

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081919\
 Data File : BF116408.D
 Acq On : 20 Aug 2019 00:38
 Operator : HP/JU
 Sample : K4223-15
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-8

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	5.434	566	569	597	rBV	1737154	2148686	59.20%	4.563%
2	6.457	740	743	761	rBV	1696845	2338187	64.42%	4.965%
3	6.581	761	764	788	rVB	2161580	2446649	67.41%	5.195%
4	6.804	799	802	812	rVB	659965	580343	15.99%	1.232%
5	6.957	825	828	838	rBV	1959826	1751668	48.26%	3.720%
6	7.369	895	898	918	rBV	1536192	1494916	41.19%	3.174%
7	8.080	1016	1019	1033	rBV	790160	776119	21.38%	1.648%
8	9.151	1198	1201	1205	rBV	2546252	2326255	64.09%	4.940%
9	9.269	1218	1221	1225	rBV	143313	133540	3.68%	0.284%
10	9.486	1256	1258	1261	rVV	98104	79349	2.19%	0.168%
11	9.551	1265	1269	1273	rVV	499784	445954	12.29%	0.947%
12	9.586	1273	1275	1280	rVB2	39184	40778	1.12%	0.087%
13	9.833	1314	1317	1320	rBV	1147128	961257	26.48%	2.041%
14	9.904	1327	1329	1332	rVB	50473	39065	1.08%	0.083%
15	9.951	1333	1337	1341	rVV	164414	158534	4.37%	0.337%
16	10.063	1351	1356	1360	rVV5	36562	60296	1.66%	0.128%
17	10.122	1363	1366	1369	rVB2	57896	59477	1.64%	0.126%
18	10.410	1412	1415	1417	rBV	69902	61613	1.70%	0.131%
19	10.498	1428	1430	1433	rVB	53627	46549	1.28%	0.099%
20	10.557	1433	1440	1443	rBV5	41545	74185	2.04%	0.158%
21	10.627	1448	1452	1460	rVB	1849695	1831598	50.46%	3.889%
22	10.739	1467	1471	1476	rVB2	58474	70906	1.95%	0.151%
23	10.986	1510	1513	1517	rBV3	46875	58458	1.61%	0.124%
24	11.033	1518	1521	1524	rVB3	40221	40412	1.11%	0.086%
