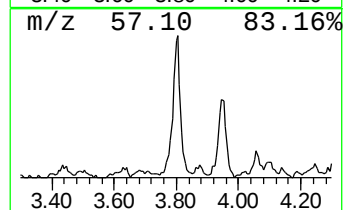
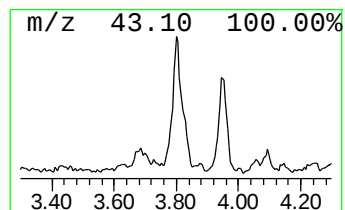
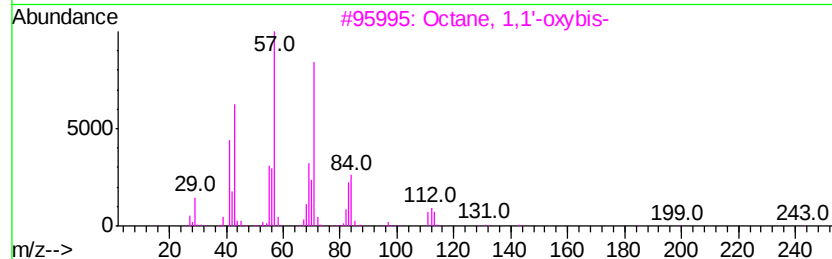
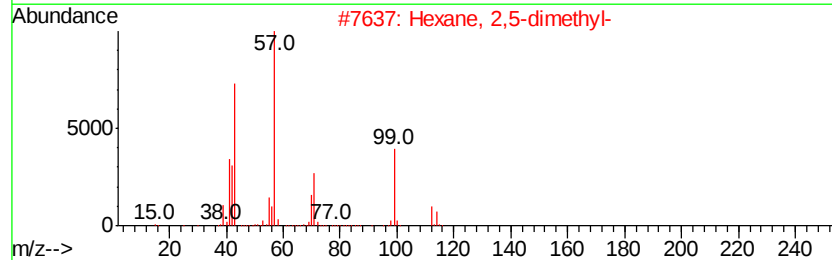
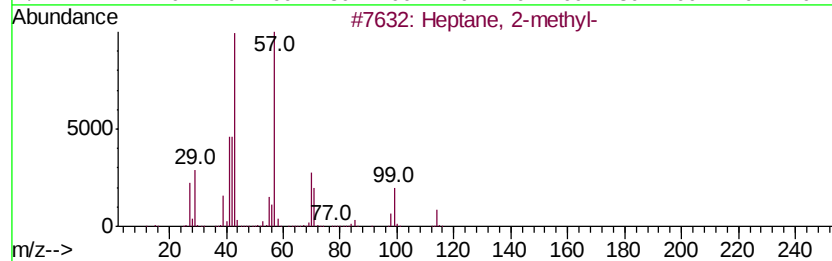
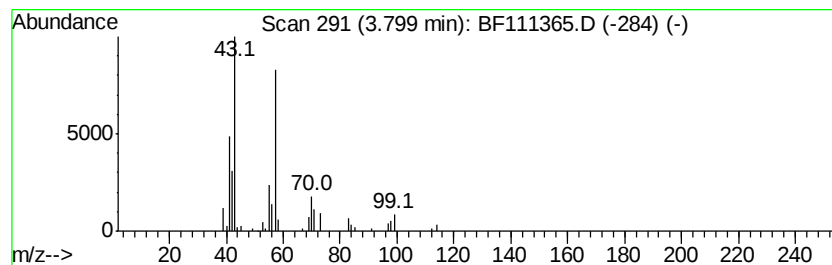
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121218.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Heptane, 2-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.80	3.27 ng	196240	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane, 2-methyl-	114	C8H18	000592-27-8	72
2		Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	64
3		Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	43
4		1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	43
5		Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	38



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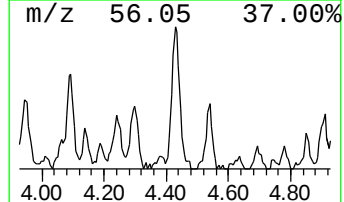
