

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081919\
 Data File : BF116388.D
 Acq On : 19 Aug 2019 14:30
 Operator : HP/JU
 Sample : K4223-27
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-14

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-BF073019.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	5.440	566	570	596	rBV	2327009	2884083	80.58%	4.393%
2	6.451	738	742	756	rBV	2730758	3059263	85.47%	4.660%
3	6.581	760	764	772	rVB	3247582	3001456	83.86%	4.572%
4	6.804	799	802	813	rBV	869738	791118	22.10%	1.205%
5	6.963	825	829	848	rVB	2339243	2394493	66.90%	3.647%
6	7.369	895	898	919	rBV	1939237	1991163	55.63%	3.033%
7	8.081	1016	1019	1036	rVB	967966	1024147	28.61%	1.560%
8	9.157	1198	1202	1205	rBV	3297640	2969227	82.96%	4.523%
9	9.463	1251	1254	1256	rBV3	69373	66472	1.86%	0.101%
10	9.486	1256	1258	1263	rVV	184343	171968	4.80%	0.262%
11	9.551	1266	1269	1272	rVV	650234	530637	14.83%	0.808%
12	9.586	1272	1275	1279	rVB3	96702	97086	2.71%	0.148%
13	9.745	1297	1302	1304	rVV3	60153	63831	1.78%	0.097%
14	9.833	1314	1317	1320	rBV	1328923	1121449	31.33%	1.708%
15	9.857	1320	1321	1327	rVB3	149702	132394	3.70%	0.202%
16	9.951	1332	1337	1341	rBV	315630	291199	8.14%	0.444%
17	9.986	1341	1343	1346	rVB	77618	64110	1.79%	0.098%
18	10.057	1348	1355	1359	rBV3	52723	94573	2.64%	0.144%
19	10.122	1364	1366	1370	rVB	69057	67269	1.88%	0.102%
20	10.386	1409	1411	1413	rBV	64992	59488	1.66%	0.091%
21	10.498	1428	1430	1433	rBV	106465	89403	2.50%	0.136%
22	10.557	1433	1440	1442	rBV5	48311	73848	2.06%	0.112%
23	10.604	1442	1448	1449	rBV4	73779	104188	2.91%	0.159%
24	10.628	1449	1452	1459	rVB	1683167	1696779	47.41%	2.585%
25	10.739	1467	1471	1475	rBV2	85418	94385	2.64%	0.144%
26	10.933	1501	1504	1508	rBV2	48615	59822	1.67%	0.091%
27	11.004	1511	1516	1520	rBV6	72716	159328	4.45%	0.243%
28	11.227	1551	1554	1559	rVB2	54061	68758	1.92%	0.105%
29	11.322	1564	1570	1572	rVV	1099964	1018605	28.46%	1.552%
30	11.345	1572	1574	1576	rVV	1047091	891490	24.91%	1.358%
31	11.363	1576	1577	1580	rVV	250816	208673	5.83%	0.318%
32	11.404	1580	1584	1587	rVV	223247	263410	7.36%	0.401%
33	11.457	1590	1593	1596	rVV	129842	143741	4.02%	0.219%
34	11.569	1609	1612	1616	rVB	61370	72033	2.01%	0.110%

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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.669	1626	1629	1632	rBV3	47792	60908	1.70%	0.093%
36	11.698	1632	1634	1638	rVB2	65117	70044	1.96%	0.107%
37	11.804	1645	1652	1654	rBV2	165095	255310	7.13%	0.389%
38	11.827	1654	1656	1657	rVV	94102	75642	2.11%	0.115%
39	11.857	1657	1661	1667	rVV	1227860	1419929	39.67%	2.163%
40	11.939	1672	1675	1677	rVV	175229	169282	4.73%	0.258%
41	12.004	1681	1686	1692	rBV2	284653	304474	8.51%	0.464%
42	12.116	1703	1705	1707	rBV	94342	76196	2.13%	0.116%
43	12.192	1716	1718	1722	rVB	78243	68476	1.91%	0.104%
44	12.251	1725	1728	1732	rBV3	59182	89358	2.50%	0.136%
45	12.380	1746	1750	1753	rBV3	139690	216171	6.04%	0.329%
46	12.404	1753	1754	1758	rVB3	115176	84903	2.37%	0.129%
47	12.457	1761	1763	1773	rVB2	465723	611130	17.07%	0.931%
