

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011119\
 Data File : BF112012.D
 Acq On : 11 Jan 2019 13:52
 Operator : JU/SJ
 Sample : K1102-06
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CPSB-13(15-20)

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-BF010719.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	2.175	11	15	28	rVB2	71425	128336	4.90%	0.422%
2	2.369	43	48	52	rBV4	16073	30210	1.15%	0.099%
3	5.092	507	511	517	rBV	130791	145282	5.54%	0.478%
4	5.510	577	582	585	rBV	2292225	2100111	80.13%	6.904%
5	6.416	733	736	742	rVB	51442	46287	1.77%	0.152%
6	6.516	748	753	764	rBV	2290797	2189589	83.55%	7.198%
7	6.645	771	775	779	rBV	2384733	2324842	88.71%	7.643%
8	6.692	781	783	789	rVB	44050	43558	1.66%	0.143%
9	6.869	810	813	817	rBV	777182	694155	26.49%	2.282%
10	7.028	836	840	844	rBV	2092011	1889926	72.11%	6.213%
11	7.433	903	909	912	rBV	1542844	1525457	58.21%	5.015%
12	8.151	1027	1031	1035	rBV	985605	884999	33.77%	2.909%
13	9.086	1187	1190	1192	rBV	29374	31784	1.21%	0.104%
14	9.116	1192	1195	1203	rVB2	69075	95868	3.66%	0.315%
15	9.227	1209	1214	1217	rBV	3055981	2620816	100.00%	8.616%
16	9.286	1221	1224	1229	rVB2	38041	34813	1.33%	0.114%
17	9.363	1235	1237	1241	rVB2	72556	65978	2.52%	0.217%
18	9.433	1246	1249	1257	rVB	40686	58404	2.23%	0.192%
19	9.616	1276	1280	1285	rVB	684530	593025	22.63%	1.950%
20	9.822	1310	1315	1318	rBV	66813	58713	2.24%	0.193%
21	9.910	1326	1330	1333	rBV	1176854	988355	37.71%	3.249%
22	9.980	1338	1342	1348	rBV	18430	38831	1.48%	0.128%
23	10.698	1460	1464	1472	rBV	1738178	1525108	58.19%	5.014%
24	10.798	1478	1481	1483	rBV	56719	52471	2.00%	0.172%
25	10.821	1483	1485	1489	rVB2	32331	34983	1.33%	0.115%
26	11.039	1518	1522	1527	rBV6	19256	31663	1.21%	0.104%
27	11.292	1562	1565	1569	rVB	56747	62005	2.37%	0.204%
28	11.398	1579	1583	1586	rBV	1025533	875445	33.40%	2.878%
29	11.921	1668	1672	1677	rBV	194118	195311	7.45%	0.642%
30	12.480	1765	1767	1773	rVB4	31278	43441	1.66%	0.143%
31	12.704	1802	1805	1811	rBV2	78189	91346	3.49%	0.300%
32	12.980	1848	1852	1855	rBV	2164364	1772493	67.63%	5.827%
33	13.210	1888	1891	1894	rVB	59658	52603	2.01%	0.173%
34	13.551	1947	1949	1950	rBV	44895	38369	1.46%	0.126%

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35	13.568	1950	1952	1955	rVB	120460	114793	4.38%	0.377%
36	13.798	1989	1991	1995	rVB5	51554	55217	2.11%	0.182%
37	13.868	2000	2003	2010	rBV	1058764	1154027	44.03%	3.794%
38	13.927	2010	2013	2015	rBV	53968	53948	2.06%	0.177%
39	14.039	2024	2032	2035	rBV	847451	957702	36.54%	3.148%
40	14.192	2055	2058	2068	rVB2	147279	202977	7.74%	0.667%
41	14.315	2077	2079	2082	rBV	88584	72586	2.77%	0.239%
42	14.345	2082	2084	2087	rBV2	46825	46085	1.76%	0.151%
43	14.457	2101	2103	2106	rBV2	43292	38981	1.49%	0.128%
44	14.504	2108	2111	2117	rBV3	844175	1233935	47.08%	4.056%
45	14.809	2160	2163	2165	rBV	84954	95477	3.64%	0.314%
46	15.151	2217	2221	2223	rBV	178455	202017	7.71%	0.664%
47	15.180	2223	2226	2231	rVB2	192508	281570	10.74%	0.926%
48	15.515	2278	2283	2292	rBV	674994	965769	36.85%	3.175%
49	15.845	2337	2339	2342	rBV3	35895	30552	1.17%	0.100%
50	15.974	2358	2361	2366	rVB	114617	155212	5.92%	0.510%
51	16.021	2366	2369	2377	rVB2	108143	158156	6.03%	0.520%
52	17.086	2545	2550	2558	rVB5	86099	179131	6.83%	0.589%
53	17.174	2561	2565	2574	rVV4	103524	232657	8.88%	0.765%
54	17.268	2575	2581	2588	rVV3	201263	488537	18.64%	1.606%
55	17.350	2589	2595	2607	rVB2	273395	688310	26.26%	2.263%
56	17.598	2631	2637	2645	rBV8	101453	278741	10.64%	0.916%
57	17.945	2690	2696	2703	rBV8	113059	321290	12.26%	1.056%
58	18.168	2728	2734	2742	rVB4	269945	622531	23.75%	2.047%
59	18.403	2768	2774	2787	rVB10	130549	424388	16.19%	1.395%

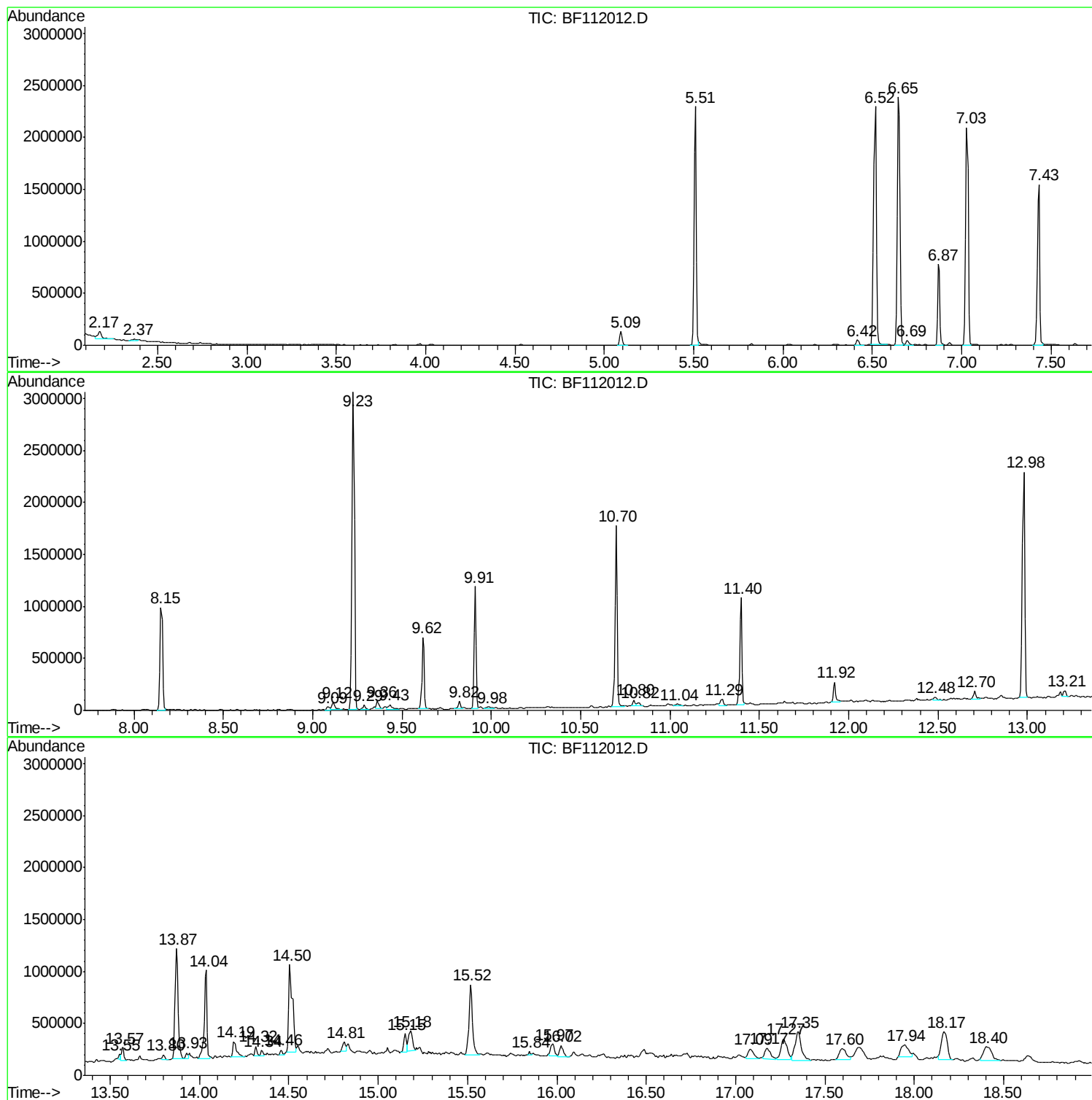
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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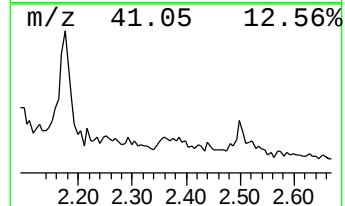
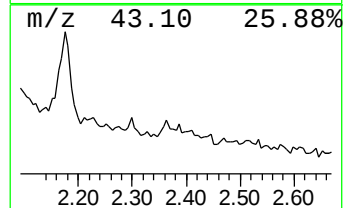
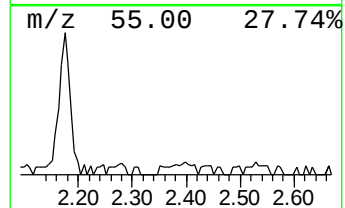
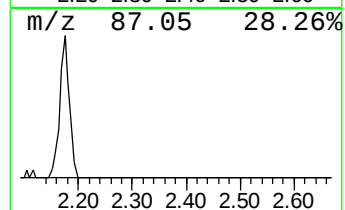
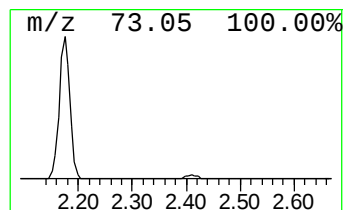
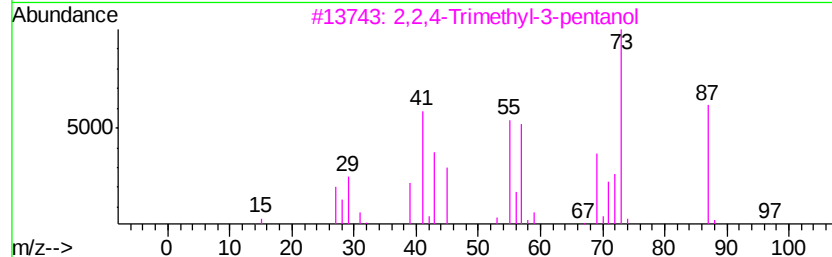
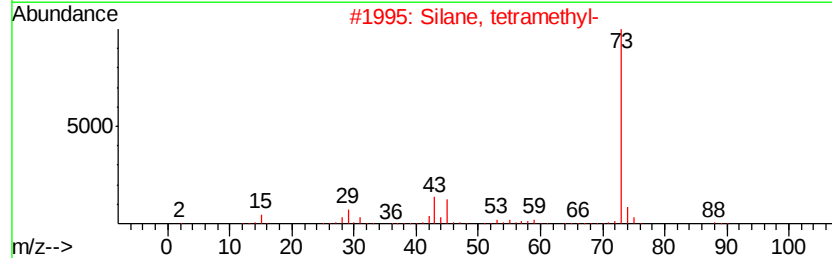
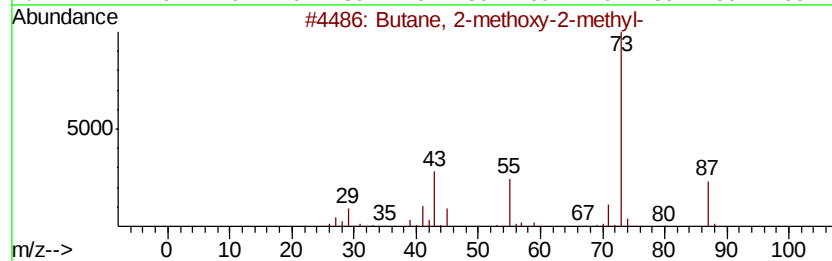
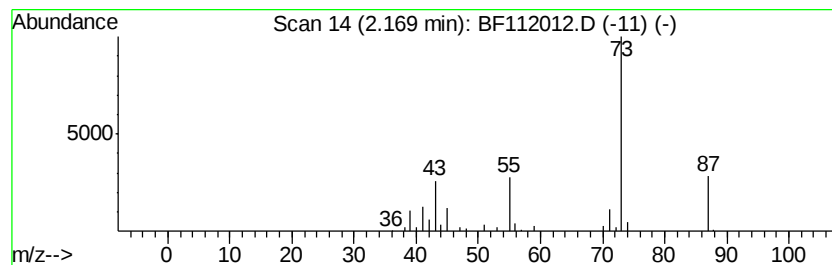
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	3.70 ng	128336	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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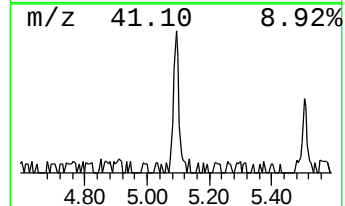
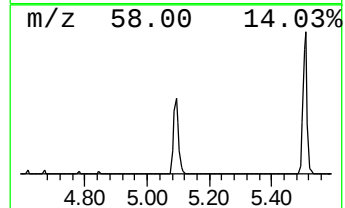
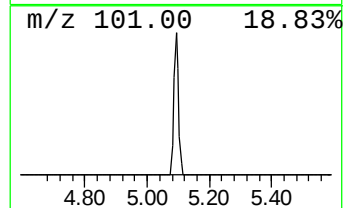
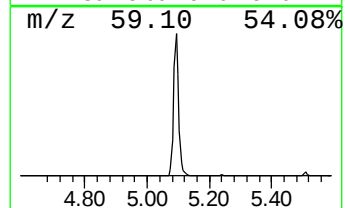
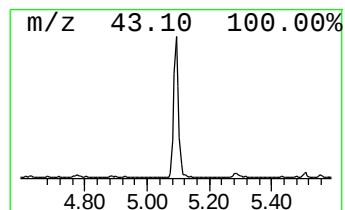
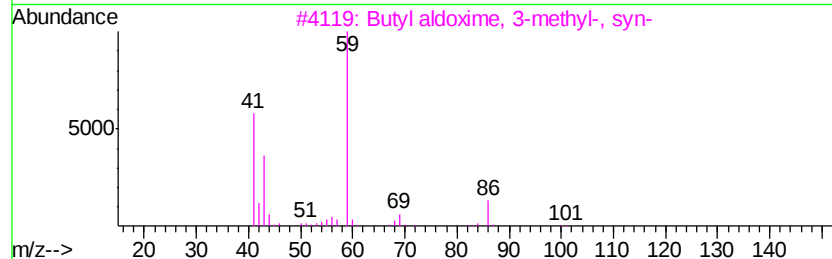
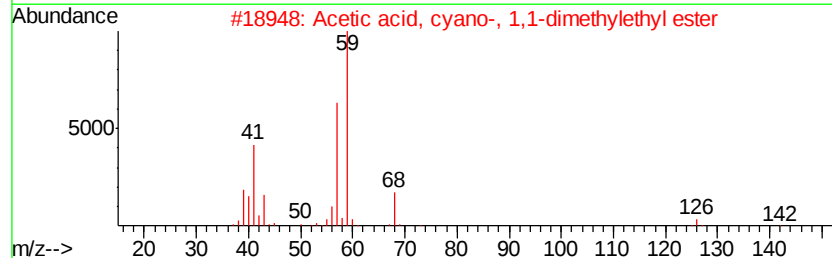
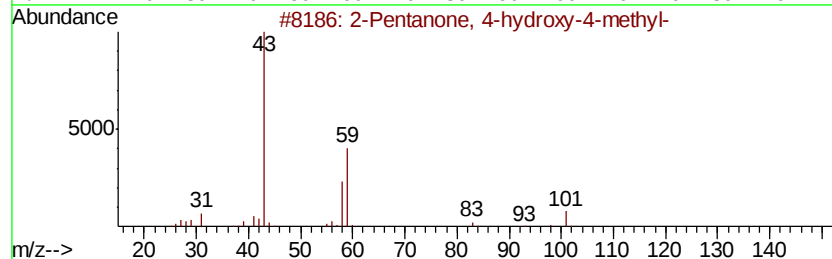
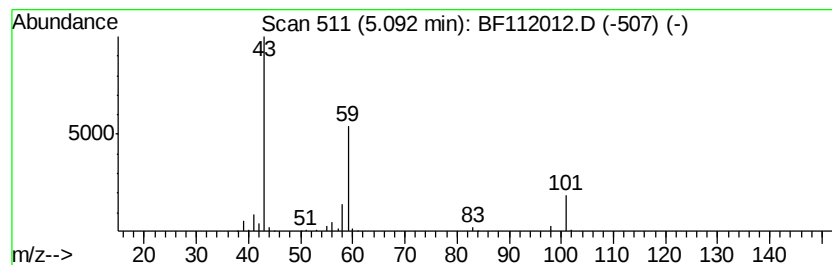
Instrument :
BNA_F
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CPSB-13(15-20)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.09	4.19 ng	145282	1,4-Dichlorobenzene-d4	6.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	9