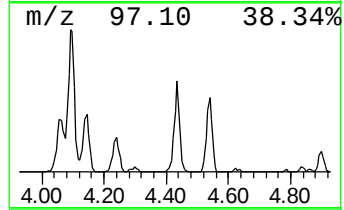
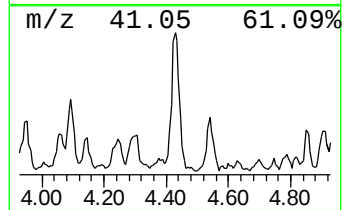
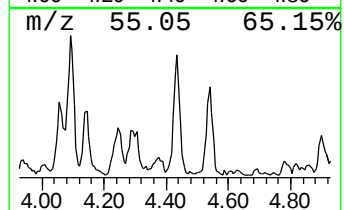
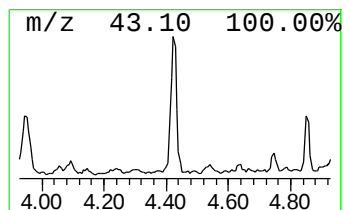
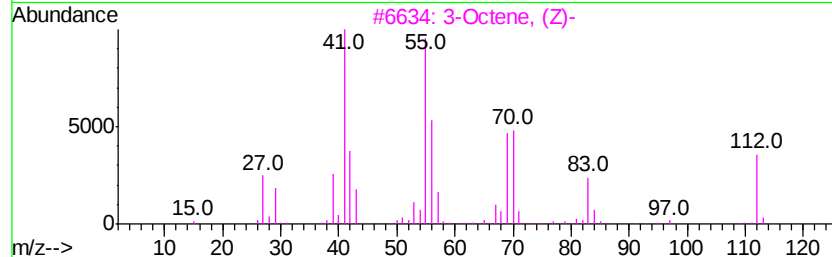
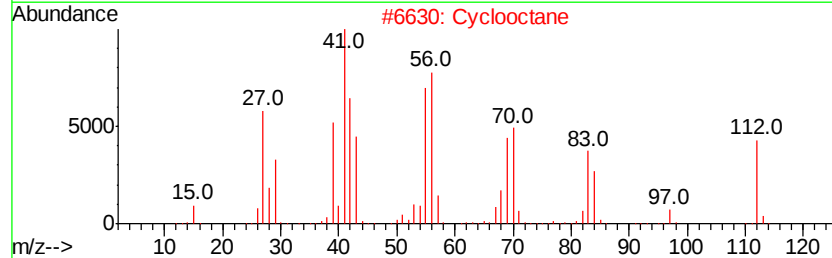
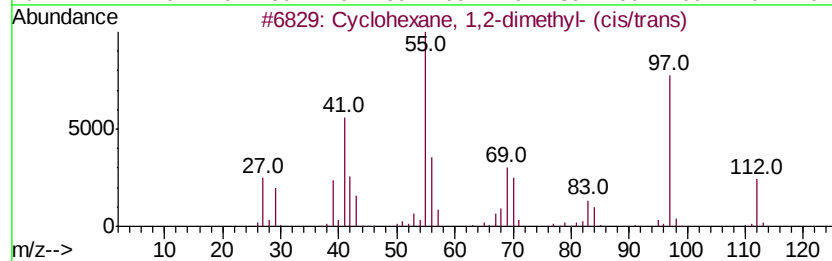
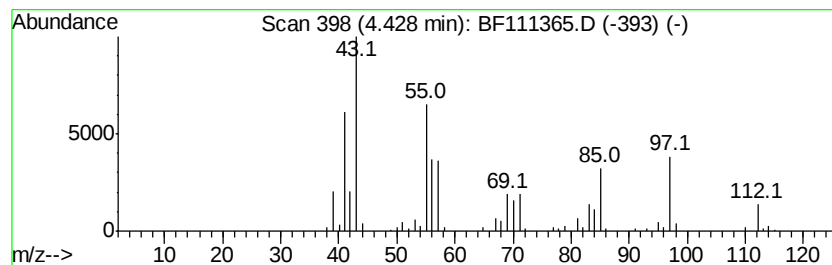
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclohexane, 1,2-dimethyl- ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.43	4.69 ng	281320	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	52
2		Cyclooctane	112	C8H16	000292-64-8	43
3		3-Octene, (Z)-	112	C8H16	014850-22-7	41
4		3-Hepten-2-one	112	C7H12O	001119-44-4	38
5		2-Octene	112	C8H16	000111-67-1	38



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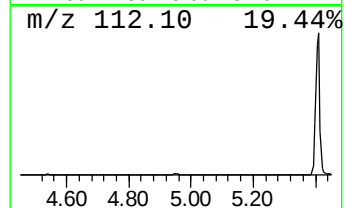
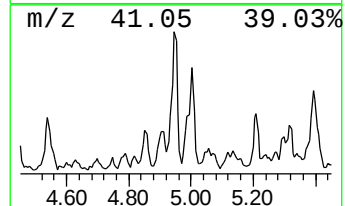
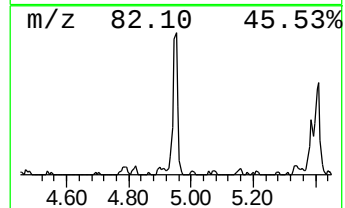
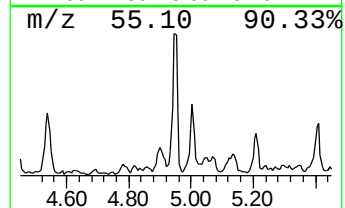
