

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012420\
 Data File : BF118697.D
 Acq On : 24 Jan 2020 20:39
 Operator : CG/JU
 Sample : L1242-14
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20200067-AMENDED-COMP-5

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-BF012020.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	2.140	3	9	15	rBV	1029708	1397550	11.37%	2.711%
2	5.116	500	515	517	rBV	5658374	12288408	100.00%	23.838%
3	5.481	572	577	581	rBV	305405	260711	2.12%	0.506%
4	6.487	743	748	758	rVB3	1350048	1625601	13.23%	3.153%
5	6.863	808	812	816	rBV	1739136	1423851	11.59%	2.762%
6	7.022	835	839	842	rVB	4466010	3677538	29.93%	7.134%
7	7.422	902	907	910	rBV	2962063	2740579	22.30%	5.316%
8	7.575	929	933	937	rBV	2159842	1915891	15.59%	3.717%
9	8.145	1026	1030	1033	rBV	2135708	1766808	14.38%	3.427%
10	9.222	1208	1213	1216	rBV	5029629	4524280	36.82%	8.776%
11	9.416	1243	1246	1250	rVB	148613	146423	1.19%	0.284%
12	9.610	1276	1279	1284	rVB	913750	775681	6.31%	1.505%
13	9.757	1301	1304	1310	rVB	150004	133635	1.09%	0.259%
14	9.898	1322	1328	1331	rBV	2402145	2020330	16.44%	3.919%
15	10.680	1457	1461	1465	rVB2	205444	201140	1.64%	0.390%
16	10.804	1478	1482	1484	rBV	269295	295406	2.40%	0.573%
17	10.898	1495	1498	1502	rVV2	105651	142296	1.16%	0.276%
18	10.998	1510	1515	1517	rVV4	68524	125711	1.02%	0.244%
19	11.045	1520	1523	1526	rVB3	129735	140052	1.14%	0.272%
20	11.239	1553	1556	1561	rBV3	233584	273269	2.22%	0.530%
21	11.380	1576	1580	1583	rBV	2102535	1989999	16.19%	3.860%
22	11.404	1583	1584	1587	rVV	385981	259444	2.11%	0.503%
23	11.457	1590	1593	1596	rVB	192314	162845	1.33%	0.316%
24	11.604	1615	1618	1622	rBV	167379	180056	1.47%	0.349%
25	11.910	1667	1670	1674	rVV2	262595	289514	2.36%	0.562%