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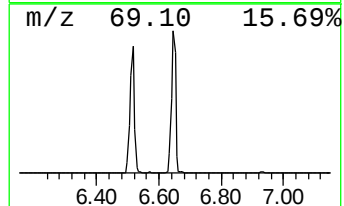
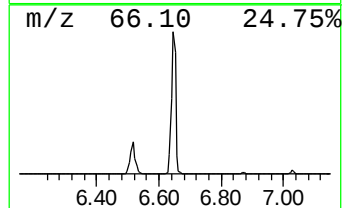
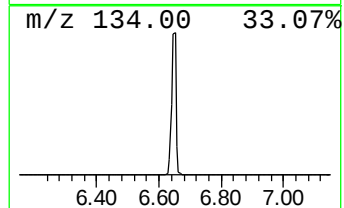
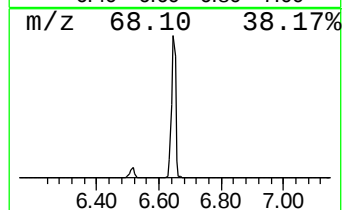
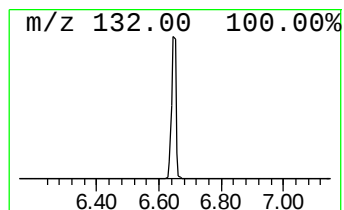
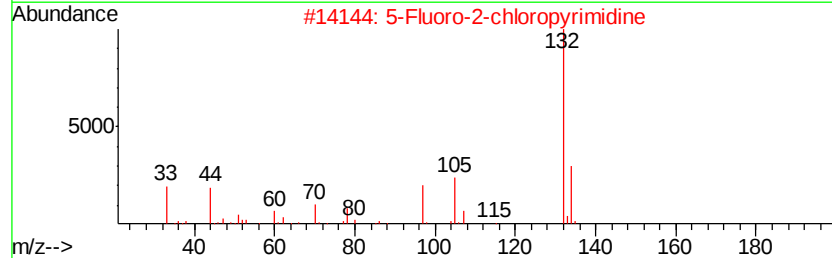
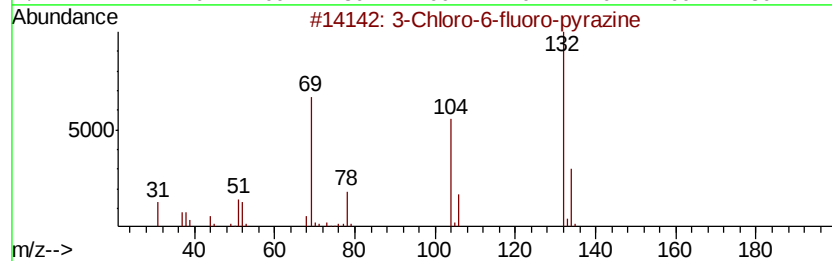
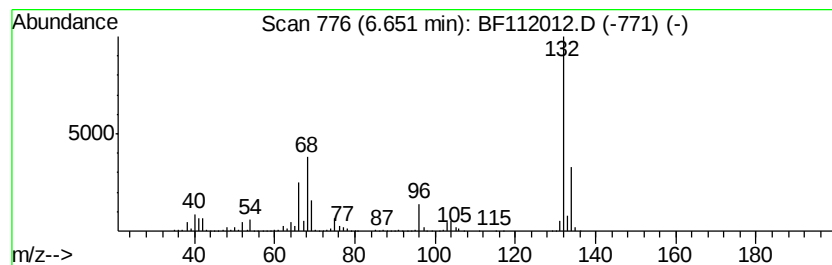
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	66.98 ng	2324840	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10
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



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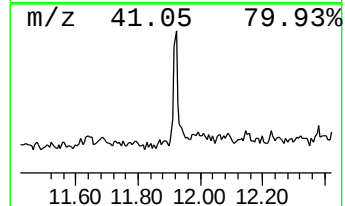
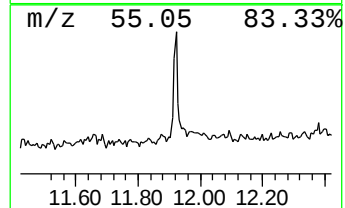
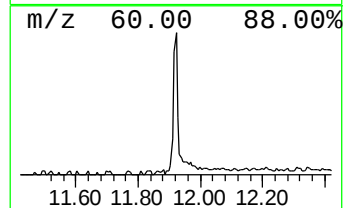
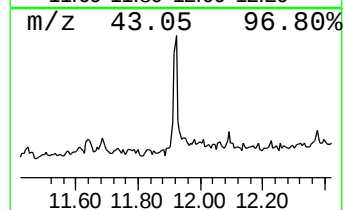
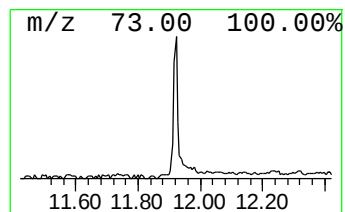
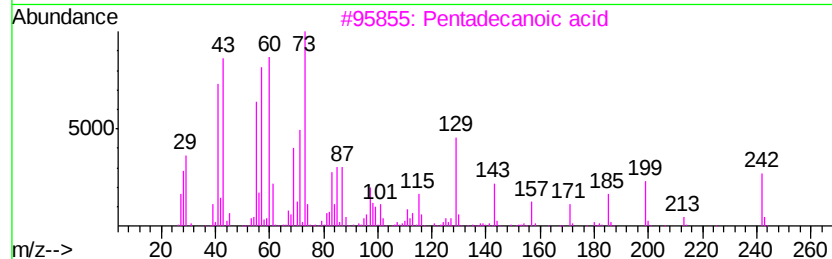
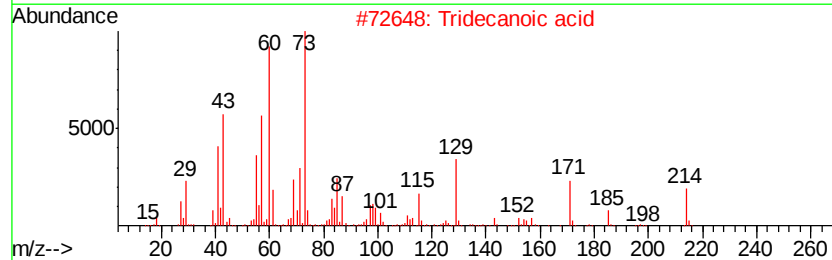
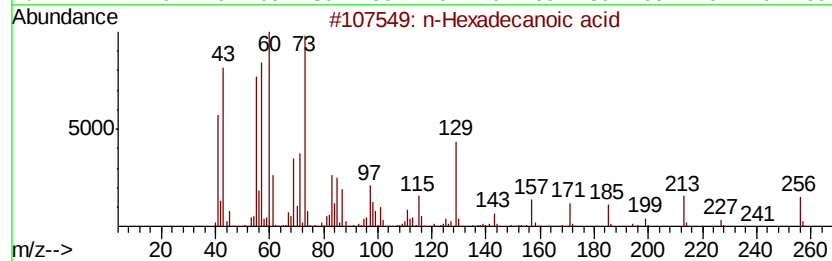
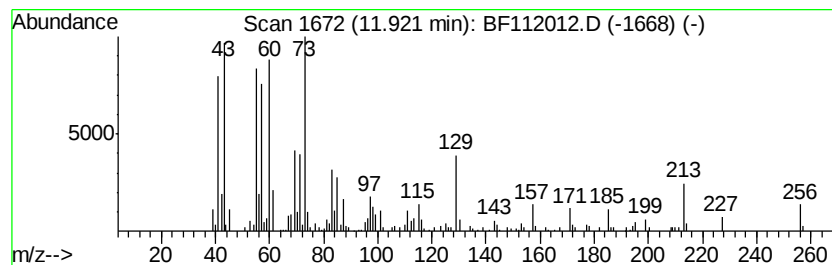
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	4.46 ng	195311	Phenanthrene-d10	11.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		n-Decanoic acid	172	C10H20O2	000334-48-5	62