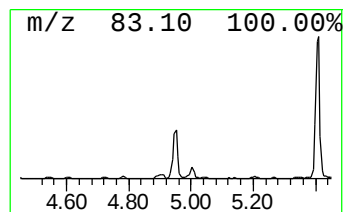
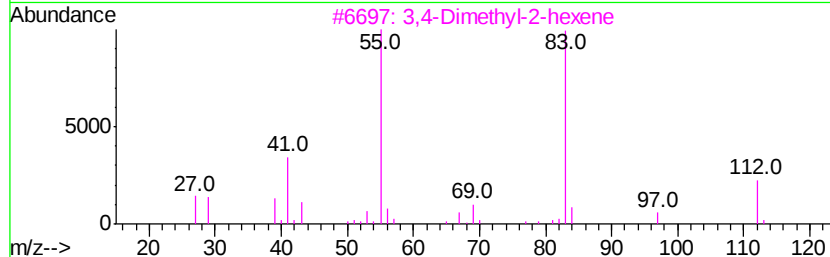
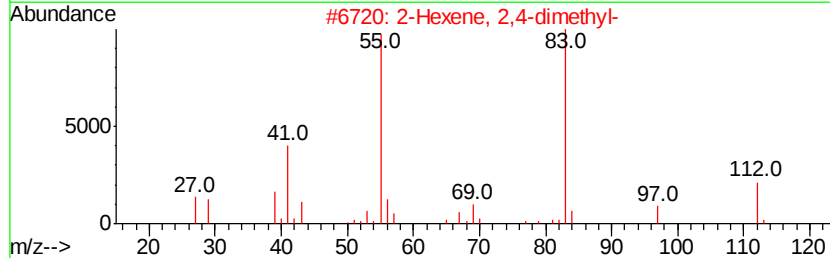
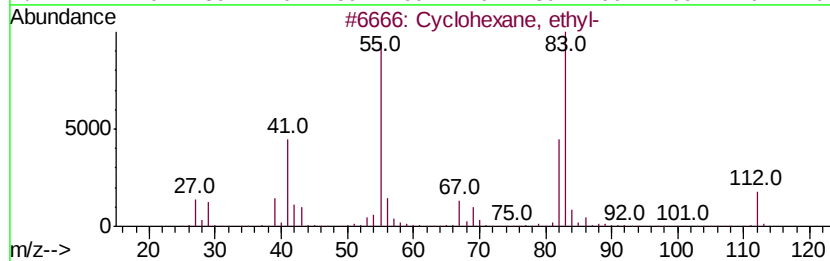
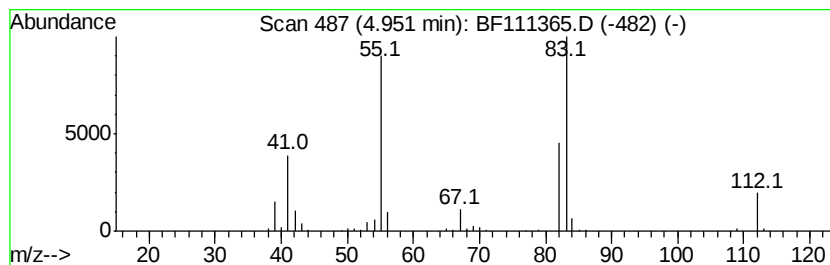
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclohexane, ethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	3.73 ng	223904	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, ethyl-	112	C8H16	001678-91-7	91
2		2-Hexene, 2,4-dimethyl-	112	C8H16	014255-23-3	68
3		3,4-Dimethyl-2-hexene	112	C8H16	002213-37-8	58
4		3-Hexene, 2,4-dimethyl-	112	C8H16	082085-14-1	58
5		2,4-Dimethyl-3-hexene(c,t)	112	C8H16	1000118-16-4	53



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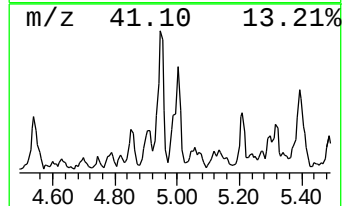
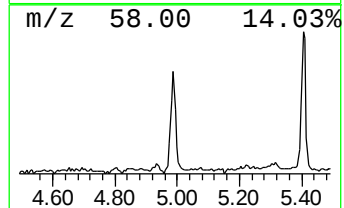
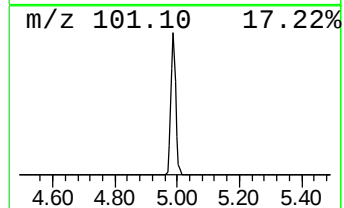
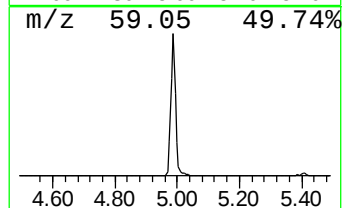
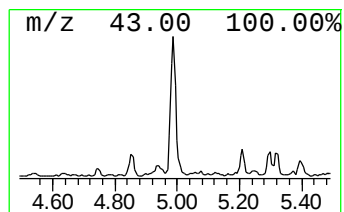