48	12.539	1773	1777	1779	rBV	1818938	2016912	56.35%	3.072%
49	12.557	1779	1780	1789	rVV2	906768	1189854	33.24%	1.812%
50	12.627	1789	1792	1800	rVV	398217	546551	15.27%	0.833%
51	12.692	1800	1803	1805	rVV2	123586	140607	3.93%	0.214%
52	12.721	1805	1808	1810	rVV2	171523	193402	5.40%	0.295%
53	12.763	1810	1815	1821	rVV	1291790	1631078	45.57%	2.485%
54	12.821	1822	1825	1828	rVB2	127040	148930	4.16%	0.227%
55	12.898	1834	1838	1842	rVB	2310912	2030560	56.73%	3.093%
56	12.992	1850	1854	1859	rVB4	84329	145503	4.07%	0.222%
57	13.074	1865	1868	1869	rBV2	92059	95170	2.66%	0.145%
58	13.098	1869	1872	1874	rVV	191990	185868	5.19%	0.283%
59	13.163	1880	1883	1886	rBV	183266	149152	4.17%	0.227%
60	13.204	1886	1890	1896	rVB2	212427	292561	8.17%	0.446%
61	13.292	1901	1905	1908	rBV2	253313	310813	8.68%	0.473%
62	13.327	1908	1911	1917	rVV3	423267	719728	20.11%	1.096%
63	13.392	1920	1922	1924	rVV	78445	82786	2.31%	0.126%
64	13.416	1924	1926	1930	rVB4	76633	81036	2.26%	0.123%
65	13.663	1966	1968	1972	rVB2	116370	110017	3.07%	0.168%
66	13.721	1975	1978	1985	rVV4	161844	330160	9.22%	0.503%
67	13.792	1987	1990	1995	rVB2	595261	601667	16.81%	0.916%
68	13.874	2001	2004	2008	rBV2	133500	189797	5.30%	0.289%
69	13.957	2015	2018	2022	rBV2	1087117	1528825	42.71%	2.329%
70	13.992	2022	2024	2030	rVB	766842	705435	19.71%	1.075%
71	14.074	2036	2038	2041	rBV	71670	63396	1.77%	0.097%

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72	14.104	2041	2043	2046	rBV2	115675	109746	3.07%	0.167%
73	14.316	2077	2079	2081	rBV	90554	87292	2.44%	0.133%
74	14.357	2081	2086	2089	rVV	358808	419551	11.72%	0.639%
75	14.410	2089	2095	2105	rVV3	665010	1292594	36.11%	1.969%
76	14.610	2126	2129	2131	rBV2	80993	87847	2.45%	0.134%
77	14.663	2136	2138	2140	rVV	113584	121865	3.40%	0.186%
78	14.710	2143	2146	2149	rVV	369652	415069	11.60%	0.632%
79	14.739	2149	2151	2154	rVV	127748	153879	4.30%	0.234%
80	14.780	2155	2158	2162	rVB2	417651	420223	11.74%	0.640%
81	15.004	2192	2196	2198	rBV	612814	738148	20.62%	1.124%
82	15.039	2198	2202	2205	rVV	2027590	2472056	69.07%	3.766%
83	15.068	2205	2207	2212	rVB2	232335	273499	7.64%	0.417%
84	15.304	2242	2247	2251	rVB2	393470	528373	14.76%	0.805%
85	15.368	2254	2258	2260	rBV	390203	474650	13.26%	0.723%
86	15.398	2260	2263	2265	rVV	309078	358972	10.03%	0.547%
87	15.421	2265	2267	2272	rVB	437997	494302	13.81%	0.753%
88	15.645	2302	2305	2312	rVB2	149408	254197	7.10%	0.387%
89	15.821	2329	2335	2340	rVB	1503875	2178453	60.86%	3.318%
90	15.874	2340	2344	2349	rBV	211701	382735	10.69%	0.583%
91	16.086	2376	2380	2393	rVB	400617	734792	20.53%	1.119%
92	16.304	2414	2417	2430	rVB2	179096	342957	9.58%	0.522%
93	16.986	2529	2533	2542	rVB5	110586	240039	6.71%	0.366%
94	17.309	2584	2588	2592	rBV3	98588	191063	5.34%	0.291%
95	17.398	2594	2603	2615	rVV7	956637	3579295	100.00%	5.452%
96	17.498	2615	2620	2631	rVV8	168970	587837	16.42%	0.895%
97	17.827	2670	2676	2685	rBV2	423071	1210857	33.83%	1.844%
98	18.162	2724	2733	2751	rBV3	815556	3513787	98.17%	5.352%
99	18.374	2765	2769	2782	rVB4	230447	642098	17.94%	0.978%
