

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
 Data File : BF110017.D
 Acq On : 19 Oct 2018 21:51
 Operator : JU/SJ
 Sample : J5588-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-6

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-BF101518.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	2.128	3	7	35	rVB	1093105	1829665	34.13%	3.079%
2	2.328	35	41	50	rVB	2156980	2835314	52.88%	4.772%
3	5.198	525	529	536	rVB	140701	146869	2.74%	0.247%
4	5.586	590	595	598	rVB	2530252	2220366	41.41%	3.737%
5	6.581	759	764	769	rBV2	1663101	1753287	32.70%	2.951%
6	6.669	777	779	782	rVB	182315	123199	2.30%	0.207%
7	6.733	785	790	794	rBV	4039462	4028656	75.14%	6.780%
8	6.969	826	830	833	rBV	1549707	1351050	25.20%	2.274%
9	7.016	835	838	842	rVB2	102802	85291	1.59%	0.144%
10	7.128	852	857	860	rVB	3755896	3686853	68.77%	6.205%
11	7.175	861	865	874	rBV	164789	295924	5.52%	0.498%
12	7.357	890	896	901	rBV	572368	468718	8.74%	0.789%
13	7.533	917	926	928	rBV	2900445	3102450	57.87%	5.222%
14	7.557	928	930	934	rVB2	222456	204914	3.82%	0.345%
15	7.992	1002	1004	1007	rVB2	70317	58749	1.10%	0.099%
16	8.151	1026	1031	1034	rBV	462945	389889	7.27%	0.656%
17	8.251	1043	1048	1051	rBV	2063682	1822058	33.99%	3.067%
18	8.392	1069	1072	1078	rBV2	107265	122143	2.28%	0.206%
19	8.457	1080	1083	1085	rBV	243567	178593	3.33%	0.301%
20	8.480	1085	1087	1090	rVB	277619	203339	3.79%	0.342%
21	8.527	1093	1095	1097	rBV	54266	57619	1.07%	0.097%
22	8.733	1126	1130	1136	rBV4	33712	64633	1.21%	0.109%
23	8.845	1145	1149	1153	rVB	406431	362309	6.76%	0.610%
24	9.192	1205	1208	1211	rBV3	66445	62670	1.17%	0.105%
25	9.327	1224	1231	1234	rBV	5747160	5361342	100.00%	9.023%
26	9.357	1234	1236	1240	rVB	183682	142939	2.67%	0.241%
27	9.427	1245	1248	1252	rBV	143352	140969	2.63%	0.237%
28	9.716	1293	1297	1300	rBV	740653	573492	10.70%	0.965%
29	10.010	1343	1347	1351	rVB2	2189046	1913360	35.69%	3.220%
30	10.380	1407	1410	1413	rVB	77045	63940	1.19%	0.108%
31	10.416	1413	1416	1420	rVB	166340	155740	2.90%	0.262%
32	10.492	1423	1429	1432	rBV5	44176	61927	1.16%	0.104%
33	10.539	1432	1437	1440	rBV2	371541	330859	6.17%	0.557%
34	10.627	1445	1452	1457	rVB2	58712	91126	1.70%	0.153%

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35	10.710	1463	1466	1467	rBV	66344	55705	1.04%	0.094%
36	10.804	1476	1482	1485	rBV	3152290	3277110	61.12%	5.516%
37	10.863	1490	1492	1494	rVV	141231	130007	2.42%	0.219%
38	10.898	1496	1498	1505	rVB4	102950	140426	2.62%	0.236%
39	11.021	1514	1519	1523	rBV6	35962	80953	1.51%	0.136%
40	11.080	1523	1529	1534	rVV2	90353	143848	2.68%	0.242%
41	11.145	1537	1540	1545	rVB3	91802	91811	1.71%	0.155%
42	11.274	1560	1562	1567	rVB	76373	69174	1.29%	0.116%
43	11.368	1576	1578	1585	rVB3	105139	145228	2.71%	0.244%
44	11.433	1586	1589	1593	rBV2	36438	60818	1.13%	0.102%
45	11.504	1596	1601	1604	rVB	2001847	1839783	34.32%	3.096%
46	11.674	1624	1630	1633	rBV	1388467	1250599	23.33%	2.105%
47	11.933	1671	1674	1680	rVB	76562	78191	1.46%	0.132%
48	12.015	1684	1688	1691	rBV2	809028	788185	14.70%	1.327%
49	12.080	1696	1699	1702	rBV	61240	64423	1.20%	0.108%
50	12.280	1730	1733	1738	rVB2	97199	117806	2.20%	0.198%
51	12.527	1772	1775	1781	rVB	116855	111394	2.08%	0.187%
52	12.715	1803	1807	1811	rBV3	40792	70613	1.32%	0.119%
53	12.757	1811	1814	1818	rVB	155281	138330	2.58%	0.233%
54	12.798	1818	1821	1825	rBV	231673	207152	3.86%	0.349%
55	13.027	1855	1860	1863	rBV5	52790	78049	1.46%	0.131%
56	13.086	1865	1870	1873	rBV	4706019	4555440	84.97%	7.667%
57	13.174	1882	1885	1888	rBV2	158733	218267	4.07%	0.367%
58	13.215	1889	1892	1895	rVV2	136008	165697	3.09%	0.279%
59	13.245	1895	1897	1900	rVV	104672	82809	1.54%	0.139%
60	13.274	1900	1902	1904	rVV	135288	144676	2.70%	0.243%
61	13.304	1904	1907	1912	rVV4	134616	190282	3.55%	0.320%
62	13.351	1912	1915	1920	rVV	186529	170678	3.18%	0.287%
63	13.398	1920	1923	1927	rVB	95271	92177	1.72%	0.155%
64	13.633	1959	1963	1968	rVB	566734	523735	9.77%	0.881%
65	13.962	2014	2019	2030	rVB	975732	976459	18.21%	1.643%
66	14.109	2038	2044	2046	rBV2	249337	276540	5.16%	0.465%
67	14.145	2046	2050	2053	rVV	1475146	1279473	23.86%	2.153%
68	14.286	2072	2074	2080	rVB2	110033	112153	2.09%	0.189%
69	14.592	2123	2126	2131	rBV2	165395	180215	3.36%	0.303%
70	14.915	2177	2181	2184	rBV	162262	166784	3.11%	0.281%
71	14.998	2190	2195	2199	rBV	1810601	1939771	36.18%	3.265%

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72	15.268	2237	2241	2245	rBV	207522	243499	4.54%	0.410%
73	15.668	2303	2309	2321	rBV2	964452	1319305	24.61%	2.220%
74	16.133	2383	2388	2393	rBV	181595	265892	4.96%	0.448%
75	16.186	2393	2397	2403	rBV2	96079	153946	2.87%	0.259%
76	16.398	2427	2433	2444	rVB2	302582	550603	10.27%	0.927%
77	16.586	2458	2465	2474	rBV2	603247	1139372	21.25%	1.918%
78	16.668	2474	2479	2485	rVB	109773	204771	3.82%	0.345%
79	17.303	2582	2587	2594	rVB4	44000	96488	1.80%	0.162%
80	17.392	2596	2602	2616	rBV3	213607	480763	8.97%	0.809%
81	17.586	2629	2635	2641	rBV6	47483	98249	1.83%	0.165%
82	17.674	2642	2650	2663	rVB6	69969	257054	4.79%	0.433%
83	17.827	2671	2676	2690	rVB5	94765	245730	4.58%	0.414%
84	18.044	2709	2713	2723	rVB5	22438	55407	1.03%	0.093%

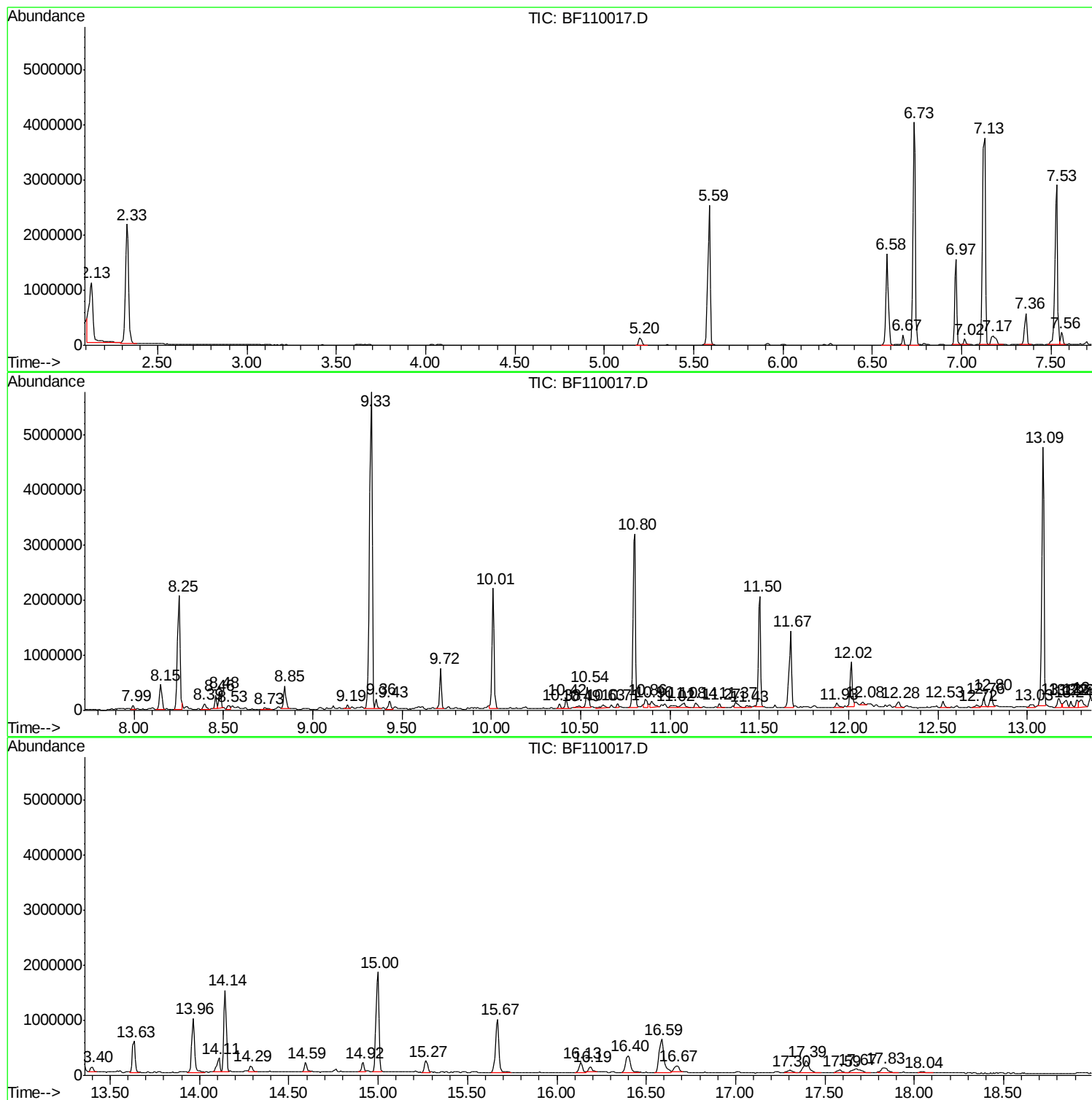
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MH-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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MH-6