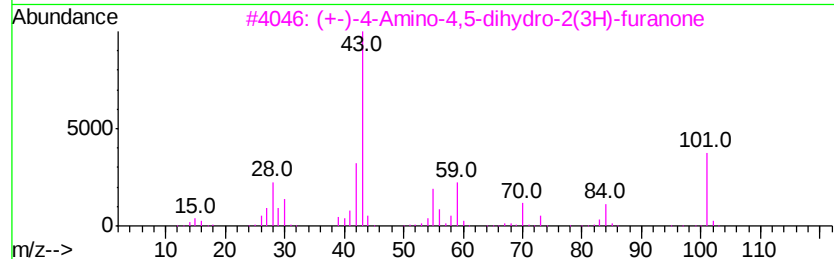
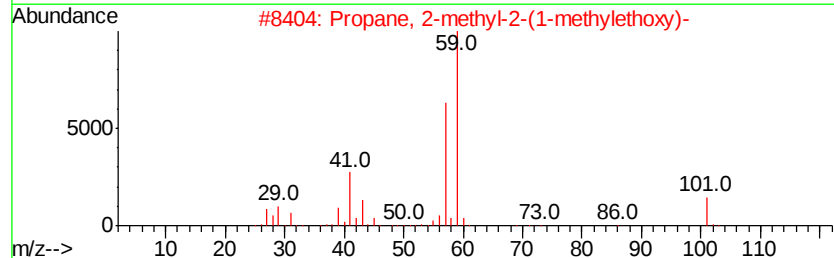
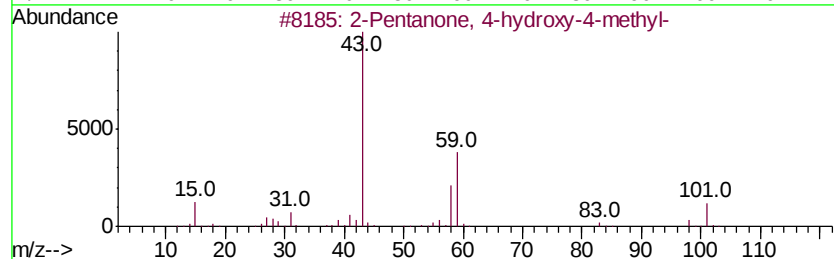
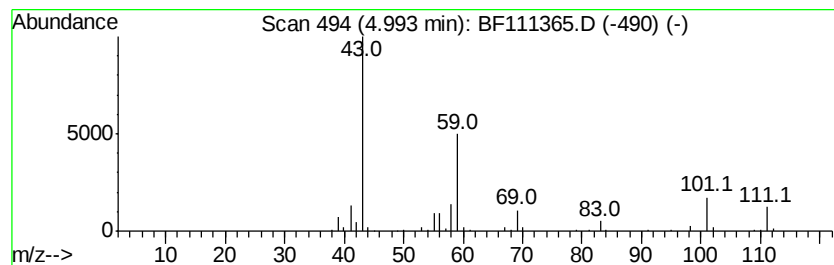
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	3.90 ng	234167	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121318\
Data File : BF111365.D
Acq On : 13 Dec 2018 12:39
Operator : JU/SJ
Sample : J6334-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

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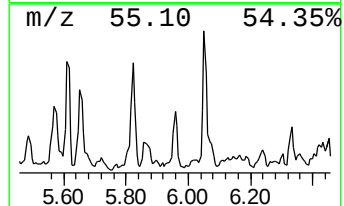
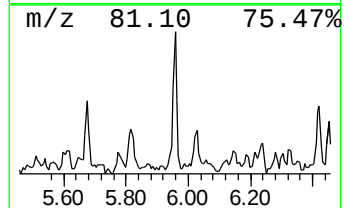
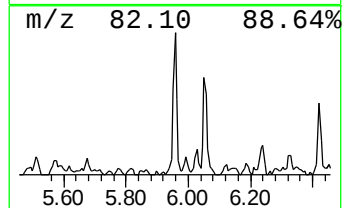
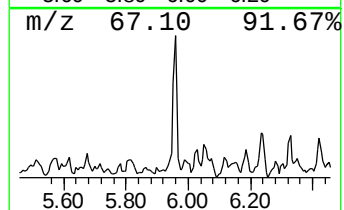
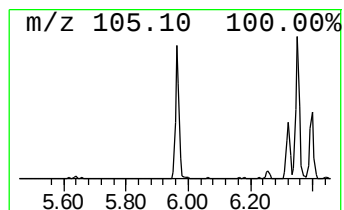
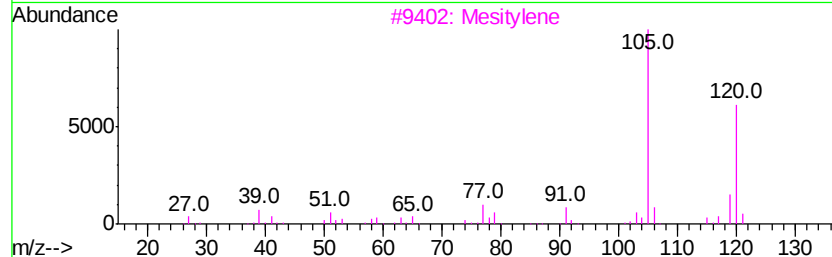
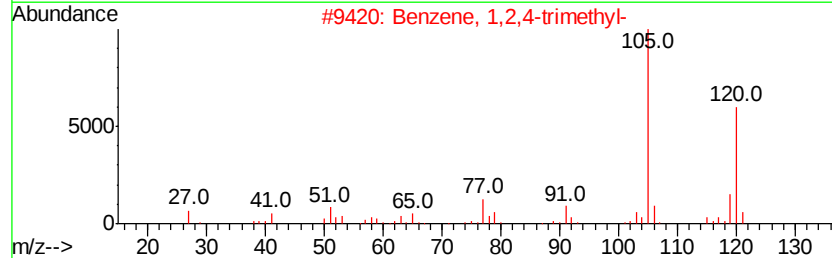
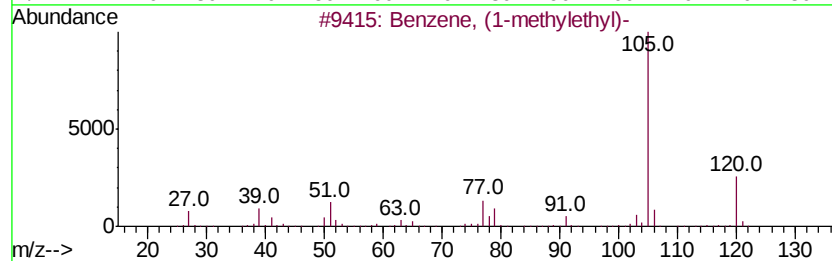
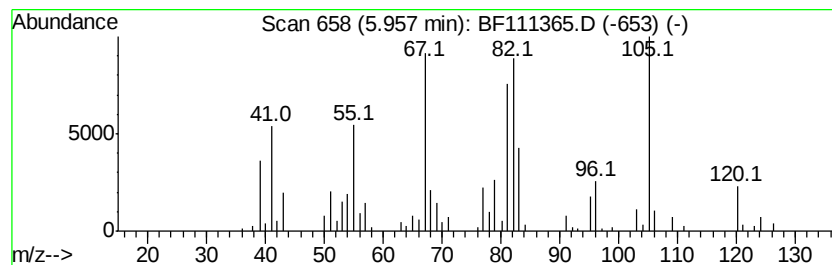