100	18.709	2821	2826	2836	rVB7	176390	531632	14.85%	0.810%

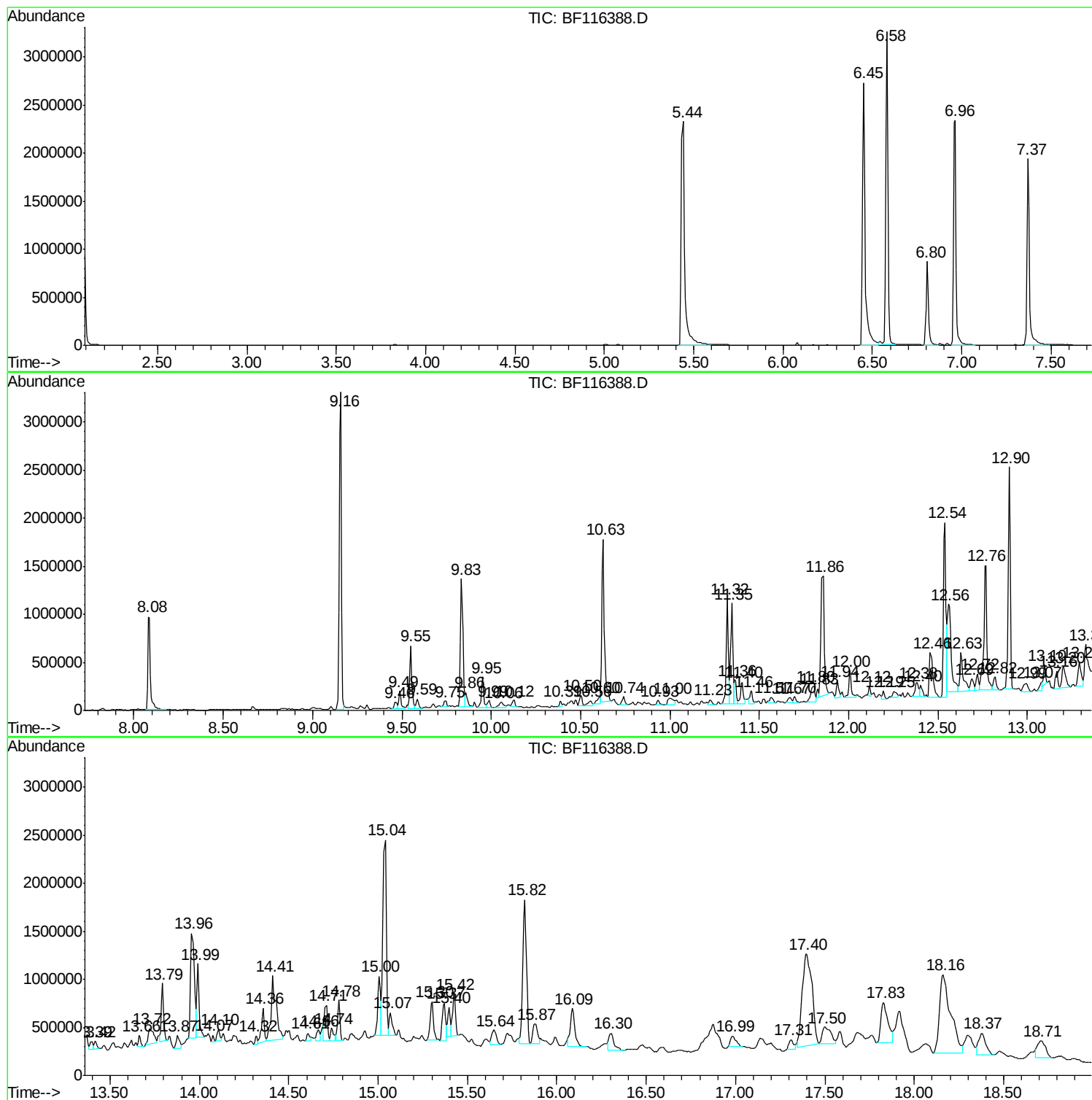
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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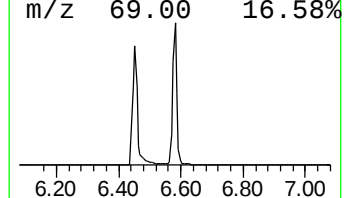
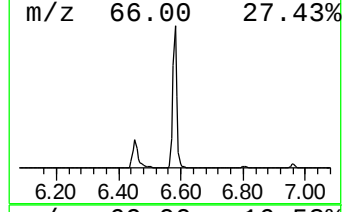
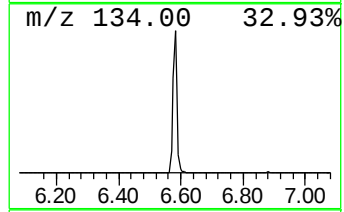
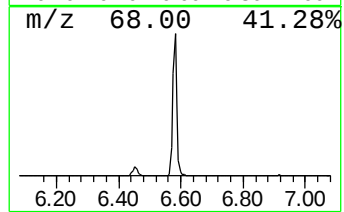
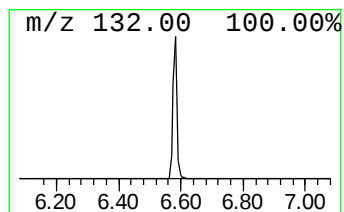
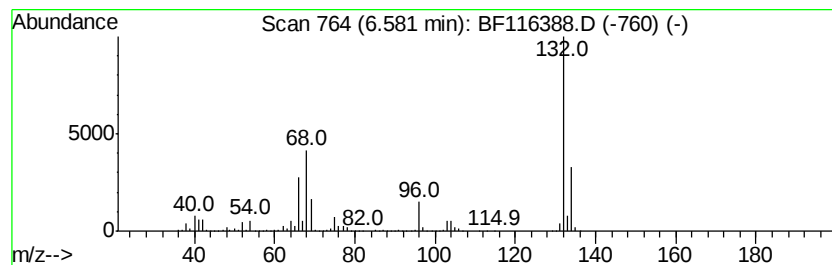
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.58 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	75.88 ng	3001460	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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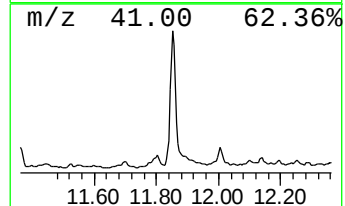
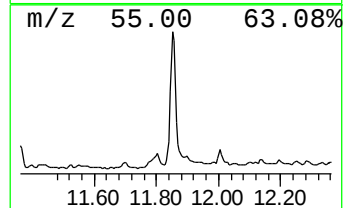
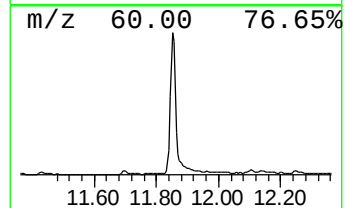
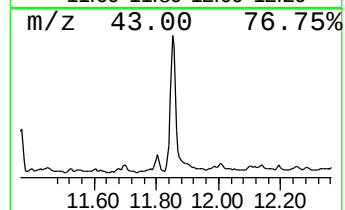
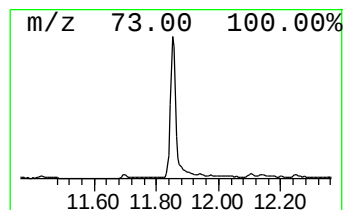
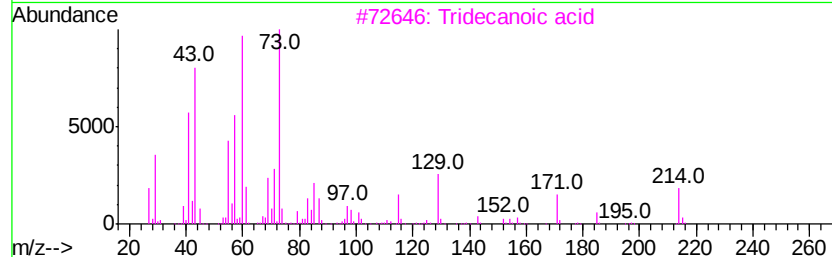
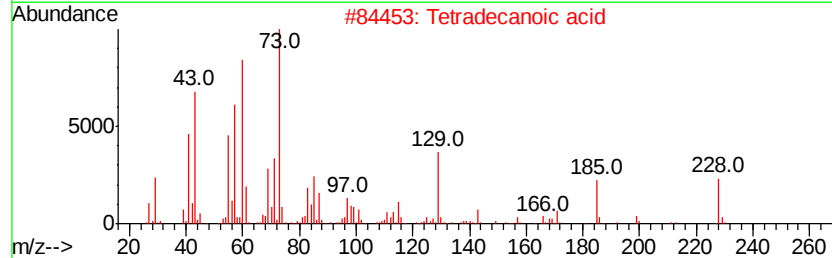
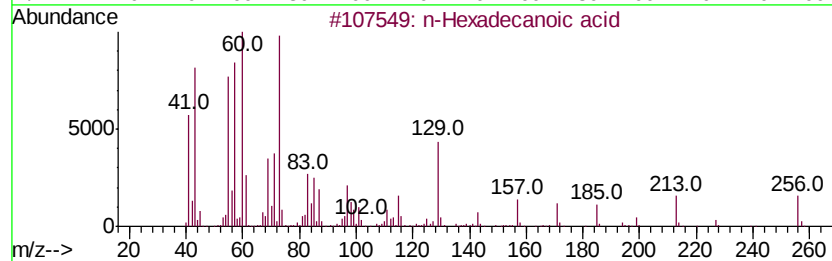
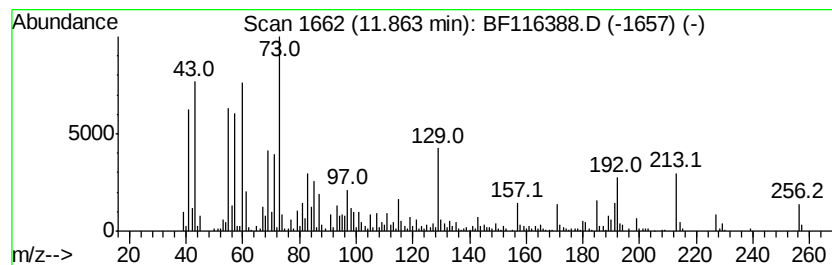
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	27.88 ng	1419930	Phenanthrene-d10	11.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3		Tridecanoic acid	214	C13H26O2	000638-53-9	90
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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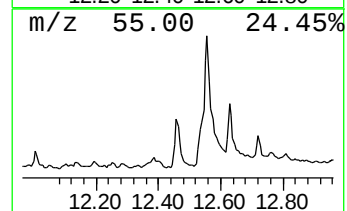
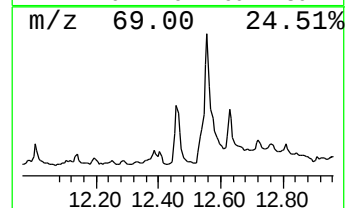
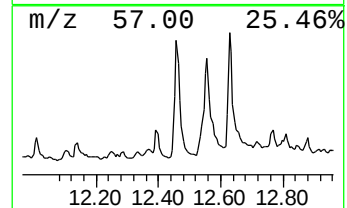
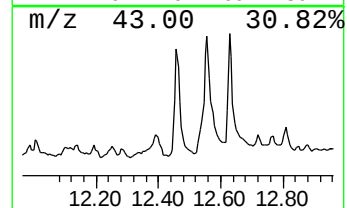
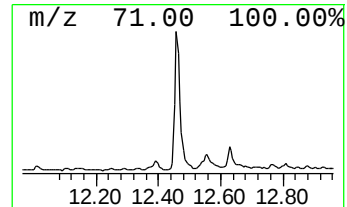
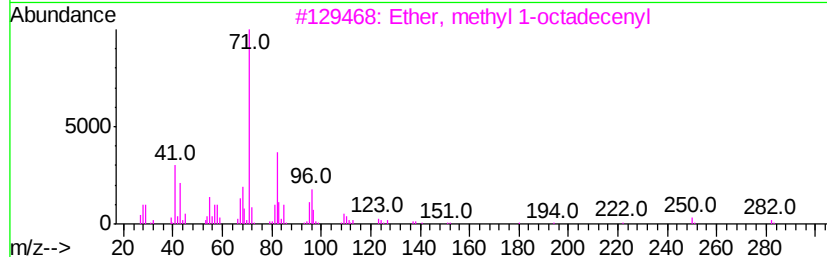
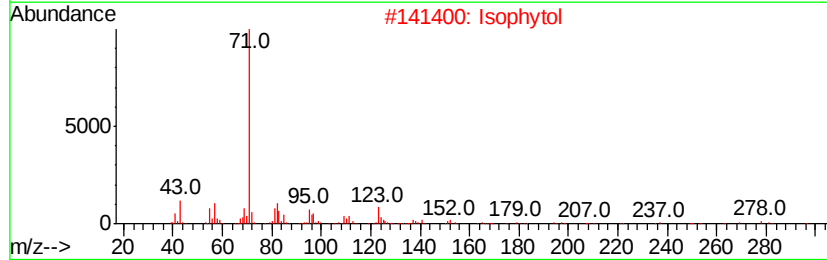
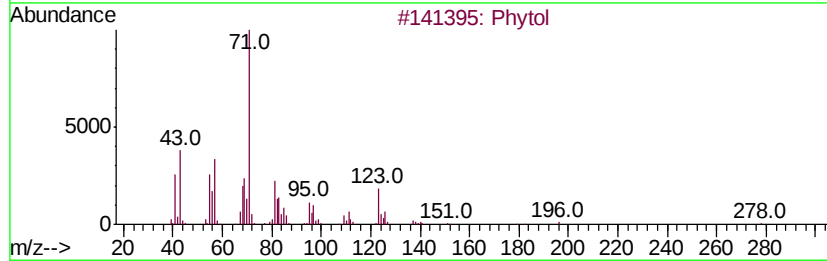
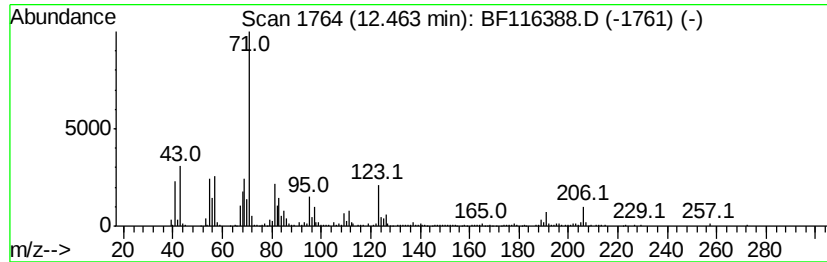
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Peak Number 4 Phytol Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	12.00 ng	611130	Phenanthrene-d10	11.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Phytol	296 C20H40O	000150-86-7	87
2	Isophytol	296 C20H40O	000505-32-8	59
3	Ether, methyl 1-octadecenyl	282 C19H38O	026537-06-4	53
4	Acetamide, N-tetrahydrofurfuryl-	197 C7H10F3N02	1000307-30-7	47
5	Butyric acid, 2-tridecyl ester	270 C17H34O2	055193-07-2	47



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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-14

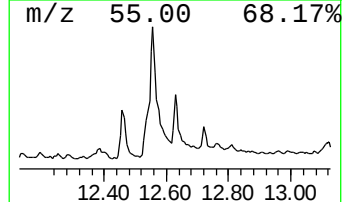
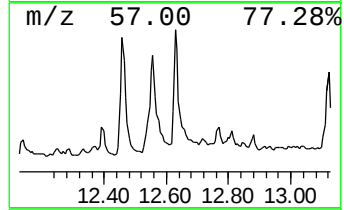
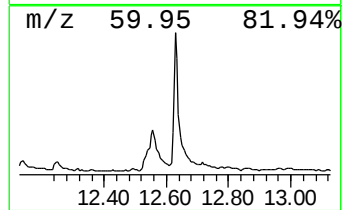
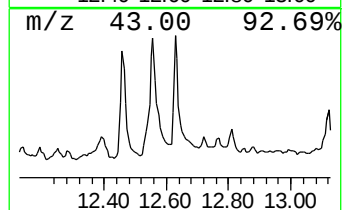
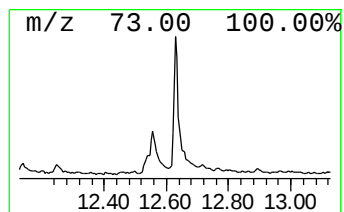
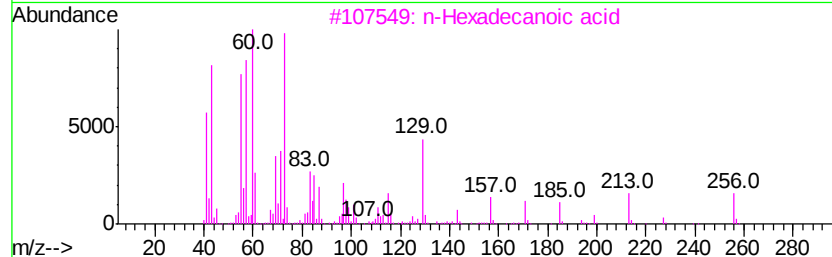
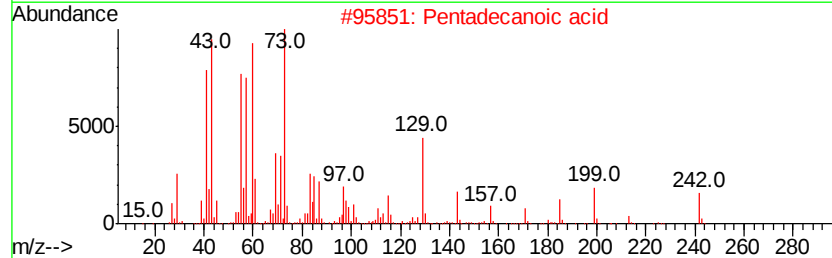
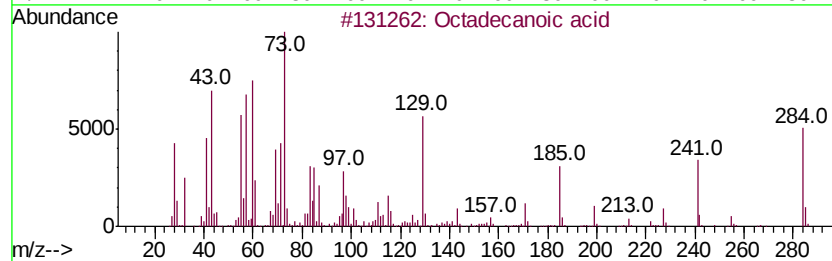
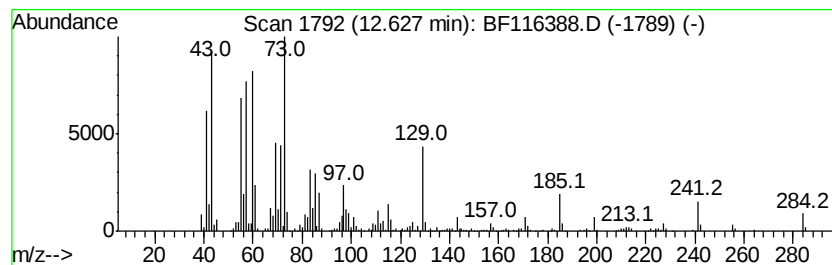
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	10.73 ng	546551	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116388.D
Acq On : 19 Aug 2019 14:30
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Sample : K4223-27
Misc :
ALS Vial : 10 Sample Multiplier: 1