25	11.269	1558	1561	1564	rBV3	29319	39005	1.07%	0.083%
26	11.321	1564	1570	1573	rBV	1155537	1097431	30.24%	2.330%
27	11.345	1573	1574	1576	rVV	133179	103024	2.84%	0.219%
28	11.363	1576	1577	1580	rVB	119115	83677	2.31%	0.178%
29	11.451	1589	1592	1595	rVB	101577	91867	2.53%	0.195%
30	11.692	1631	1633	1637	rVB3	37006	44751	1.23%	0.095%
31	11.774	1644	1647	1648	rBV	98246	87280	2.40%	0.185%
32	11.798	1648	1651	1655	rVV2	153045	213368	5.88%	0.453%
33	11.851	1655	1660	1672	rVV	1343724	1520585	41.89%	3.229%
34	12.004	1683	1686	1689	rVB	216914	165764	4.57%	0.352%

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 Integrator: RTE
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.098	1698	1702	1703	rBV3	41784	43598	1.20%	0.093%
36	12.192	1716	1718	1722	rVB3	52879	52376	1.44%	0.111%
37	12.251	1722	1728	1731	rBV6	61145	99571	2.74%	0.211%
38	12.351	1742	1745	1752	rBV	674143	771906	21.27%	1.639%
39	12.451	1759	1762	1773	rVB	390349	479179	13.20%	1.017%
40	12.568	1773	1782	1789	rBV4	1012377	2080800	57.33%	4.418%
41	12.627	1789	1792	1800	rVB	379195	436312	12.02%	0.926%
42	12.721	1805	1808	1811	rVB3	54882	52916	1.46%	0.112%
43	12.768	1813	1816	1819	rVB	208858	206456	5.69%	0.438%
44	12.898	1834	1838	1842	rBV	2653299	2364832	65.15%	5.022%
45	13.068	1864	1867	1869	rBV3	33842	49504	1.36%	0.105%
46	13.098	1869	1872	1875	rBV	150729	178605	4.92%	0.379%
47	13.163	1881	1883	1887	rBV3	43196	55571	1.53%	0.118%
48	13.292	1902	1905	1907	rBV2	99106	118252	3.26%	0.251%
49	13.321	1908	1910	1912	rBV	224485	225093	6.20%	0.478%
50	13.392	1920	1922	1924	rBV	74620	50566	1.39%	0.107%
51	13.580	1952	1954	1958	rBV4	41233	43553	1.20%	0.092%