26	11.957	1676	1678	1681	rVV2	129152	151960	1.24%	0.295%
27	11.998	1681	1685	1693	rVB2	209390	347421	2.83%	0.674%
28	12.163	1710	1713	1718	rBV2	212573	225074	1.83%	0.437%
29	12.433	1756	1759	1761	rBV	132653	137940	1.12%	0.268%
30	12.592	1783	1786	1790	rBV	482478	427960	3.48%	0.830%
31	12.710	1803	1806	1811	rVB	430326	401448	3.27%	0.779%
32	12.821	1819	1825	1827	rBV	499872	517031	4.21%	1.003%
33	12.963	1845	1849	1853	rVB	4353427	3720420	30.28%	7.217%
34	13.039	1859	1862	1869	rBV4	86874	130171	1.06%	0.253%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.151	1878	1881	1884	rVB	184055	169401	1.38%	0.329%
36	13.216	1889	1892	1895	rVB	177401	147597	1.20%	0.286%
37	13.857	1998	2001	2007	rVB2	458021	472241	3.84%	0.916%
38	14.015	2023	2028	2031	rBV2	1684840	1977864	16.10%	3.837%
39	14.039	2031	2032	2041	rVB	405521	330654	2.69%	0.641%
40	14.492	2106	2109	2112	rVB2	179341	186402	1.52%	0.362%
41	14.792	2158	2160	2164	rBV	145411	139911	1.14%	0.271%
42	14.874	2170	2174	2177	rBV	306625	374315	3.05%	0.726%
43	15.051	2201	2204	2207	rBV	219652	287847	2.34%	0.558%
44	15.133	2215	2218	2220	rBV	173092	174165	1.42%	0.338%
45	15.357	2253	2256	2262	rVB	195354	264852	2.16%	0.514%
46	15.415	2262	2266	2272	rVB	299911	354290	2.88%	0.687%
47	15.480	2272	2277	2281	rBV	1291762	1667123	13.57%	3.234%
48	15.951	2354	2357	2362	rVB	137030	186867	1.52%	0.362%

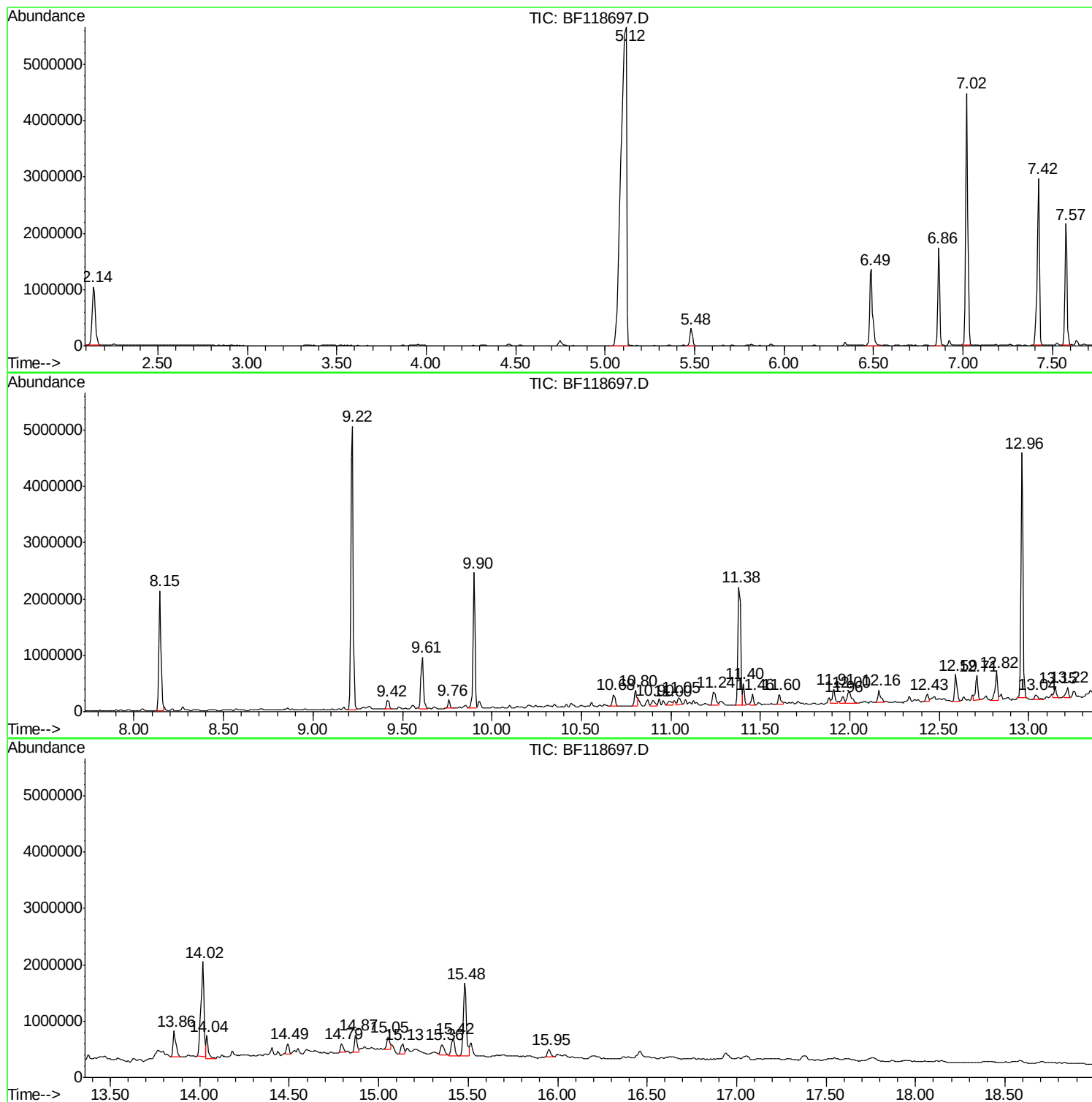
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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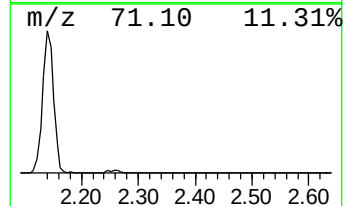
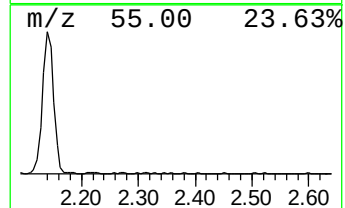
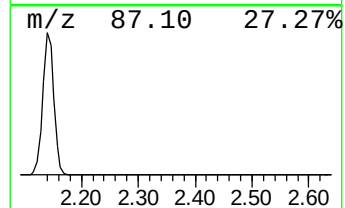
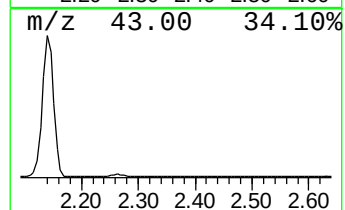
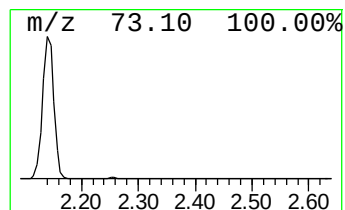
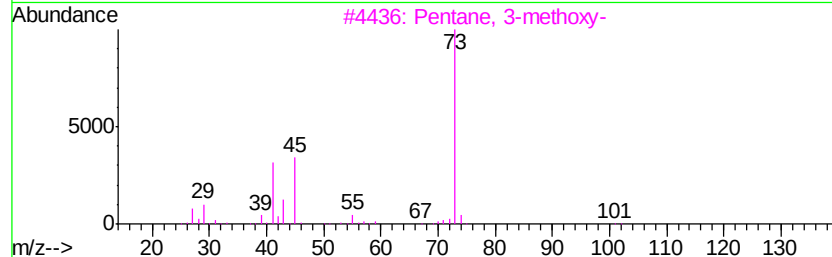