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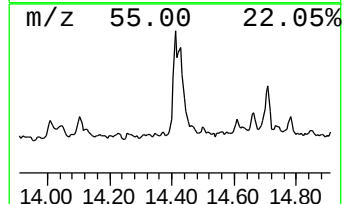
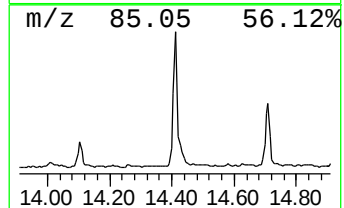
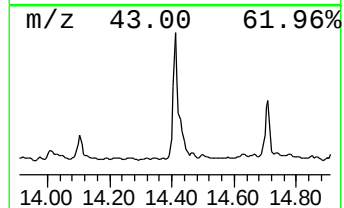
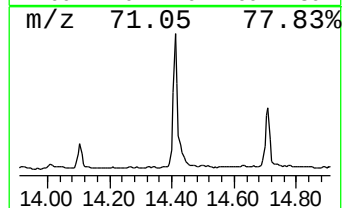
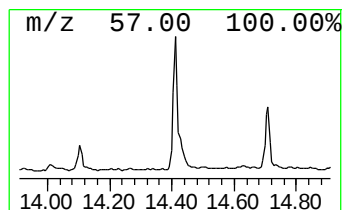
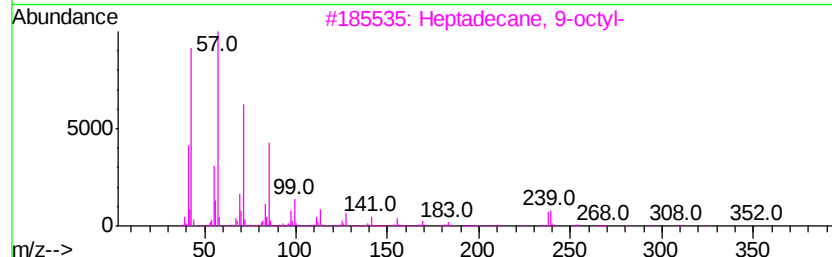
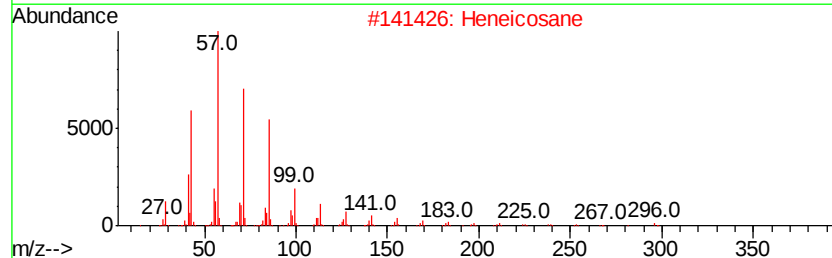
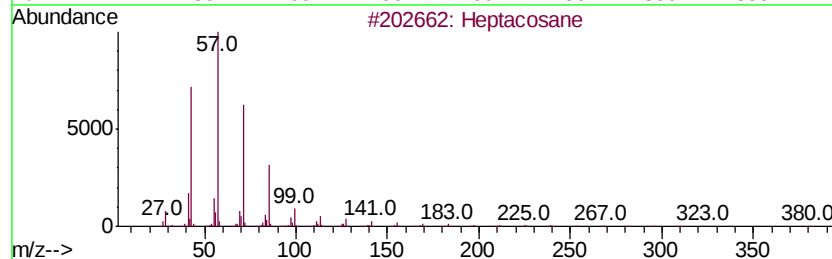
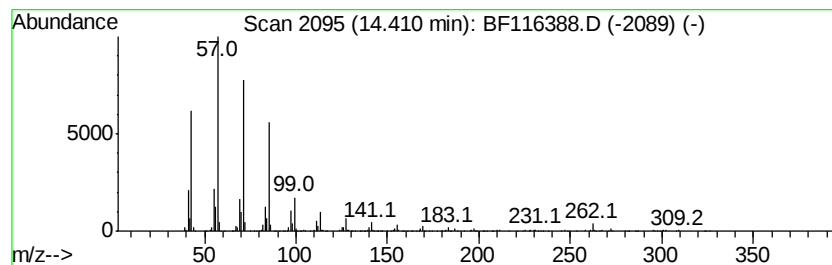
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	16.91 ng	1292590	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Hexadecane	226	C16H34	000544-76-3	87
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116388.D
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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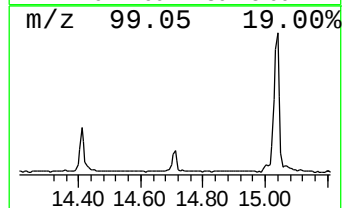
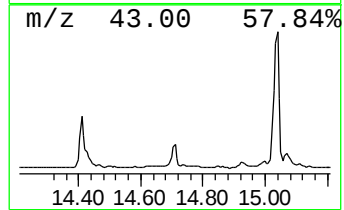
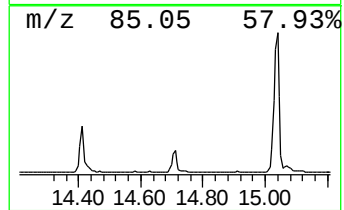
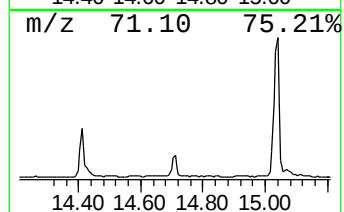
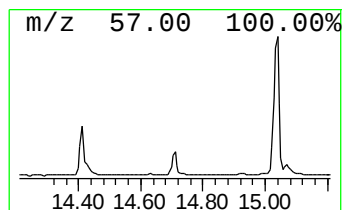
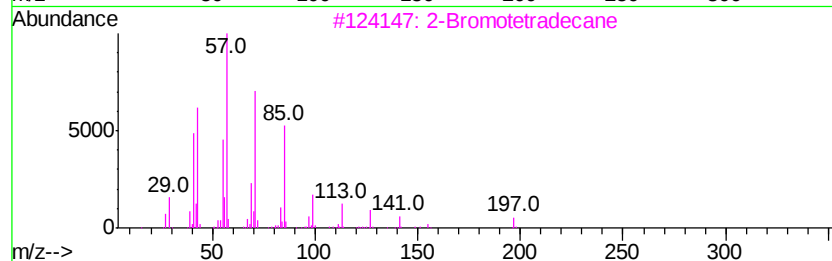
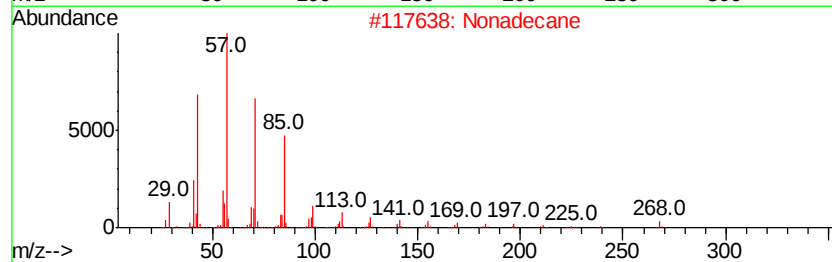
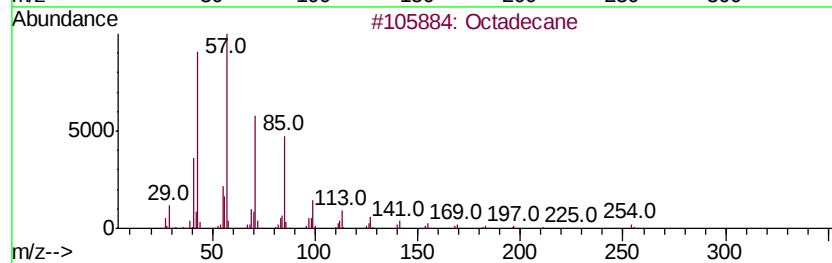
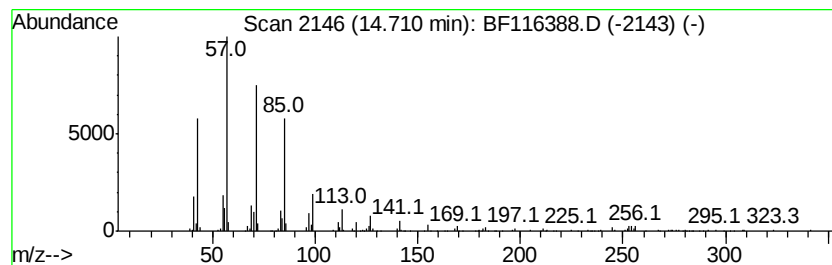
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	16.79 ng	415069	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	94
2		Nonadecane	268	C19H40	000629-92-5	91
3		2-Bromotetradecane	276	C14H29Br	074036-95-6	91
4		Heneicosane	296	C21H44	000629-94-7	90
5		Octacosane	394	C28H58	000630-02-4	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116388.D
Acq On : 19 Aug 2019 14:30
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Misc :
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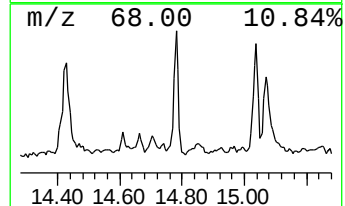
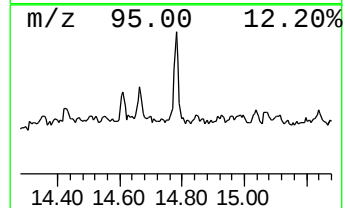
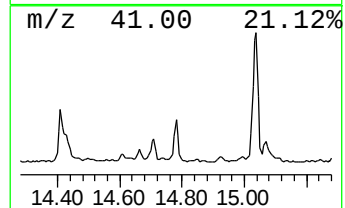
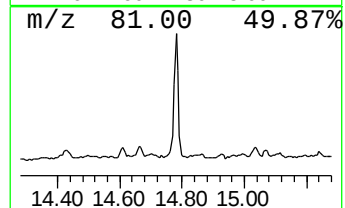
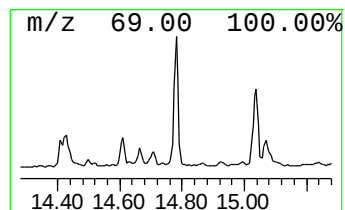
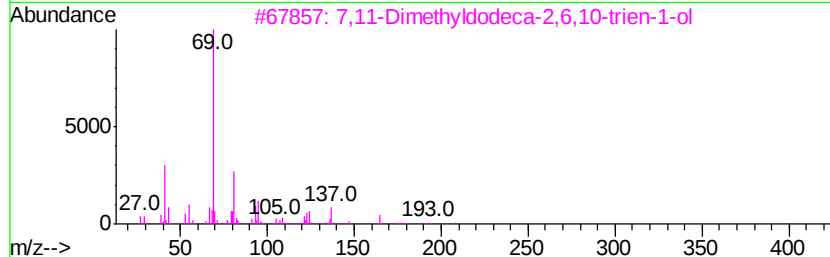
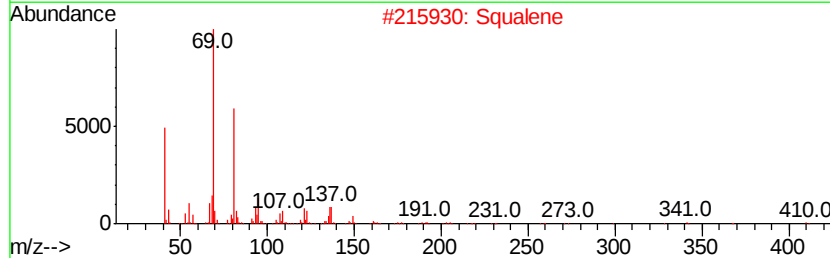
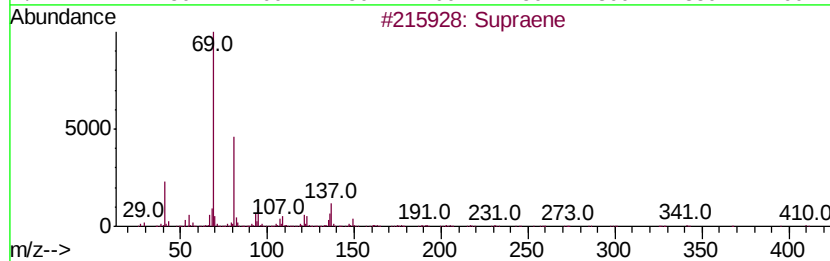
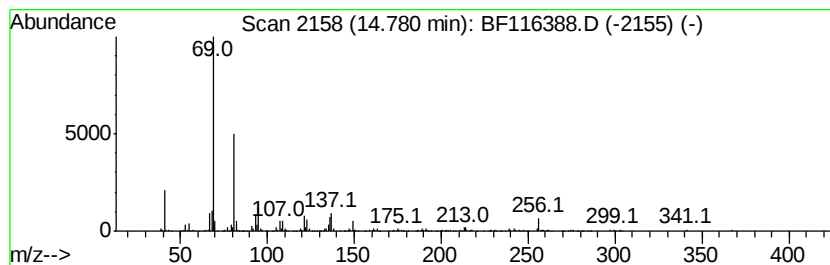
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.78	17.00 ng	420223	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4		3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	72
5		trans-Farnesol	222	C15H26O	000106-28-5	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
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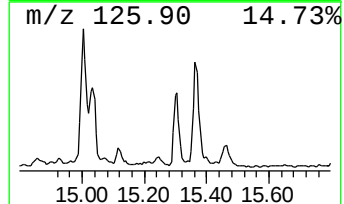
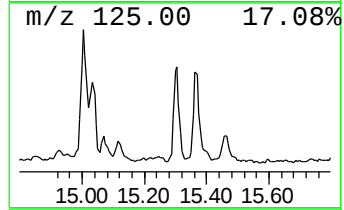
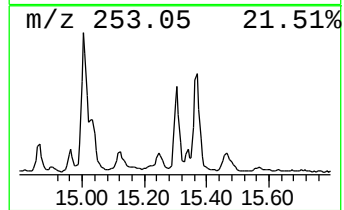
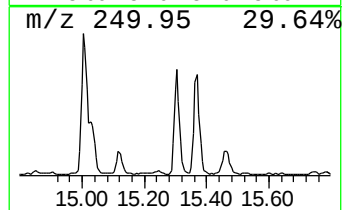
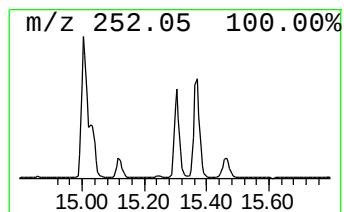
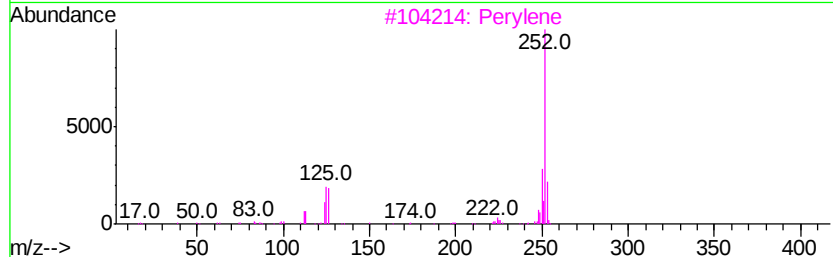
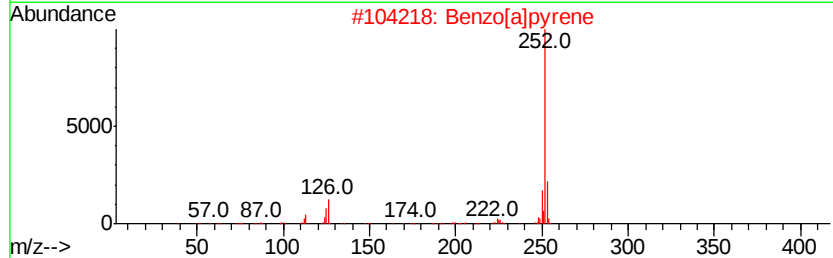
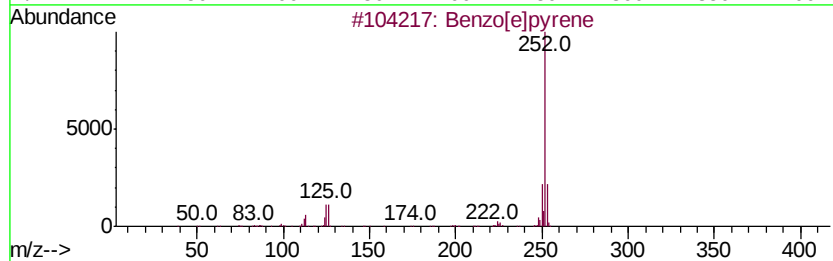
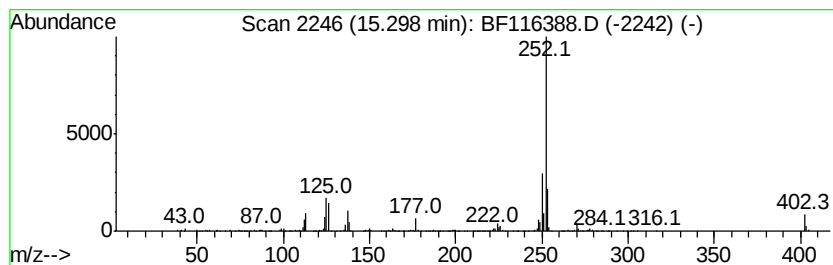
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzo[e]pyrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.30	21.38 ng	528373	Perylene-d12	15.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	99
2		Benzo[a]pyrene	252	C20H12	000050-32-8	98
3		Perylene	252	C20H12	000198-55-0	97
4		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	94