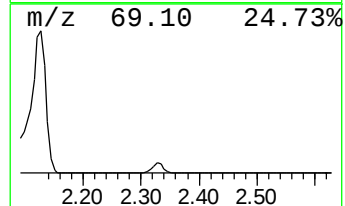
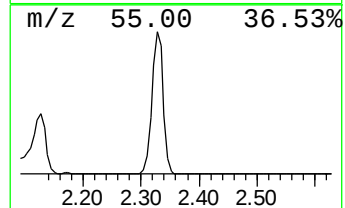
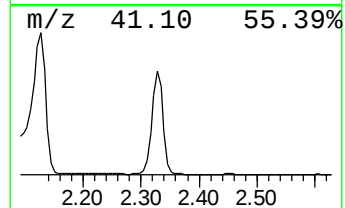
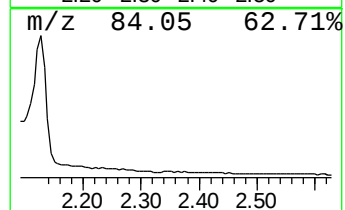
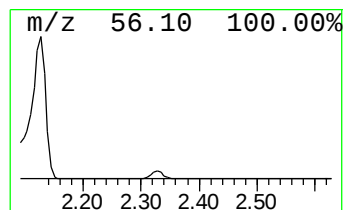
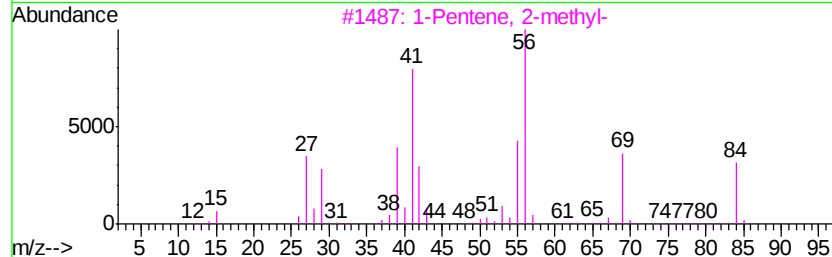
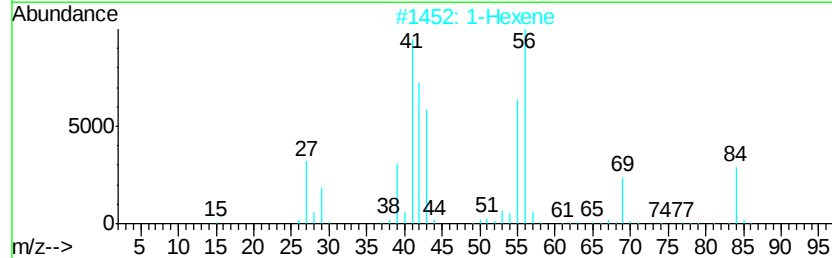
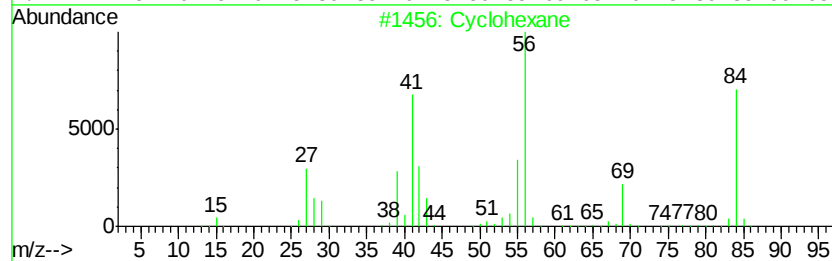
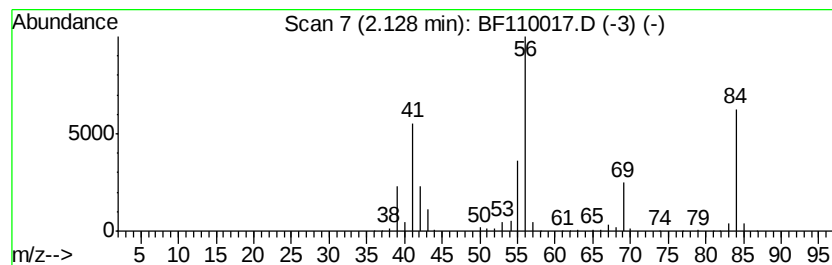
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclohexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	27.09 ng	1829670	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane	84	C6H12	000110-82-7	91
2		1-Hexene	84	C6H12	000592-41-6	59
3		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	56
4		2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	53
5		Cyclopentane, methyl-	84	C6H12	000096-37-7	45



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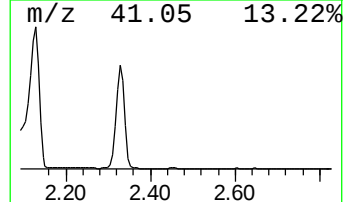
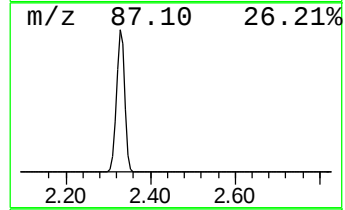
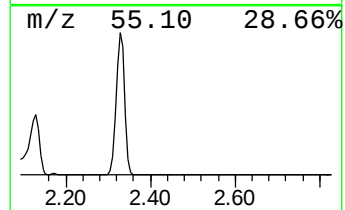
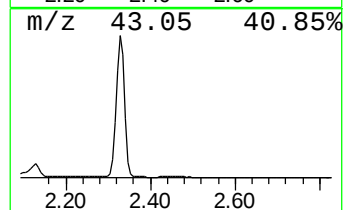
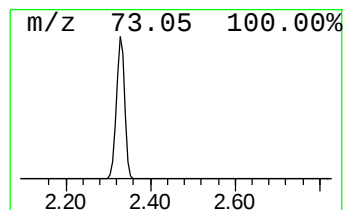
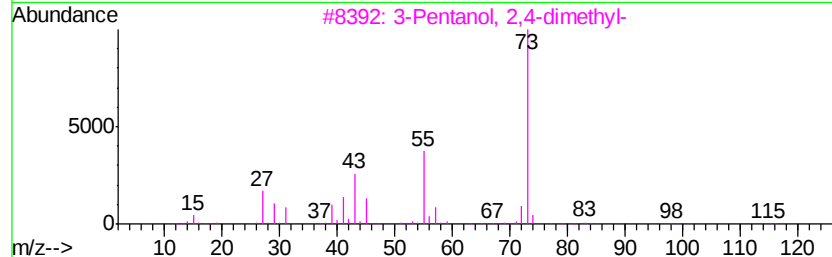
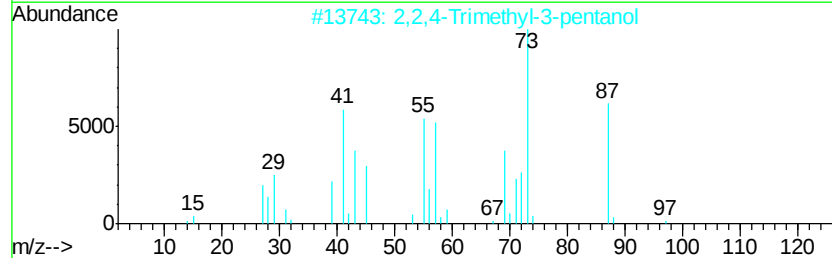
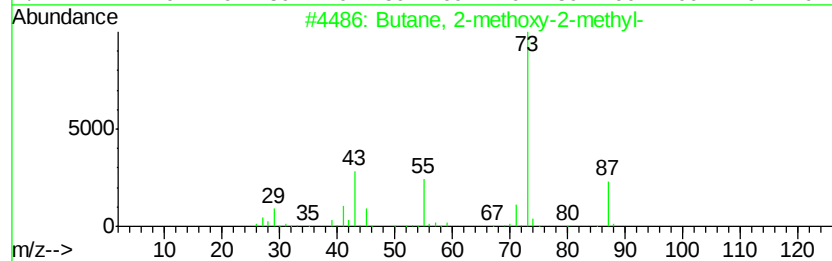
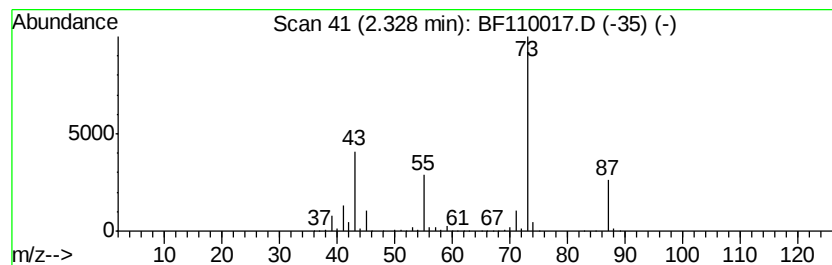
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	41.97 ng	2835310	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22



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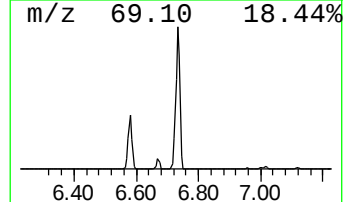
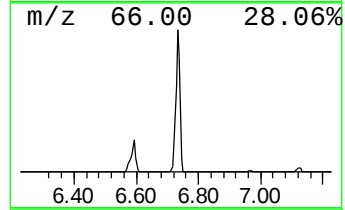
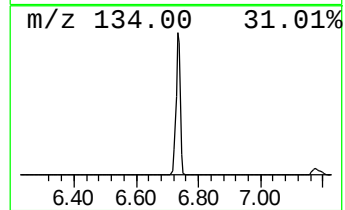
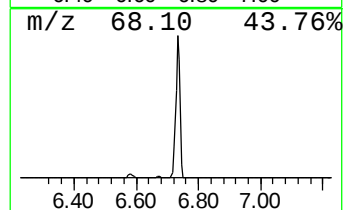
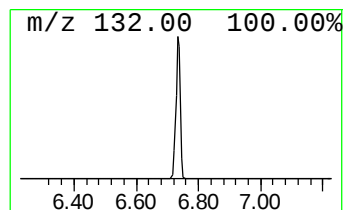
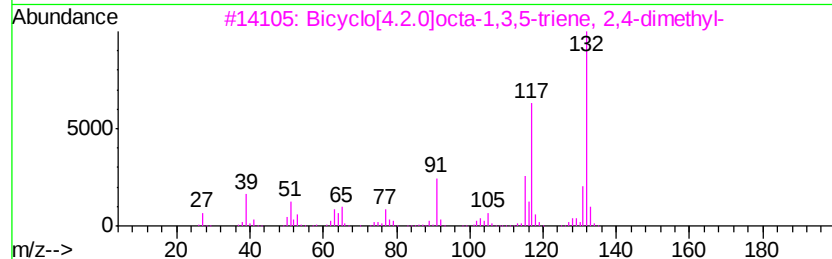
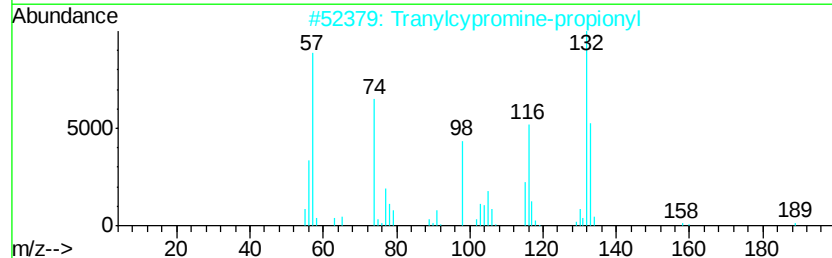
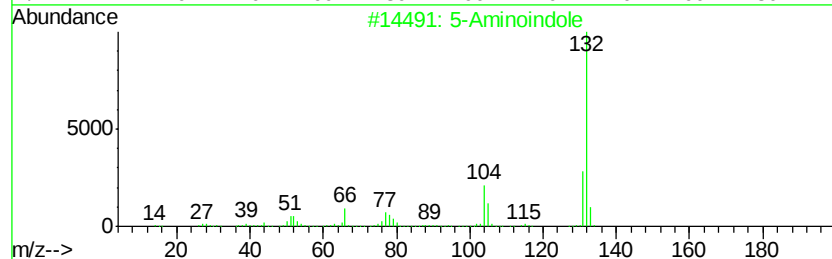
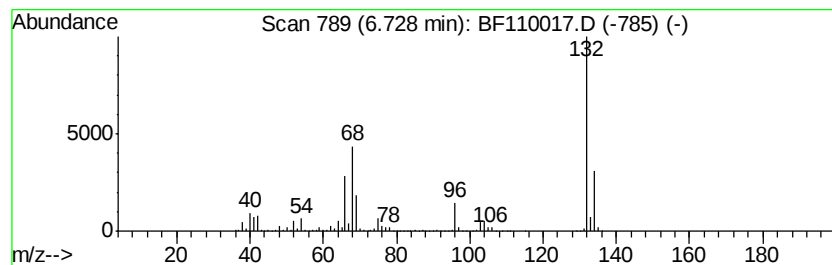
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	59.64 ng	4028660	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene, ...	132	C10H12	028749-81-7	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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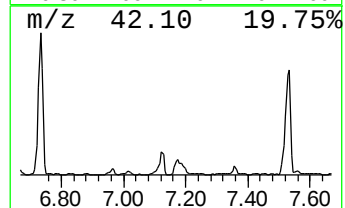
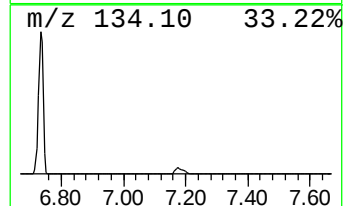
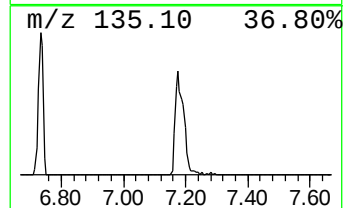
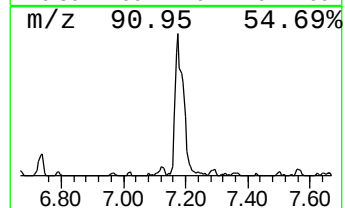
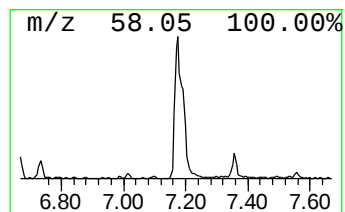
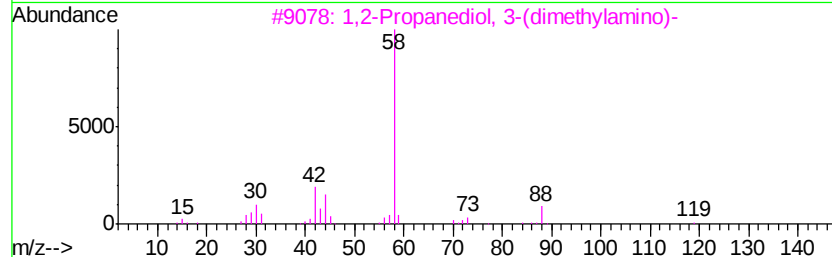
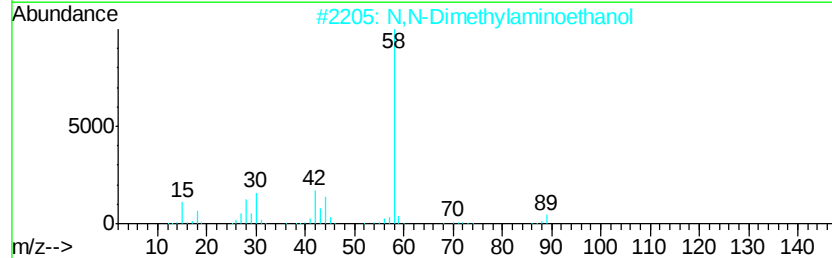
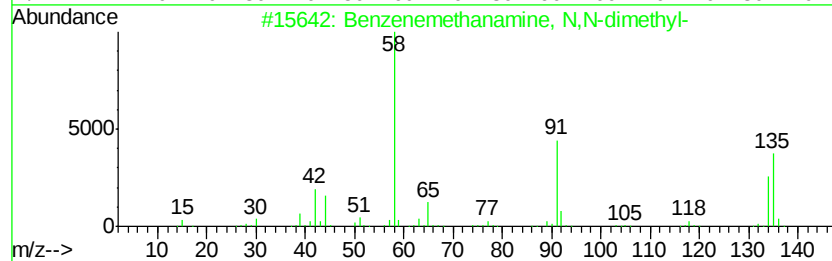
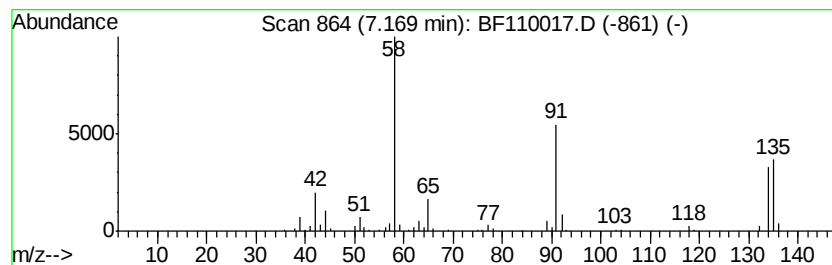
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzenemethanamine, N,N-dim... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.17	4.38 ng	295924	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenemethanamine, N,N-dimethyl-	135	C9H13N	000103-83-3	91
2		N,N-Dimethylaminoethanol	89	C4H11NO	000108-01-0	43
3		1,2-Propanediol, 3-(dimethylamino)-	119	C5H13NO2	000623-57-4	38
4		N-Methyl-3-methoxy-4-methylmetam...	193	C12H19NO	1000367-31-4	33
5		2-(2-Dimethylaminoethyl)isothioure...	147	C5H13N3S	086114-63-8	32