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzene, (1-methylethyl)- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.96	3.75 ng	224700	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	89
2		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	38
3		Mesitylene	120	C9H12	000108-67-8	38
4		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	38
5		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121318\
Data File : BF111365.D
Acq On : 13 Dec 2018 12:39
Operator : JU/SJ
Sample : J6334-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

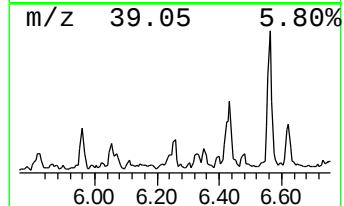
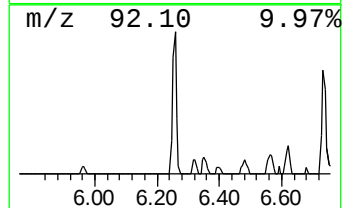
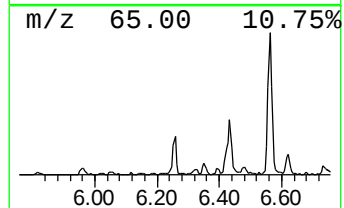
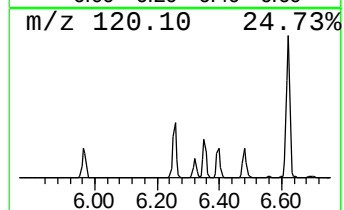
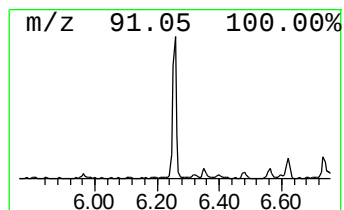
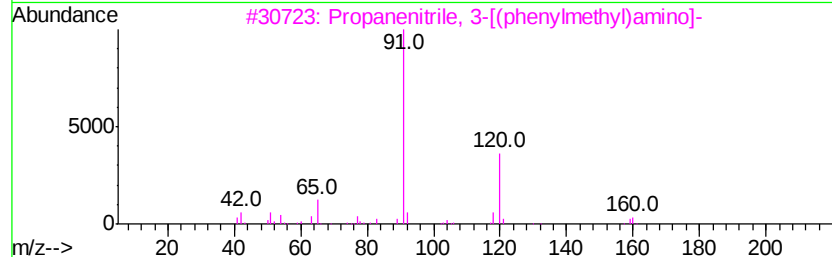
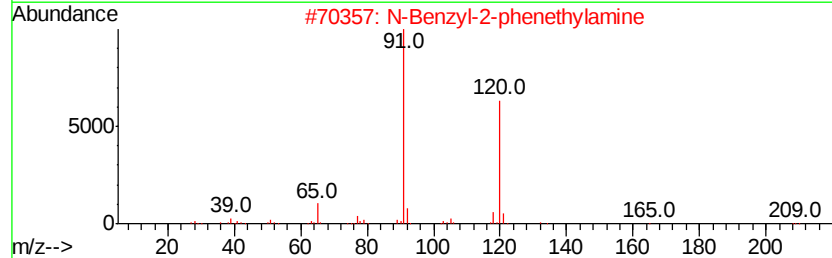
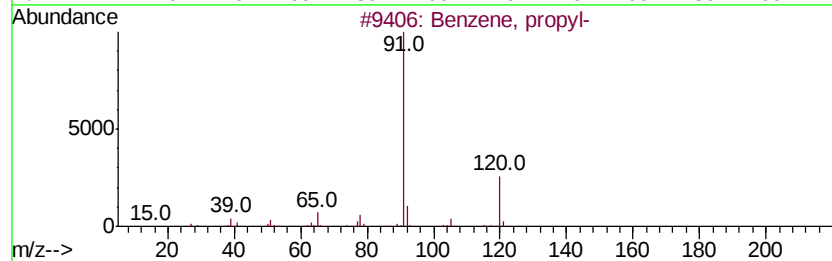