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
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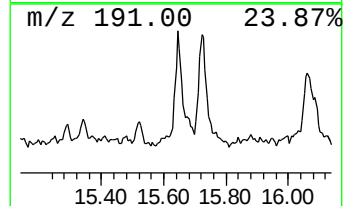
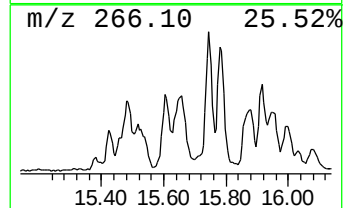
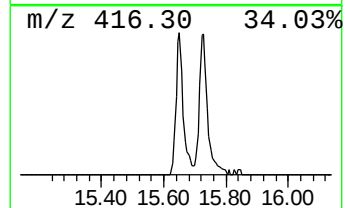
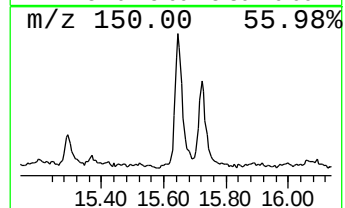
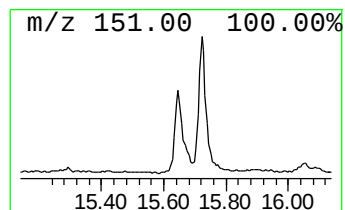
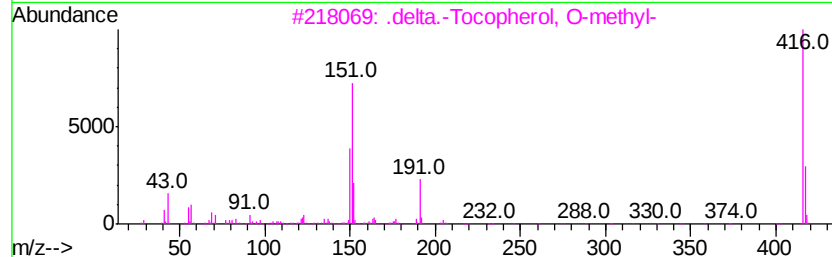
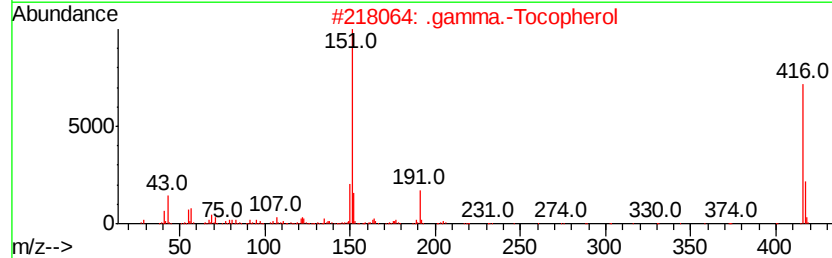
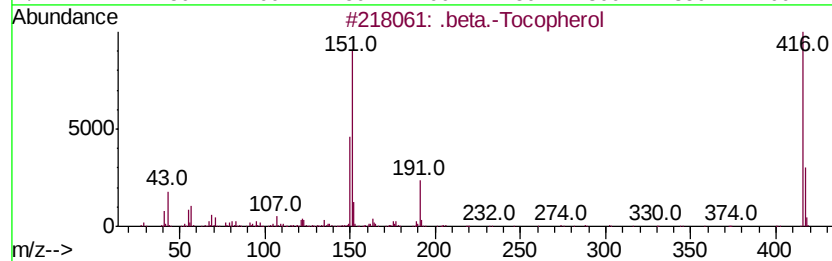
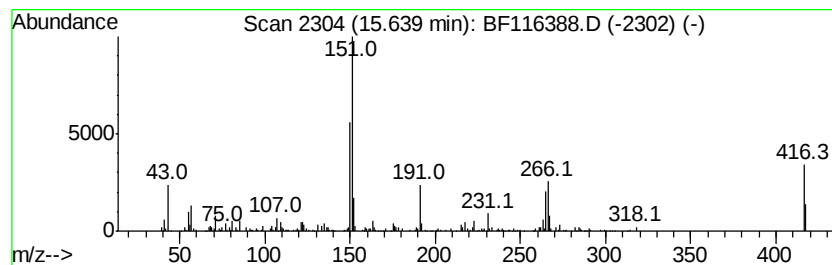
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 .beta.-Tocopherol Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	10.29 ng	254197	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Tocopherol	416	C28H48O2	000148-03-8	93
2		.gamma.-Tocopherol	416	C28H48O2	007616-22-0	91
3		.delta.-Tocopherol, 0-methyl-	416	C28H48O2	1000374-72-8	81
4		N,N'-Bis(3-methoxyfluoren-9-ylid...	416	C28H20N2O2	1000210-76-6	43
5		3,4-Dihydro-3,5,8-trimethyl-3-(4...	458	C30H50O3	1000105-71-9	40



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
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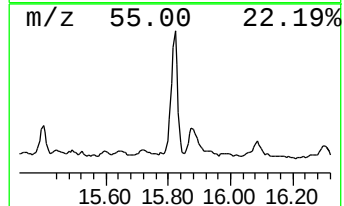
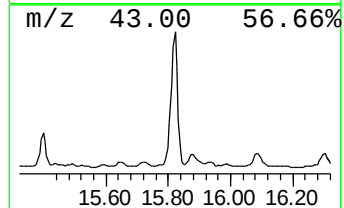
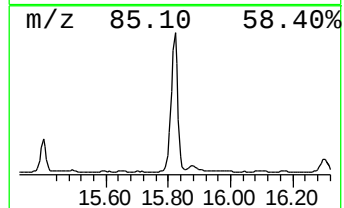
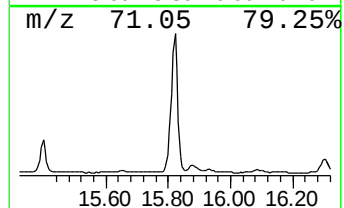
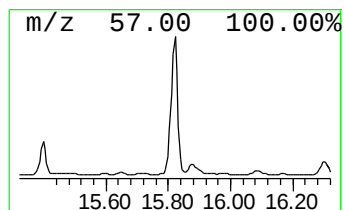
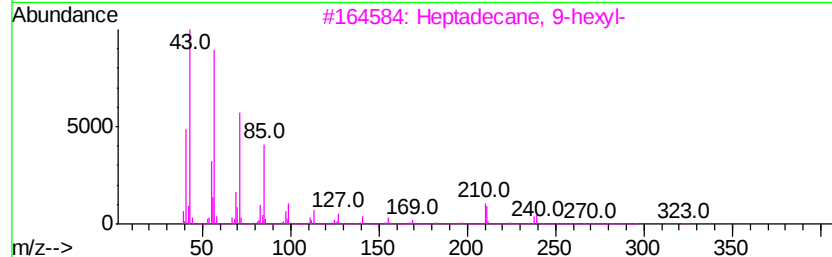
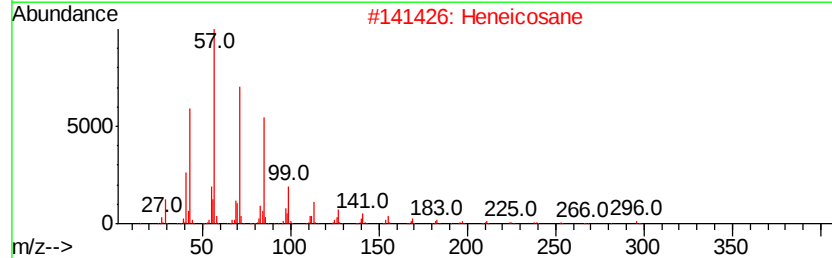
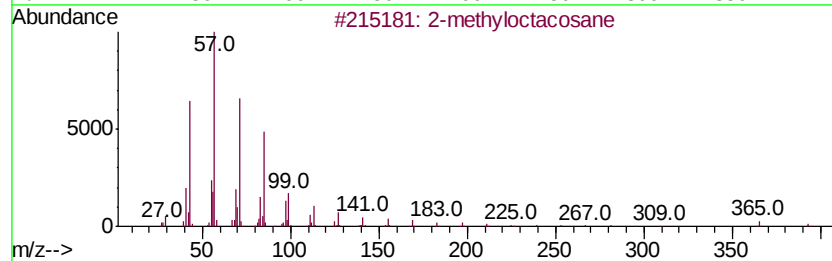
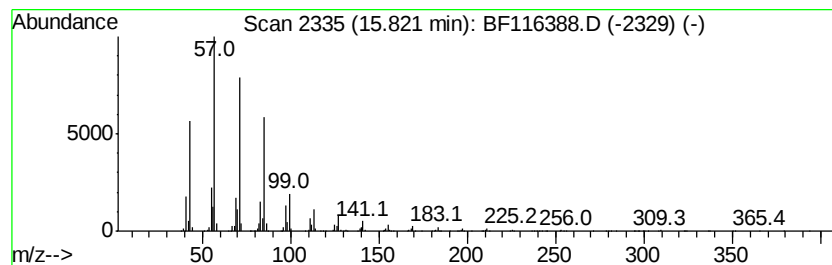
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-methyloctacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.82	88.14 ng	2178450	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	90
4		Hexacosane	366	C26H54	000630-01-3	90
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116388.D
Acq On : 19 Aug 2019 14:30
Operator : HP/JU
Sample : K4223-27
Misc :
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ClientSampleId :
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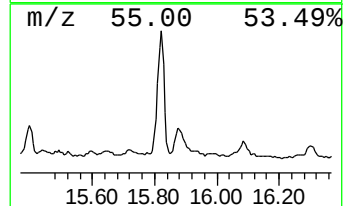
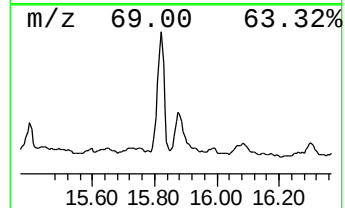
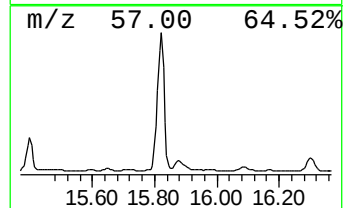
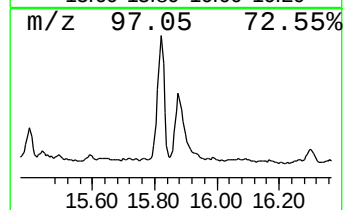
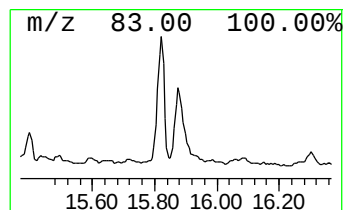
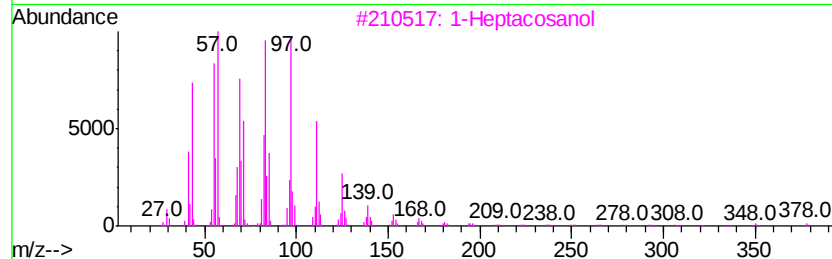
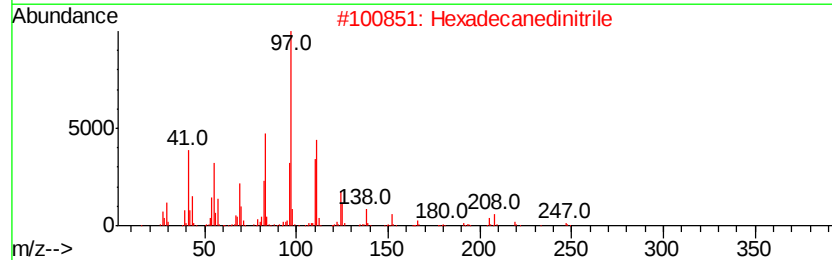
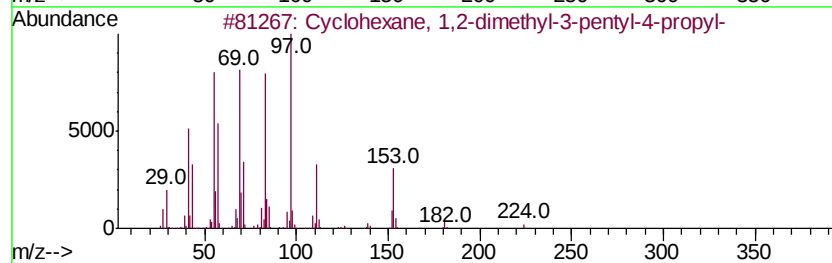
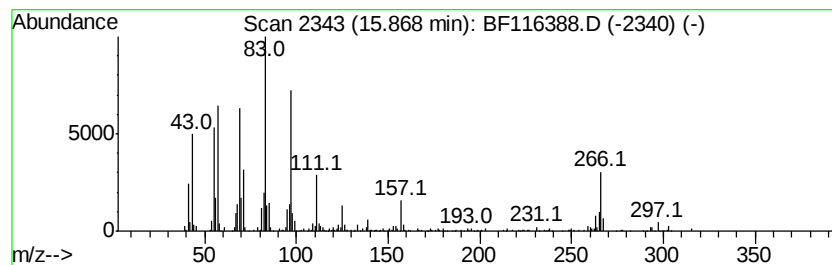
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown15.87 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	15.49 ng	382735	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	49
2		Hexadecanedinitrile	248	C16H28N2	006812-44-8	46
3		1-Heptacosanol	396	C27H56O	002004-39-9	41
4		2-Aziridinone, 1-tert-butyl-3-(1...	223	C14H25NO	026944-18-3	38
5		Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116388.D
Acq On : 19 Aug 2019 14:30
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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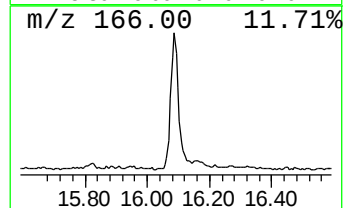
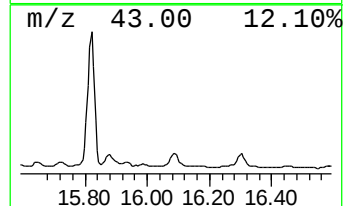
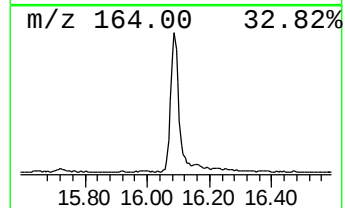
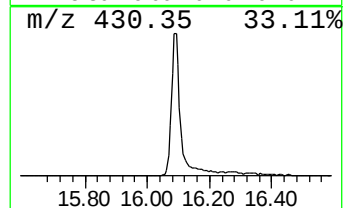
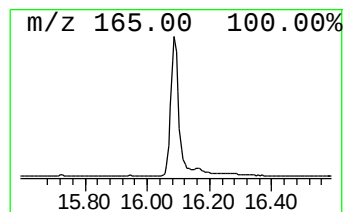