52	13.745	1976	1982	1984	rBV4	73446	140302	3.87%	0.298%
53	13.786	1985	1989	1996	rVV2	646853	754251	20.78%	1.602%
54	13.868	2001	2003	2008	rBV	98952	113838	3.14%	0.242%
55	13.921	2009	2012	2015	rBV	534182	474051	13.06%	1.007%
56	13.962	2015	2019	2023	rBV	806455	793174	21.85%	1.684%
57	14.104	2041	2043	2045	rVB	58018	43653	1.20%	0.093%
58	14.409	2091	2095	2102	rBV2	565393	788908	21.74%	1.675%
59	14.604	2126	2128	2130	rBV	76893	66597	1.83%	0.141%
60	14.662	2135	2138	2140	rVV	81926	77464	2.13%	0.164%
61	14.704	2143	2145	2148	rVB	106214	93920	2.59%	0.199%
62	14.780	2154	2158	2166	rVB	239344	272562	7.51%	0.579%
63	14.921	2179	2182	2187	rBV3	93443	142635	3.93%	0.303%
64	15.033	2197	2201	2204	rBV	1387603	1466146	40.39%	3.113%
65	15.057	2204	2205	2211	rVB	201203	233173	6.42%	0.495%
66	15.286	2241	2244	2255	rVB2	98999	188293	5.19%	0.400%
67	15.368	2256	2258	2260	rVV	58547	70670	1.95%	0.150%
68	15.421	2264	2267	2275	rVB	564433	735228	20.26%	1.561%
69	15.639	2301	2304	2311	rVB2	79624	124957	3.44%	0.265%
70	15.715	2314	2317	2324	rVV2	78132	132376	3.65%	0.281%
71	15.815	2328	2334	2339	rVV	927090	1339380	36.90%	2.844%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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72	15.868	2339	2343	2351	rVB	129636	240538	6.63%	0.511%
73	15.986	2360	2363	2370	rVB7	64742	94174	2.59%	0.200%
74	16.080	2374	2379	2388	rVB2	253762	463081	12.76%	0.983%
75	16.968	2525	2530	2546	rVB8	134463	374204	10.31%	0.795%
76	17.139	2554	2559	2564	rBV4	77020	161110	4.44%	0.342%
77	17.303	2582	2587	2591	rBV2	118009	216508	5.97%	0.460%