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
Data File : BF110017.D
Acq On : 19 Oct 2018 21:51
Operator : JU/SJ
Sample : J5588-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-6

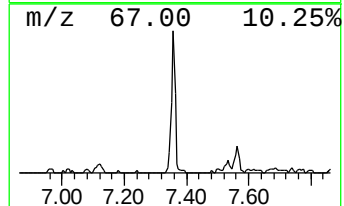
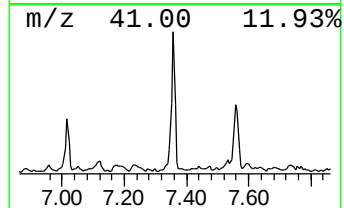
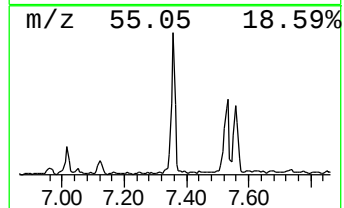
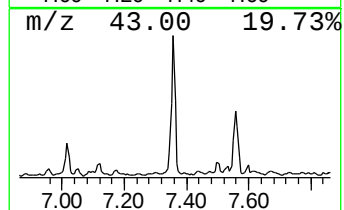
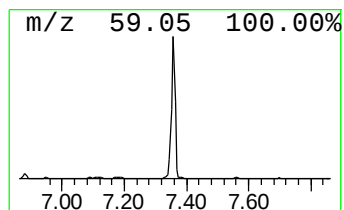
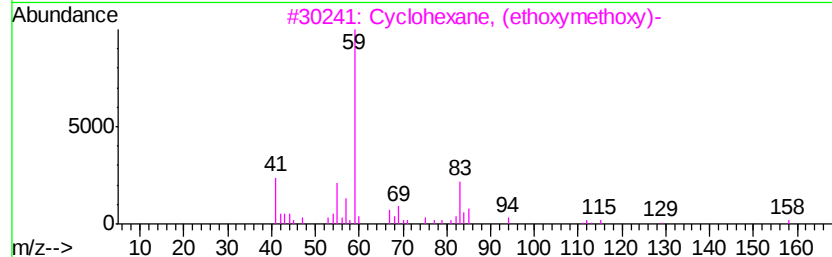
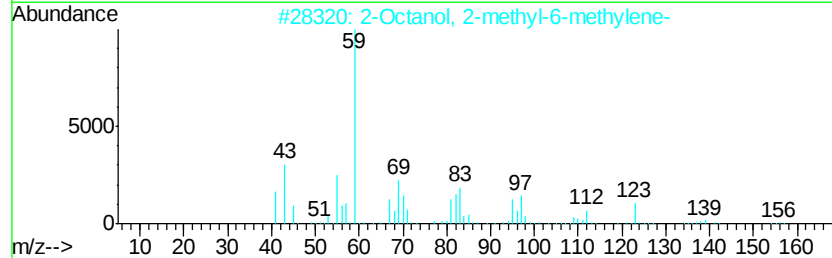
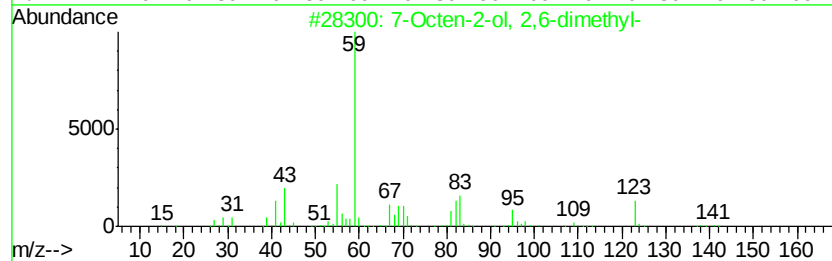
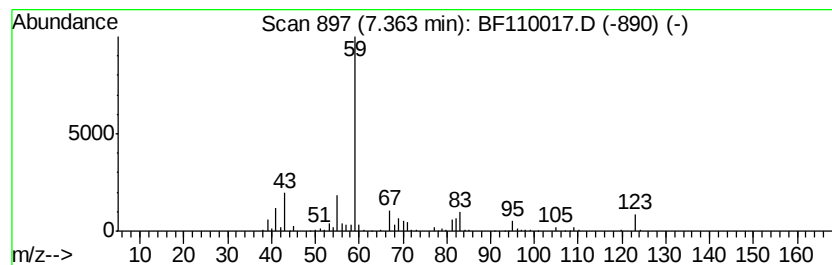
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.36	6.94 ng	468718	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	83
2			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	78
3			Cyclohexane, (ethoxymethoxy)-	158	C9H18O2	054699-29-5	50
4			2-Heptanol, 2-methyl-	130	C8H18O	000625-25-2	40
5			1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	40



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
Data File : BF110017.D
Acq On : 19 Oct 2018 21:51
Operator : JU/SJ
Sample : J5588-01
Misc :
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ClientSampleId :
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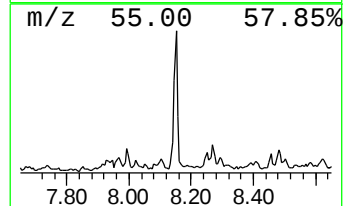
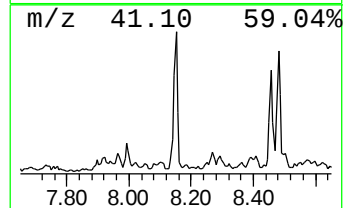
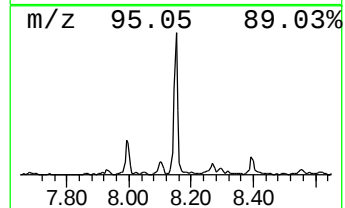
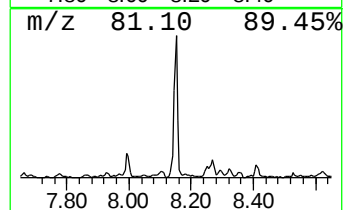
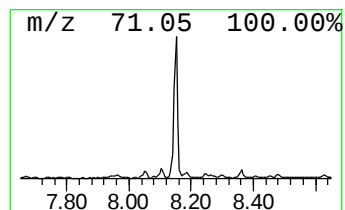
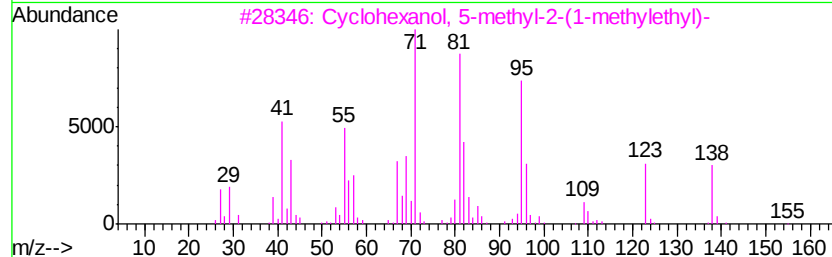
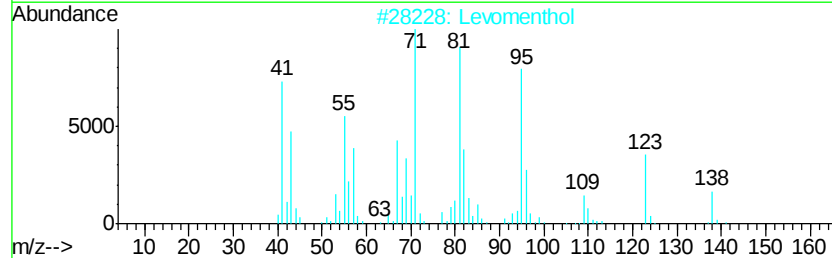
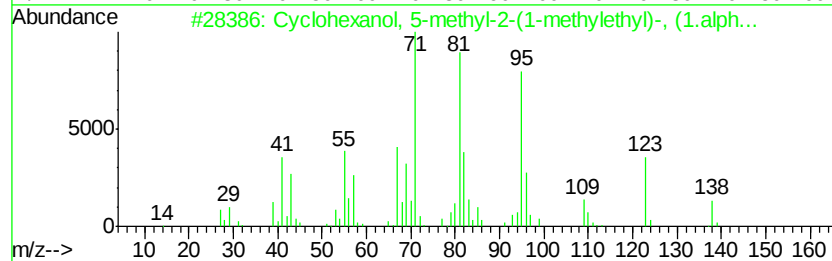
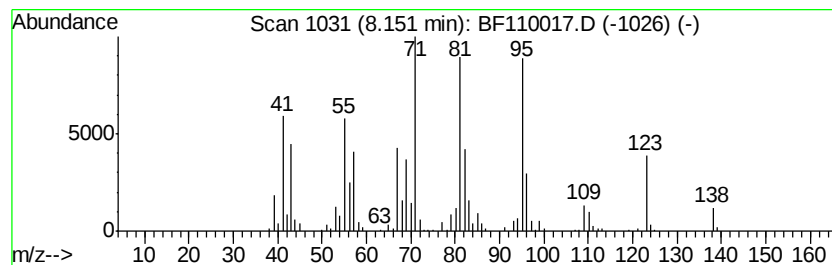
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclohexanol, 5-methyl-2-(1... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	4.28 ng	389889	Naphthalene-d8	8.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	91
2		Levomenthol	156	C10H20O	002216-51-5	91
3		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	91
4		d-Menthol	156	C10H20O	015356-60-2	90
5		dl-Menthol	156	C10H20O	000089-78-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
Data File : BF110017.D
Acq On : 19 Oct 2018 21:51
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Sample : J5588-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