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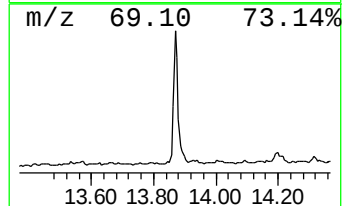
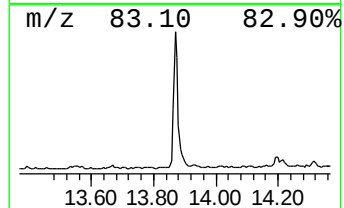
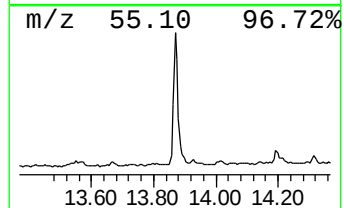
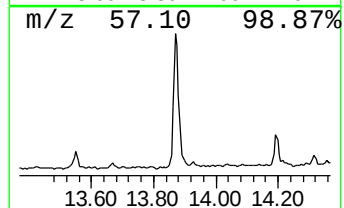
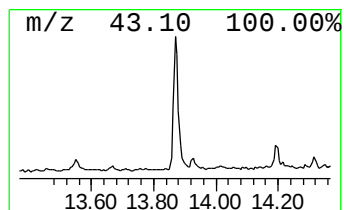
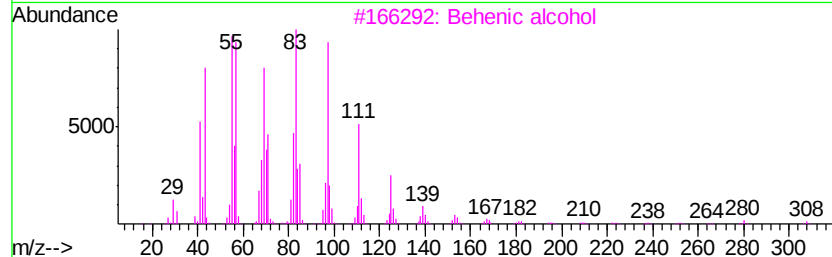
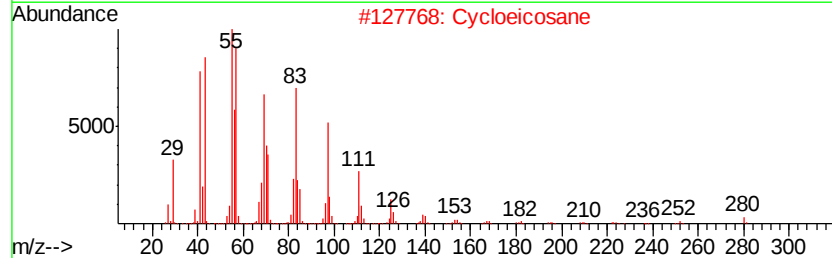
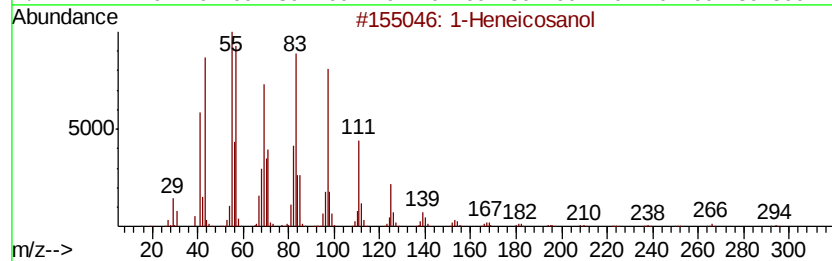
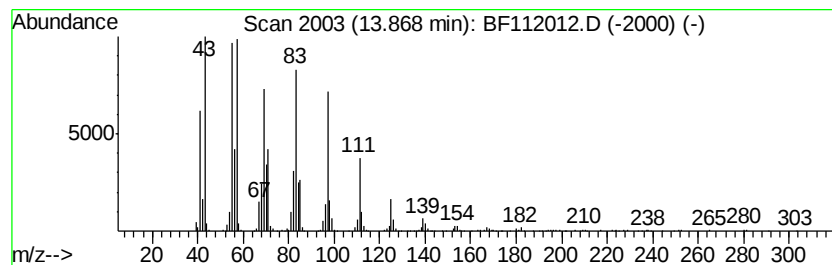
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ClientSampleId :
CPSB-13(15-20)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	24.10 ng	1154030	Chrysene-d12	14.04
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Heneicosanol	312 C21H44O	015594-90-8 95
2		Cycloeicosane	280 C20H40	000296-56-0 95
3		Behenic alcohol	326 C22H46O	000661-19-8 94
4		1-Heptacosanol	396 C27H56O	002004-39-9 91
5		Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1 91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011119\
Data File : BF112012.D
Acq On : 11 Jan 2019 13:52
Operator : JU/SJ
Sample : K1102-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

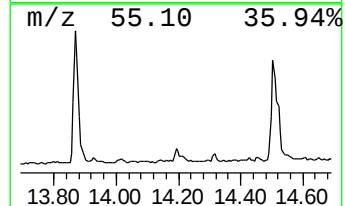
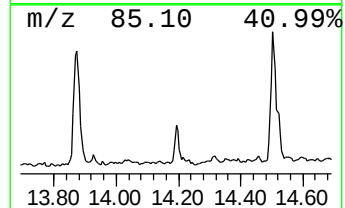
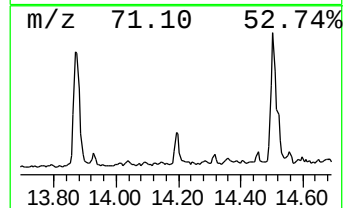
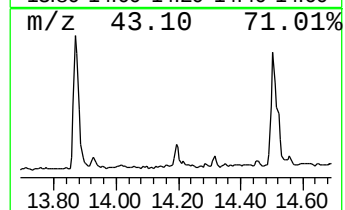
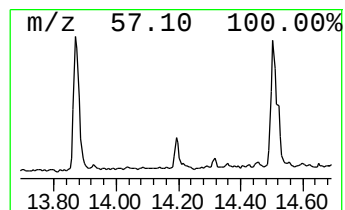
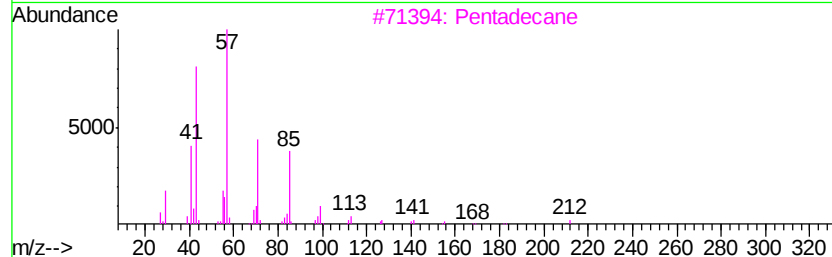
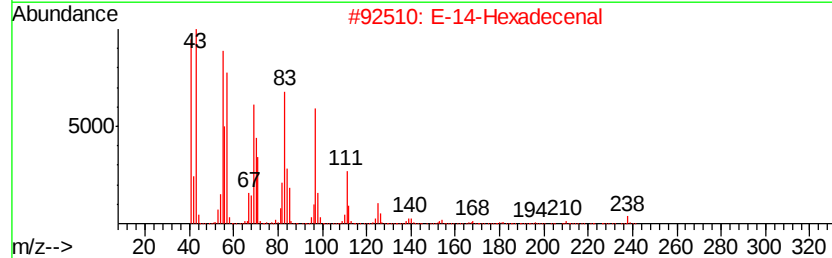
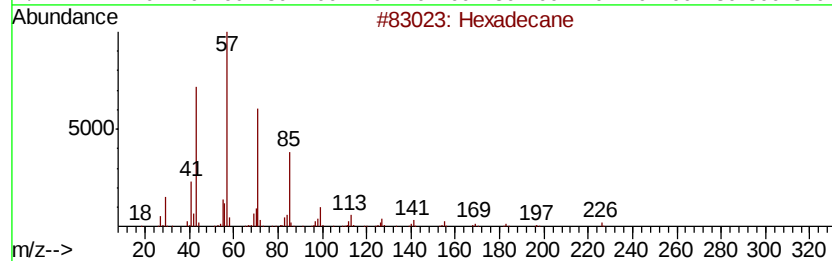
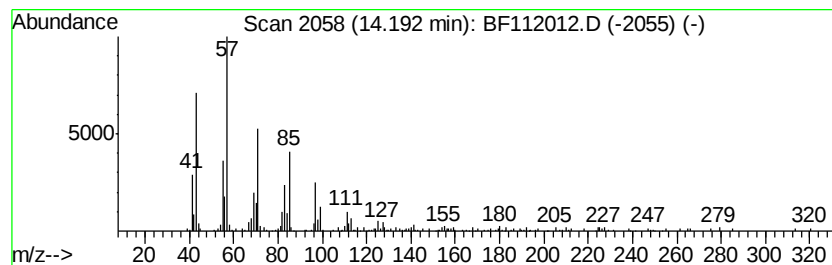
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ClientSampleId :
CPSB-13(15-20)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	4.24 ng	202977	Chrysene-d12	14.04
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	96
2	E-14-Hexadecenal	238 C16H30O	330207-53-9	94
3	Pentadecane	212 C15H32	000629-62-9	92
4	Cetene	224 C16H32	000629-73-2	86
5	Sulfurous acid, butyl hexadecyl ...	362 C20H42O3S	1000309-18-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011119\
Data File : BF112012.D
Acq On : 11 Jan 2019 13:52
Operator : JU/SJ
Sample : K1102-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CPSB-13(15-20)

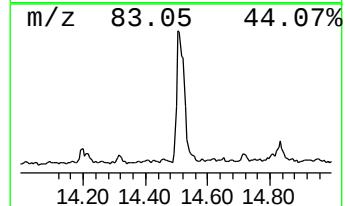
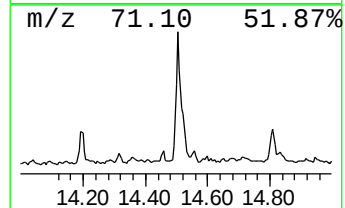
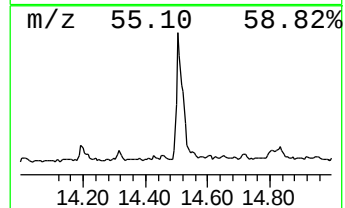
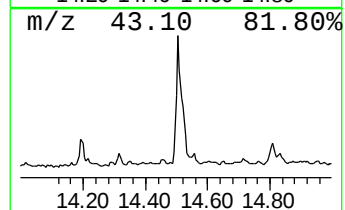
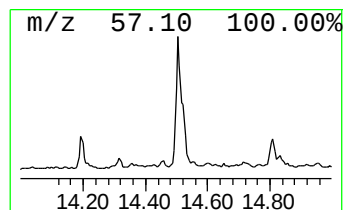
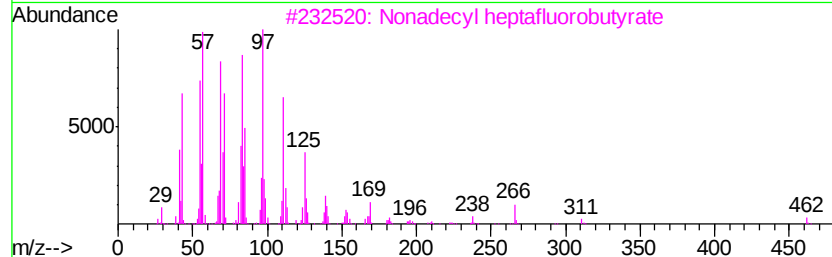
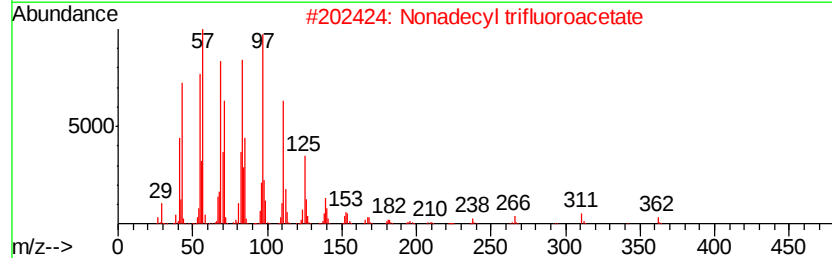
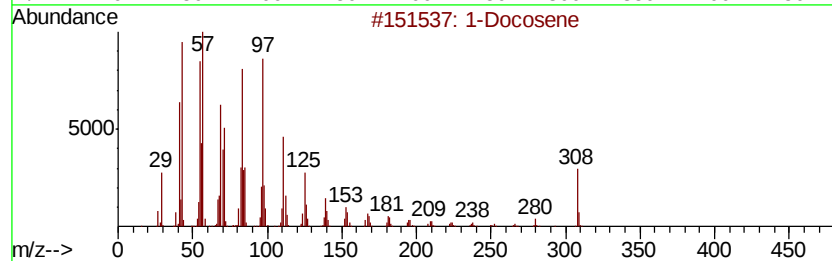
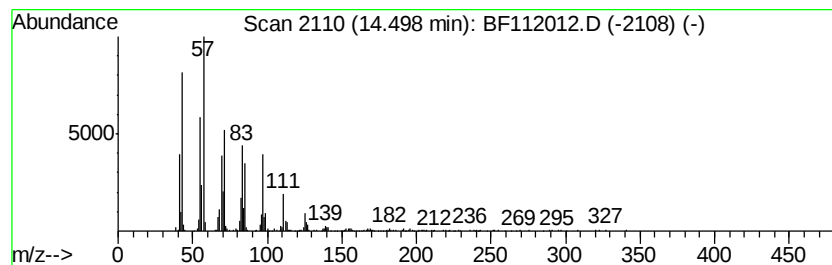
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	25.77 ng	1233940	Chrysene-d12	14.04