78	17.386	2592	2601	2613	rVV8	963884	3629618	100.00%	7.707%
79	17.486	2613	2618	2629	rVB5	193117	580348	15.99%	1.232%
80	17.815	2668	2674	2684	rBV	442704	1203108	33.15%	2.555%
81	18.150	2723	2731	2736	rBV2	566683	1648168	45.41%	3.500%
82	18.292	2750	2755	2762	rVB5	163952	391115	10.78%	0.830%
83	18.368	2763	2768	2778	rVB4	208859	550118	15.16%	1.168%
84	18.697	2819	2824	2836	rVB5	228755	709659	19.55%	1.507%

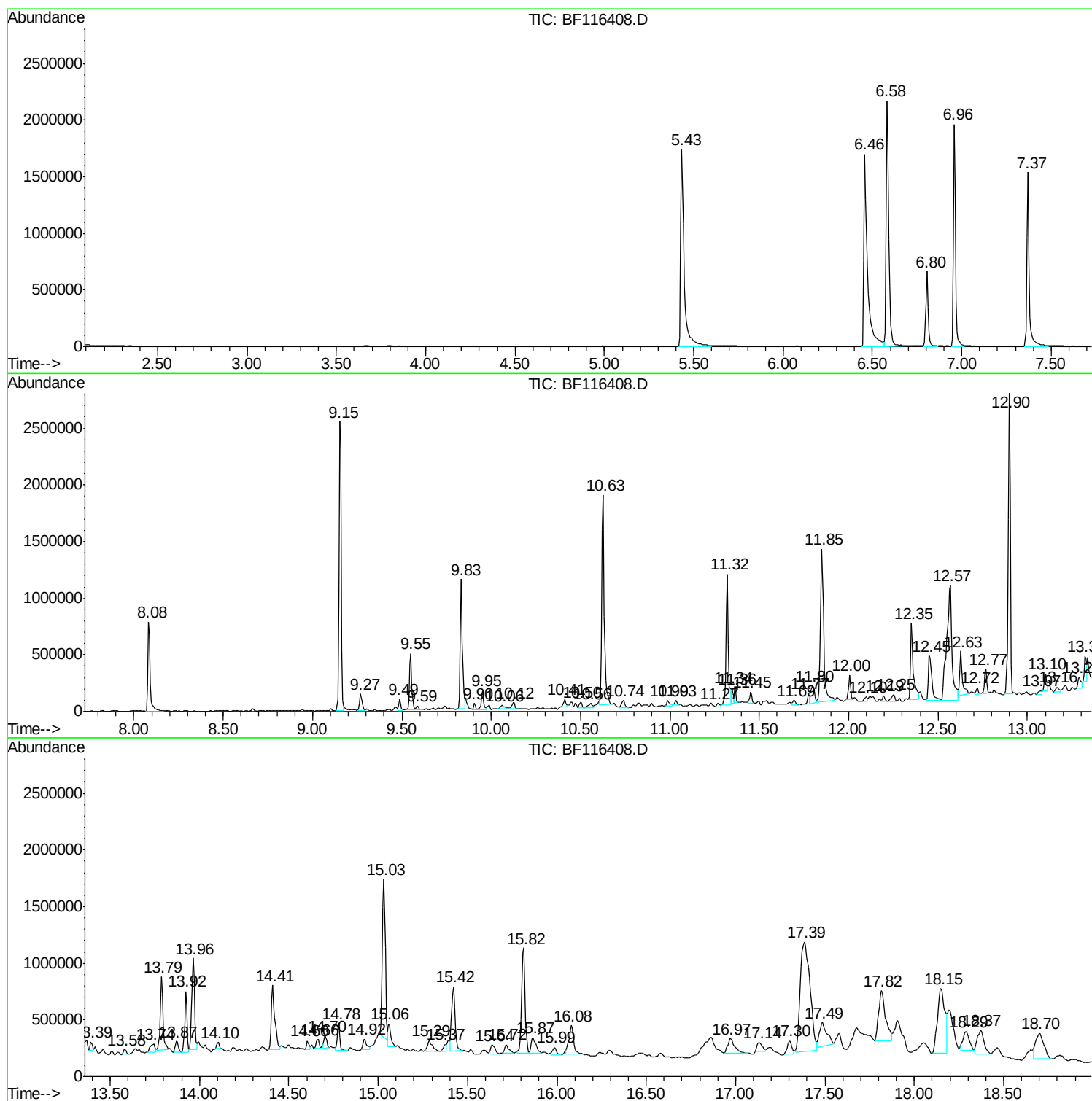
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Instrument :
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : K4223-15
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Instrument :
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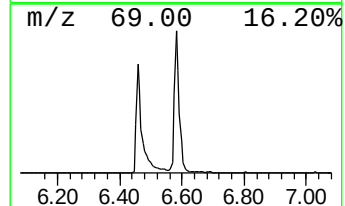
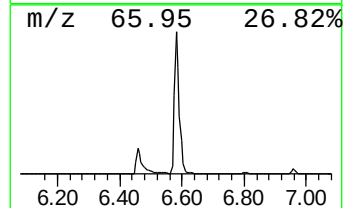
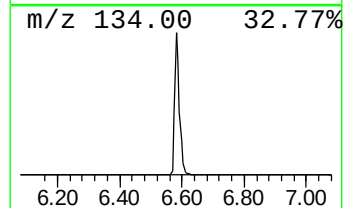
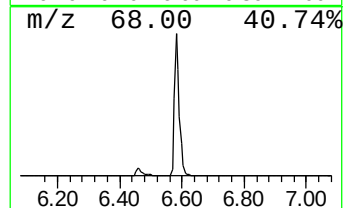
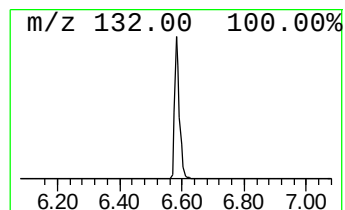
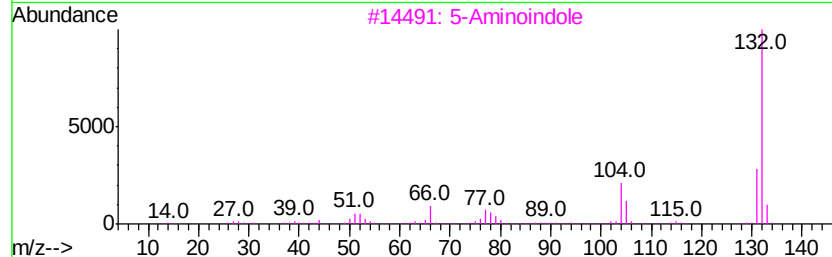
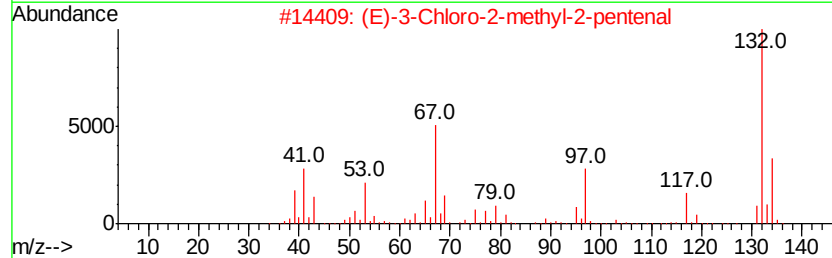
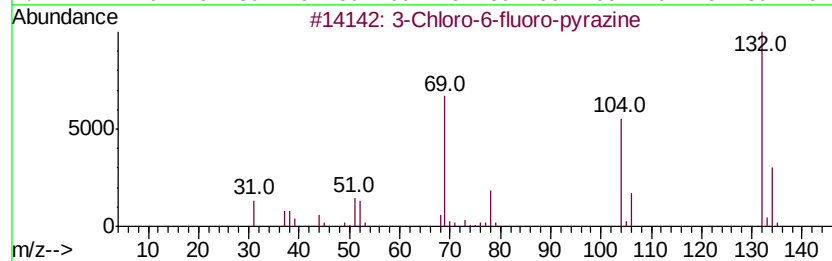
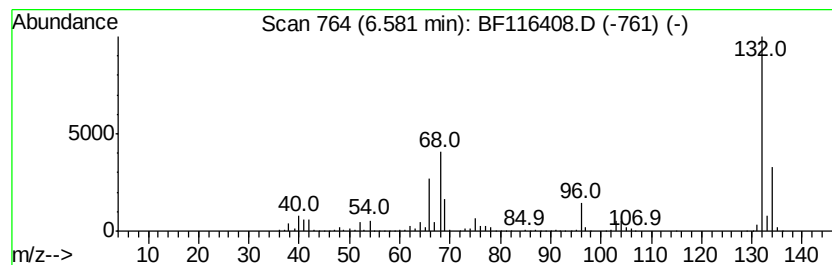
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	84.32 ng	2446650	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	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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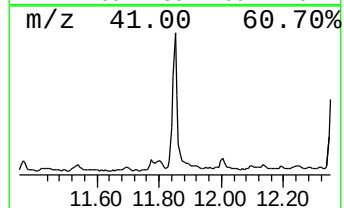
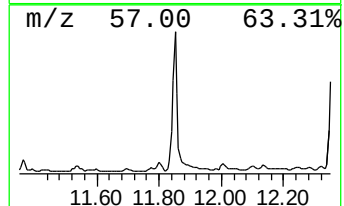
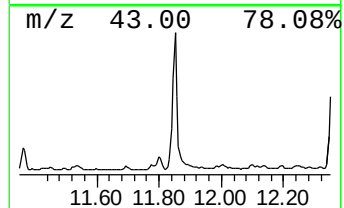
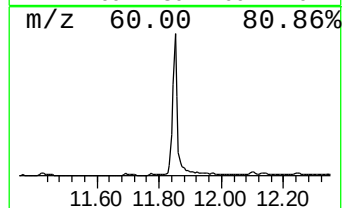
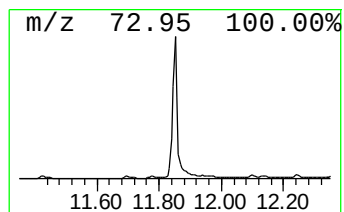
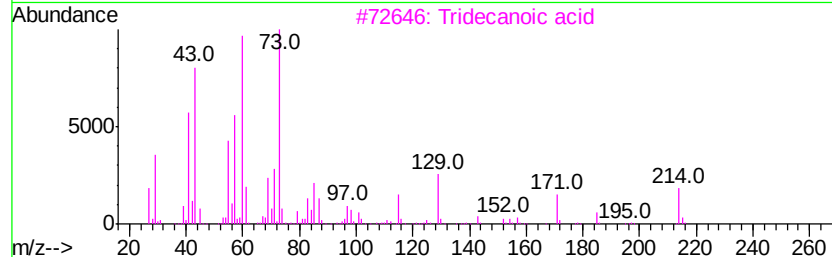
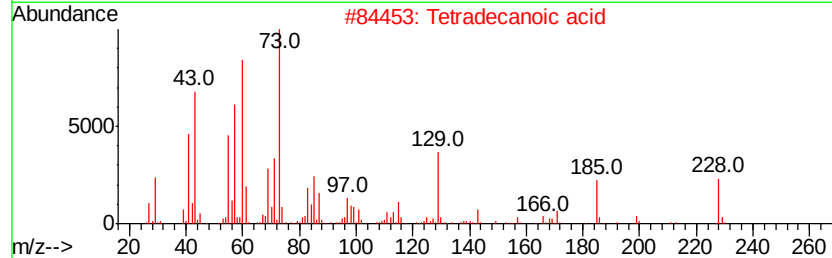