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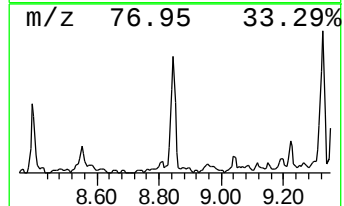
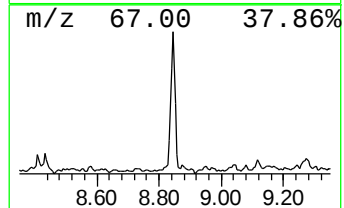
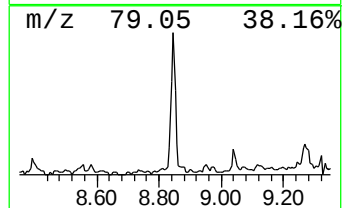
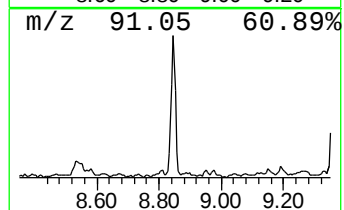
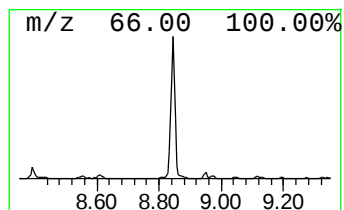
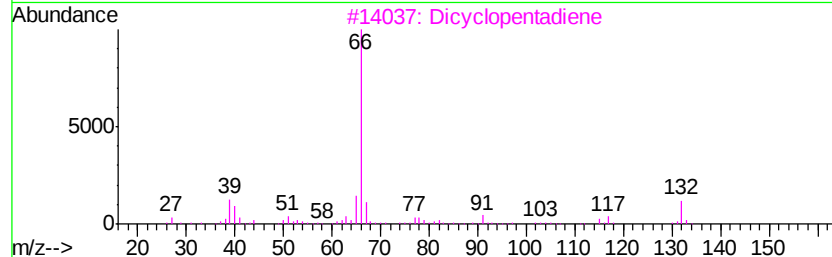
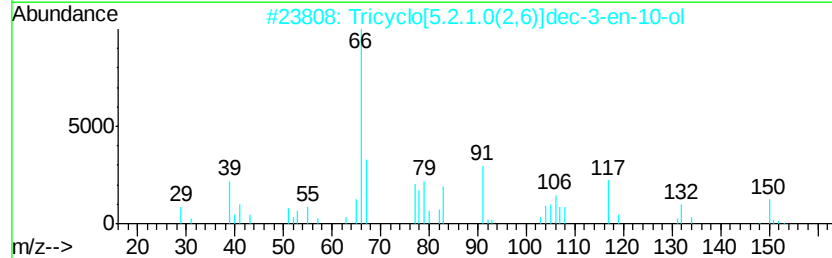
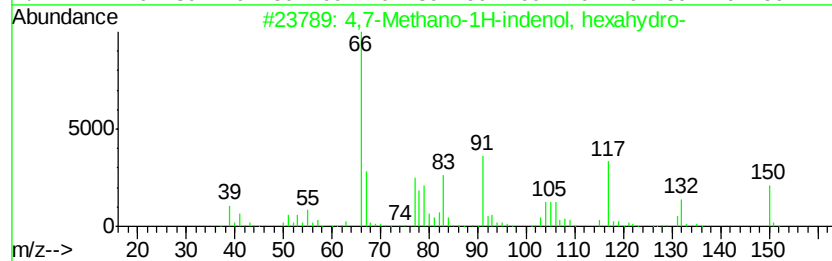
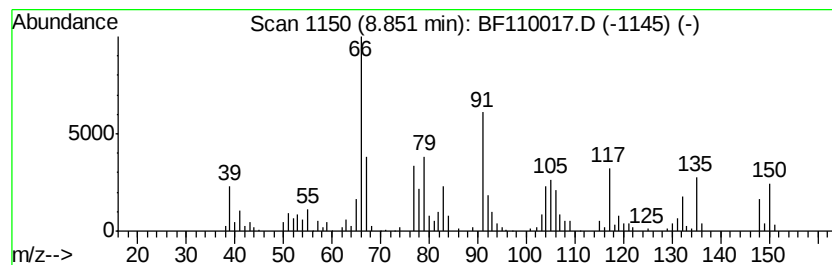
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4,7-Methano-1H-indenol, hex... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.85	3.98 ng	362309	Napthalene-d8	8.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4,7-Methano-1H-indenol, hexahydro-	150	C10H14O	037275-49-3	96
2		Tricyclo[5.2.1.0(2,6)]dec-3-en-1...	150	C10H14O	039852-87-4	93
3		Dicyclopentadiene	132	C10H12	000077-73-6	72
4		Bicyclo[3.2.0]hept-2-en-6-one	108	C7H8O	013173-09-6	64
5		1,2,4-Metheno-1H-cyclobuta[cd]pe...	148	C10H12O	015776-05-3	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
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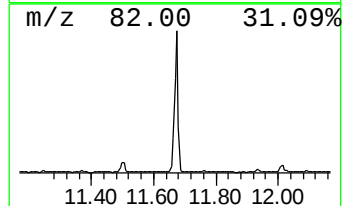
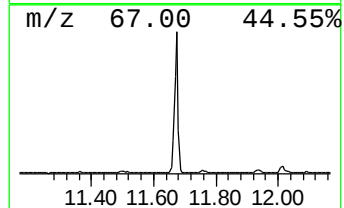
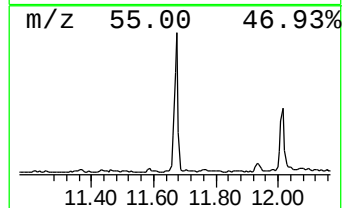
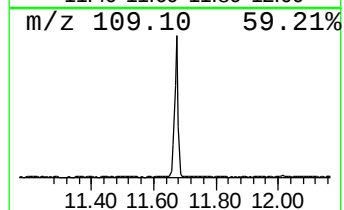
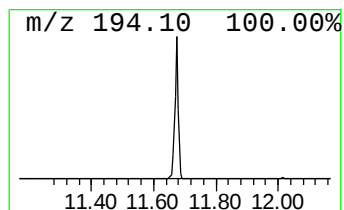
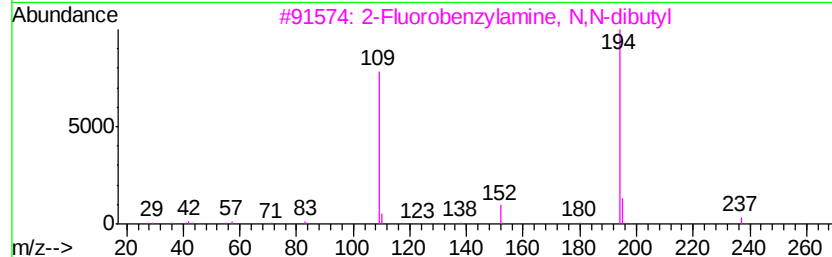
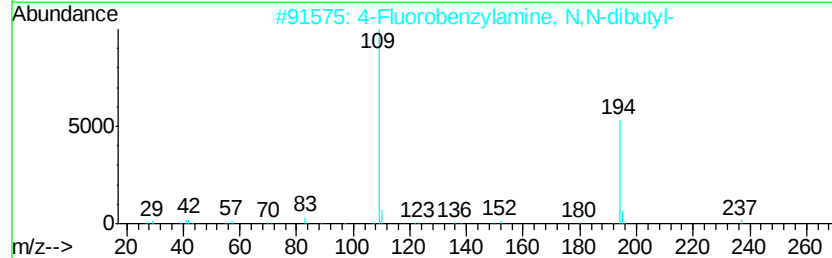
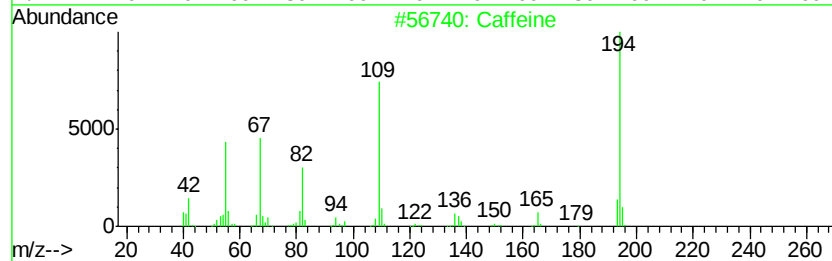
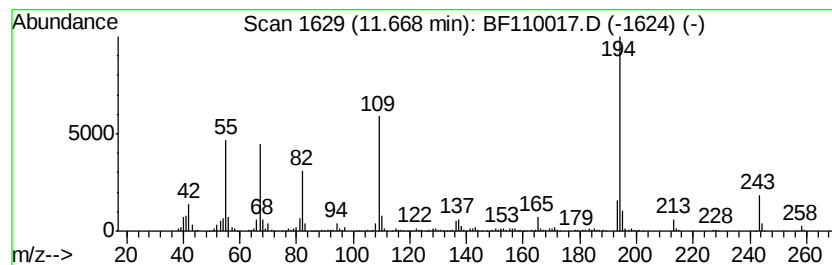
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Caffeine Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	13.60 ng	1250600	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Caffeine	194	C8H10N4O2	000058-08-2	98
2		4-Fluorobenzylamine, N,N-dibutyl-	237	C15H24FN	1000310-47-8	50
3		2-Fluorobenzylamine, N,N-dibutyl	237	C15H24FN	1000310-31-2	50
4		3(2H)-Benzofuranone, 4,6-dimethoxy-	194	C10H10O4	004225-35-8	47
5		4-Iodoimidazole	194	C3H3IN2	071759-89-2	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
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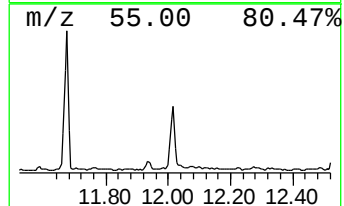
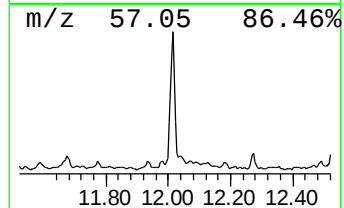
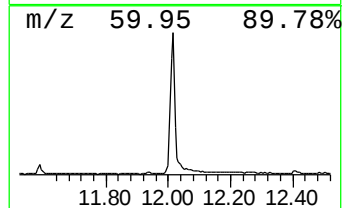
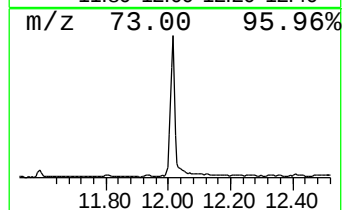
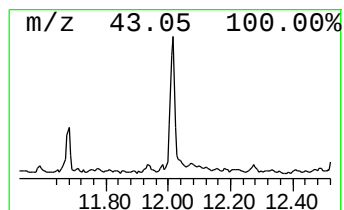
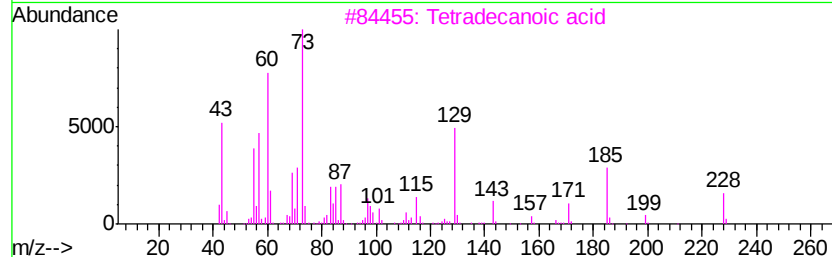
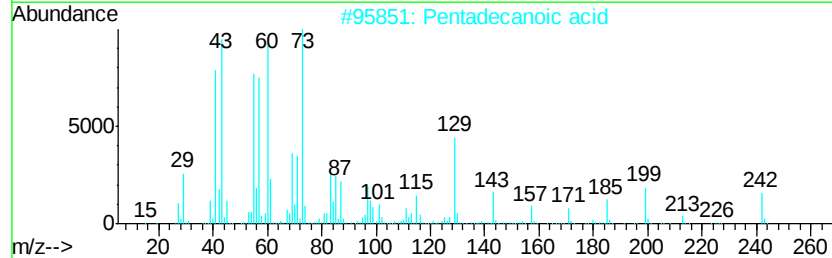
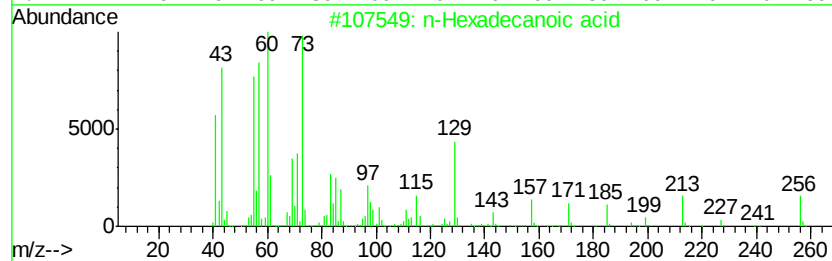
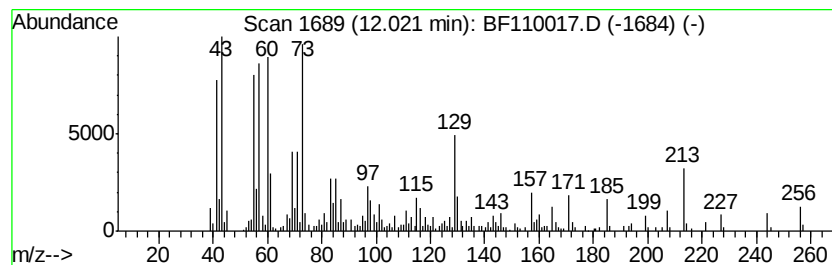
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	8.57 ng	788185	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
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Misc :
ALS Vial : 22 Sample Multiplier: 1