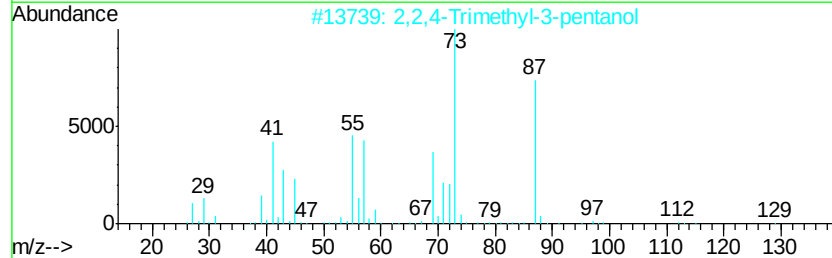
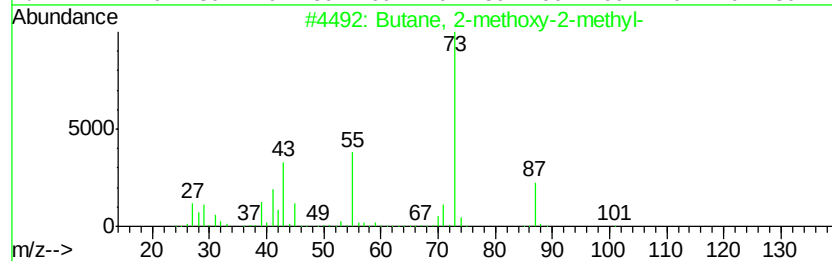
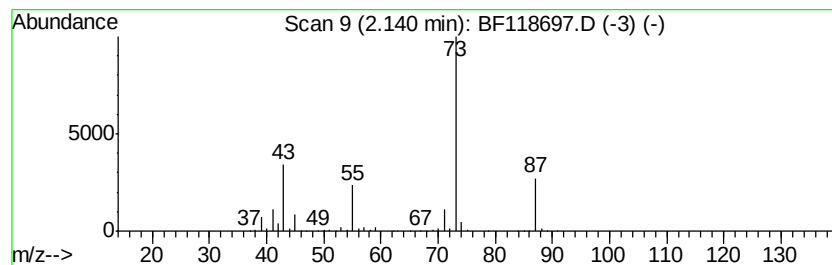
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	19.63 ng	1397550	1,4-Dichlorobenzene-d4	6.86

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	39
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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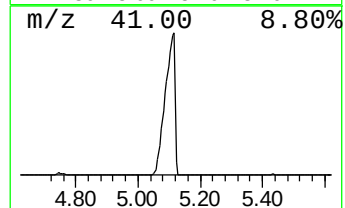
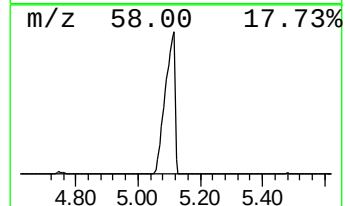
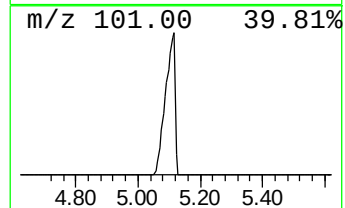
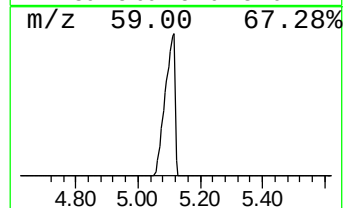
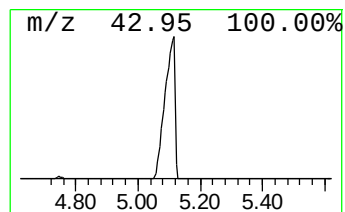
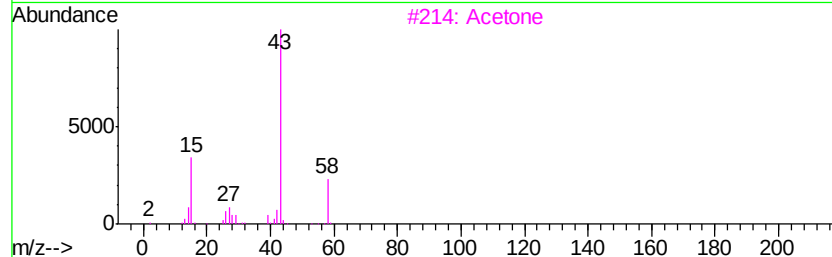
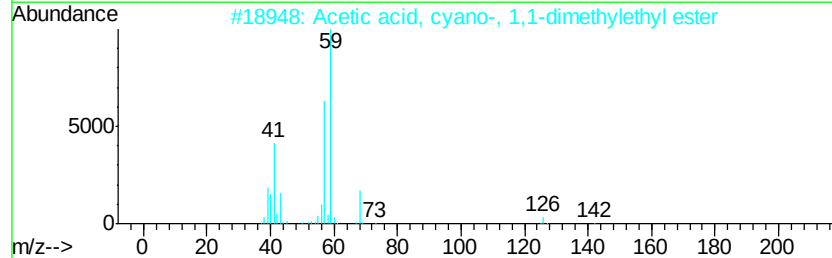
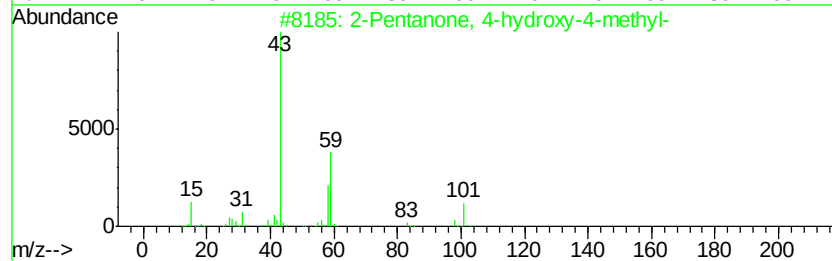
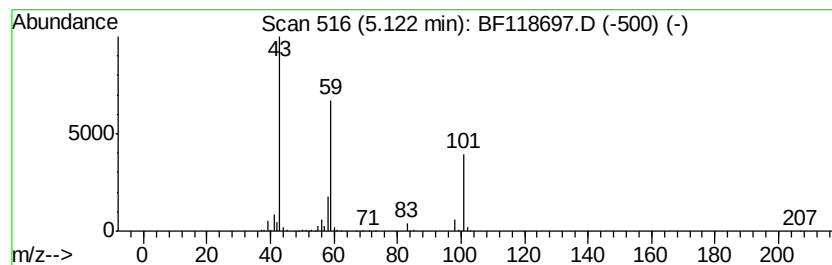
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012020.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	172.61 ng	12288400	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Acetone	58	C3H6O	000067-64-1	10
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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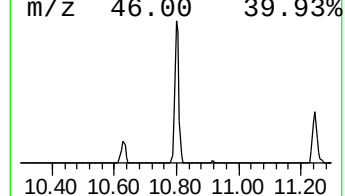
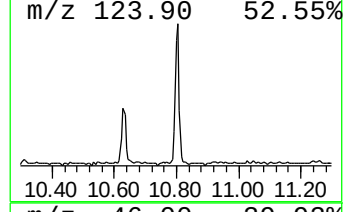
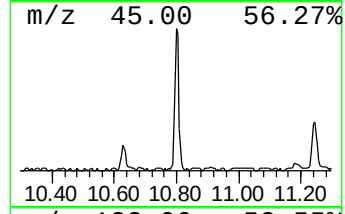
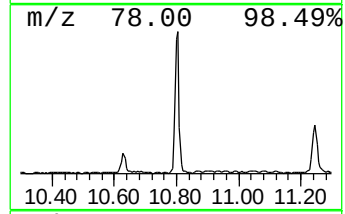
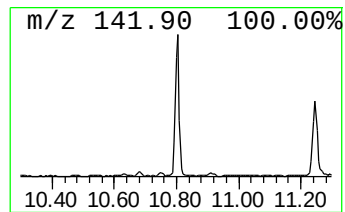
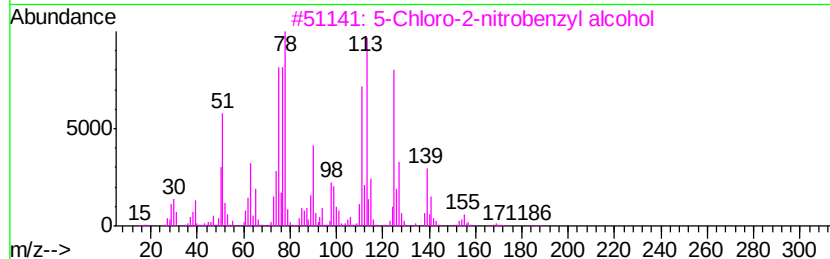
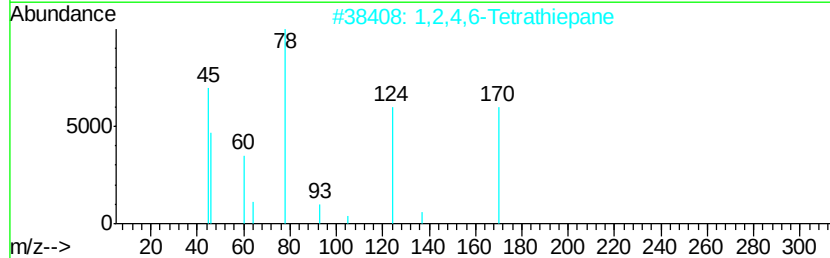
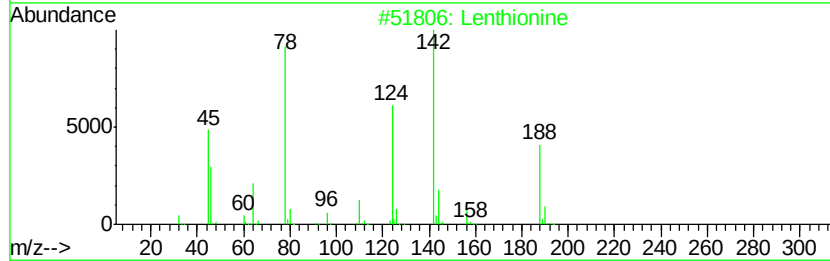
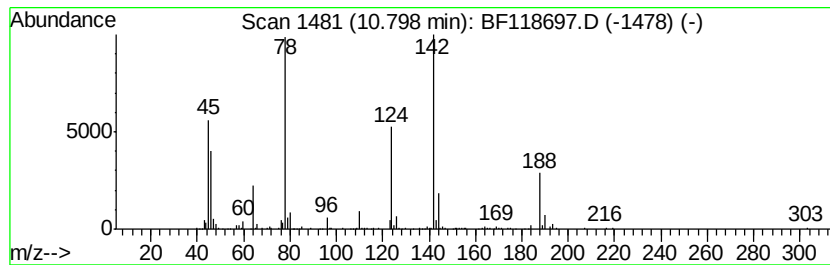
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Lenthionine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	2.97 ng	295406	Phenanthrene-d10	11.38
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Lenthionine	188 C2H4S5	000292-46-6	98
2	1,2,4,6-Tetrathiepane	170 C3H6S4	000292-45-5	38