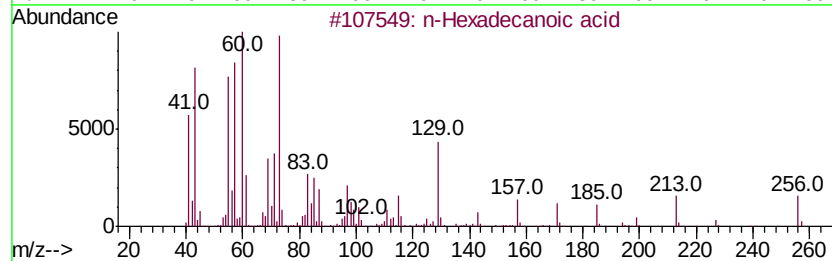
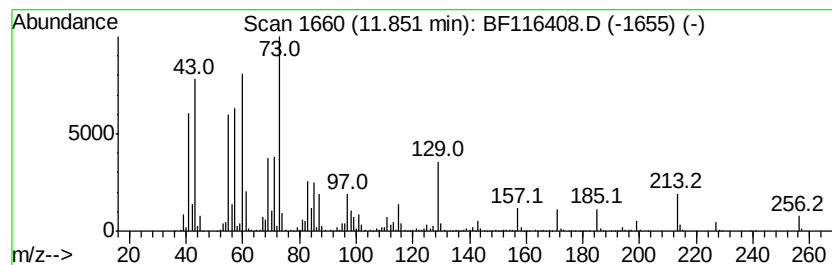
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073019.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	27.71 ng	1520590	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3		Tridecanoic acid	214	C13H26O2	000638-53-9	90
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5		Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	18



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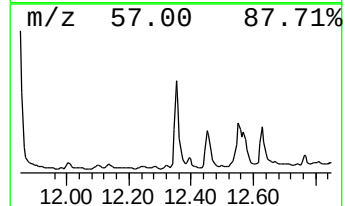
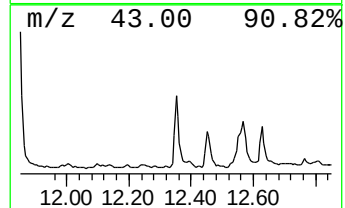
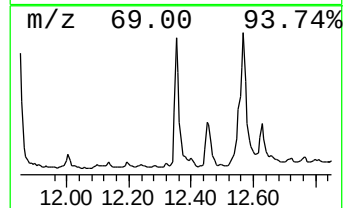
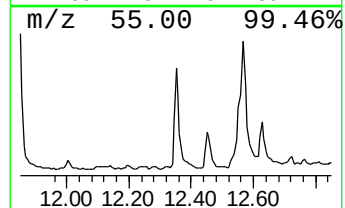
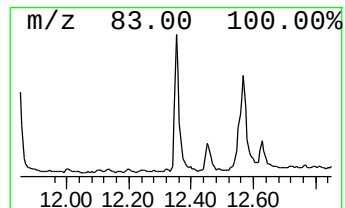
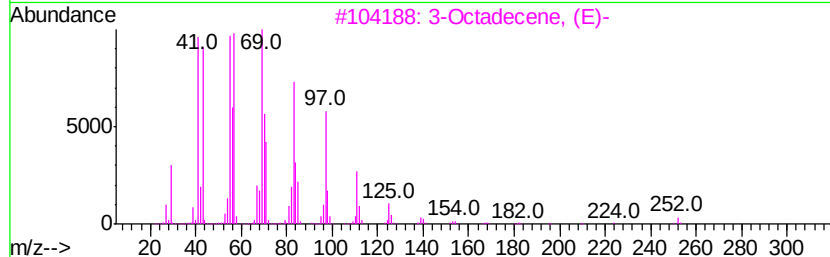
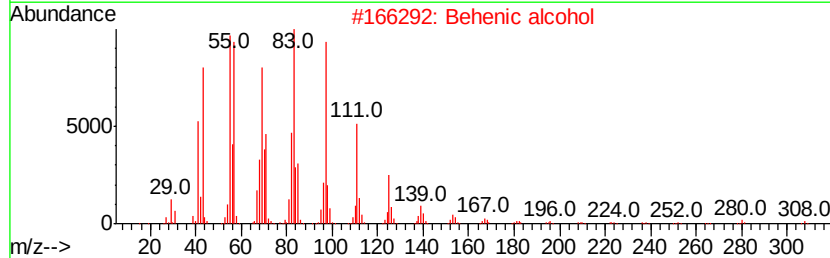
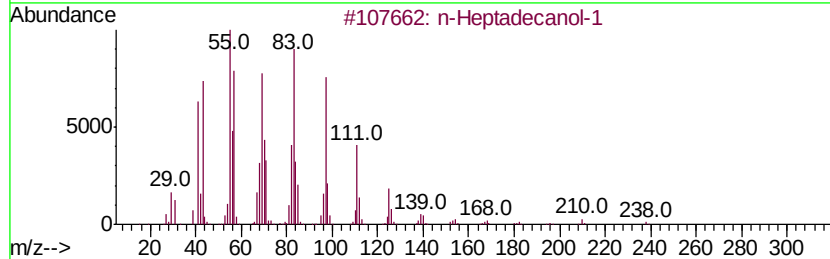
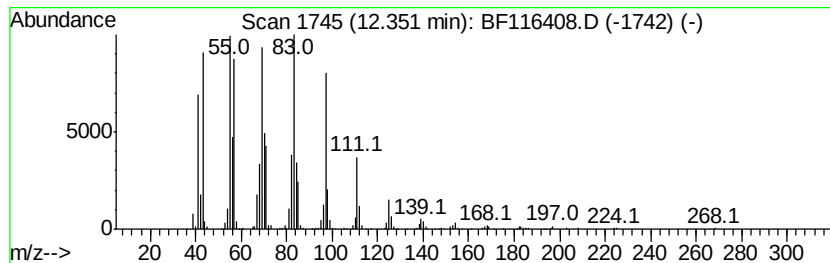
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Heptadecanol-1 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.35	14.07 ng	771906	Phenanthrene-d10	11.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		n-Heptadecanol-1	256 C17H36O	001454-85-9 95
2		Behenic alcohol	326 C22H46O	000661-19-8 91
3		3-Octadecene, (E)-	252 C18H36	007206-19-1 91
4		5-Octadecene, (E)-	252 C18H36	007206-21-5 91
5		1-Nonadecene	266 C19H38	018435-45-5 91



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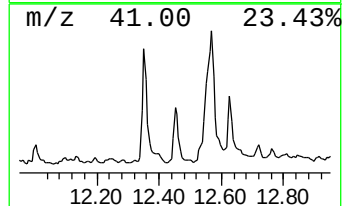
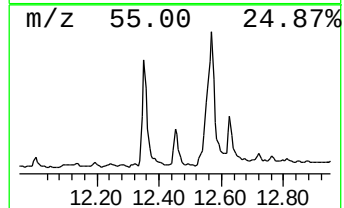
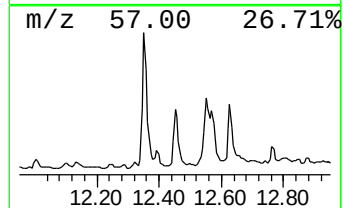
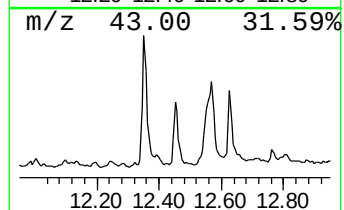
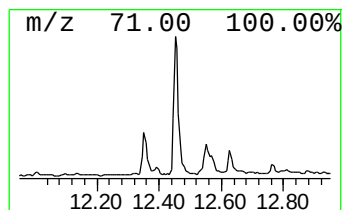
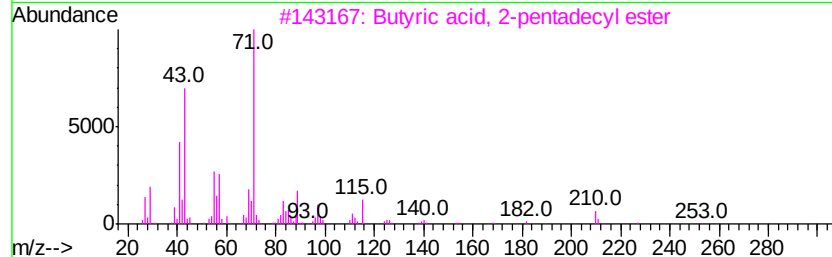