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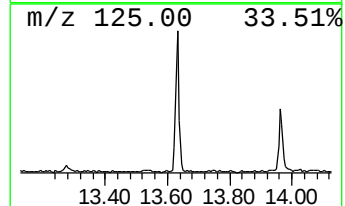
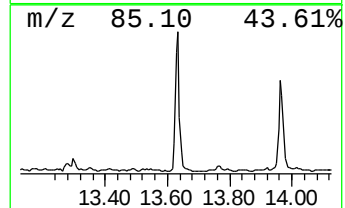
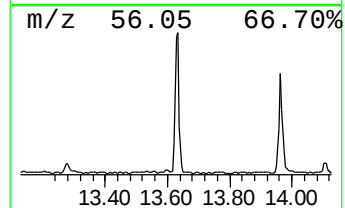
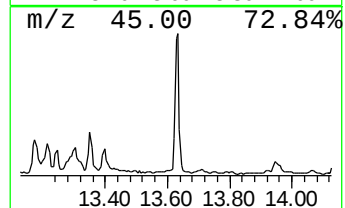
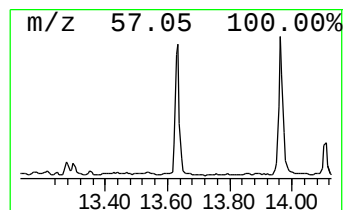
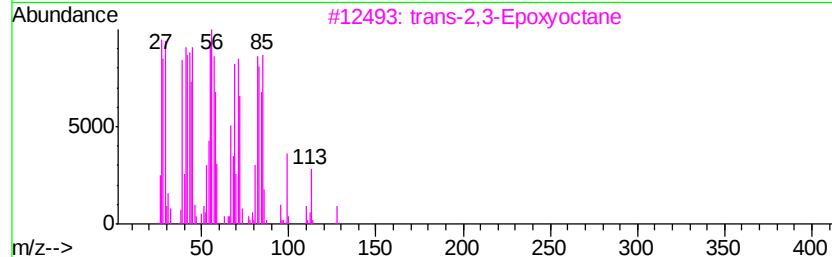
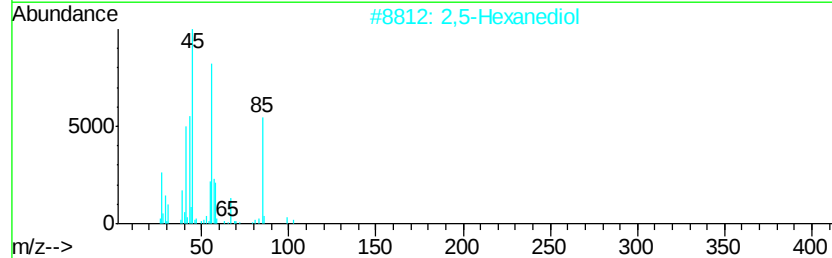
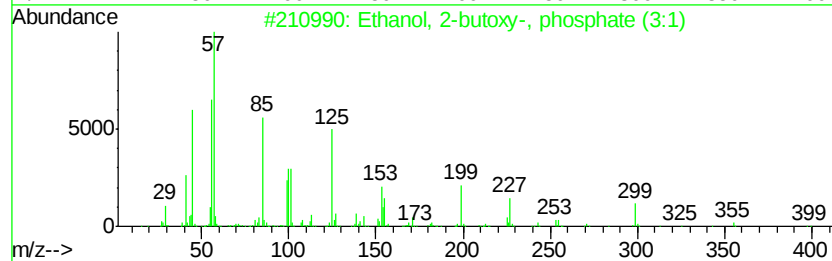
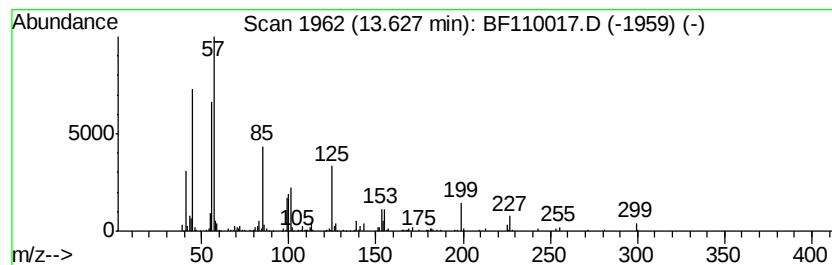
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Ethanol, 2-butoxy-, phospho... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	8.19 ng	523735	Chrysene-d12	14.14

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	87
2			2,5-Hexanediol	118	C6H14O2	002935-44-6	35
3			trans-2,3-Epoxyoctane	128	C8H16O	028180-70-3	35
4			2-Propanone, ethylhydrazone	100	C5H12N2	007422-99-3	14
5			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	10



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
Data File : BF110017.D
Acq On : 19 Oct 2018 21:51
Operator : JU/SJ
Sample : J5588-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-6