3	5-Chloro-2-nitrobenzyl alcohol	187 C7H6ClN03	073033-58-6	37
4	Phenylphosphonous acid	142 C6H7O2P	001779-48-2	36
5	7-Oxabicyclo[4.2.1]nona-2,4-dien...	212 C14H12O2	056771-84-7	33



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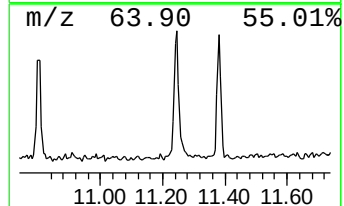
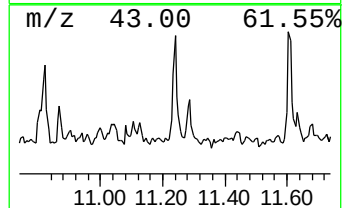
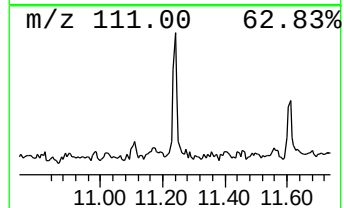
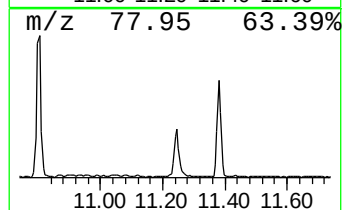
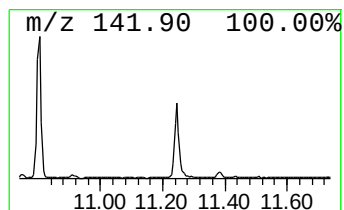
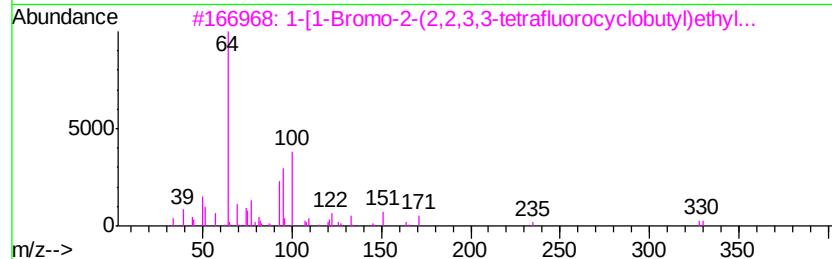
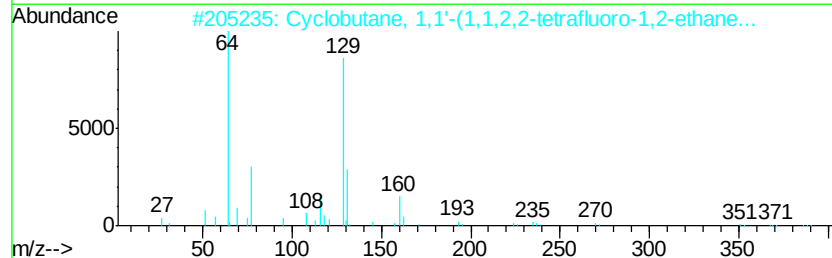
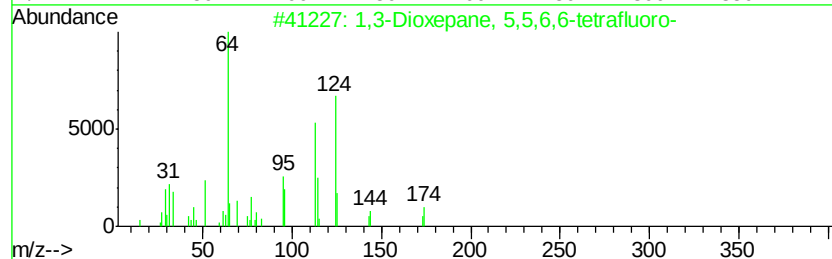
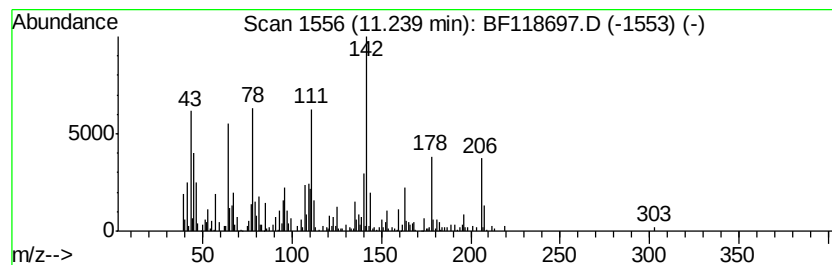
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown11.24 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.24	2.75 ng	273269	Phenanthrene-d10	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxepane, 5,5,6,6-tetrafluoro-	174	C5H6F4O2	001547-52-0	25
2		Cyclobutane, 1,1'-(1,1,2,2-tetra...	386	C10H6Cl2F10	035208-02-7	22
3		1-[1-Bromo-2-(2,2,3,3-tetrafluor...	328	C12H10BrF5	1000223-18-3	12
4		S-2-[3-Succinimidopropylamino]et...	296	C9H16N2O5S2	031701-75-4	12
5		Ethyl Chloride	64	C2H5Cl	000075-00-3	12



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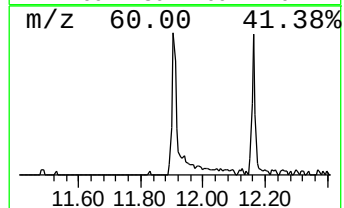
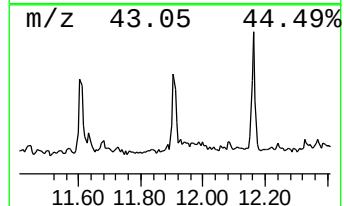
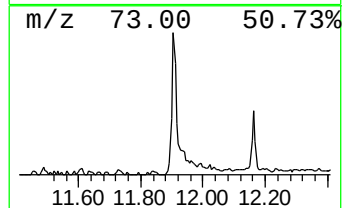
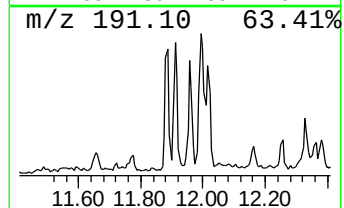
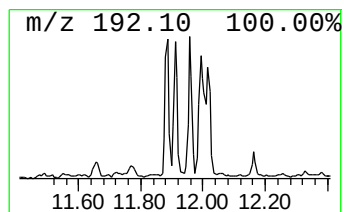
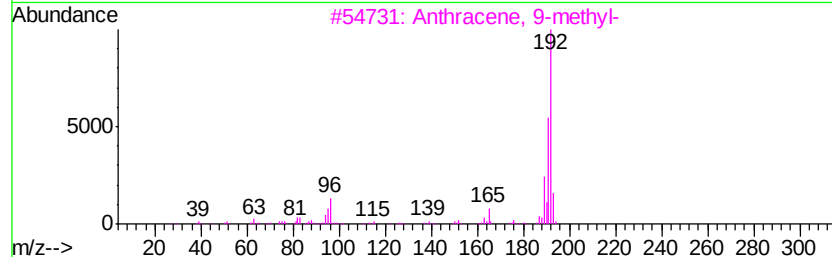
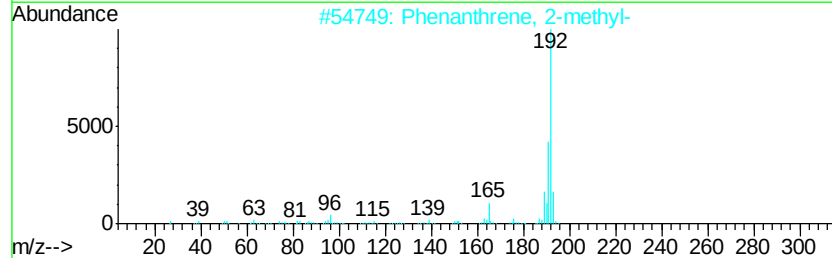
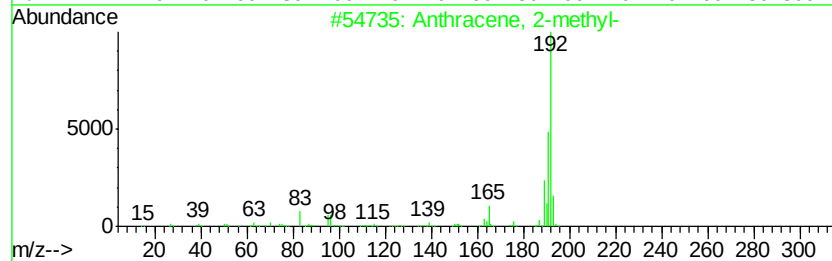
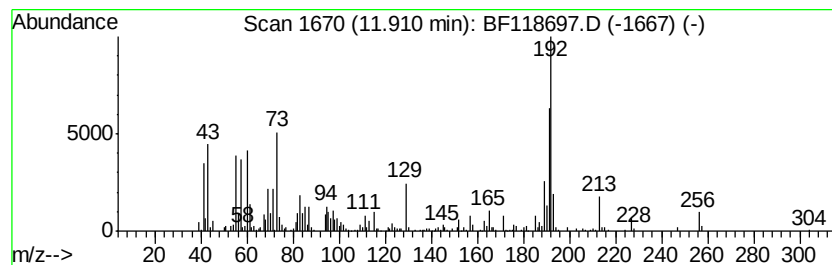
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Anthracene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.91	2.91 ng	289514	Phenanthrene-d10	11.38	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	87