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	98
2	Nonadecyl trifluoroacetate		380	C21H39F3O2	1000351-76-3	91
3	Nonadecyl heptafluorobutyrat		480	C23H39F7O2	1000351-83-9	91
4	Heptafluorobutyric acid, n-octad...		466	C22H37F7O2	000400-57-7	91
5	Eicosyl pentafluoropropionate		444	C23H41F5O2	1000351-80-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011119\
Data File : BF112012.D
Acq On : 11 Jan 2019 13:52
Operator : JU/SJ
Sample : K1102-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

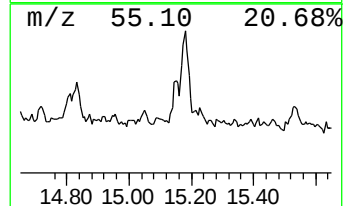
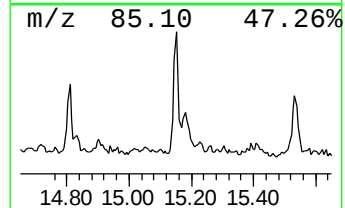
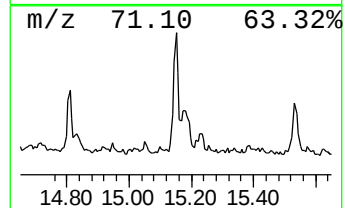
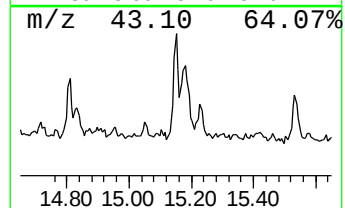
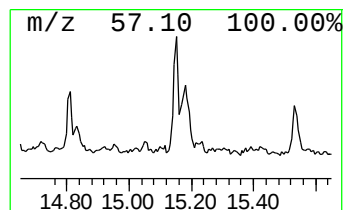
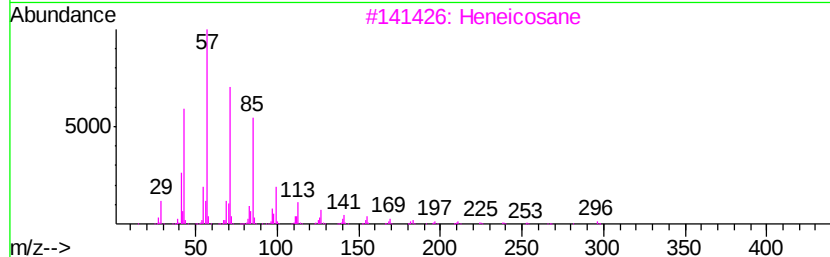
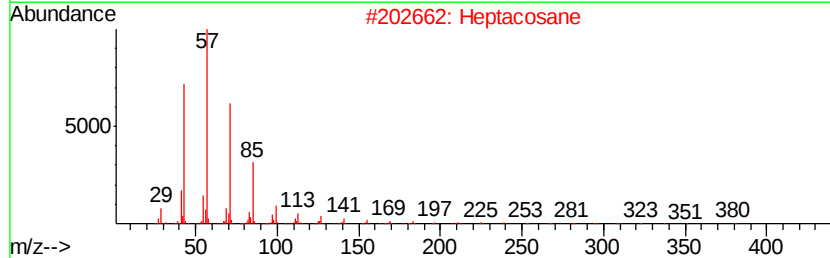
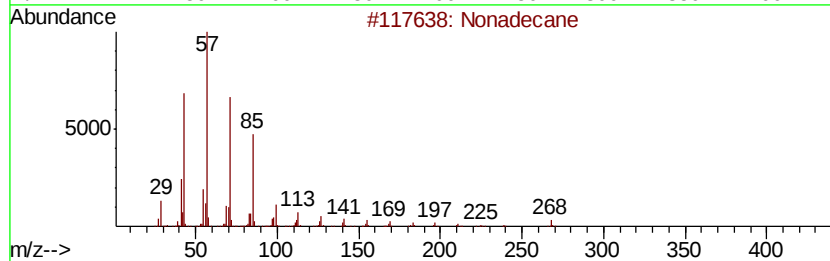
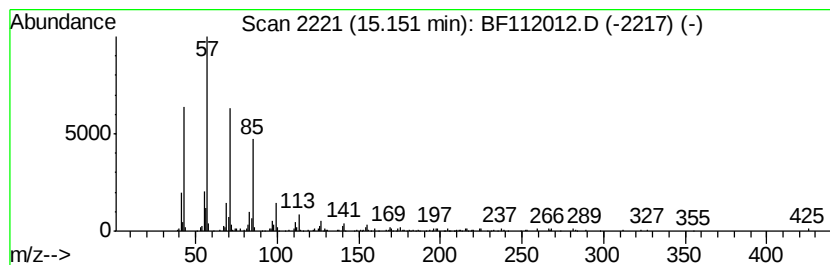
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	4.18 ng	202017	Perylene-d12	15.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonadecane	268	C19H40	000629-92-5 91
2	Heptacosane	380	C27H56	000593-49-7 83
3	Heneicosane	296	C21H44	000629-94-7 81
4	Octadecane	254	C18H38	000593-45-3 80
5	2-Bromo dodecane	248	C12H25Br	013187-99-0 80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011119\
Data File : BF112012.D
Acq On : 11 Jan 2019 13:52
Operator : JU/SJ
Sample : K1102-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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CPSB-13(15-20)