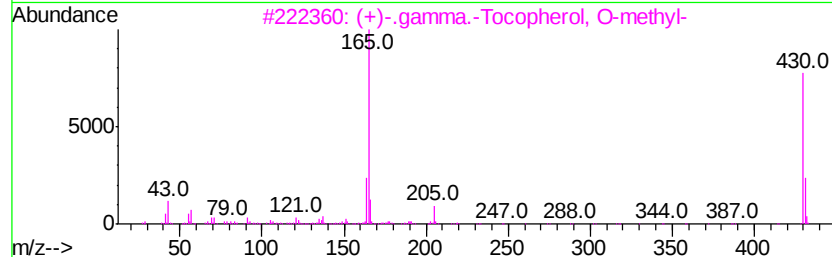
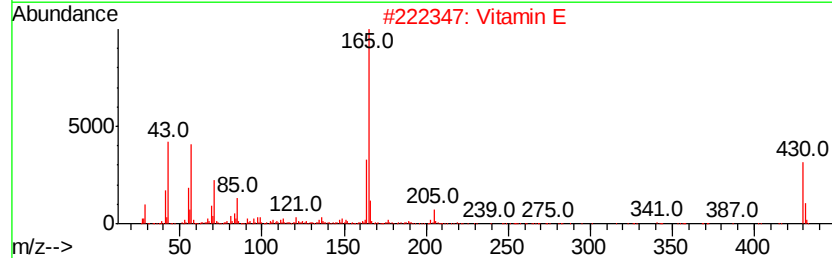
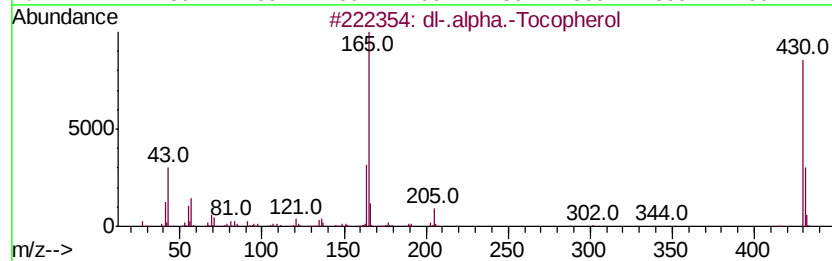
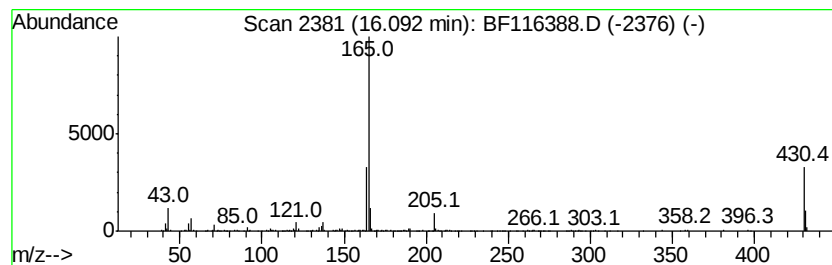
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 dl-.alpha.-Tocopherol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	29.73 ng	734792	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	dl-.alpha.-Tocopherol	430	C29H50O2	010191-41-0	94
2		Vitamin E	430	C29H50O2	000059-02-9	94
3		(+)-.gamma.-Tocopherol, O-methyl-	430	C29H50O2	1000374-72-2	93
4		Piperazine, 1-(3,4-dimethoxybenz...	430	C26H26N2O4	333756-87-9	59
5		4-Amino-3-methoxypyrazolo[3,4-d]...	165	C6H7N5O	111375-22-5	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116388.D
Acq On : 19 Aug 2019 14:30
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Sample : K4223-27
Misc :
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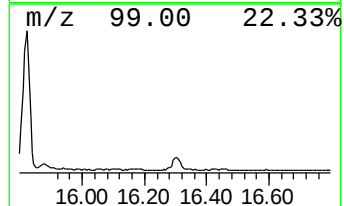
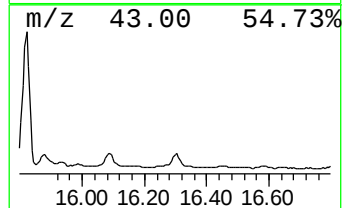
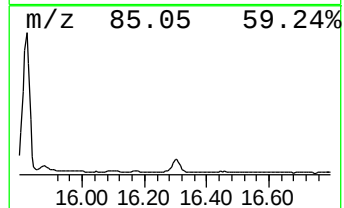
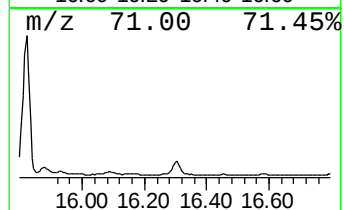
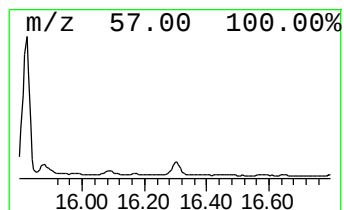
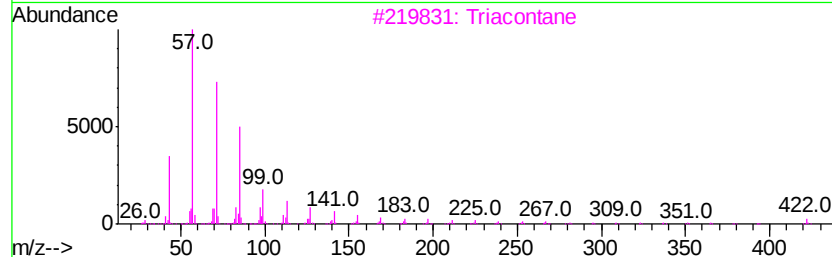
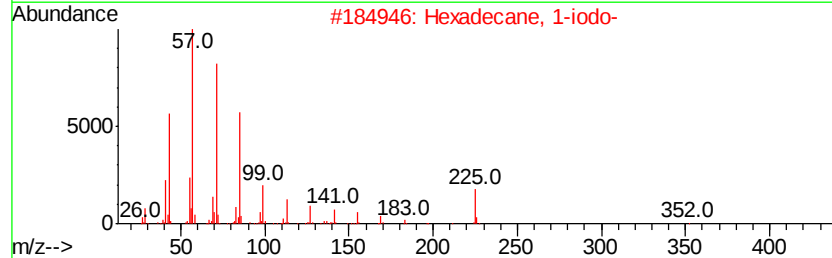
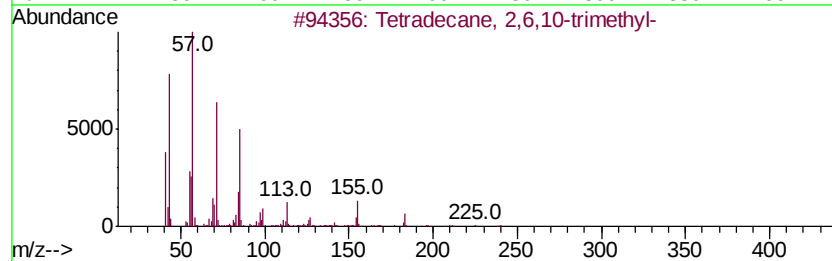
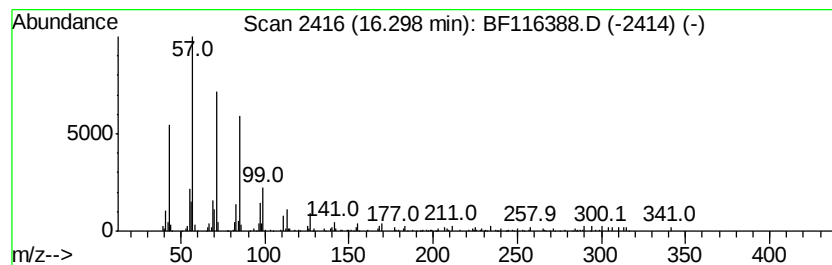
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Tetradecane, 2,6,10-trimethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.30	13.88 ng	342957	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87
2		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87
3		Triacontane	422	C30H62	000638-68-6	87
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5		Hentriacontane	437	C31H64	000630-04-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116388.D
Acq On : 19 Aug 2019 14:30
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Sample : K4223-27
Misc :
ALS Vial : 10 Sample Multiplier: 1

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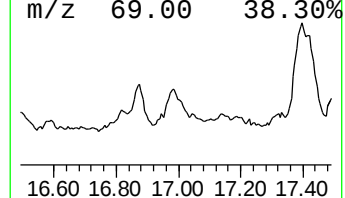
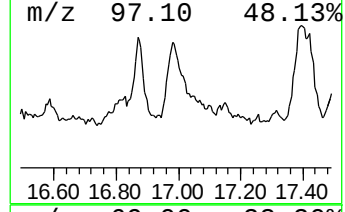
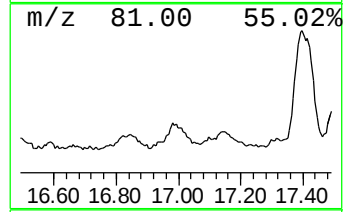
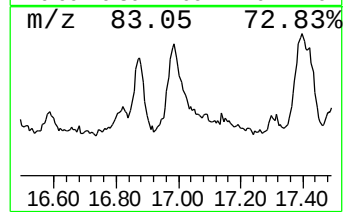
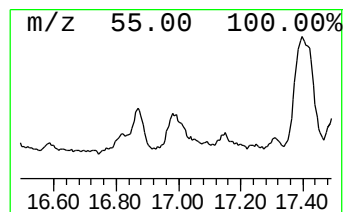
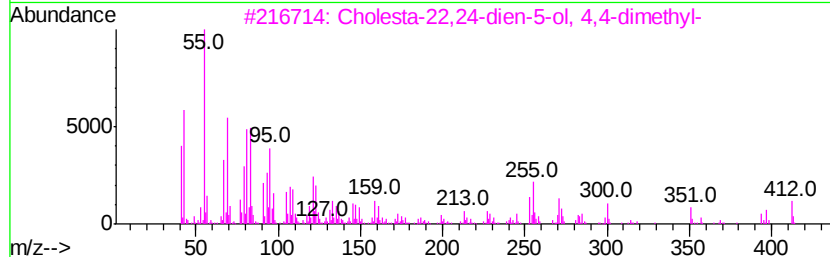
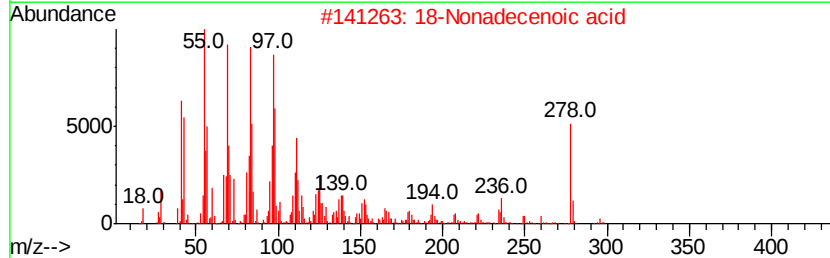
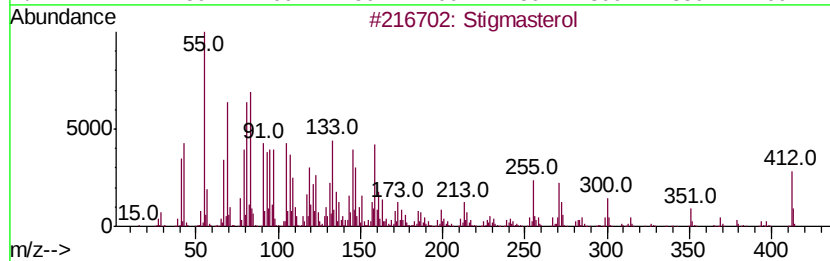
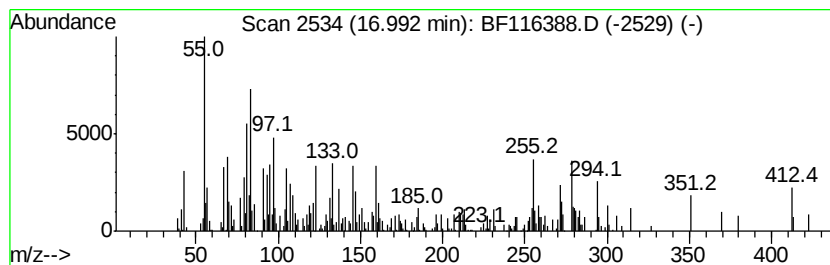
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Stigmasterol Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.99	9.71 ng	240039	Perylene-d12	15.42

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Stigmasterol	412	C29H48O	000083-48-7	92
2			18-Nonadecenoic acid	296	C19H36O2	076998-87-3	35
3			Cholesta-22,24-dien-5-ol, 4,4-di...	412	C29H48O	1000128-66-1	20
4			Ergosta-5,22-dien-3-ol, 24-methy...	412	C29H48O	053755-22-9	20
5			Decanoic acid, 10-(2-hexylcyclop...	296	C19H36O2	1000197-99-5	10



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116388.D
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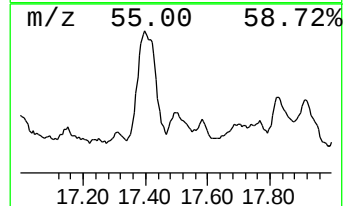
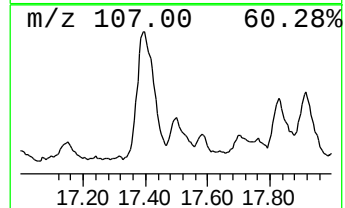
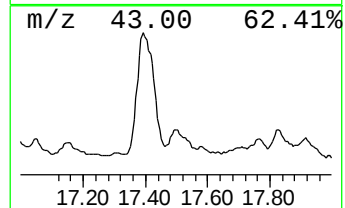