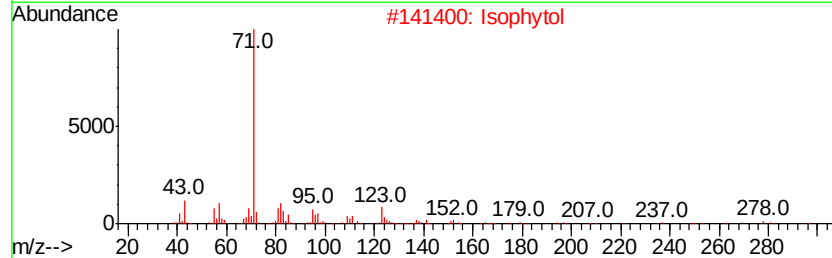
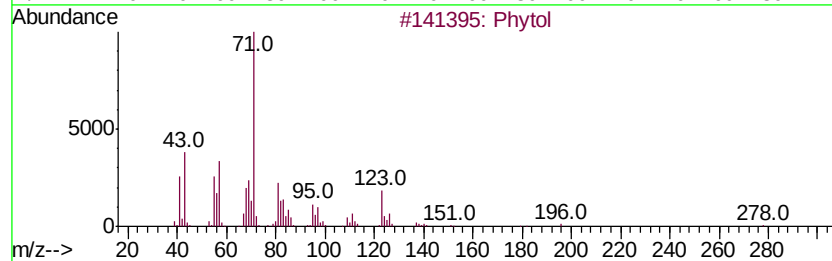
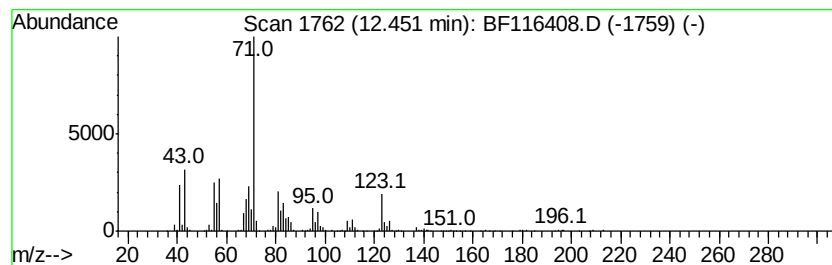
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Phytol Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.45	8.73 ng	479179	Phenanthrene-d10	11.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phytol	296	C20H40O	000150-86-7	90
2	Isophytol	296	C20H40O	000505-32-8	72
3	Butyric acid, 2-pentadecyl ester	298	C19H38O2	107853-73-6	58
4	Butyric acid, 3-tridecyl ester	270	C17H34O2	1000280-56-8	50
5	Butyric acid, 3-tetradecyl ester	284	C18H36O2	1000280-57-1	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116408.D
Acq On : 20 Aug 2019 00:38
Operator : HP/JU
Sample : K4223-15
Misc :
ALS Vial : 17 Sample Multiplier: 1

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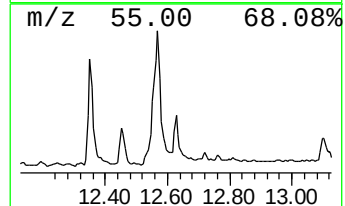
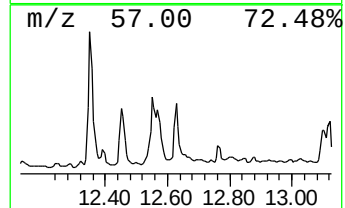
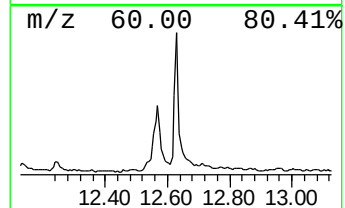
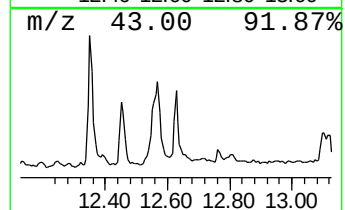
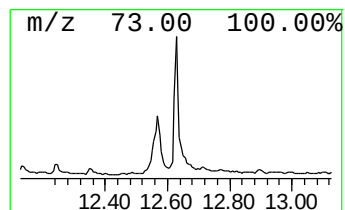
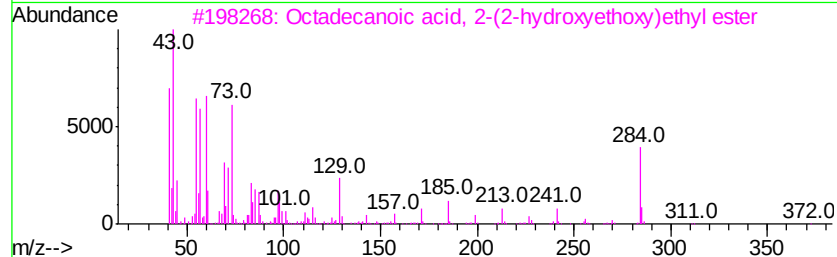
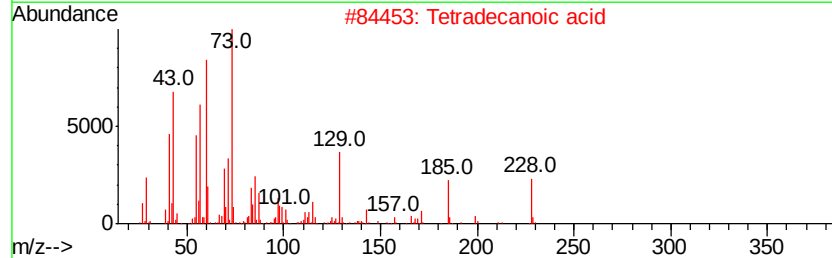
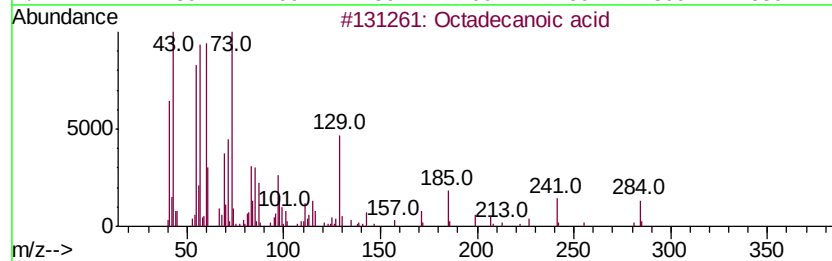
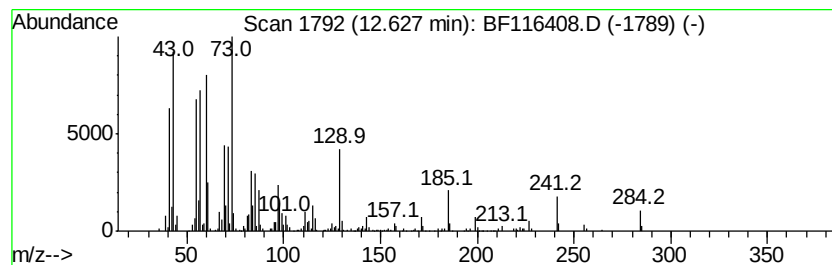
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	7.95 ng	436312	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	87
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5		n-Decanoic acid	172	C10H20O2	000334-48-5	68



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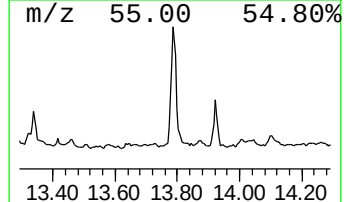
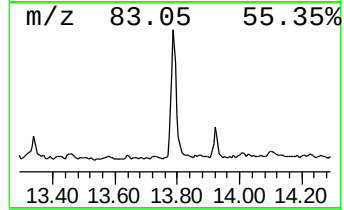
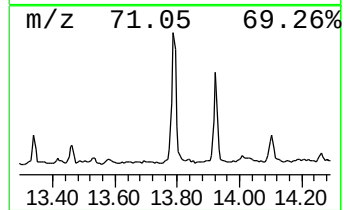