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	70
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	70
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012420\
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Acq On : 24 Jan 2020 20:39
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Sample : L1242-14
Misc :
ALS Vial : 17 Sample Multiplier: 1

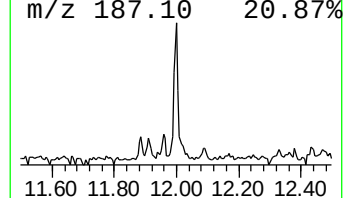
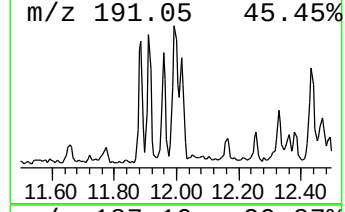
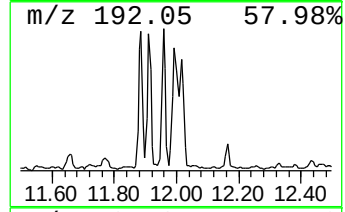
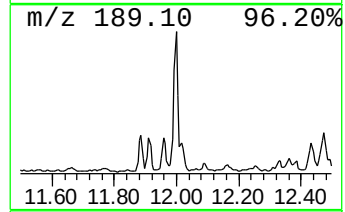
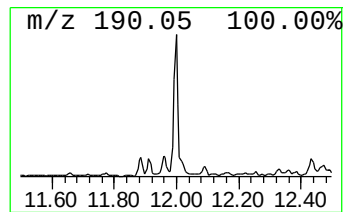
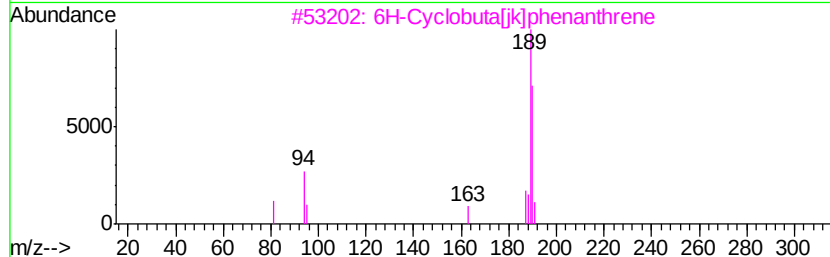
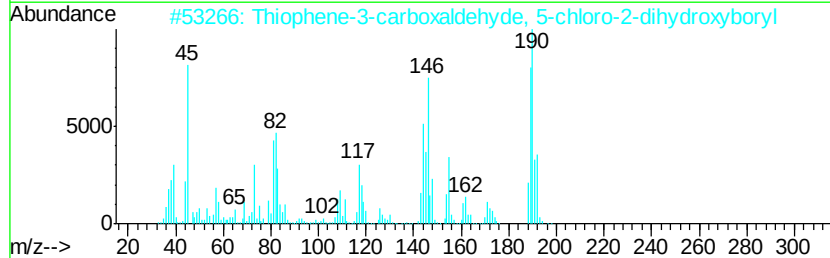
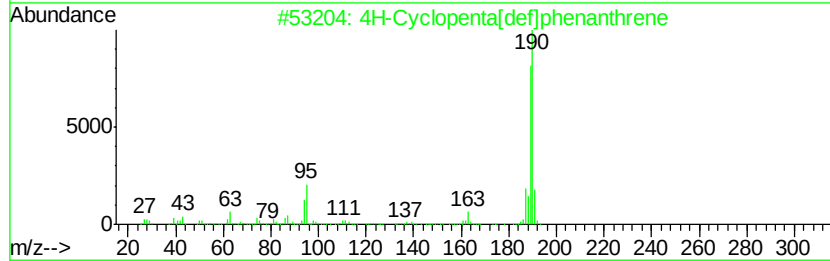
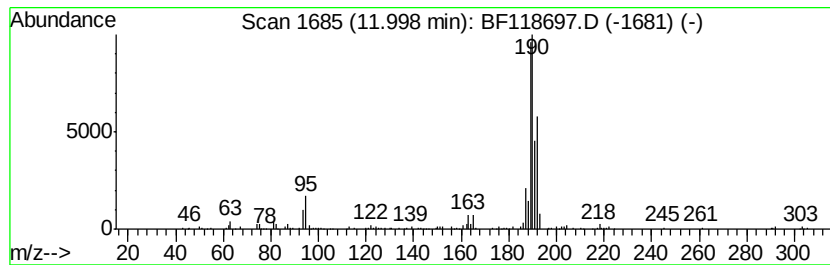
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.00	3.49 ng	347421	Phenanthrene-d10	11.38	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	83
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	53
3	6H-Cyclobuta[f]phenanthrene	190	C15H10	083469-43-6	53
4	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	47
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012420\
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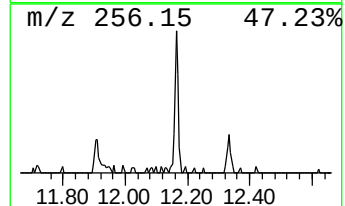
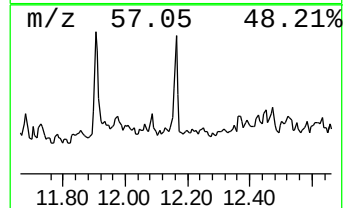
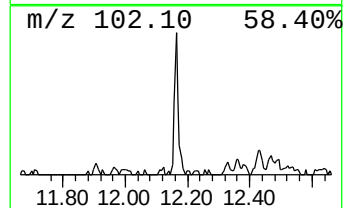
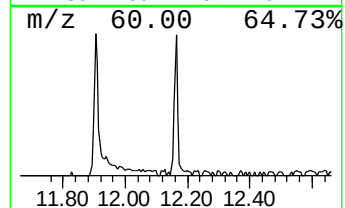
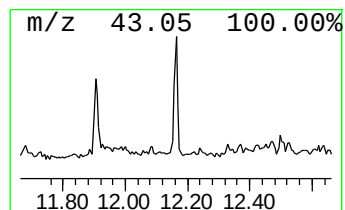
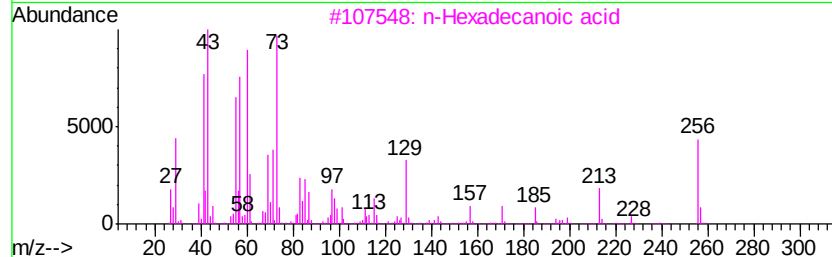
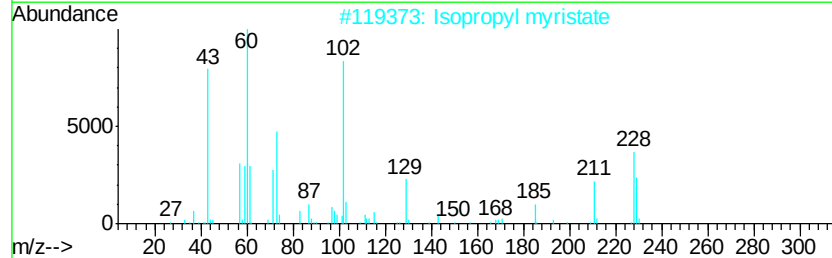
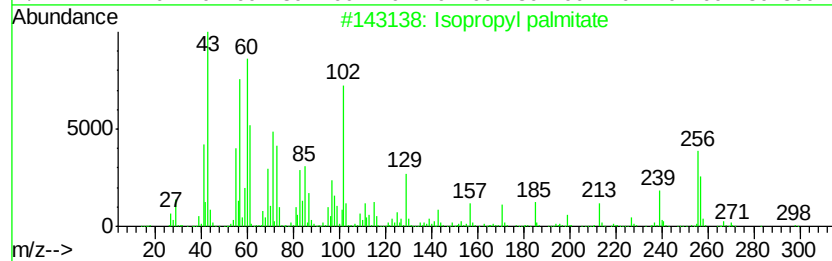
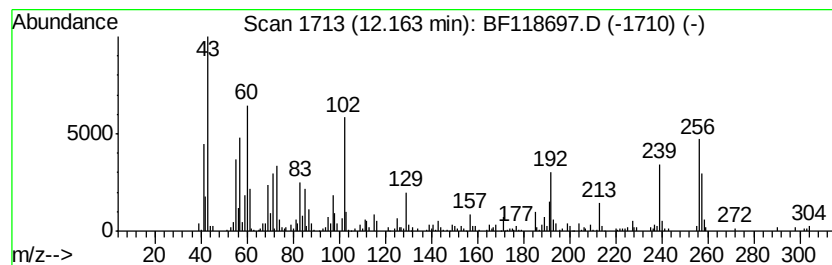
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Isopropyl palmitate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.16	2.26 ng	225074	Phenanthrene-d10		11.38