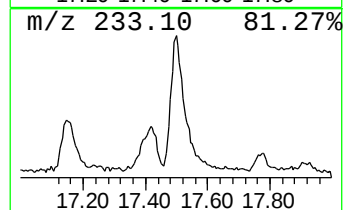
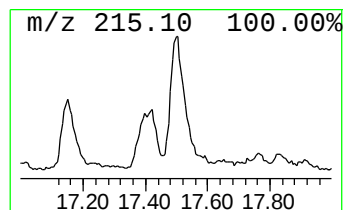
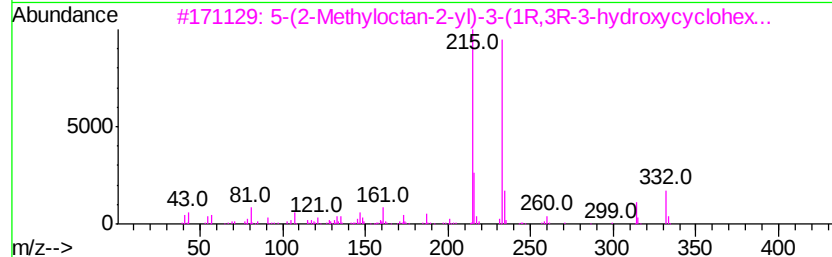
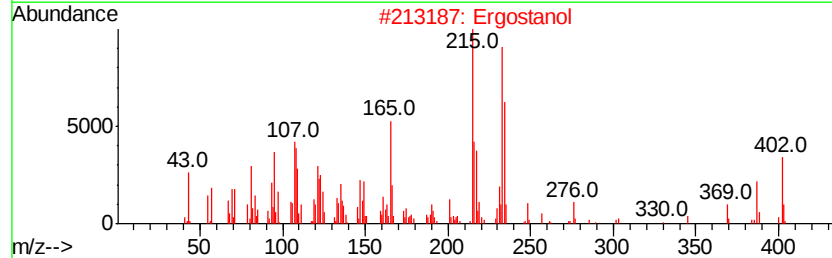
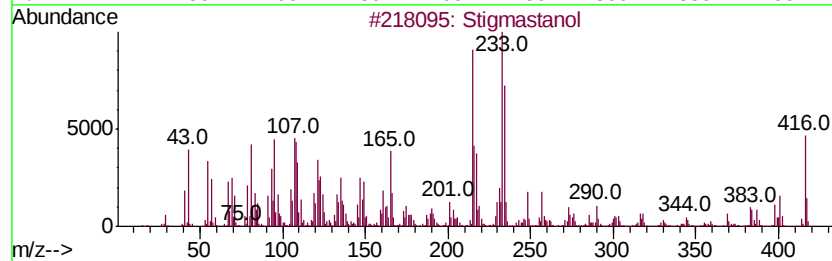
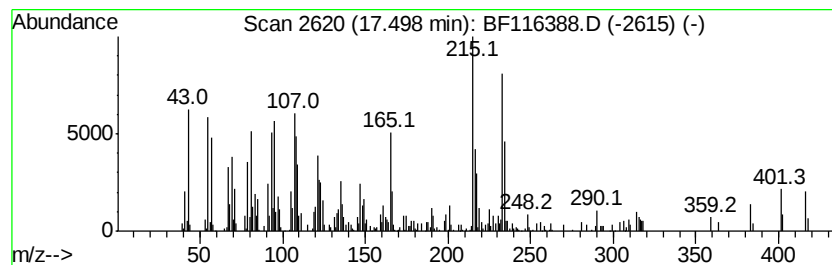
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Stigmastanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.50	23.78 ng	587837	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Stigmastanol	416	C29H52O	019466-47-8	83
2		Ergostanol	402	C28H50O	006538-02-9	49
3		5-(2-Methyloctan-2-yl)-3-(1R,3R-...	332	C22H36O2	070434-92-3	35
4		2-((1S,3S)-3-hydroxycyclohexyl)-...	332	C22H36O2	1000372-26-3	27
5		2-((1S,3R)-3-hydroxycyclohexyl)-...	332	C22H36O2	1000372-26-4	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
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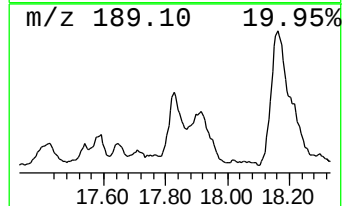
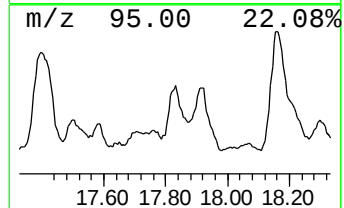
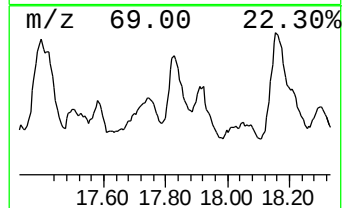
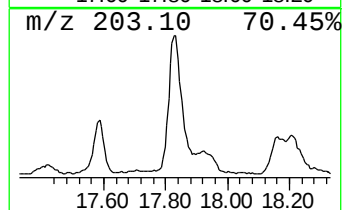
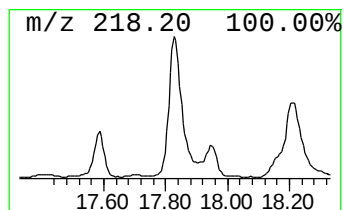
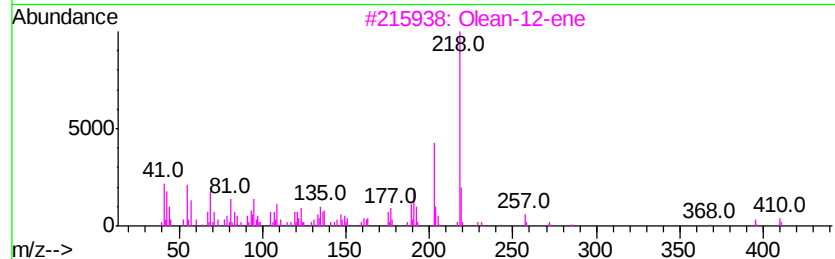
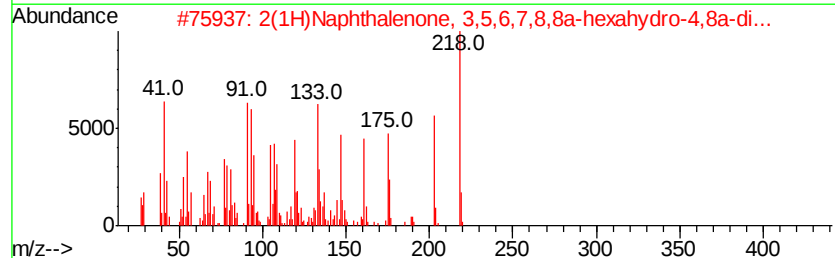
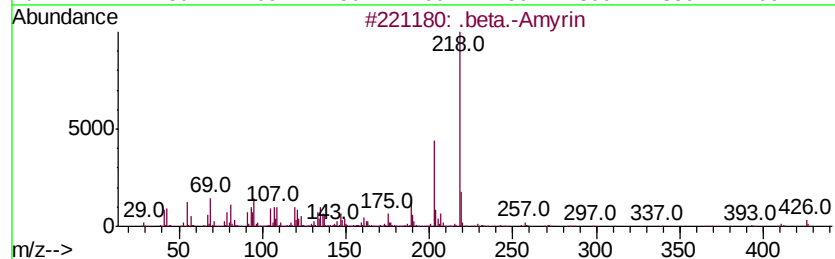
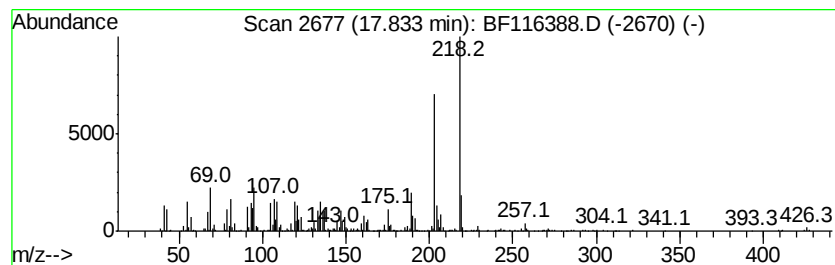
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 .beta.-Amyrin Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	48.99 ng	1210860	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Amyrin	426	C30H500	000559-70-6	87
2		2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H220	1000188-66-5	81
3		Olean-12-ene	410	C30H50	000471-68-1	72
4		2H-Cyclopropafalnaphthalen-2-one...	218	C15H220	006831-17-0	62
5		2,4(1H,3H)-Quinazolidinedione, 1,3...	218	C12H14N2O2	002049-84-5	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
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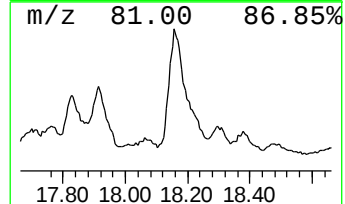
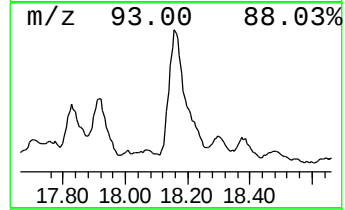
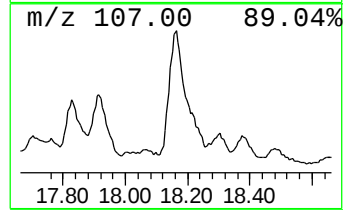
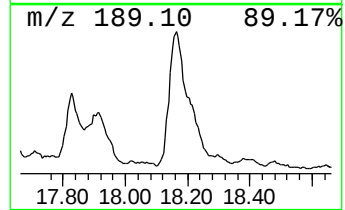
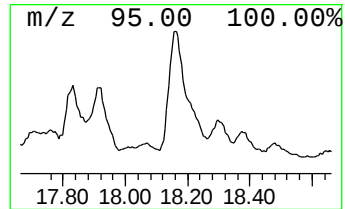
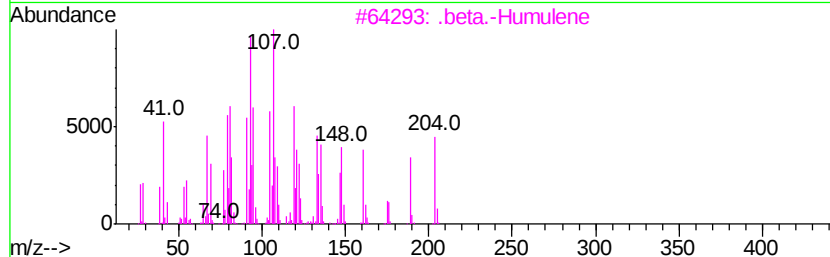
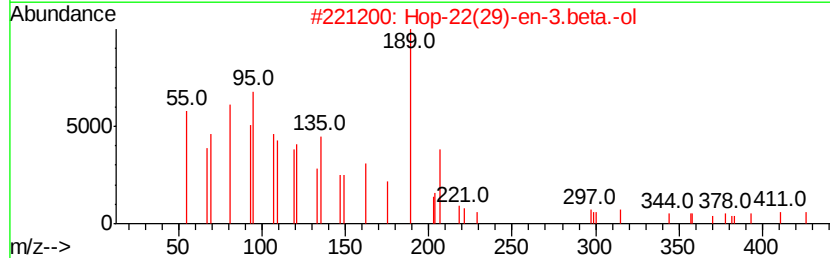
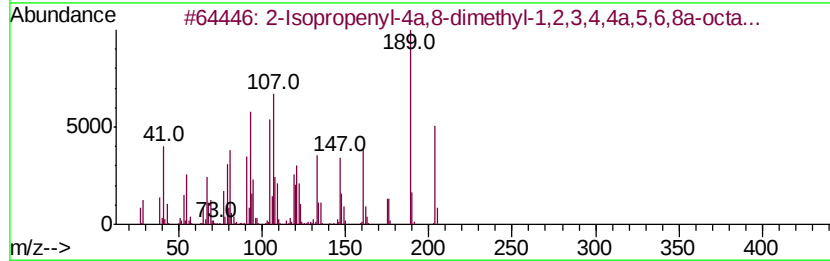
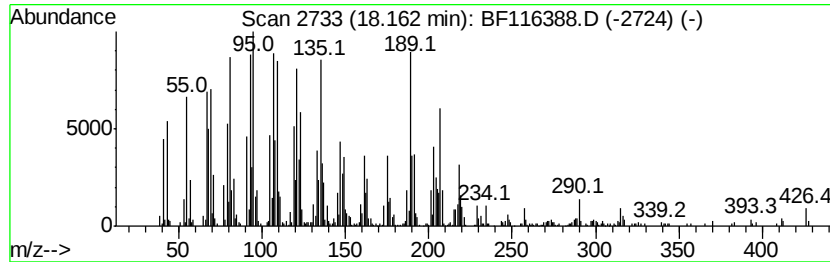
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 2-Isopropenyl-4a,8-dimethyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.16	142.17 ng	3513790	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0	93
2		Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	92
3		.beta.-Humulene	204	C15H24	000116-04-1	64
4		Taraxasterol	426	C30H50O	001059-14-9	62
5		Caparratriene	206	C15H26	1000374-08-7	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116388.D
Acq On : 19 Aug 2019 14:30
Operator : HP/JU
Sample : K4223-27
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-14

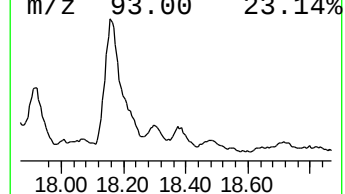
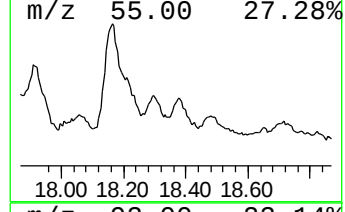
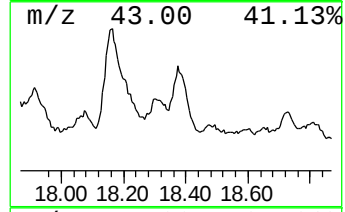
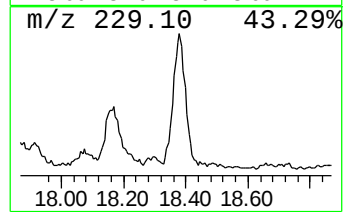
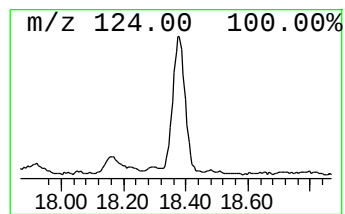
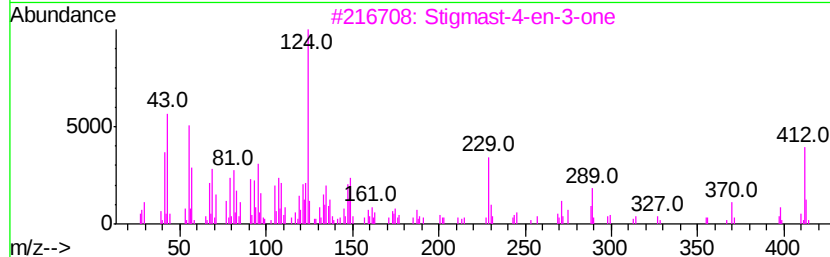
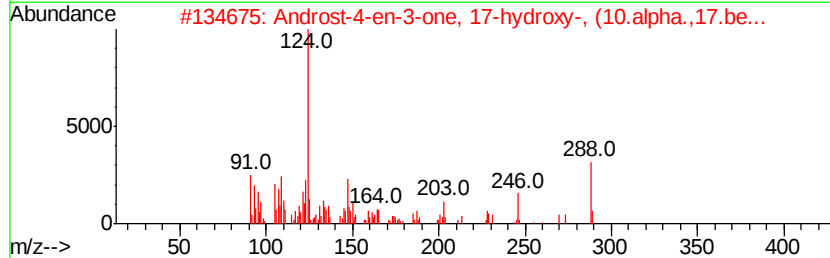