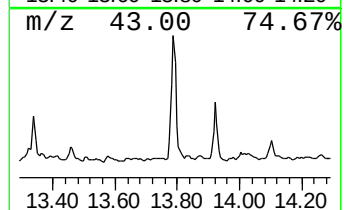
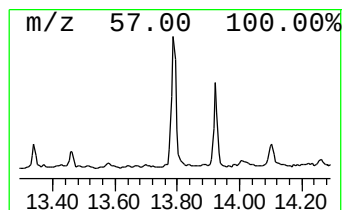
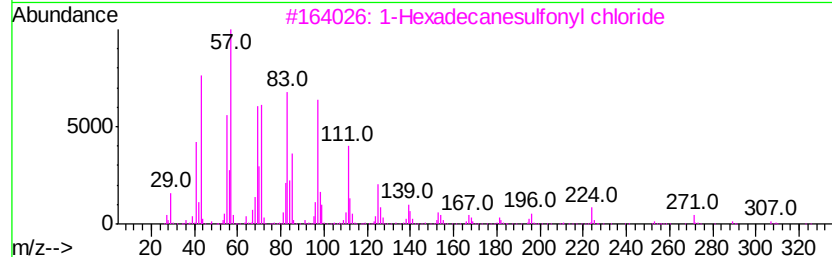
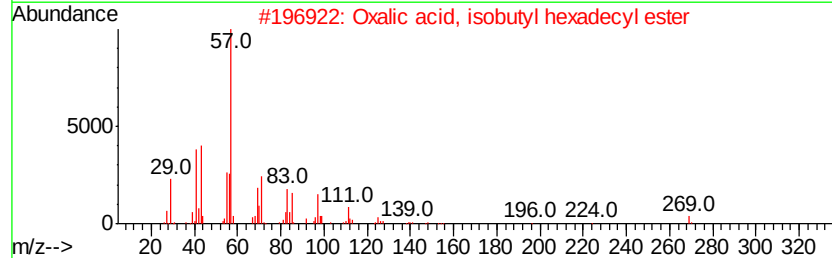
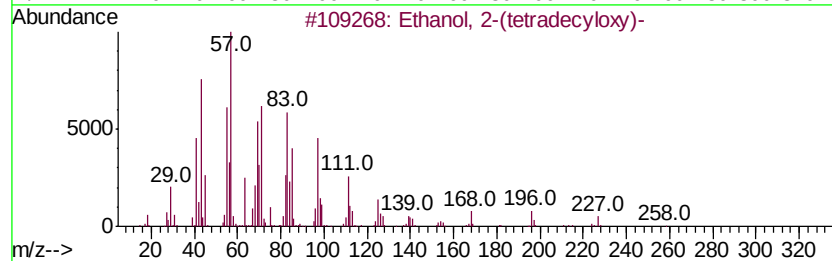
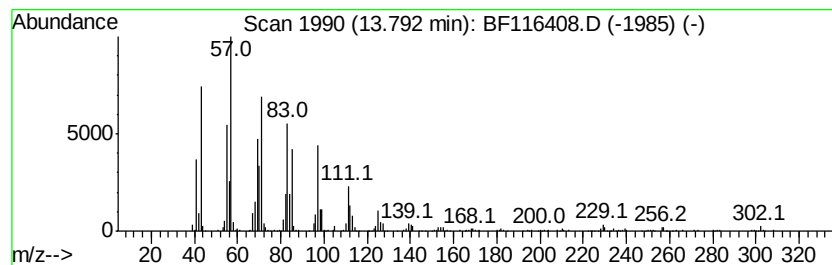
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	19.02 ng	754251	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2		Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
3		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	90
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
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Sample : K4223-15
Misc :
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ClientSampleId :
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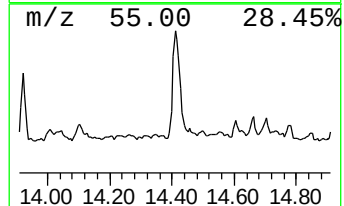
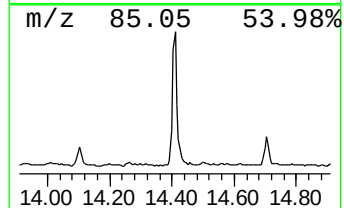
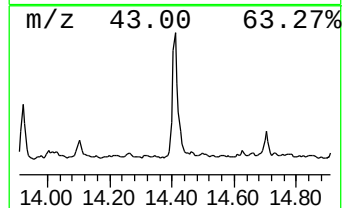
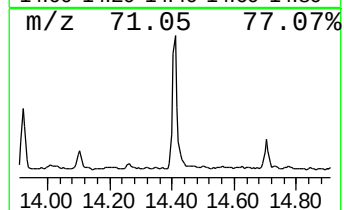
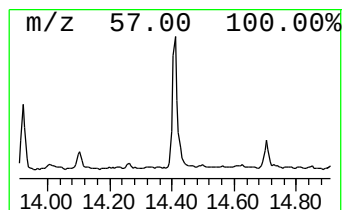
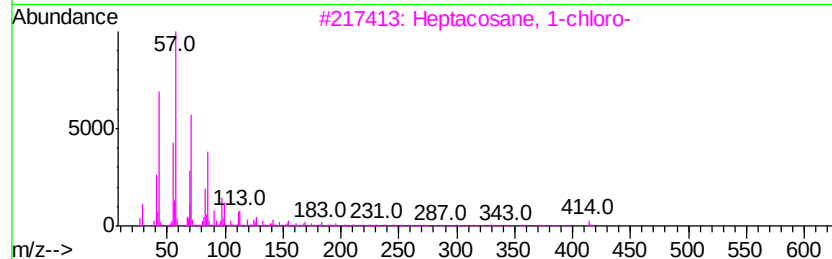
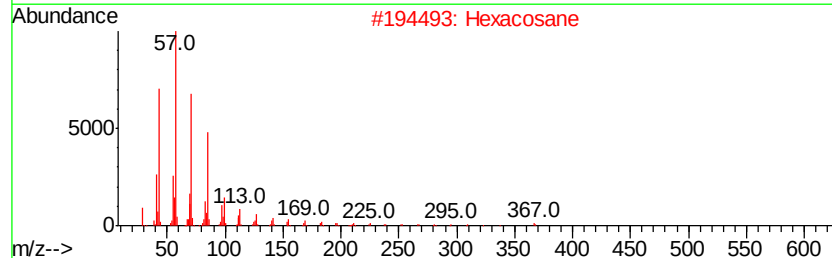
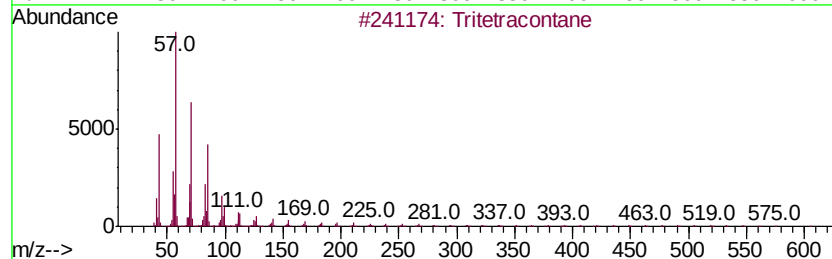
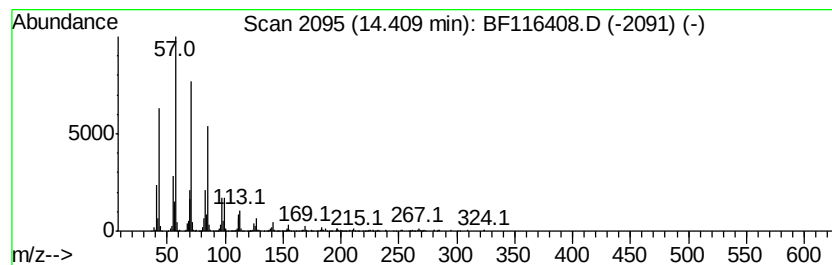
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tritetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	19.89 ng	788908	Chrysene-d12	13.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tritetracontane	605	C43H88	007098-21-7	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	91
4		Octacosane	394	C28H58	000630-02-4	87
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86



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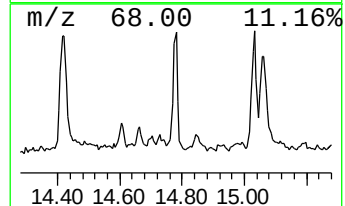