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl palmitate	298	C19H38O2	000142-91-6	86
2	Isopropyl myristate	270	C17H34O2	000110-27-0	45
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	41
4	Nonadecanoic acid	298	C19H38O2	000646-30-0	38
5	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012420\
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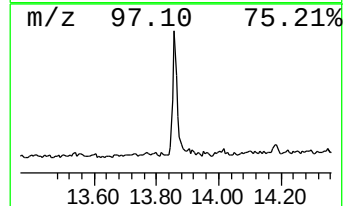
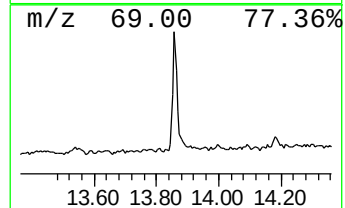
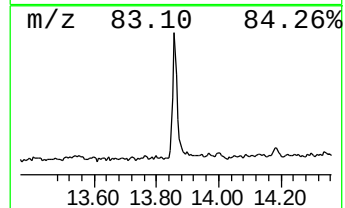
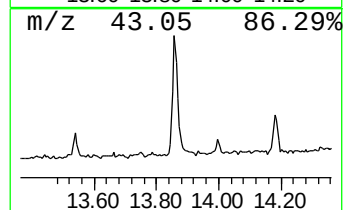
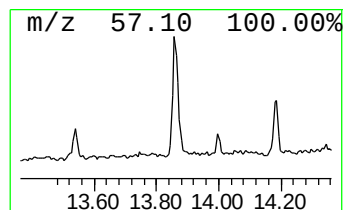
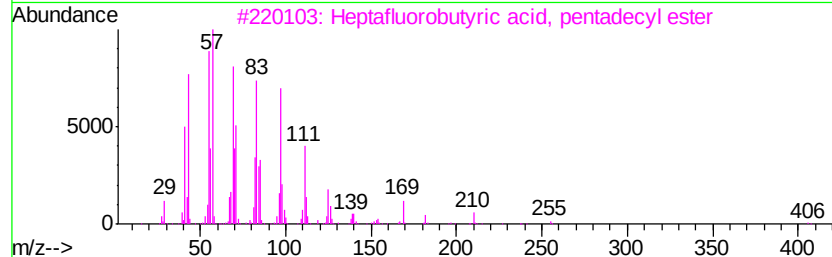
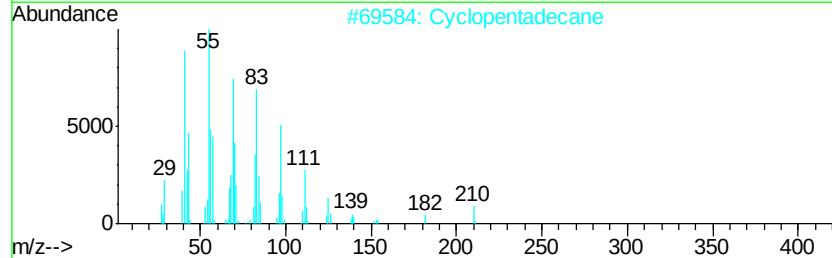
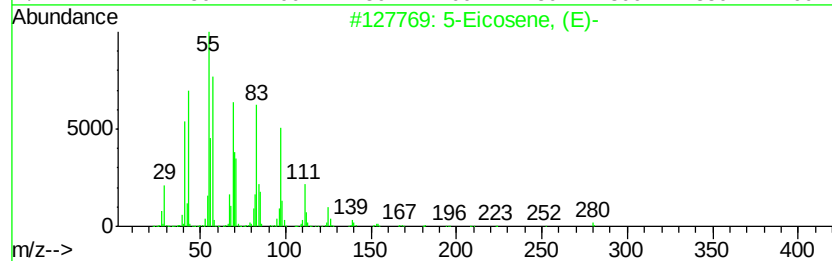
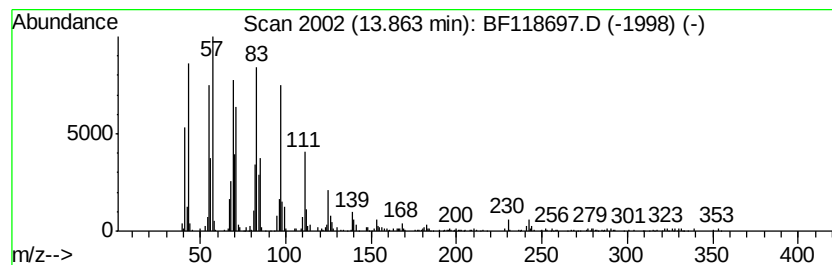
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.86	4.78 ng	472241	Chrysene-d12	14.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	96
2	Cyclopentadecane	210	C15H30	000295-48-7	95
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012420\
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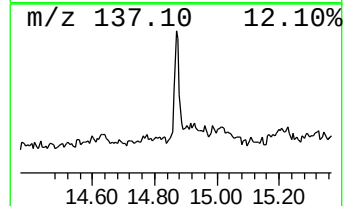
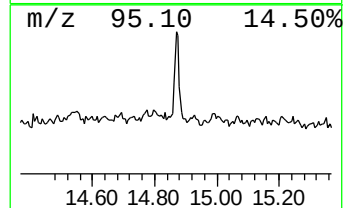
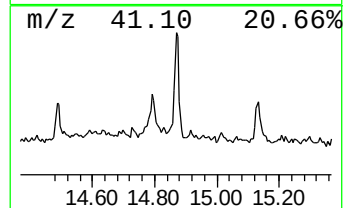
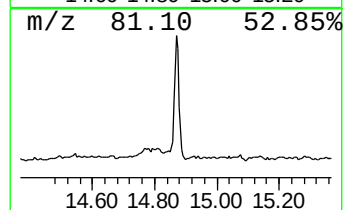
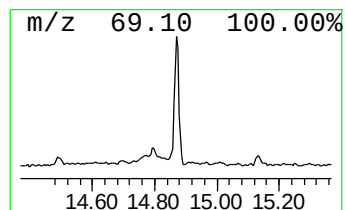
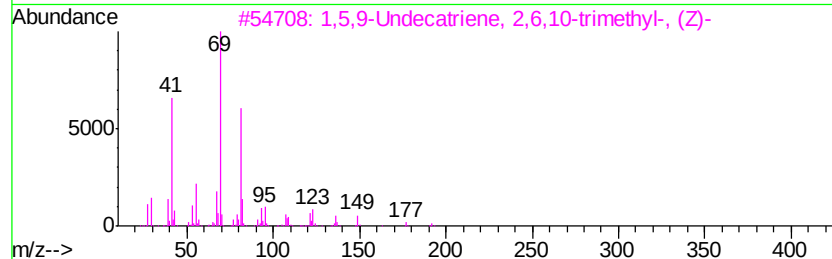
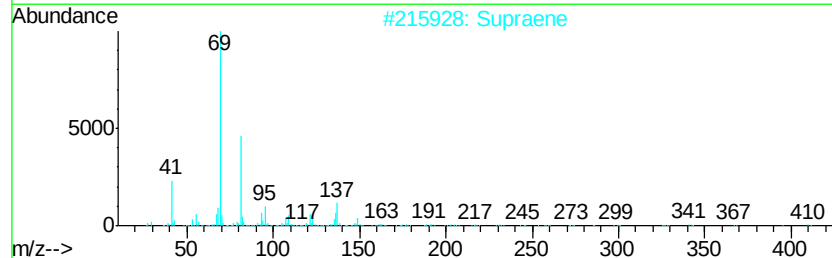
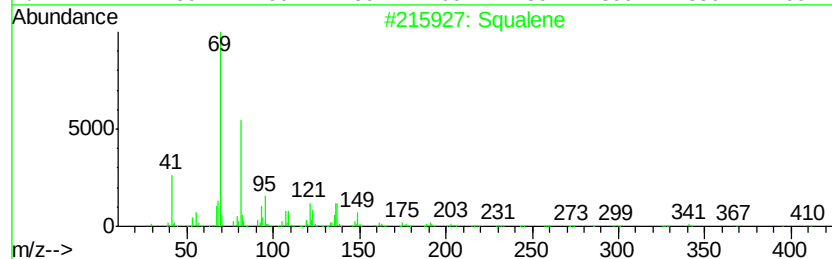
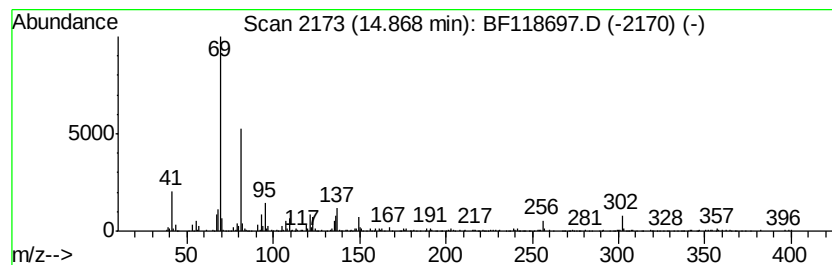
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	4.49 ng	374315	Perylene-d12	15.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	000111-02-4	87
2	Supraene	410 C30H50	007683-64-9	74
3	1,5,9-Undecatriene, 2,6,10-trime...	192 C14H24	062951-96-6	68
4	Trifluoroacetyl-lavandulol	250 C12H17F3O2	028673-24-7	59