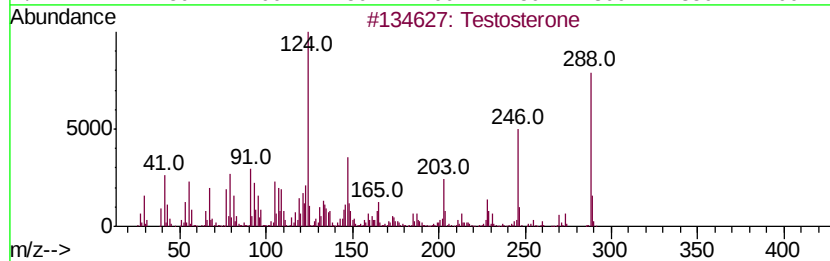
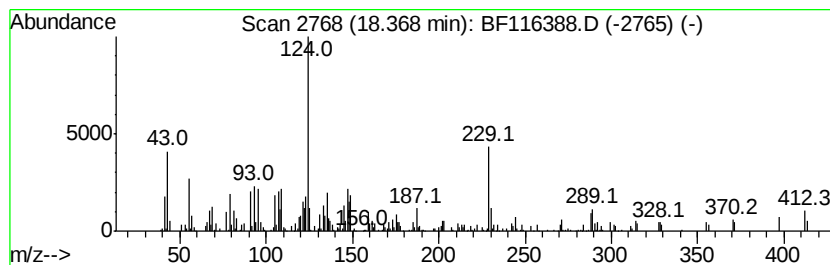
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Testosterone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	25.98 ng	642098	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Testosterone	288	C19H28O2	000058-22-0	92
2		Androst-4-en-3-one, 17-hydroxy-,...	288	C19H28O2	000604-39-7	70
3		Stigmast-4-en-3-one	412	C29H48O	001058-61-3	55
4		Androst-4-en-3-one, 17-hydroxy-,...	288	C19H28O2	000481-30-1	38
5		(2,3-Dichlorophenyl)carbamic aci...	311	C14H11Cl2N03	1000305-08-9	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116388.D
Acq On : 19 Aug 2019 14:30
Operator : HP/JU
Sample : K4223-27
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-14

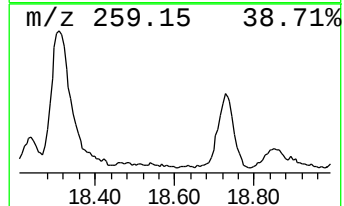
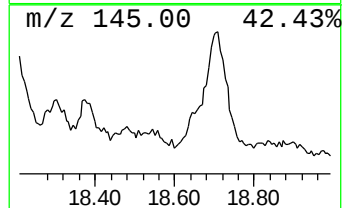
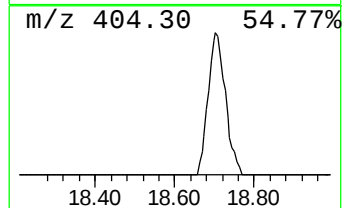
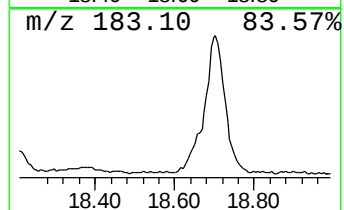
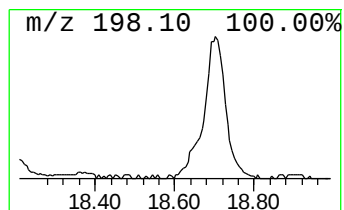
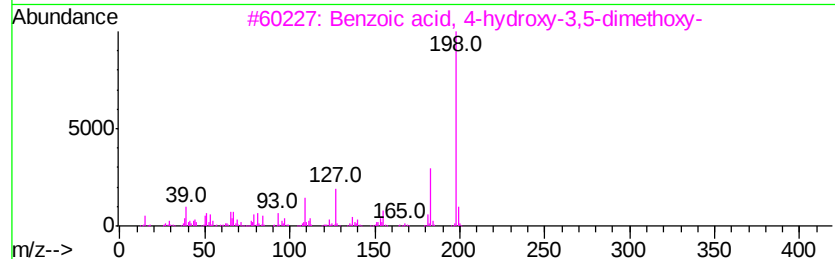
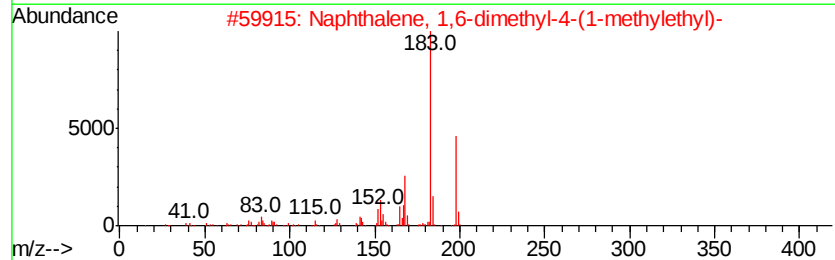
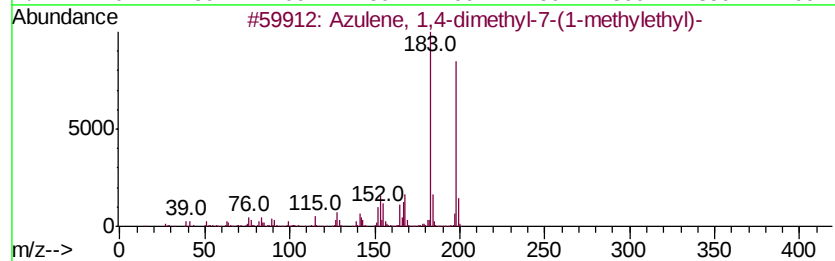
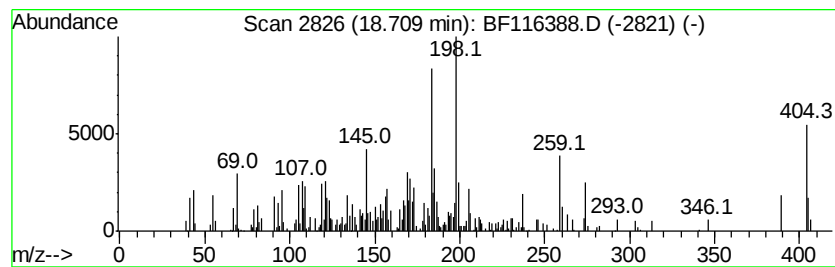
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Azulene, 1,4-dimethyl-7-(1-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.71	21.51 ng	531632	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Azulene, 1,4-dimethyl-7-(1-methyl-...	198	C15H18	000489-84-9	50
2		Naphthalene, 1,6-dimethyl-4-(1-methyl-...	198	C15H18	000483-78-3	50
3		Benzoic acid, 4-hydroxy-3,5-dimethoxy-	198	C9H10O5	000530-57-4	25
4		Benzenemethanol, 3,4,5-trimethoxy-	198	C10H14O4	003840-31-1	25
5		3H-Indol-3-one, 1,2-dihydro-2-(2-methyl-...	228	C14H16N2O	112338-29-1	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081919\
 Data File : BF116388.D
 Acq On : 19 Aug 2019 14:30
 Operator : HP/JU
 Sample : K4223-27
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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
unknown6.58	6.58	75.9	ng	3001460	1	6.80	791118	20.0
n-Hexadecanoic acid	11.86	27.9	ng	1419930	4	11.32	1018610	20.0
Phytol	12.46	12.0	ng	611130	4	11.32	1018610	20.0
Octadecanoic acid	12.63	10.7	ng	546551	4	11.32	1018610	20.0
Heptacosane	14.41	16.9	ng	1292590	5	13.96	1528830	20.0
Octadecane	14.71	16.8	ng	415069	6	15.42	494302	20.0
Supraene	14.78	17.0	ng	420223	6	15.42	494302	20.0
Benzo[e]pyrene	15.30	21.4	ng	528373	6	15.42	494302	20.0
.beta.-Tocopherol	15.64	10.3	ng	254197	6	15.42	494302	20.0
2-methyloctacosane	15.82	88.1	ng	2178450	6	15.42	494302	20.0
unknown15.87	15.87	15.5	ng	382735	6	15.42	494302	20.0
dl-.alpha.-Tocoph...	16.09	29.7	ng	734792	6	15.42	494302	20.0
Tetradecane, 2,6,...	16.30	13.9	ng	342957	6	15.42	494302	20.0
Stigmasterol	16.99	9.7	ng	240039	6	15.42	494302	20.0
Stigmastanol	17.50	23.8	ng	587837	6	15.42	494302	20.0
.beta.-Amyrin	17.83	49.0	ng	1210860	6	15.42	494302	20.0
2-Isopropenyl-4a,...	18.16	142.2	ng	3513790	6	15.42	494302	20.0
Testosterone	18.37	26.0	ng	642098	6	15.42	494302	20.0
Azulene, 1,4-dime...	18.71	21.5	ng	531632	6	15.42	494302	20.0