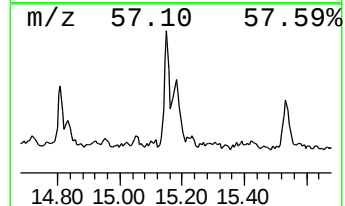
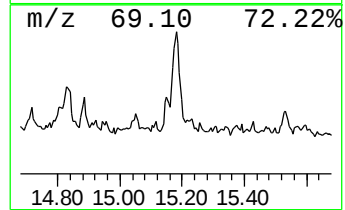
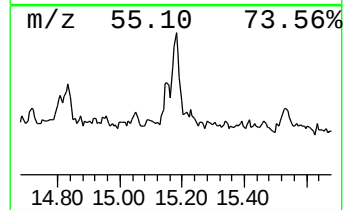
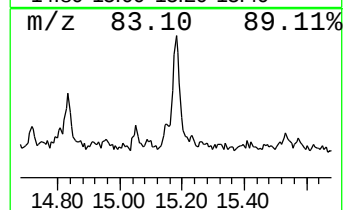
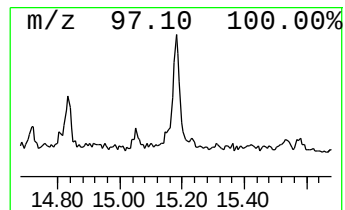
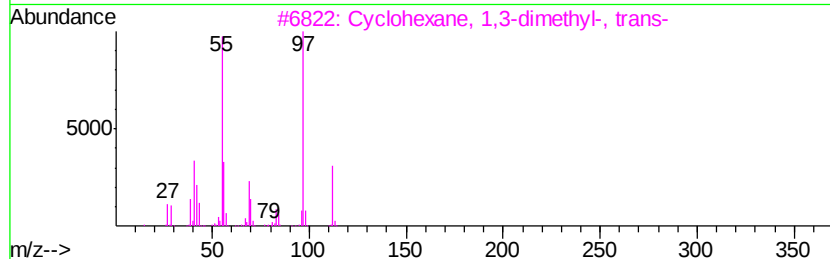
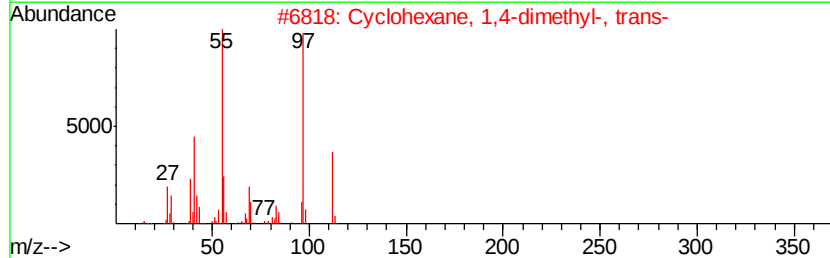
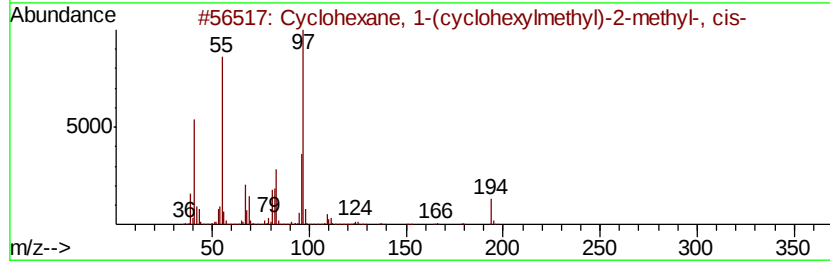
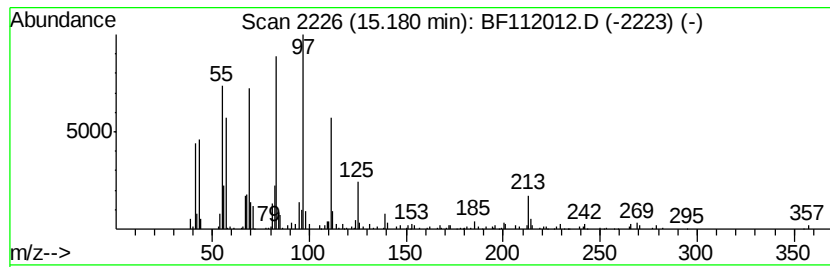
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.18 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	5.83 ng	281570	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-(cyclohexylmethyl)...	194	C14H26	054824-04-3	35
2		Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	30
3		Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	25
4		Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	25
5		Cyclopentane, (1-methylbutyl)-	140	C10H20	004737-43-3	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011119\
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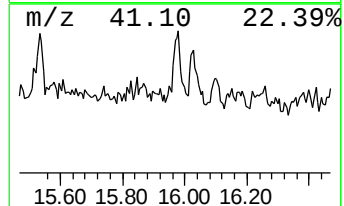
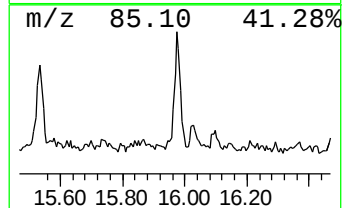
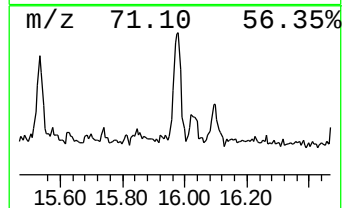
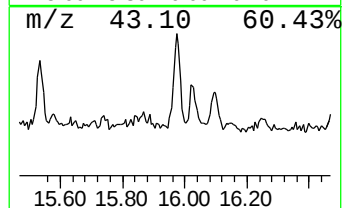
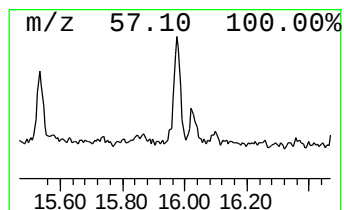
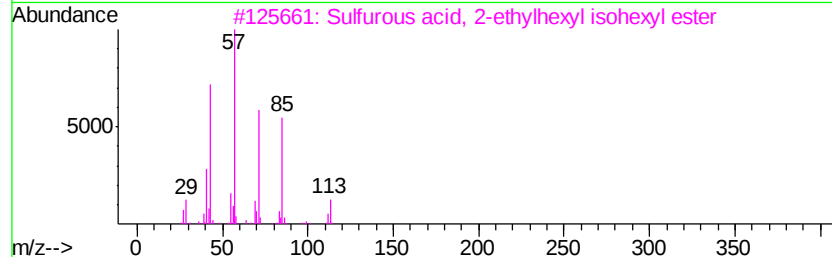
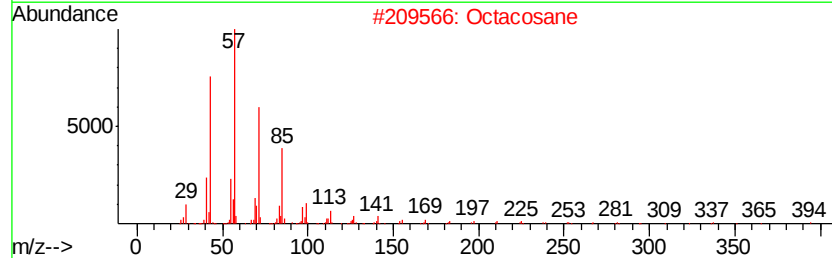
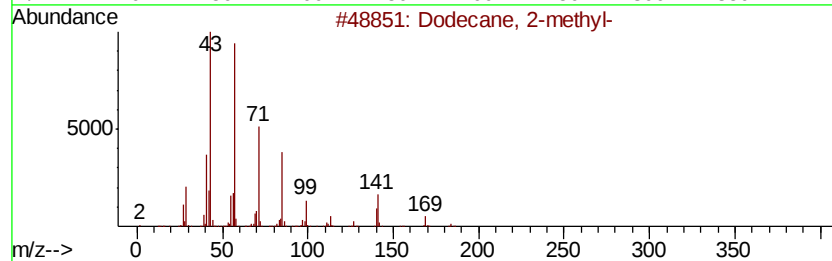
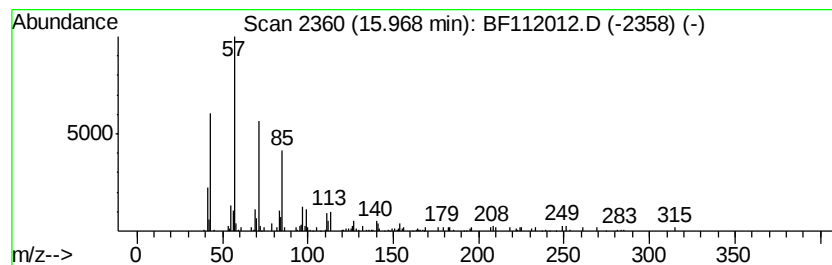
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ClientSampleId :
CPSB-13(15-20)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Dodecane, 2-methyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	3.21 ng	155212	Perylene-d12	15.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Dodecane, 2-methyl-	184 C13H28	001560-97-0	72
2	Octacosane	394 C28H58	000630-02-4	68
3	Sulfurous acid, 2-ethylhexyl iso...	278 C14H30O3S	1000309-19-0	64
4	Sulfurous acid, butyl tetradecyl...	334 C18H38O3S	1000309-18-1	64
5	Tetracosane	338 C24H50	000646-31-1	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011119\
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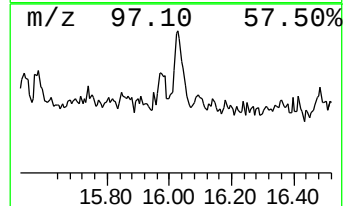
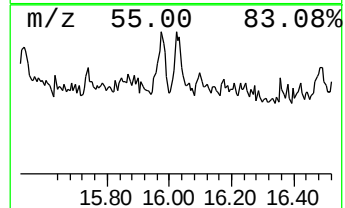
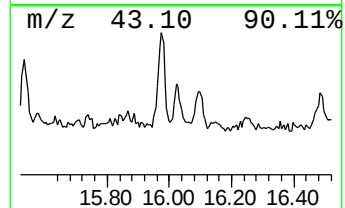
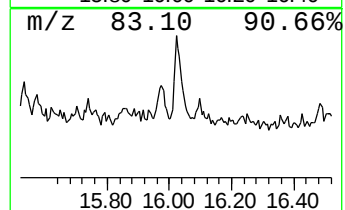
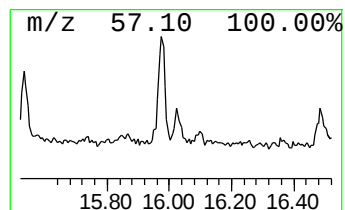
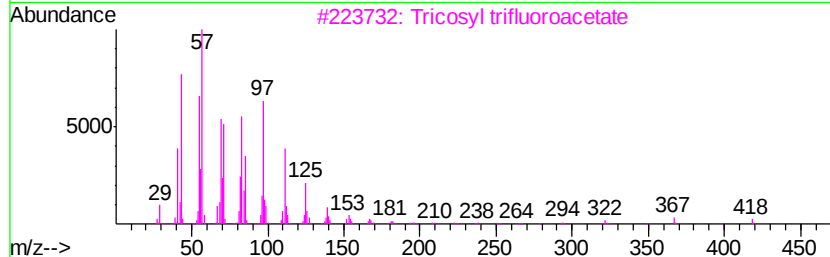
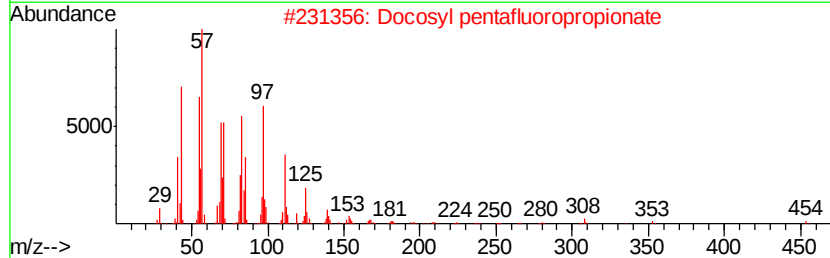
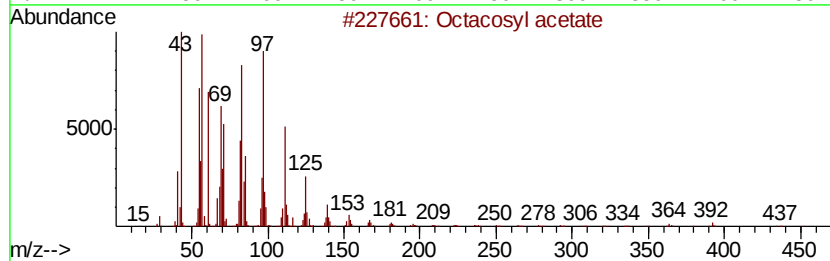
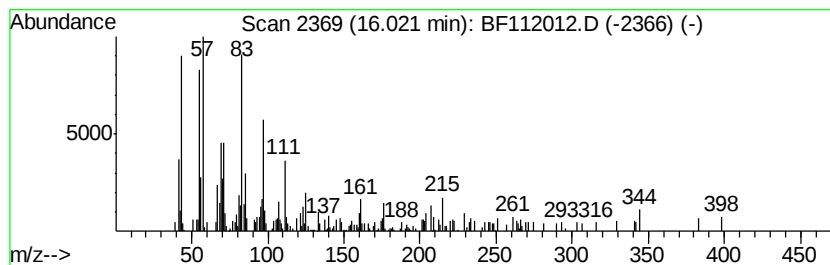
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octacosyl acetate Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	3.28 ng	158156	Perylene-d12	15.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Octacosyl acetate	452 C30H60O2	018206-97-8 62
2		Docosyl pentafluoropropionate	472 C25H45F5O2	1000351-80-9 62
3		Tricosyl trifluoroacetate	436 C25H47F3O2	1000351-75-1 58
4		1-Hexacosene	364 C26H52	018835-33-1 58
5		Tricosyl pentafluoropropionate	486 C26H47F5O2	1000351-81-0 58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011119\
Data File : BF112012.D
Acq On : 11 Jan 2019 13:52
Operator : JU/SJ
Sample : K1102-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CPSB-13(15-20)

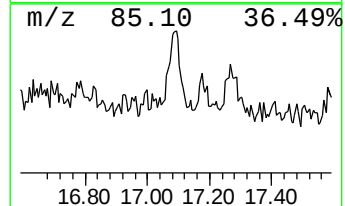
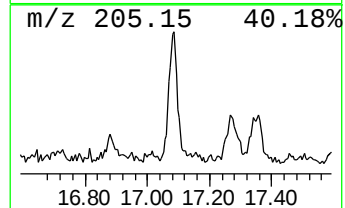
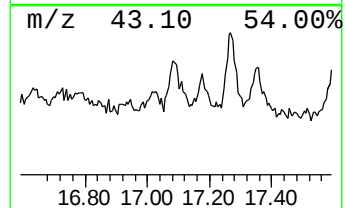
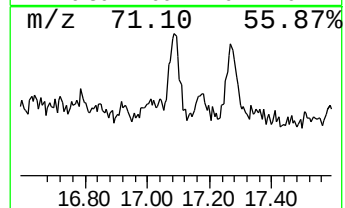
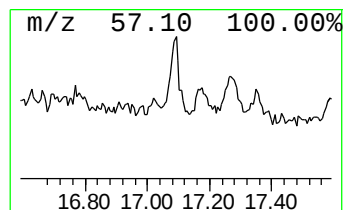
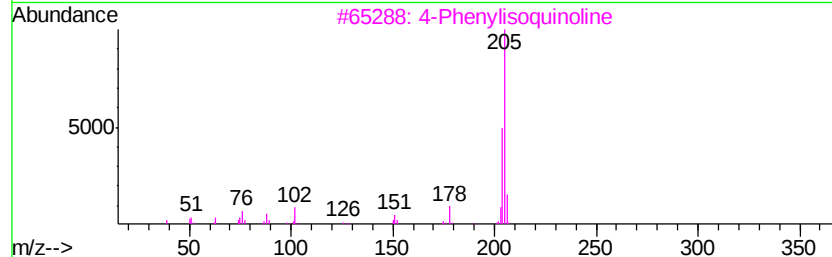
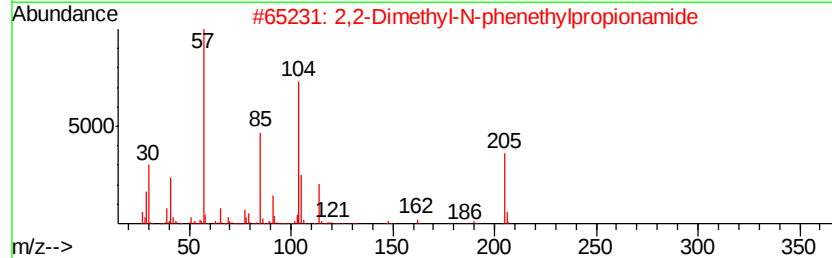
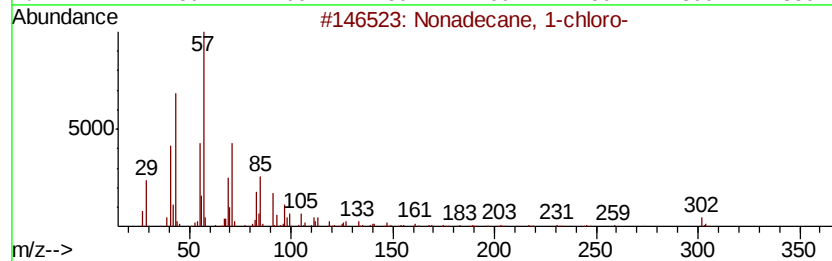
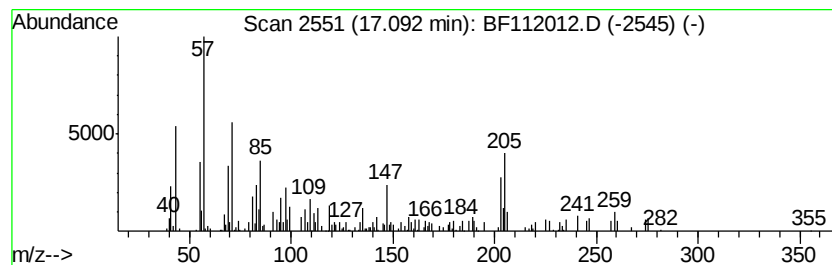
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.09 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.09	3.71 ng	179131	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	44
2		2,2-Dimethyl-N-phenethylpropionam...	205	C13H19NO	062056-54-6	18
3		4-Phenylisoquinoline	205	C15H11N	019571-30-3	18
4		Chromone, 3-methyl-7-nitro-	205	C10H7NO4	253668-57-4	18
5		4H-Benzo[def]carbazole, 4-methyl-	205	C15H11N	084819-26-1	18