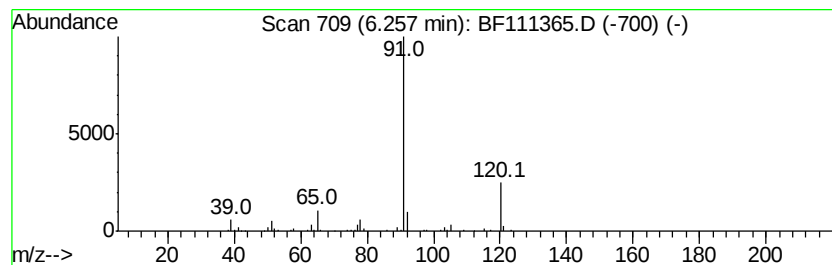
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzene, propyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.26	3.83 ng	230054	1,4-Dichlorobenzene-d4	6.79	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, propyl-	120	C9H12	000103-65-1	90
2	N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	72
3	Propanenitrile, 3-[(phenylmethyl)amino]-	160	C10H12N2	000706-03-6	64
4	Oxirane, phenyl-	120	C8H8O	000096-09-3	58
5	1,2-Ethanediamine, N,N'-bis(phenyl)-	240	C16H20N2	000140-28-3	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121318\
Data File : BF111365.D
Acq On : 13 Dec 2018 12:39
Operator : JU/SJ
Sample : J6334-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

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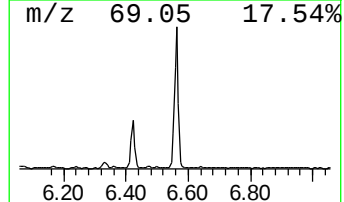
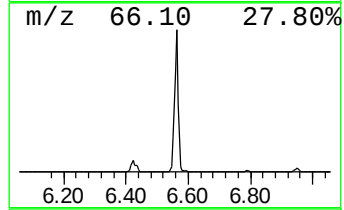
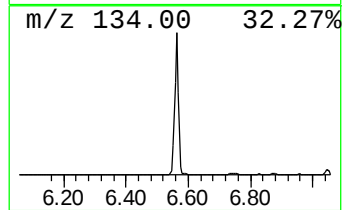