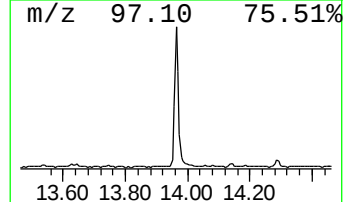
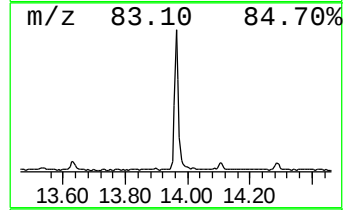
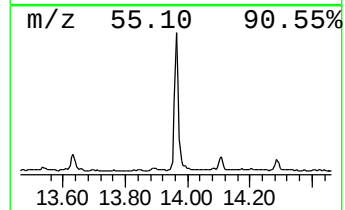
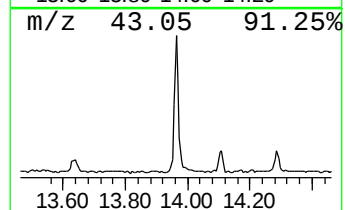
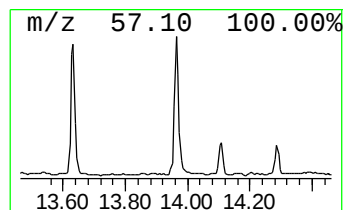
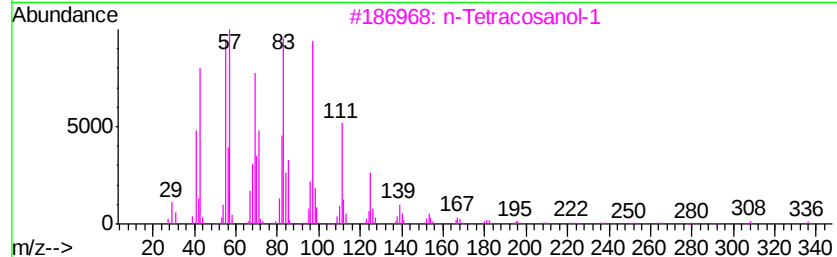
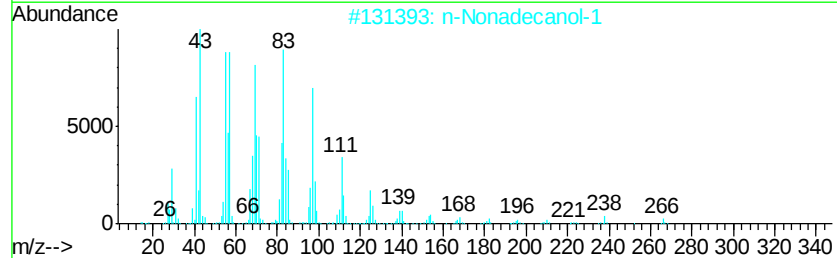
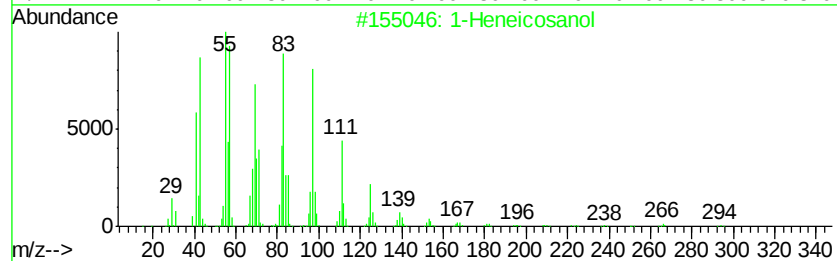
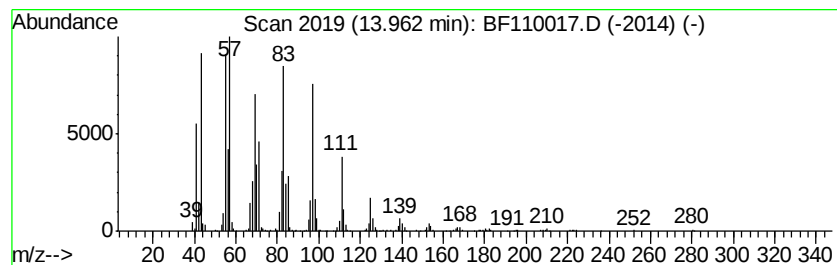
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	15.26 ng	976459	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
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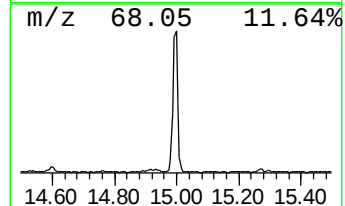
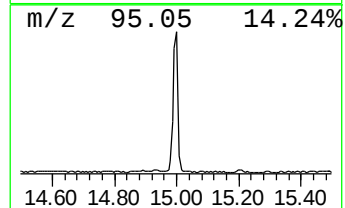
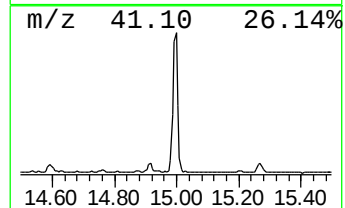
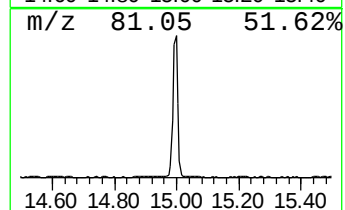
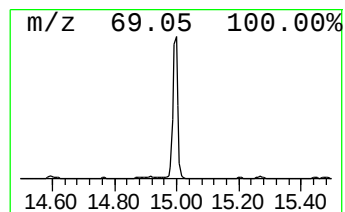
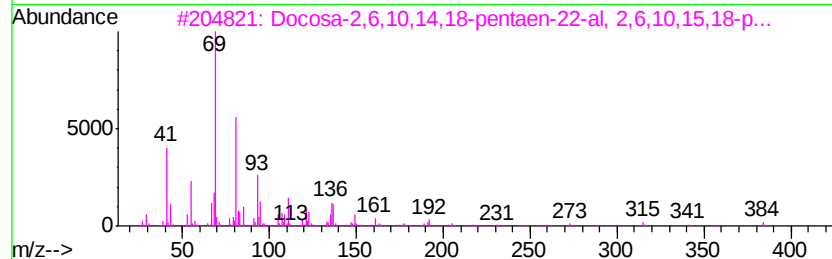
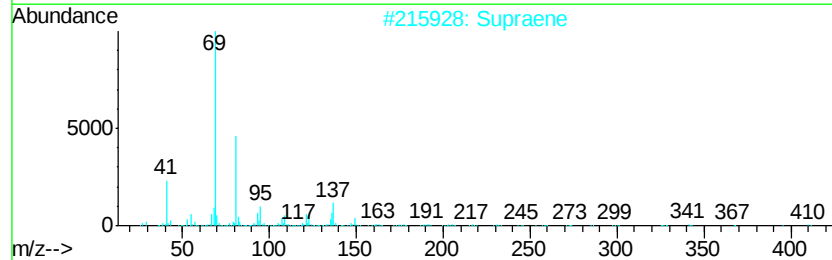
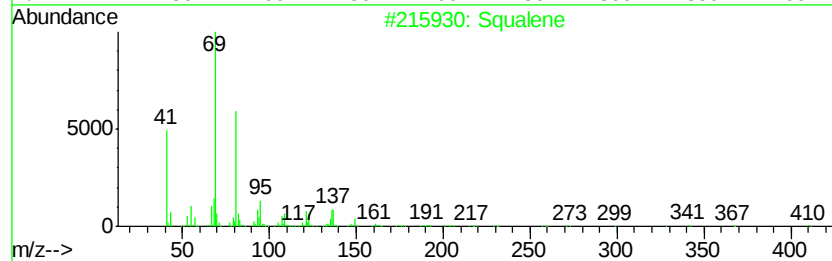
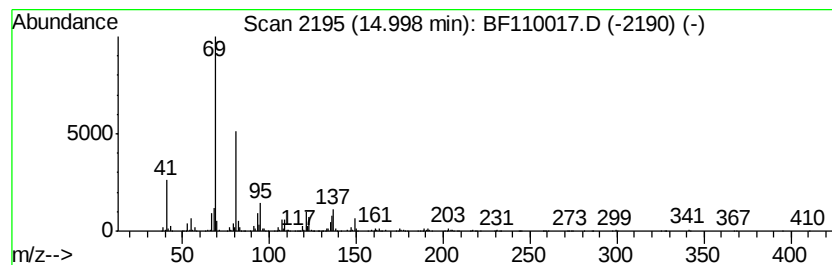
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	29.41 ng	1939770	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
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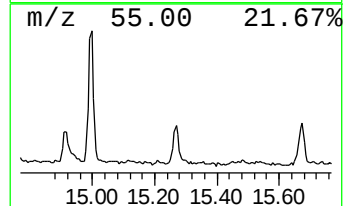
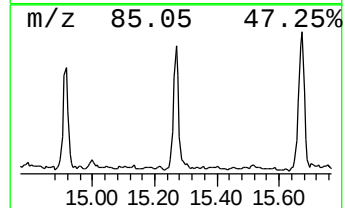
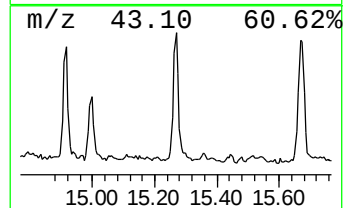
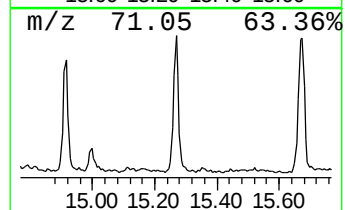
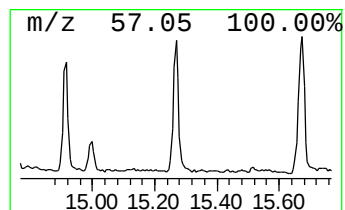
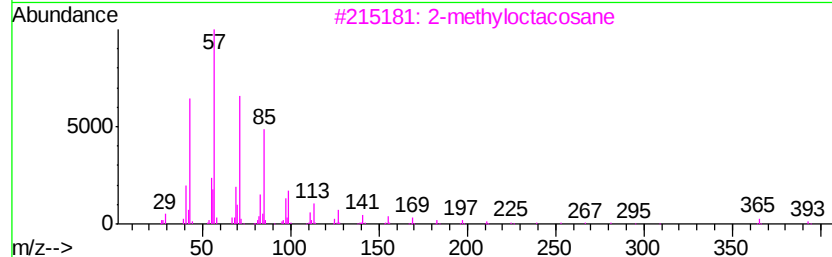
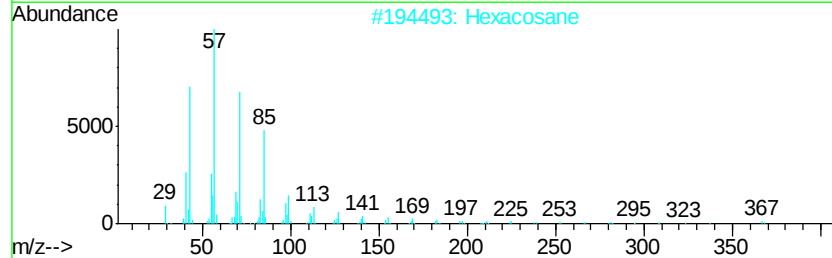
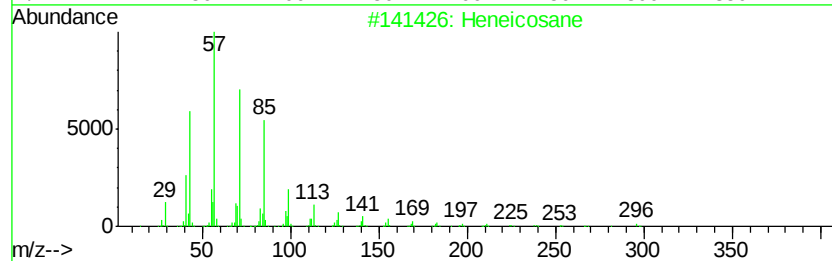
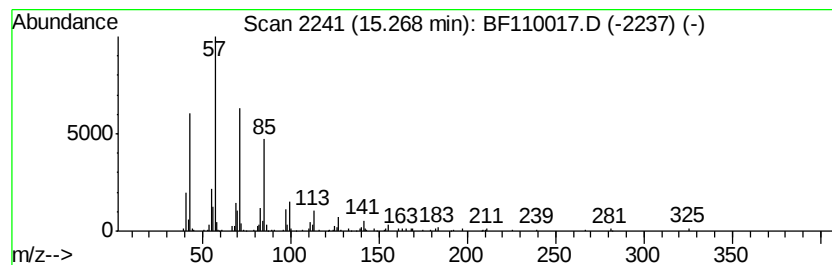
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Heneicosane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	3.69 ng	243499	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			2-methyloctacosane	408	C29H60	1000376-72-8	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Docosane, 11-butyl-	366	C26H54	013475-76-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
Data File : BF110017.D
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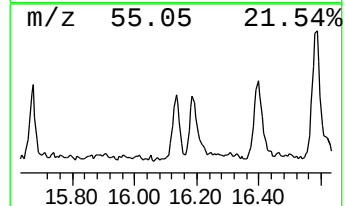
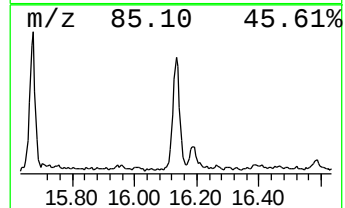
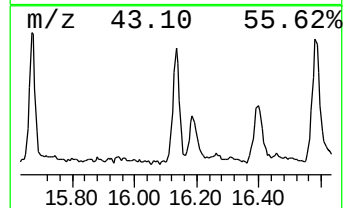
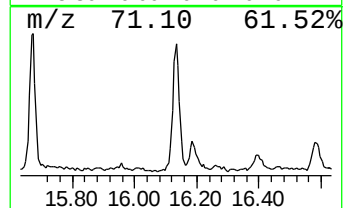
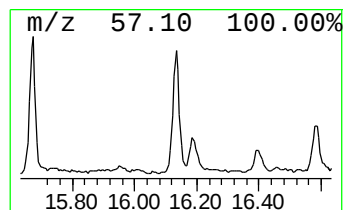
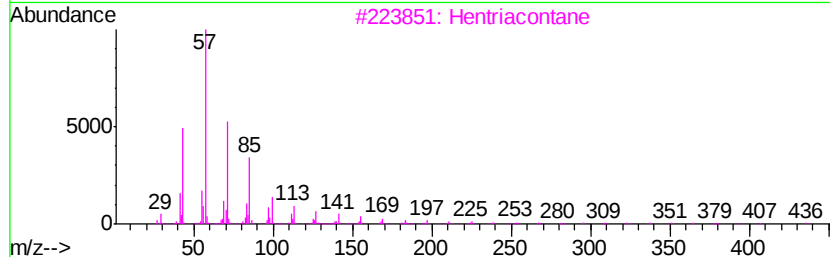
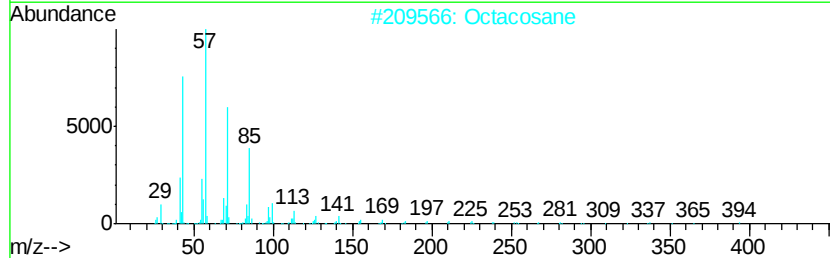
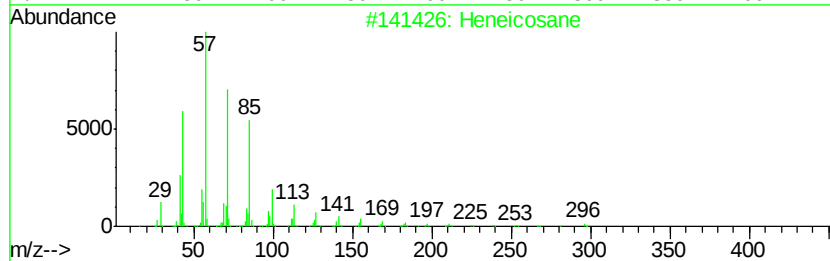
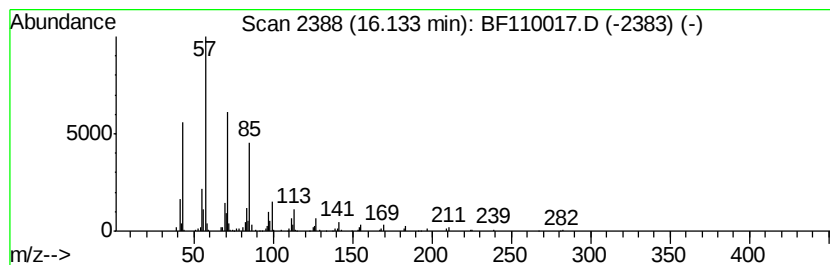
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Octacosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	4.03 ng	265892	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Hentriacontane	437	C31H64	000630-04-6	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Eicosane	282	C20H42	000112-95-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
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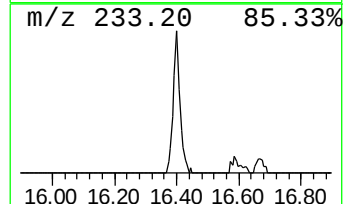
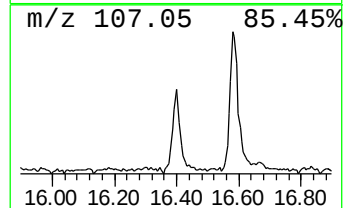
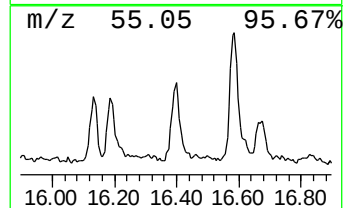
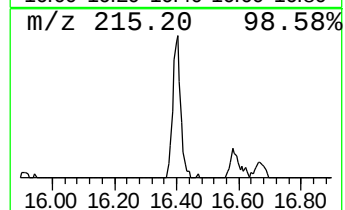
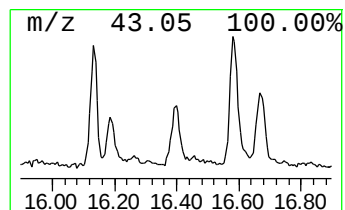
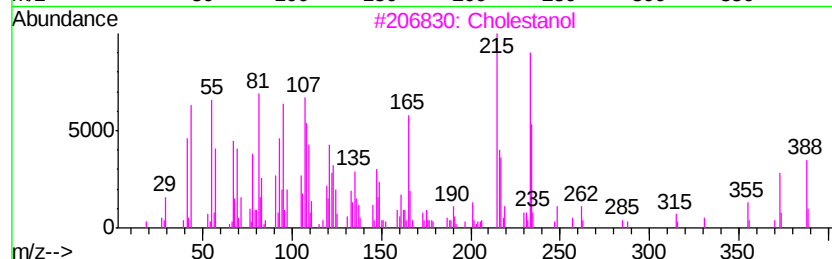
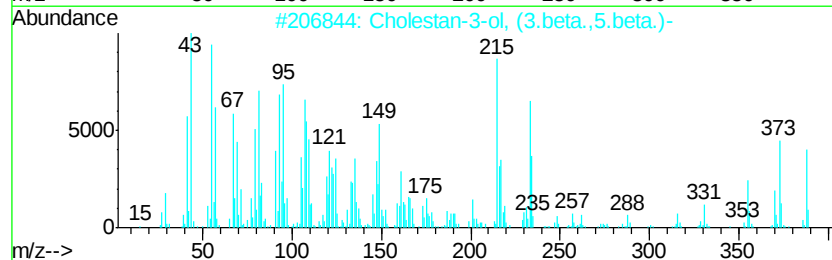
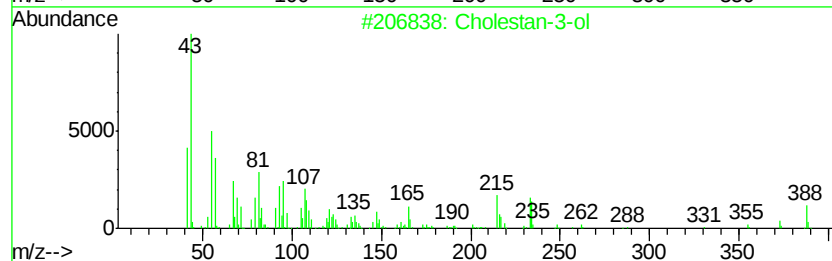
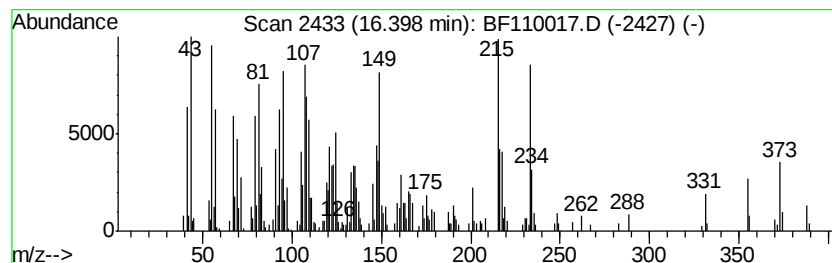
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Cholestan-3-ol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	8.35 ng	550603	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholestan-3-ol	388	C27H48O	027409-41-2	86
2			Cholestan-3-ol, (3.beta.,5.beta.)-	388	C27H48O	000360-68-9	86
3			Cholestanol	388	C27H48O	000080-97-7	64
4			Pentanenitrile, 2-(4-fluoropheny...	233	C12H12FN3O	1000269-22-3	35
5			Cyclohexane, 1,2-dimethyl-3,5-bi...	192	C14H24	074806-55-6	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
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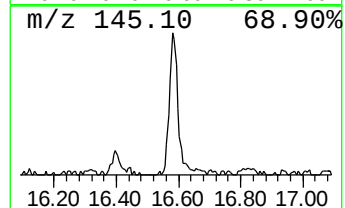
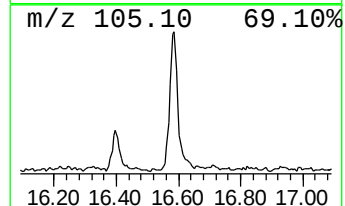
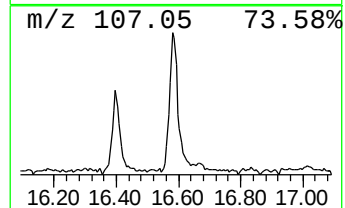
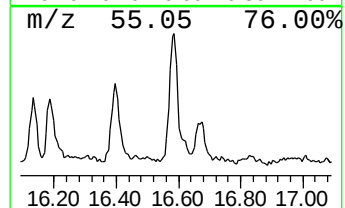
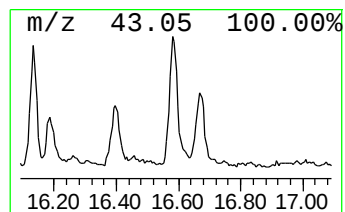
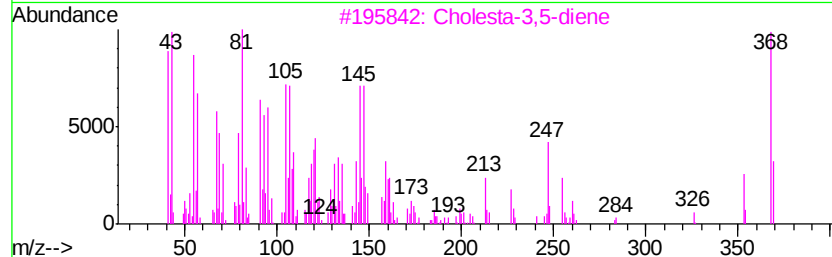
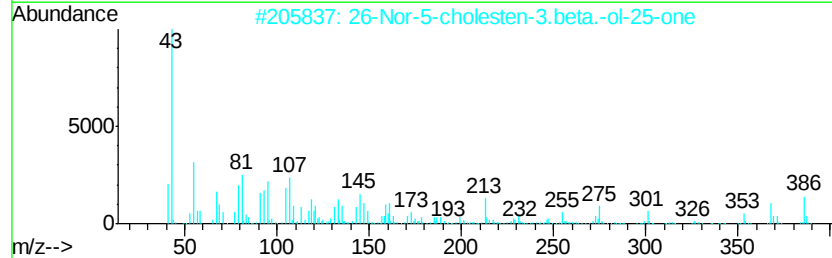
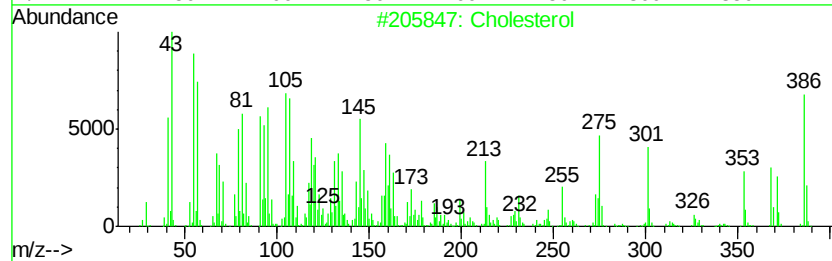
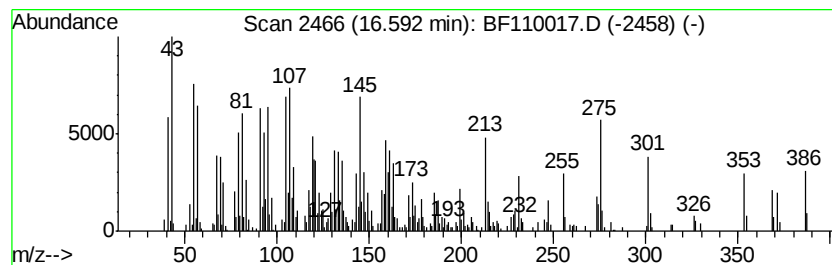
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Cholesterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	17.27 ng	1139370	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cholesterol	386	C27H46O	000057-88-5	99
2		26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	99
3		Cholesta-3,5-diene	368	C27H44	000747-90-0	50
4		1H-Indole, 1-[[3-(trifluoromethy...	275	C16H12F3N	1000337-43-9	25
5		Cholest-5-en-3-ol (3.beta.)-, te...	597	C41H72O2	001989-52-2	16