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011119\
Data File : BF112012.D
Acq On : 11 Jan 2019 13:52
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Sample : K1102-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

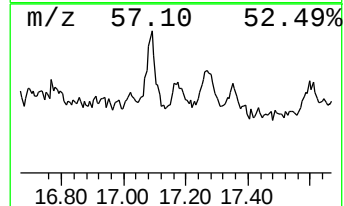
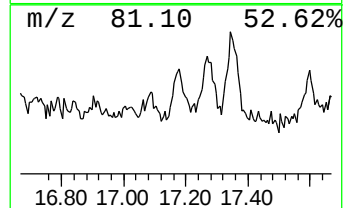
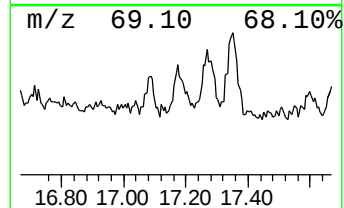
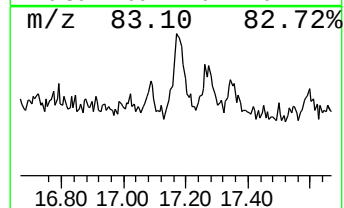
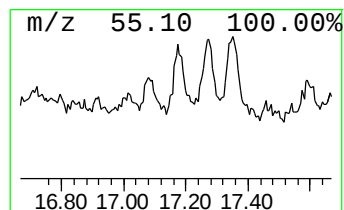
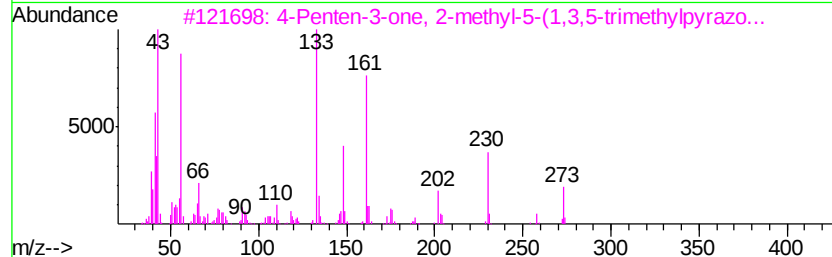
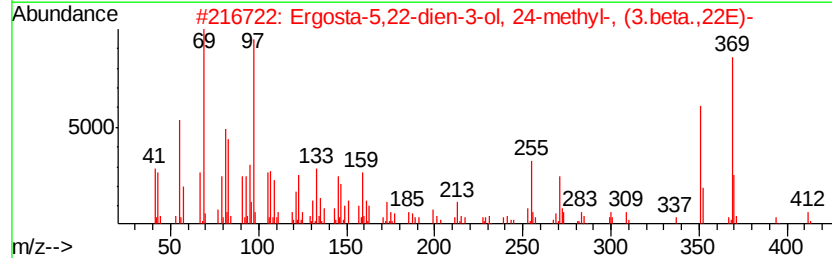
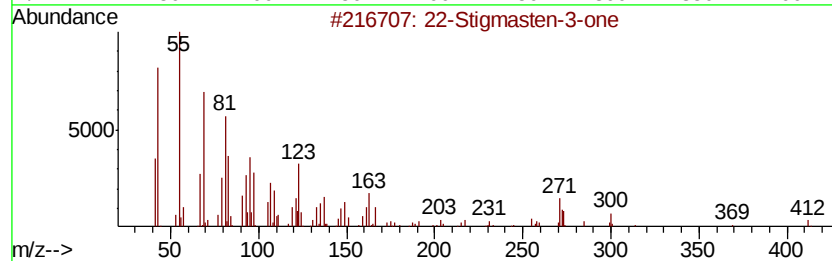
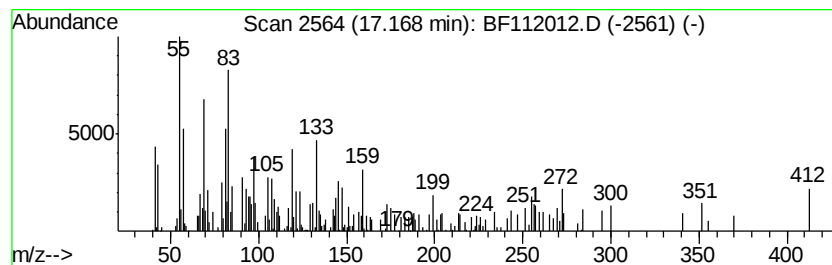
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ClientSampleId :
CPSB-13(15-20)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown17.17 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.17	4.82 ng	232657	Perylene-d12	15.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	22-Stigmasten-3-one	412	C29H48O	004736-95-2 38
2	Ergosta-5,22-dien-3-ol, 24-methy...	412	C29H48O	053755-22-9 12
3	4-Penten-3-one, 2-methyl-5-(1,3,...	273	C14H19N5O	312311-98-1 9
4	Benzeneacetamide, .alpha.-cyano-...	256	C14H12N2OS	1000337-17-1 9
5	Kaur-16-ene, (8.beta.,13.beta.)-	272	C20H32	020070-61-5 9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011119\
Data File : BF112012.D
Acq On : 11 Jan 2019 13:52
Operator : JU/SJ
Sample : K1102-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CPSB-13(15-20)

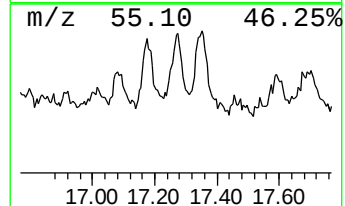
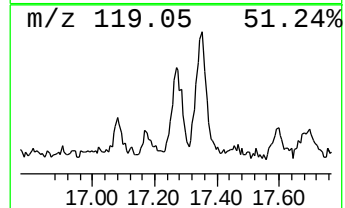
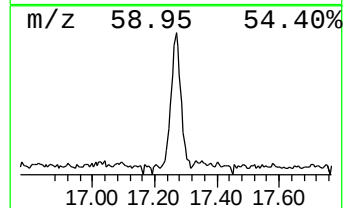
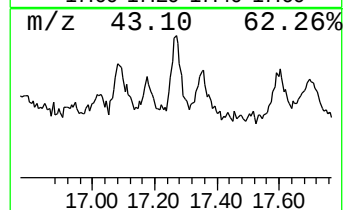
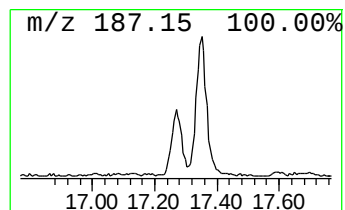
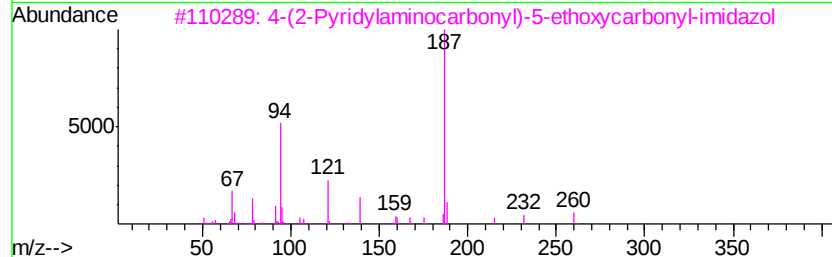
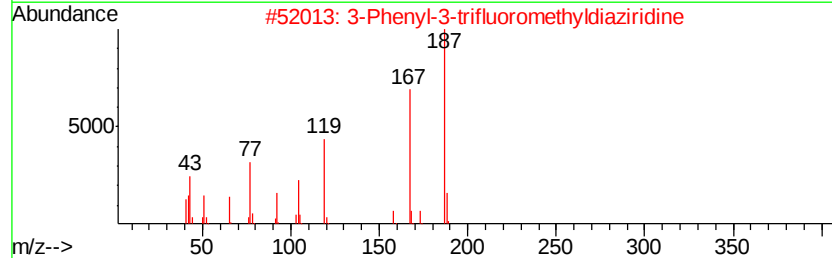
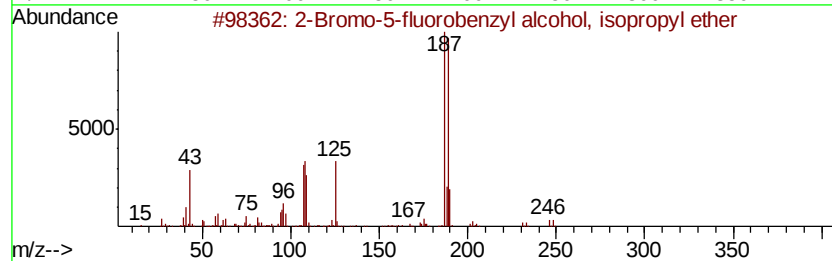
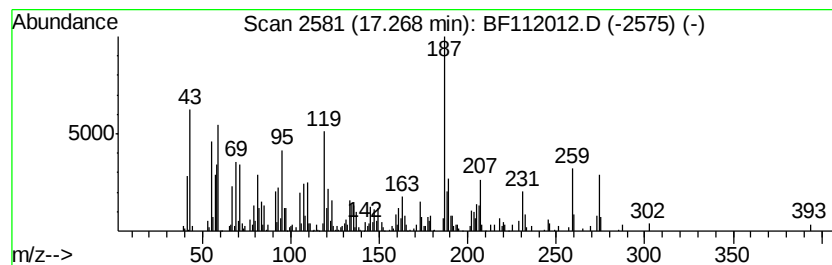
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown17.27 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.27	10.12 ng	488537	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Bromo-5-fluorobenzyl alcohol, ...	246	C10H12BrFO	1000375-22-8	38
2		3-Phenyl-3-trifluoromethylidiazir...	188	C8H7F3N2	040618-96-0	25
3		4-(2-Pyridylaminocarbonyl)-5-eth...	260	C12H12N4O3	312758-82-0	18
4		1H-Pyrrole-2,5-dione, 1-(4-methy...	187	C11H9NO2	001631-28-3	14
5		Silane, trimethyl(3-phenyl-1-but...	202	C13H18Si	028129-04-6	12



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011119\
Data File : BF112012.D
Acq On : 11 Jan 2019 13:52
Operator : JU/SJ
Sample : K1102-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CPSB-13(15-20)