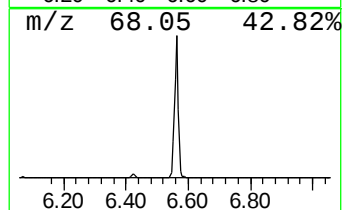
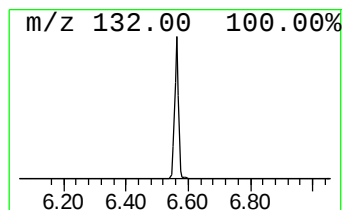
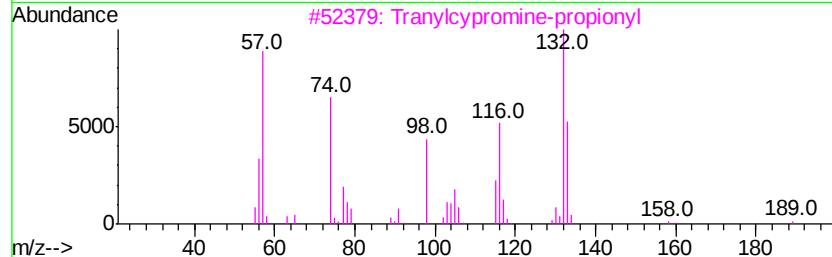
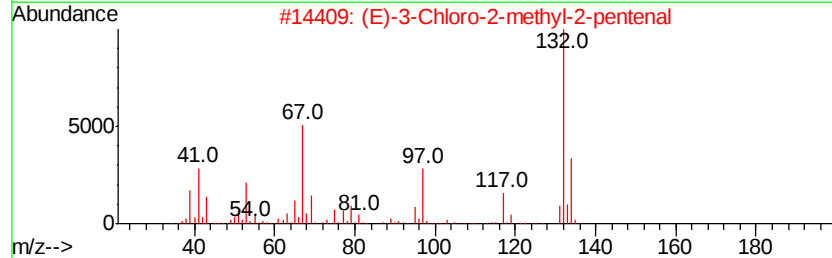
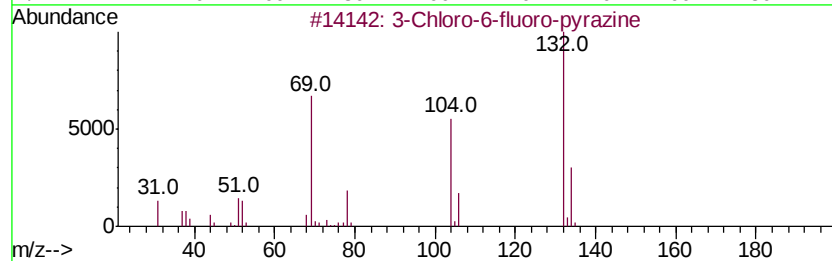
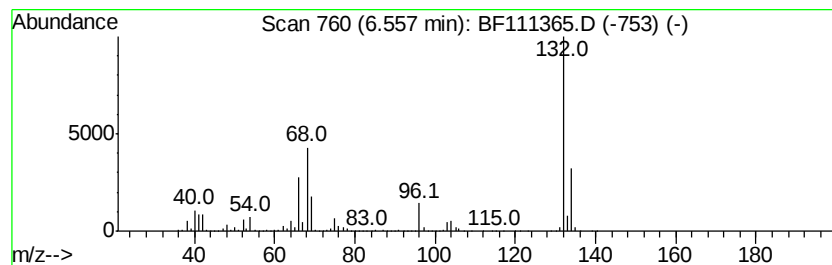
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	79.44 ng	4765500	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121318\
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Misc :
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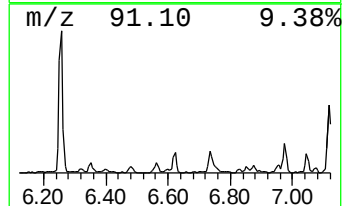
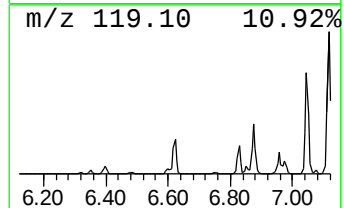
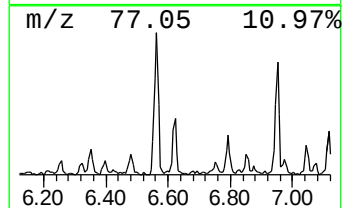
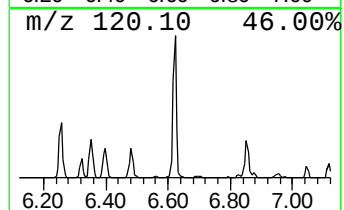
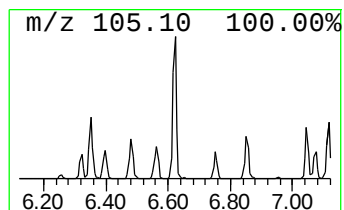
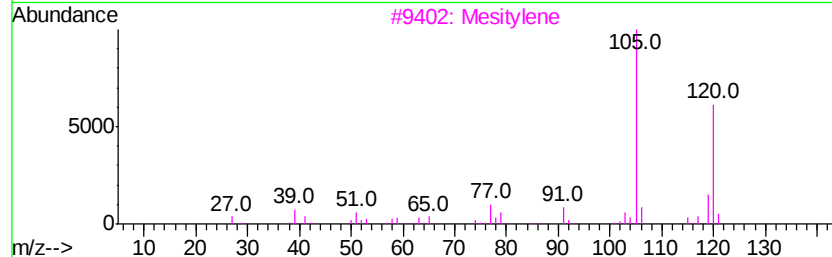
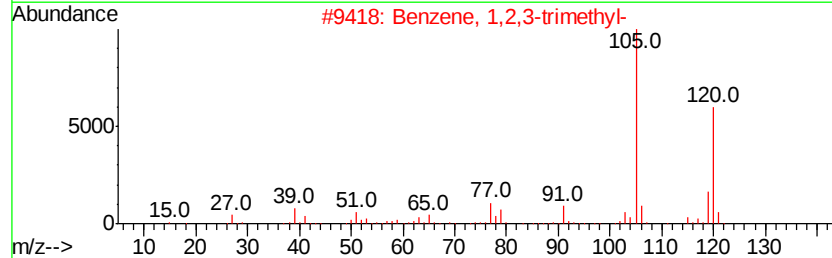
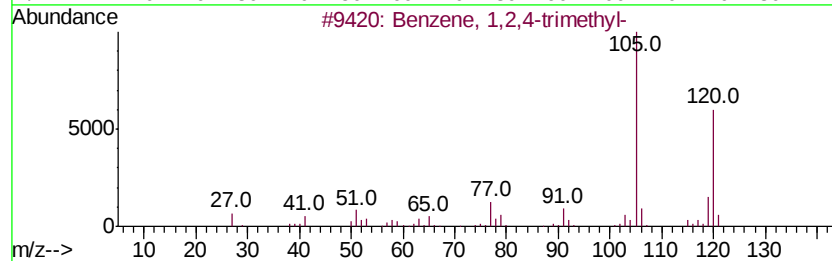
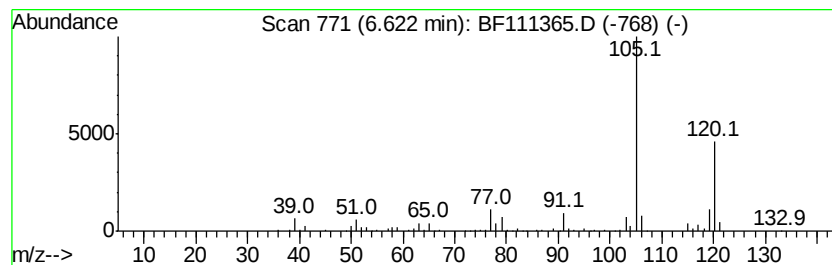
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzene, 1,2,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	4.67 ng	280261	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Mesitylene	120	C9H12	000108-67-8	93
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121318\
Data File : BF111365.D
Acq On : 13 Dec 2018 12:39
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Sample : J6334-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

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

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

Peak Number 12 Benzene, 2-propenyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.97	3.55 ng	212759	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
2		Benzene, 1-propenyl-	118	C9H10	000637-50-3	74
3		Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
4		Indane	118	C9H10	000496-11-7	64
5		Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	59