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
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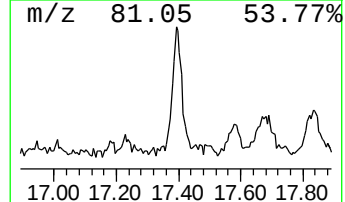
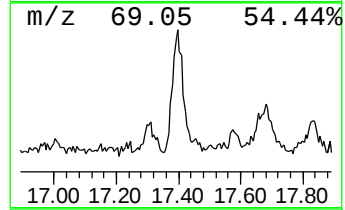
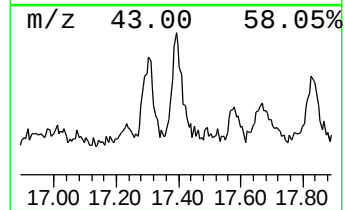
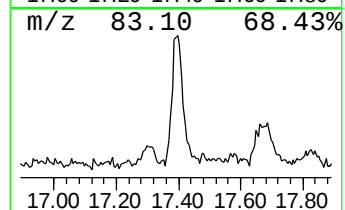
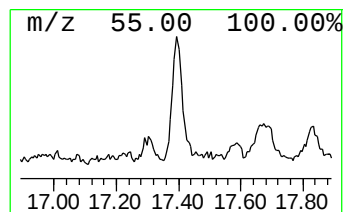
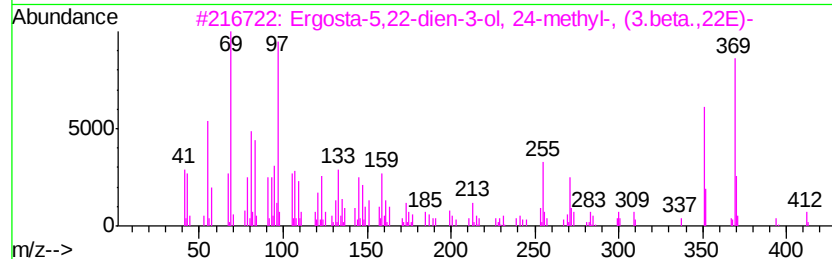
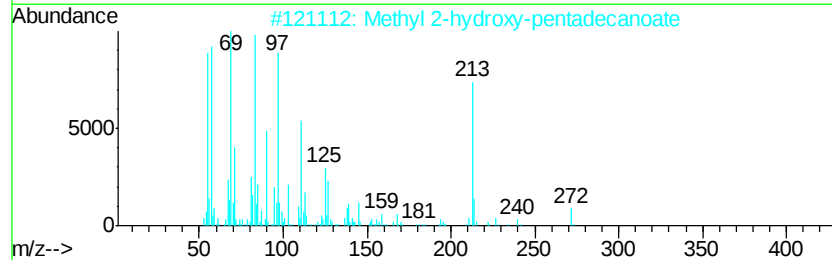
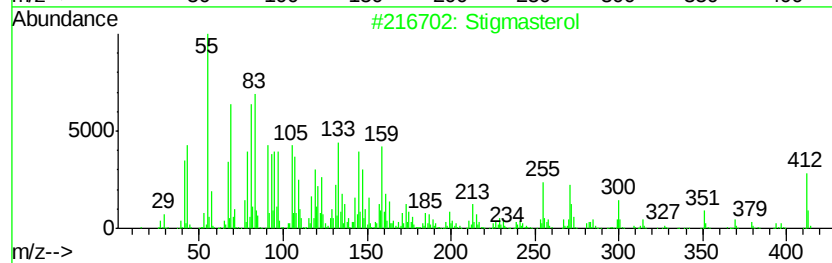
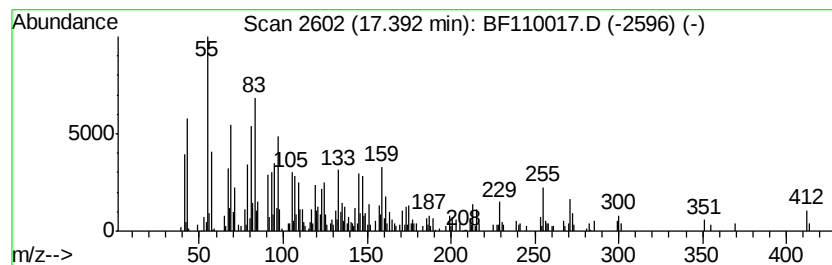
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Stigmasterol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.39	7.29 ng	480763	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Stigmasterol	412	C29H48O	000083-48-7	94
2		Methyl 2-hydroxy-pentadecanoate	272	C16H32O3	1000336-35-7	35
3		Ergosta-5,22-dien-3-ol, 24-methy...	412	C29H48O	053755-22-9	35
4		Cholesta-22,24-dien-5-ol, 4,4-di...	412	C29H48O	1000128-66-1	25
5		Cholest-5-en-3-ol (3.beta.)-, te...	597	C41H72O2	001989-52-2	14