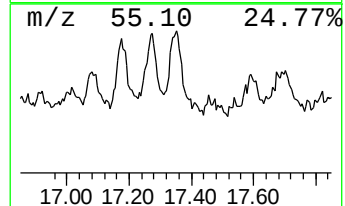
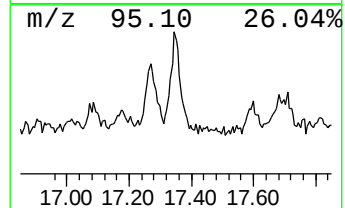
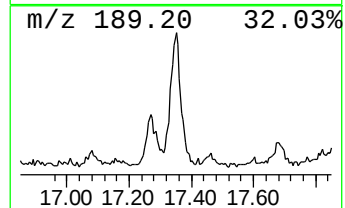
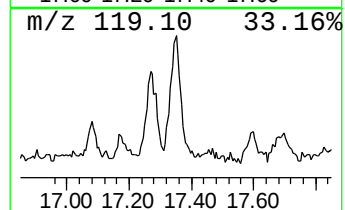
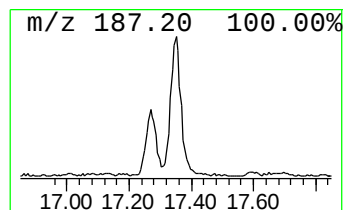
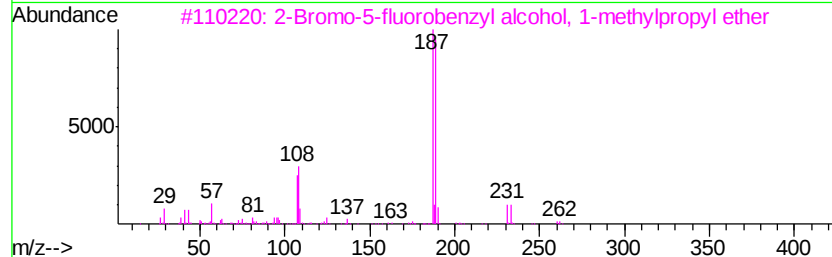
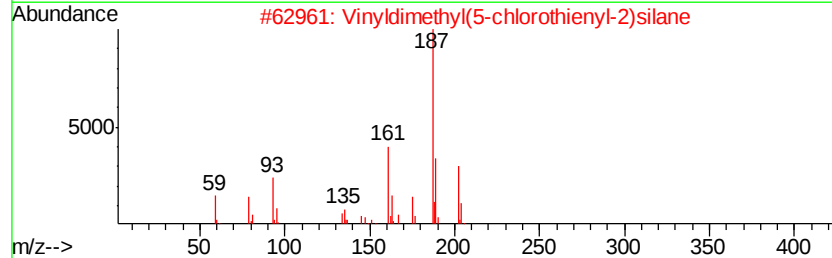
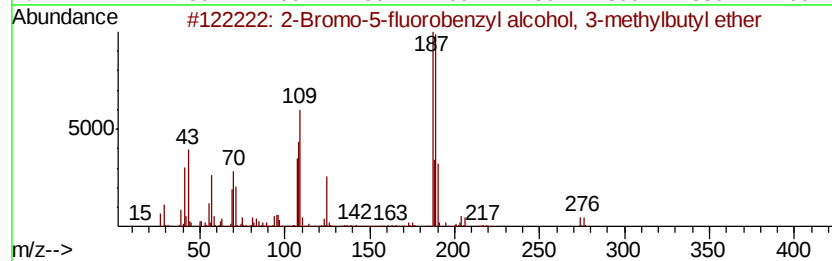
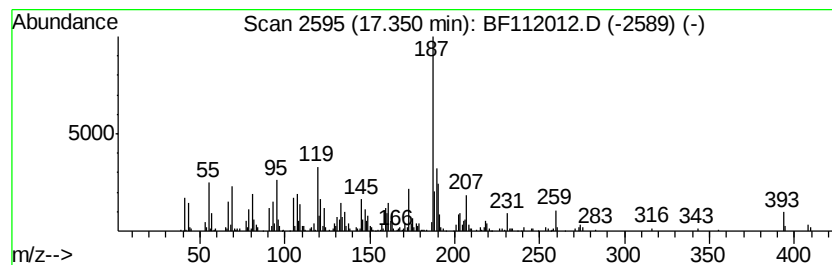
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown17.35 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.35	14.25 ng	688310	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Bromo-5-fluorobenzyl alcohol, ...	274	C12H16BrFO	1000375-22-3	38
2		Vinyl dimethyl(5-chlorothieryl-2)...	202	C8H11ClSSi	180140-41-4	35
3		2-Bromo-5-fluorobenzyl alcohol, ...	260	C11H14BrFO	1000375-22-5	35
4		Phenol, 4-chloro-5-methyl-2-nitro-	187	C7H6ClNO3	007147-89-9	35
5		Pyridine, 4-[3,4-dihydroxyphenyl]-	187	C11H9NO2	079445-43-5	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011119\
 Data File : BF112012.D
 Acq On : 11 Jan 2019 13:52
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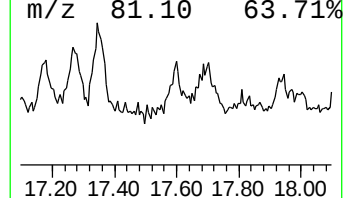
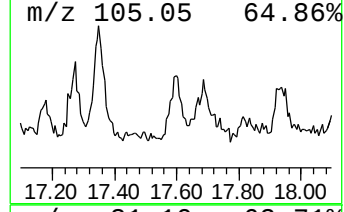
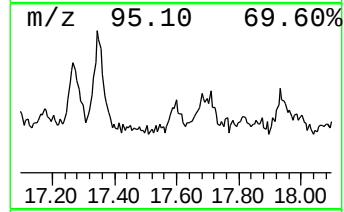
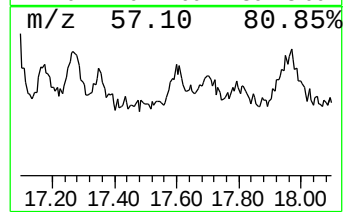
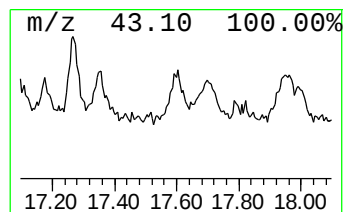
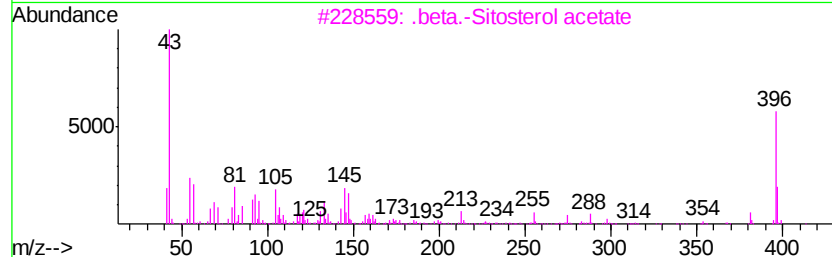
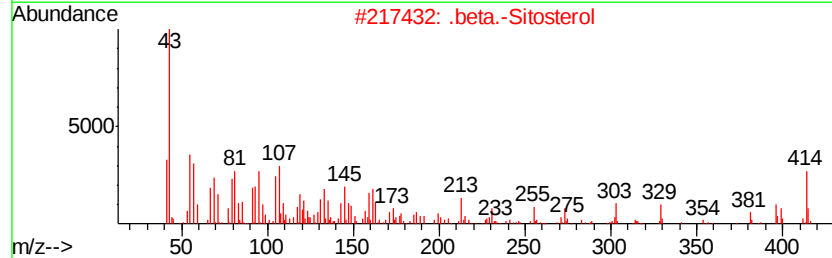
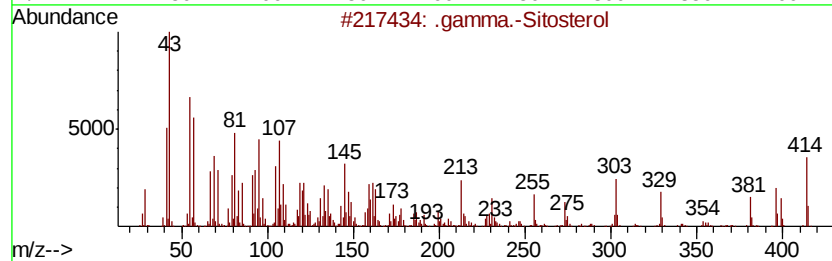
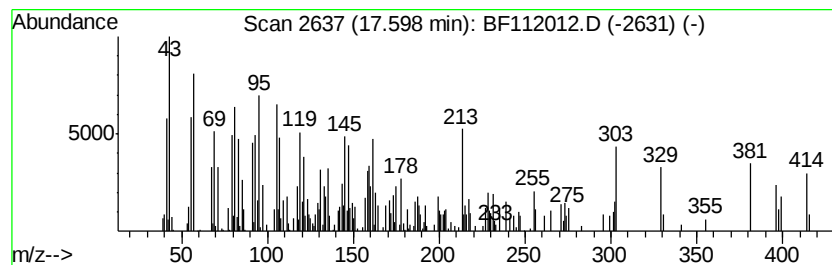
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 17 .gamma.-Sitosterol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.60	5.77 ng	278741	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.gamma.-Sitosterol	414	C29H50O	000083-47-6	64
2		.beta.-Sitosterol	414	C29H50O	000083-46-5	30
3		.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	27
4		Stigmastan-3,5-diene	396	C29H48	1000214-16-4	27
5		Cholest-7-en-3-ol, 4,4-dimethyl-...	414	C29H50O	006384-28-7	15



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011119\
Data File : BF112012.D
Acq On : 11 Jan 2019 13:52
Operator : JU/SJ
Sample : K1102-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CPSB-13(15-20)