5	7,11-Dimethyldodeca-2,6,10-trien...	208 C14H24O	125529-10-4	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012420\
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Acq On : 24 Jan 2020 20:39
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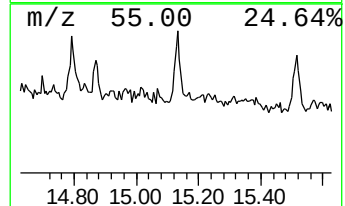
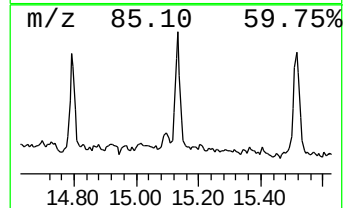
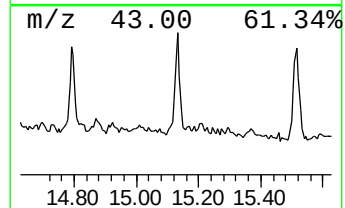
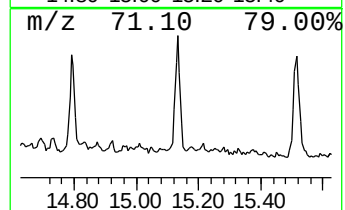
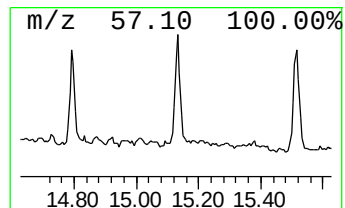
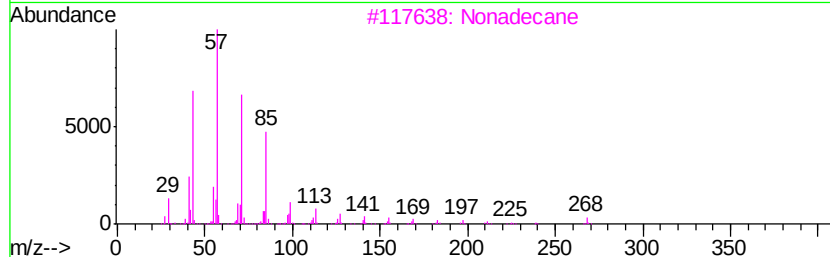
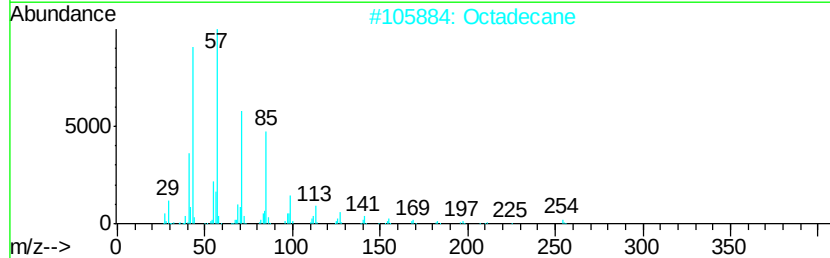
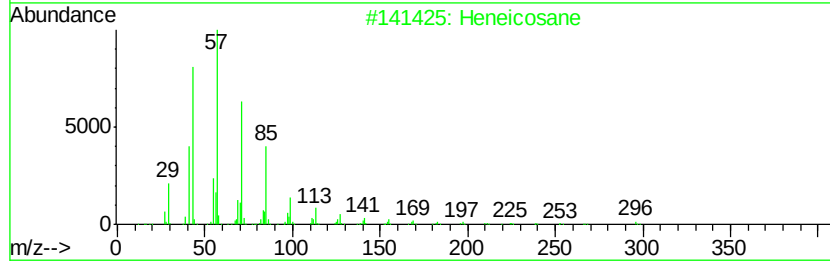
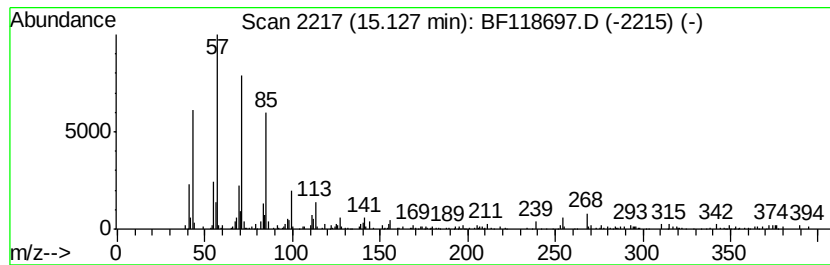
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heneicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	2.09 ng	174165	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	96
2		Octadecane	254	C18H38	000593-45-3	93
3		Nonadecane	268	C19H40	000629-92-5	93
4		Tetracosane	338	C24H50	000646-31-1	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



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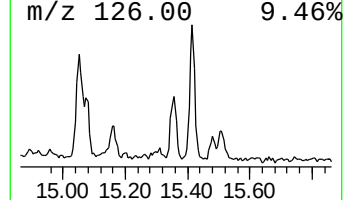
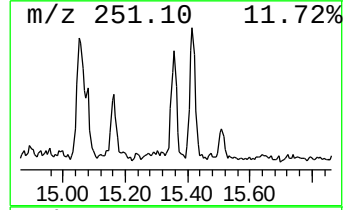
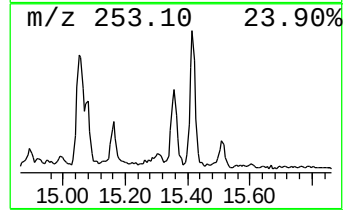
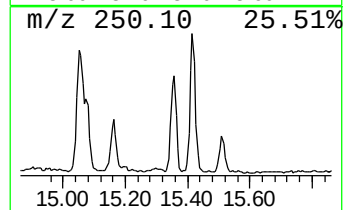
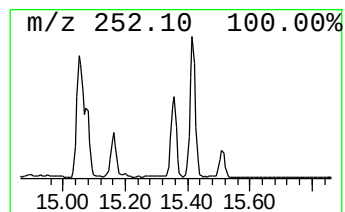
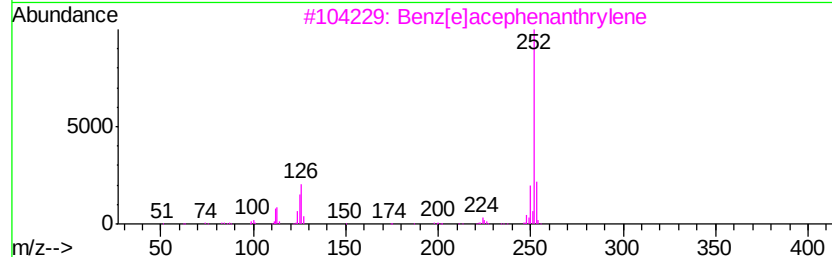
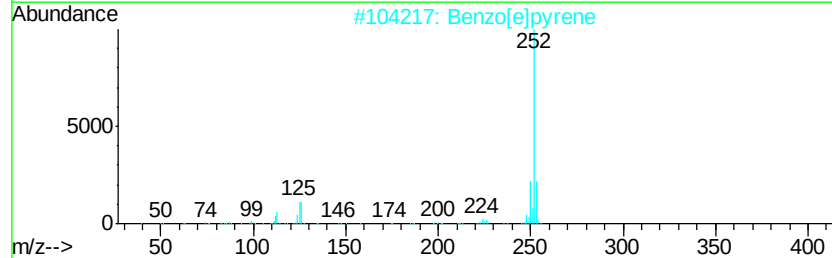
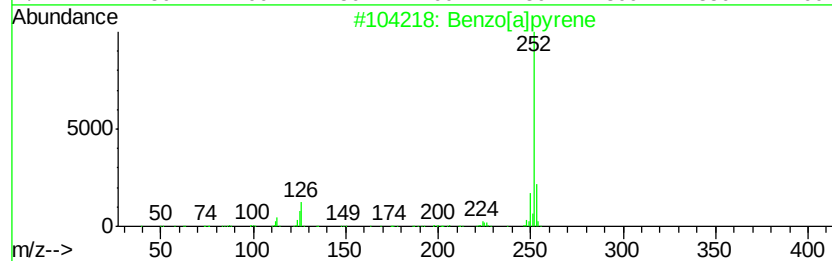
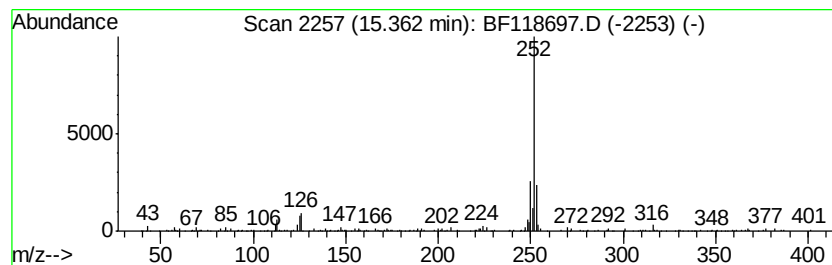
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	3.18 ng	264852	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[a]pyrene	252	C20H12	000050-32-8	97
2		Benzo[e]pyrene	252	C20H12	000192-97-2	96
3		Benz[el]acephenanthrylene	252	C20H12	000205-99-2	95
4		Perylene	252	C20H12	000198-55-0	90