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
Data File : BF110017.D
Acq On : 19 Oct 2018 21:51
Operator : JU/SJ
Sample : J5588-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-6

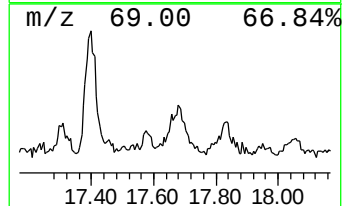
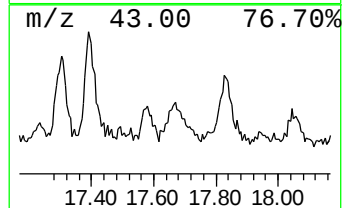
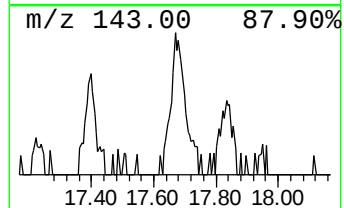
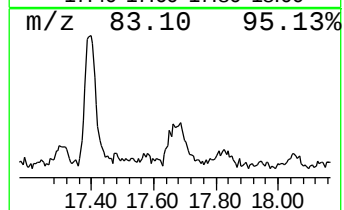
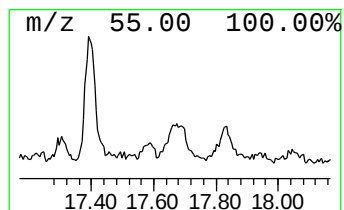
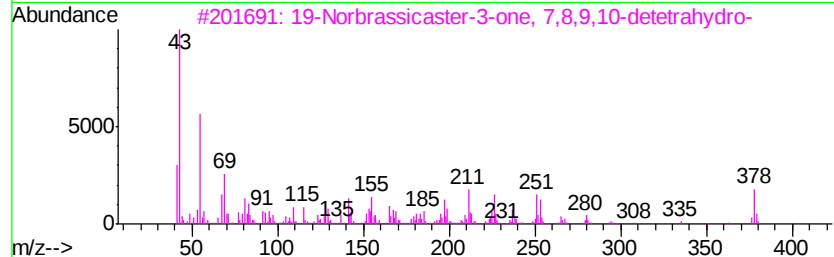
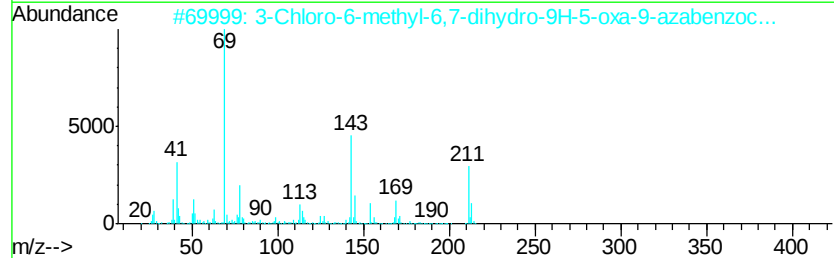
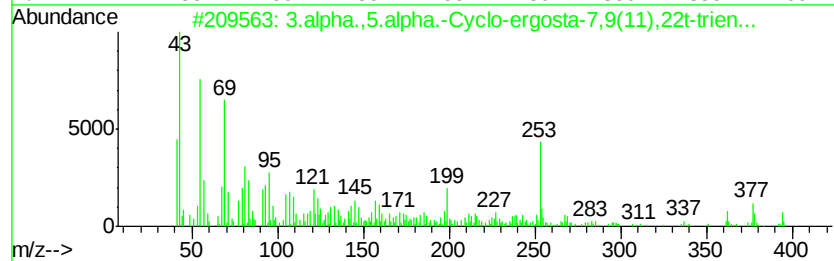
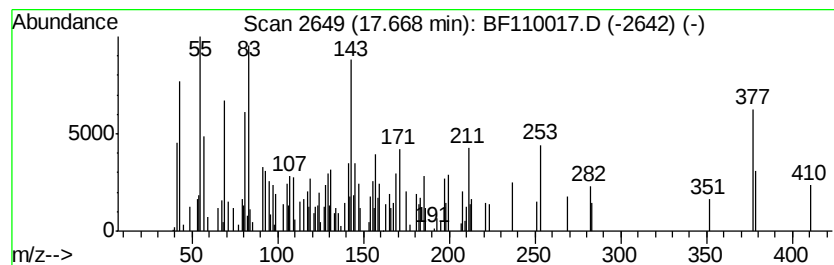
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown17.67 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.67	3.90 ng	257054	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3.alpha.,5.alpha.-Cyclo-ergosta-...	394	C28H42O	118978-72-6	25		
2	3-Chloro-6-methyl-6,7-dihydro-9H...	211	C10H10ClNO2	134076-61-2	18		
3	19-Norbrassicaster-3-one, 7,8,9,...	378	C27H38O	032277-76-2	18		
4	3.alpha.,5-Cyclo-5.alpha.-ergost...	378	C28H42	024352-51-0	12		
5	3-Heptyne, 7-chloro-2,2-dimethyl-	158	C9H15Cl	055402-10-3	11		



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
Data File : BF110017.D
Acq On : 19 Oct 2018 21:51
Operator : JU/SJ
Sample : J5588-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-6

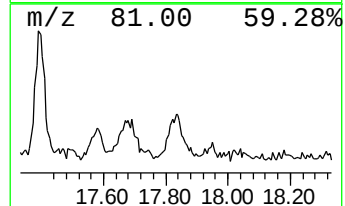
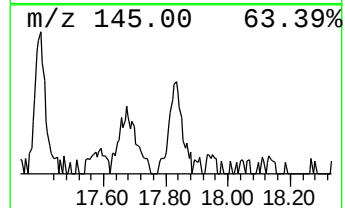
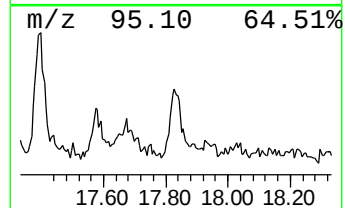
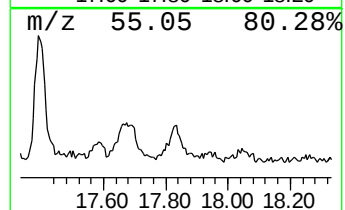
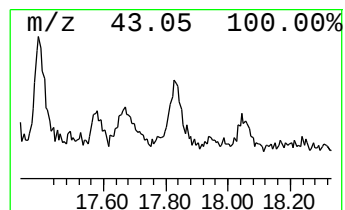
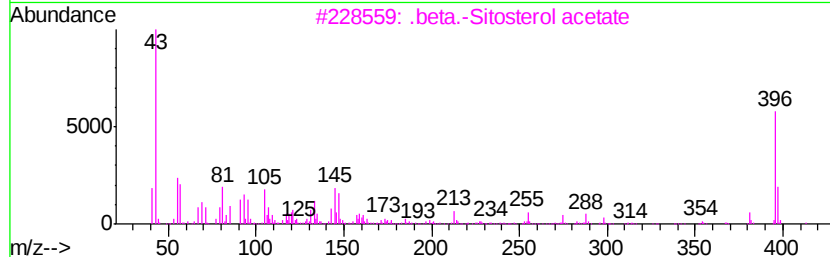
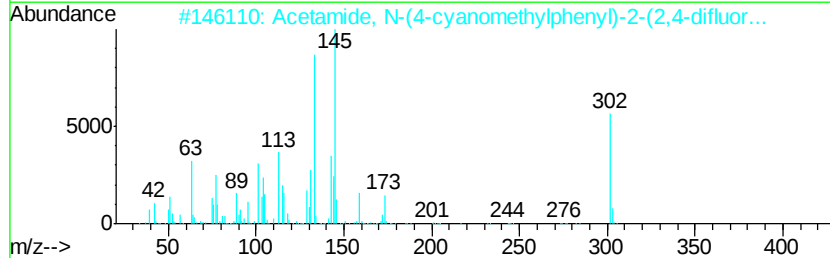
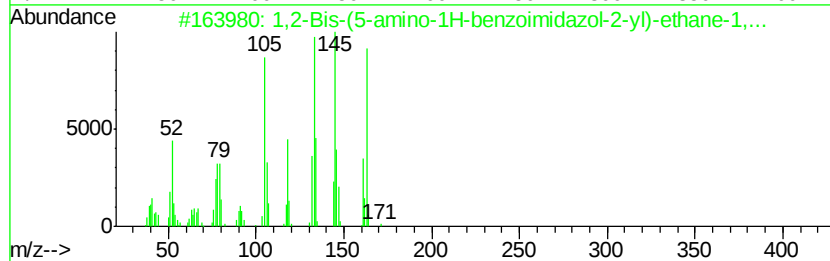
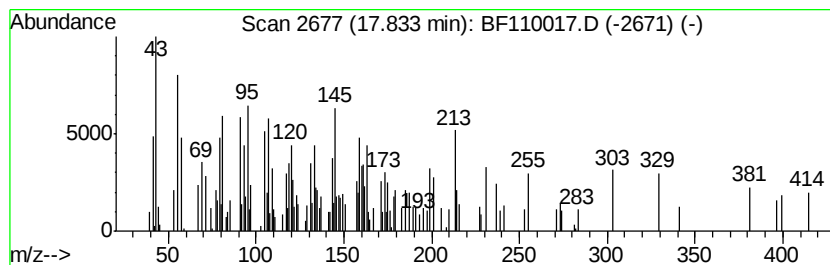
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown17.83 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	3.73 ng	245730	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Bis-(5-amino-1H-benzoimidazo...	324	C16H16N6O2	031545-09-2	22
2		Acetamide, N-(4-cyanomethylpheny...	302	C16H12F2N2O2	1000303-56-0	14
3		.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	12
4		Stigmastan-3,5-diene	396	C29H48	1000214-16-4	10
5		1H-Pyrazole-4-sulfonamide, N-(2,...	273	C10H9F2N3O2S	1000319-53-0	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101918\
 Data File : BF110017.D
 Acq On : 19 Oct 2018 21:51
 Operator : JU/SJ
 Sample : J5588-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexane	2.13	27.1 ng		1829670	1	6.97	1351050	20.0
Butane, 2-methoxy...	2.33	42.0 ng		2835310	1	6.97	1351050	20.0
unknown6.73	6.73	59.6 ng		4028660	1	6.97	1351050	20.0
Benzenemethanamin...	7.17	4.4 ng		295924	1	6.97	1351050	20.0
7-Octen-2-ol, 2,6...	7.36	6.9 ng		468718	1	6.97	1351050	20.0
Cyclohexanol, 5-m...	8.15	4.3 ng		389889	2	8.25	1822060	20.0
4,7-Methano-1H-in...	8.85	4.0 ng		362309	2	8.25	1822060	20.0
Caffeine	11.67	13.6 ng		1250600	4	11.50	1839780	20.0
n-Hexadecanoic acid	12.02	8.6 ng		788185	4	11.50	1839780	20.0
Ethanol, 2-butoxy...	13.63	8.2 ng		523735	5	14.14	1279470	20.0
1-Heneicosanol	13.96	15.3 ng		976459	5	14.14	1279470	20.0
Squalene	15.00	29.4 ng		1939770	6	15.67	1319310	20.0
Heneicosane	15.27	3.7 ng		243499	6	15.67	1319310	20.0
Octacosane	16.13	4.0 ng		265892	6	15.67	1319310	20.0
Cholestan-3-ol	16.40	8.3 ng		550603	6	15.67	1319310	20.0
Cholesterol	16.59	17.3 ng		1139370	6	15.67	1319310	20.0
Stigmasterol	17.39	7.3 ng		480763	6	15.67	1319310	20.0
unknown17.67	17.67	3.9 ng		257054	6	15.67	1319310	20.0
unknown17.83	17.83	3.7 ng		245730	6	15.67	1319310	20.0