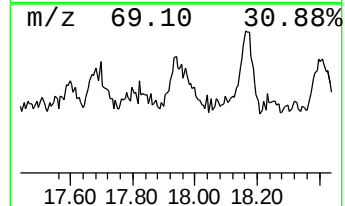
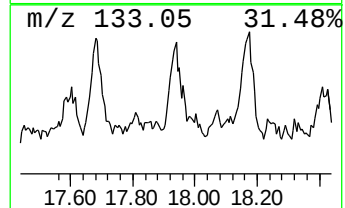
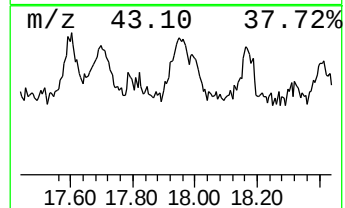
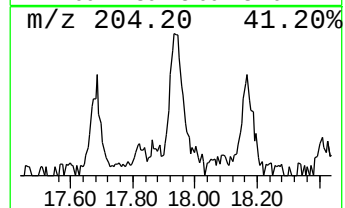
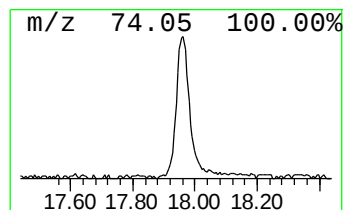
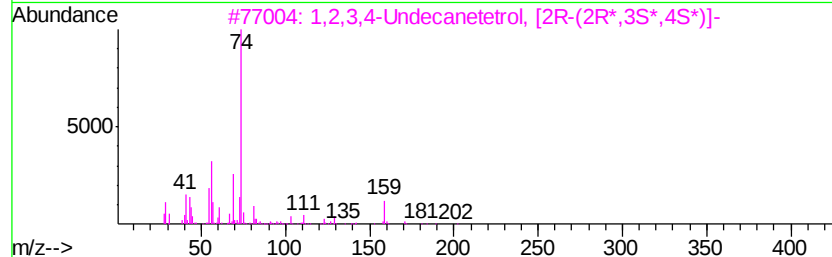
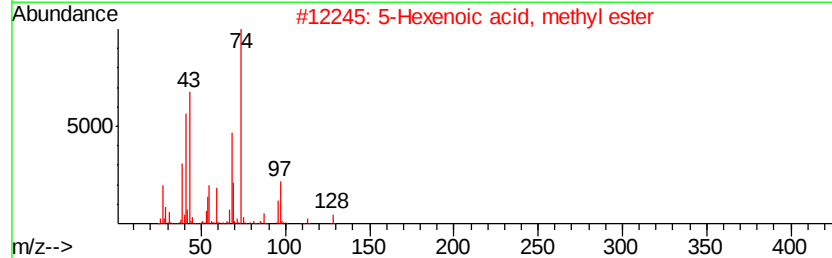
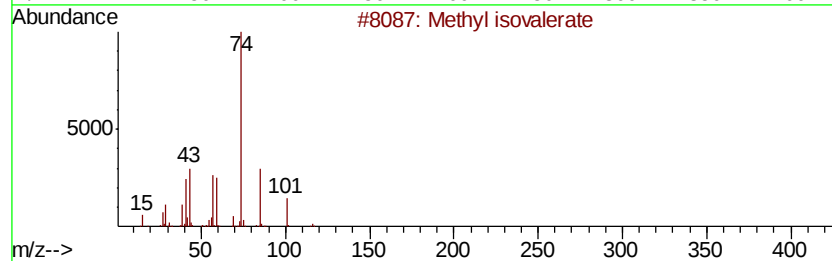
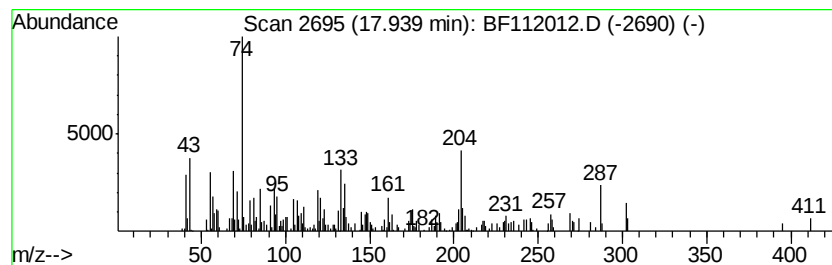
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown17.94 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.94	6.65 ng	321290	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl isovalerate	116	C6H12O2	000556-24-1	37
2		5-Hexenoic acid, methyl ester	128	C7H12O2	002396-80-7	35
3		1,2,3,4-Undecanetetrol, [2R-(2R*...	220	C11H24O4	137036-71-6	35
4		1,2,3,4-Dodecanetetrol, [2R-(2R*...	234	C12H26O4	136953-02-1	35
5		Octanoic acid, 2-methyl-	158	C9H18O2	003004-93-1	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011119\
Data File : BF112012.D
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Operator : JU/SJ
Sample : K1102-06
Misc :
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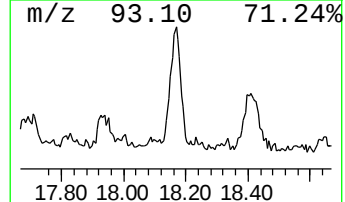
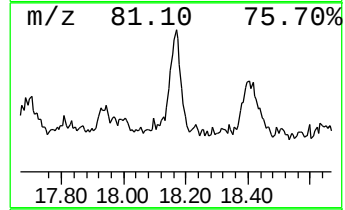
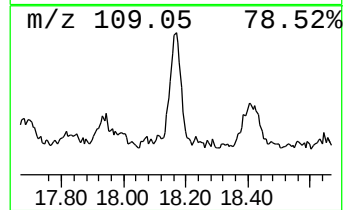
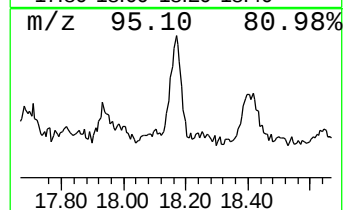
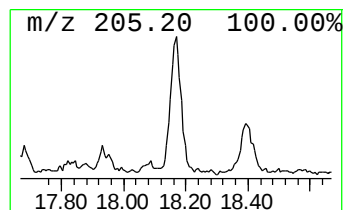
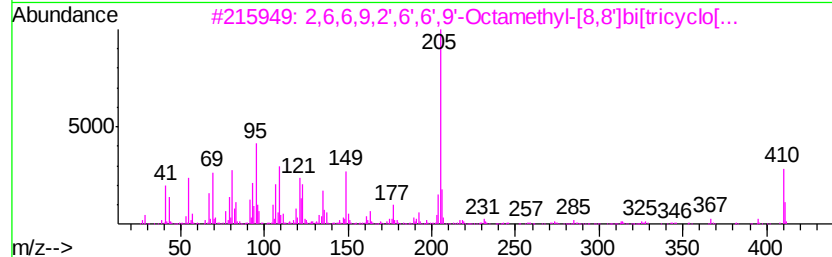
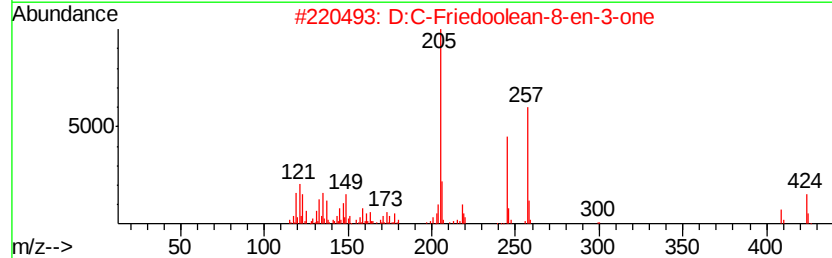
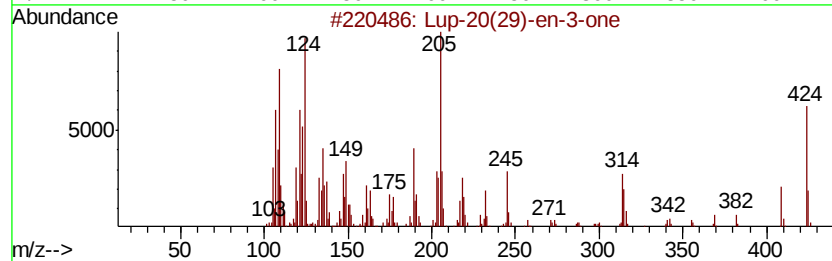
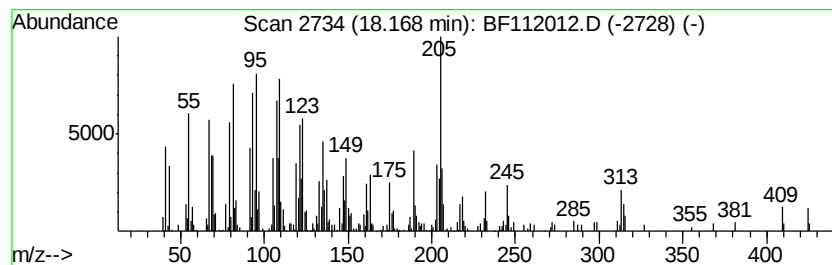
Instrument :
BNA_F
ClientSampleId :
CPSB-13(15-20)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Lup-20(29)-en-3-one Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.17	12.89 ng	622531	Perylene-d12	15.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Lup-20(29)-en-3-one	424 C30H48O	001617-70-5 91
2		D:C-Friedoolean-8-en-3-one	424 C30H48O	022611-26-3 62
3		2,6,6,9,2',6',6',9'-Octamethyl-[...]	410 C30H50	1000189-48-2 52
4		1H-Cycloprop[elazulene, 1a,2,3,5...	204 C15H24	021747-46-6 42
5		(5,6-Dihydro-4H-[1,3]thiazin-2-y...	206 C11H14N2S	1000300-96-9 25



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011119\
Data File : BF112012.D
Acq On : 11 Jan 2019 13:52
Operator : JU/SJ
Sample : K1102-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CPSB-13(15-20)

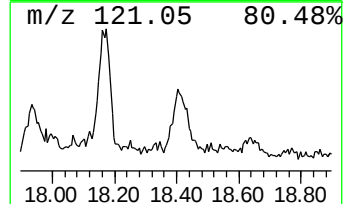
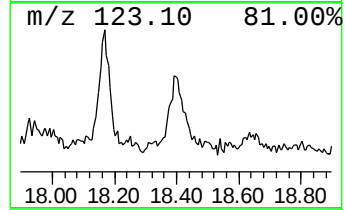
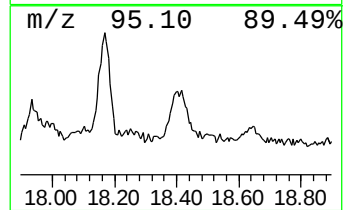
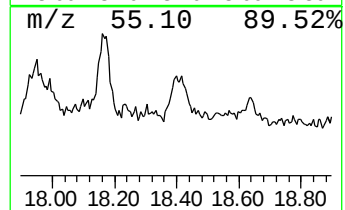
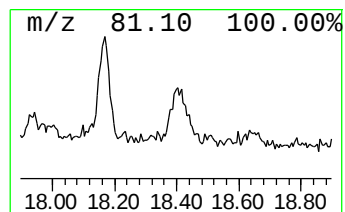
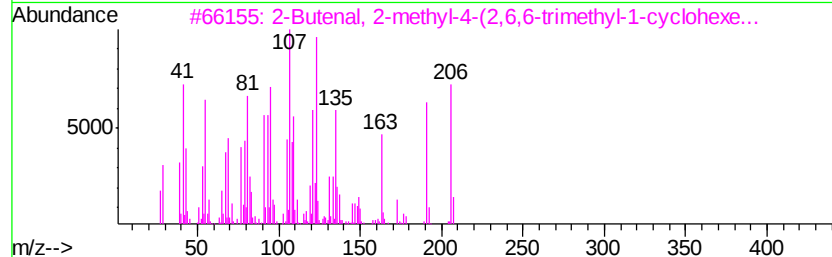
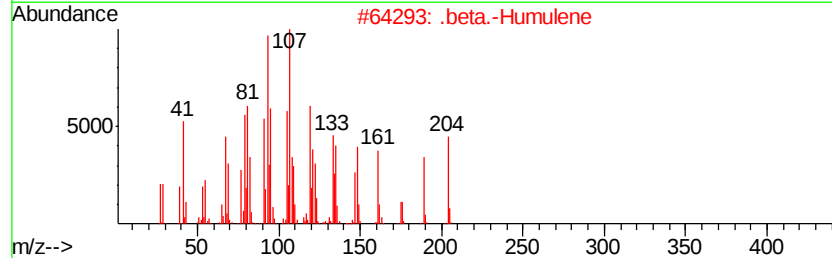
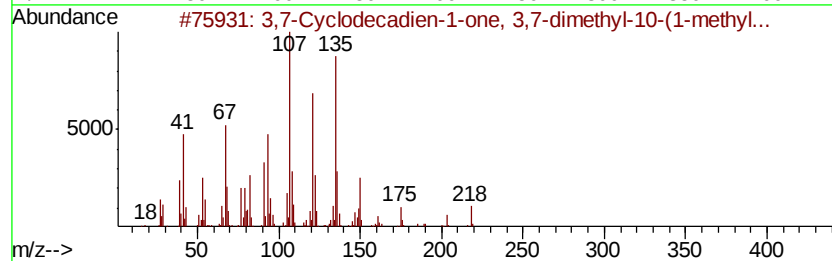
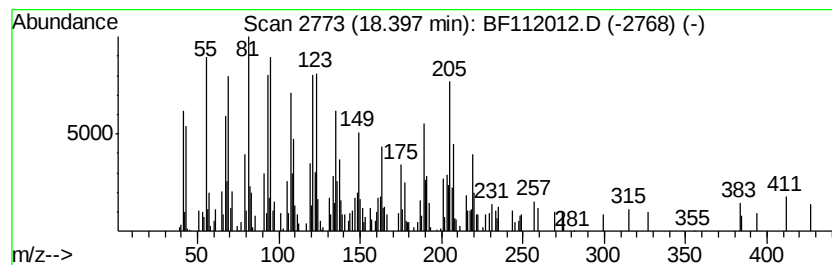
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 3,7-Cyclodecadien-1-one, 3,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.40	8.79 ng	424388	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,7-Cyclodecadien-1-one, 3,7-dim...	218	C15H22O	006902-91-6	64
2		.beta.-Humulene	204	C15H24	000116-04-1	60
3		2-Butenal, 2-methyl-4-(2,6,6-tri...	206	C14H22O	003155-71-3	60
4		2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0	59
5		1,3,3-Trimethyl-2-hydroxymethyl-...	222	C15H26O	1000144-10-7	55



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011119\
 Data File : BF112012.D
 Acq On : 11 Jan 2019 13:52
 Operator : JU/SJ
 Sample : K1102-06
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CPSB-13(15-20)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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
Butane, 2-methoxy...	2.17	3.7	ng	128336	1	6.87	694155	20.0
2-Pentanone, 4-hy...	5.09	4.2	ng	145282	1	6.87	694155	20.0
unknown6.65	6.65	67.0	ng	2324840	1	6.87	694155	20.0
n-Hexadecanoic acid	11.92	4.5	ng	195311	4	11.40	875445	20.0
1-Heneicosanol	13.87	24.1	ng	1154030	5	14.04	957702	20.0
Hexadecane	14.19	4.2	ng	202977	5	14.04	957702	20.0
1-Docosene	14.50	25.8	ng	1233940	5	14.04	957702	20.0
Nonadecane	15.15	4.2	ng	202017	6	15.52	965769	20.0
unknown15.18	15.18	5.8	ng	281570	6	15.52	965769	20.0
Dodecane, 2-methyl-	15.97	3.2	ng	155212	6	15.52	965769	20.0
Octacosyl acetate	16.02	3.3	ng	158156	6	15.52	965769	20.0
unknown17.09	17.09	3.7	ng	179131	6	15.52	965769	20.0
unknown17.17	17.17	4.8	ng	232657	6	15.52	965769	20.0
unknown17.27	17.27	10.1	ng	488537	6	15.52	965769	20.0
unknown17.35	17.35	14.3	ng	688310	6	15.52	965769	20.0
.gamma.-Sitosterol	17.60	5.8	ng	278741	6	15.52	965769	20.0
unknown17.94	17.94	6.7	ng	321290	6	15.52	965769	20.0
Lup-20(29)-en-3-one	18.17	12.9	ng	622531	6	15.52	965769	20.0
3,7-Cyclodecadien...	18.40	8.8	ng	424388	6	15.52	965769	20.0