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	89



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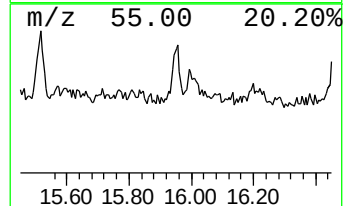
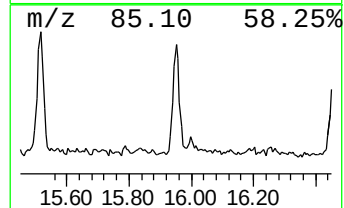
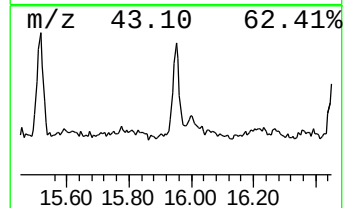
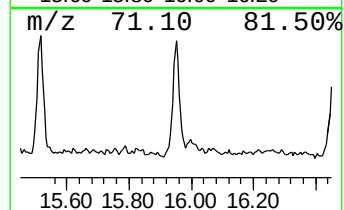
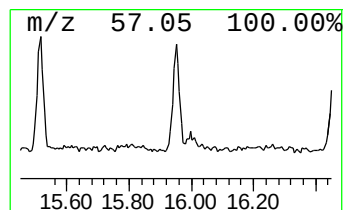
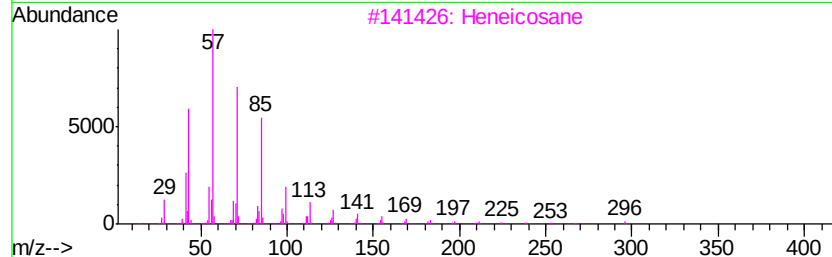
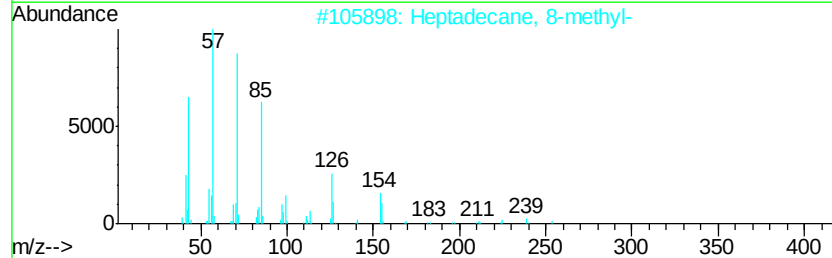
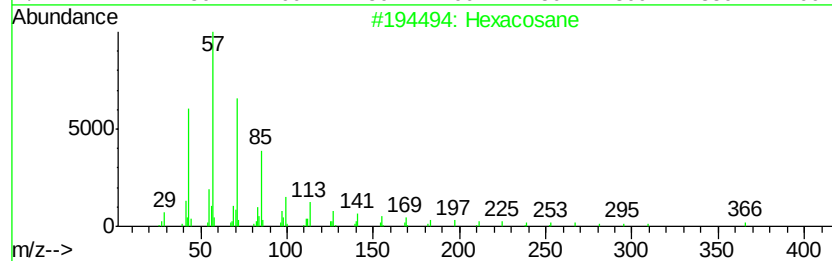
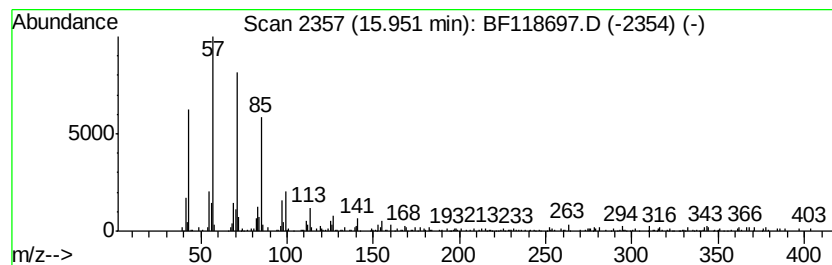
Instrument :
BNA_F
ClientSampleId :
20200067-AMENDED-COMP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Hexacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.95	2.24 ng	186867	Perylene-d12		15.48
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	93
2	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012420\
 Data File : BF118697.D
 Acq On : 24 Jan 2020 20:39
 Operator : CG/JU
 Sample : L1242-14
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20200067-AMENDED-COMP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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...	2.14	19.6	ng	1397550	1	6.86	1423850	20.0
2-Pentanone, 4-hy...	5.12	172.6	ng	12288400	1	6.86	1423850	20.0
Lenthionine	10.80	3.0	ng	295406	4	11.38	1990000	20.0
unknown11.24	11.24	2.8	ng	273269	4	11.38	1990000	20.0
Anthracene, 2-met...	11.91	2.9	ng	289514	4	11.38	1990000	20.0
4H-Cyclopenta[def...	12.00	3.5	ng	347421	4	11.38	1990000	20.0
Isopropyl palmitate	12.16	2.3	ng	225074	4	11.38	1990000	20.0
5-Eicosene, (E)-	13.86	4.8	ng	472241	5	14.02	1977860	20.0
Squalene	14.87	4.5	ng	374315	6	15.48	1667120	20.0
Heneicosane	15.13	2.1	ng	174165	6	15.48	1667120	20.0
Benzo[e]pyrene	15.36	3.2	ng	264852	6	15.48	1667120	20.0
Hexacosane	15.95	2.2	ng	186867	6	15.48	1667120	20.0