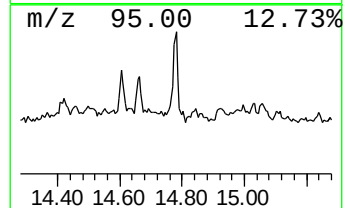
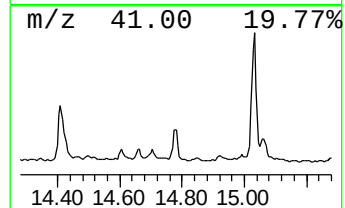
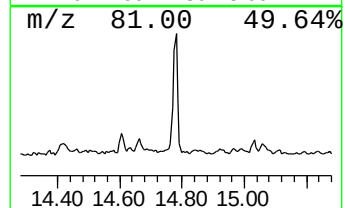
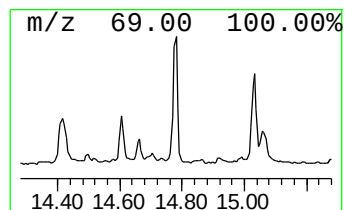
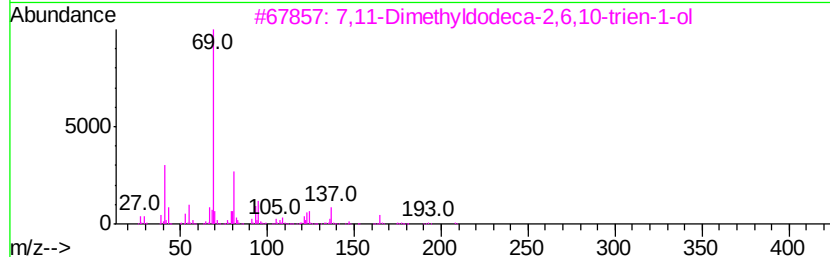
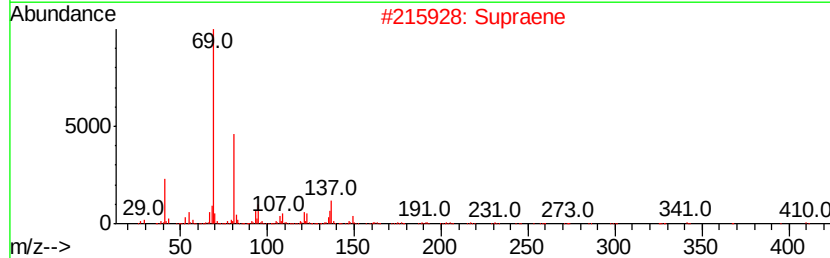
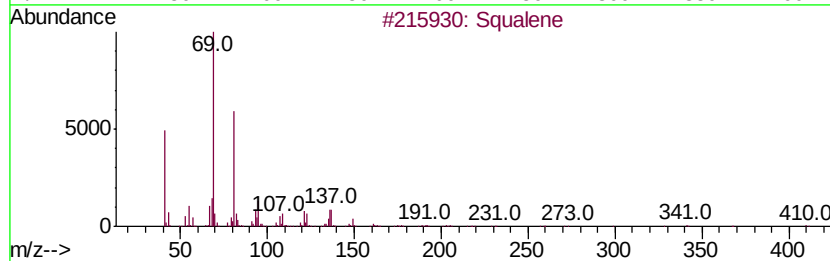
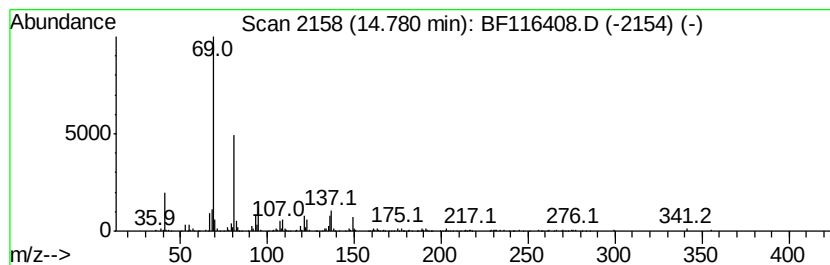
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.78	7.41 ng	272562	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	78
4		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	74
5		3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	56



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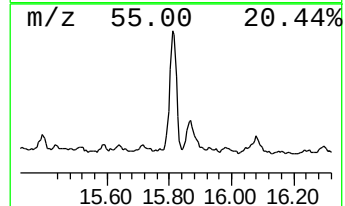
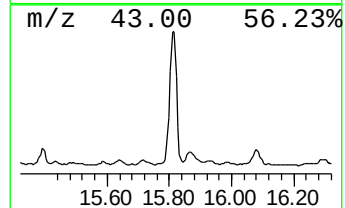
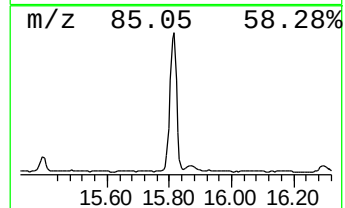
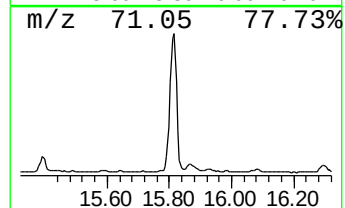
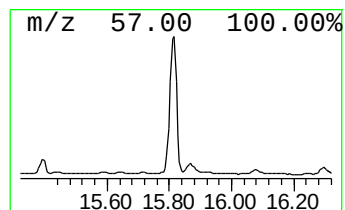
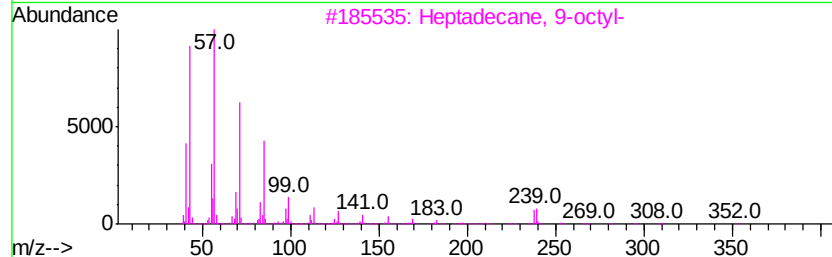
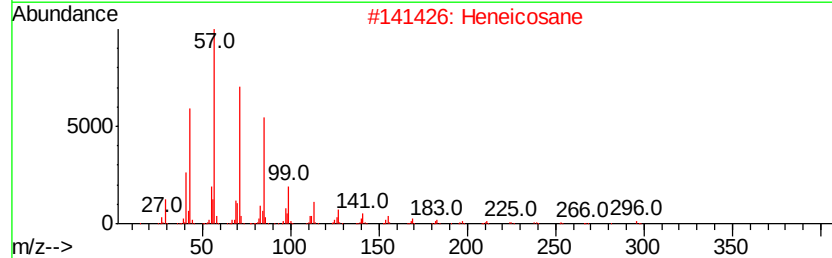
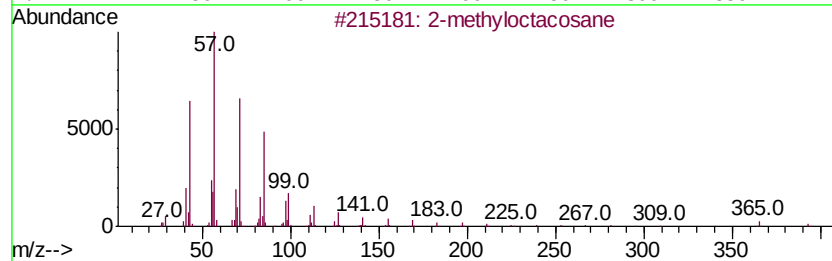
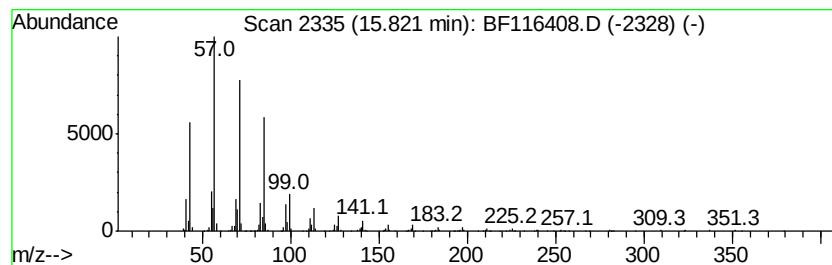
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.82	36.43 ng	1339380	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-octyl-	352	C25H52	007225-64-1	91
4		Hexacosane	366	C26H54	000630-01-3	90
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90



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Data File : BF116408.D
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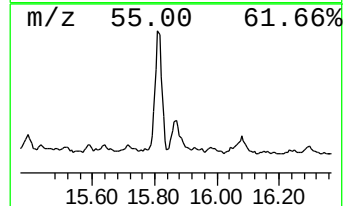
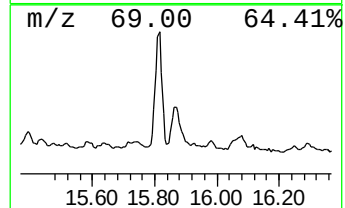
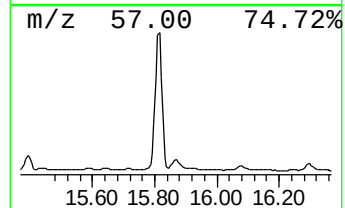
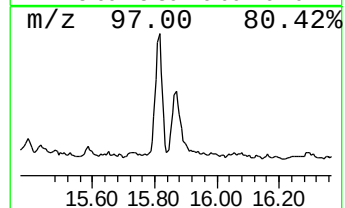
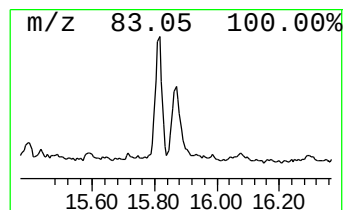
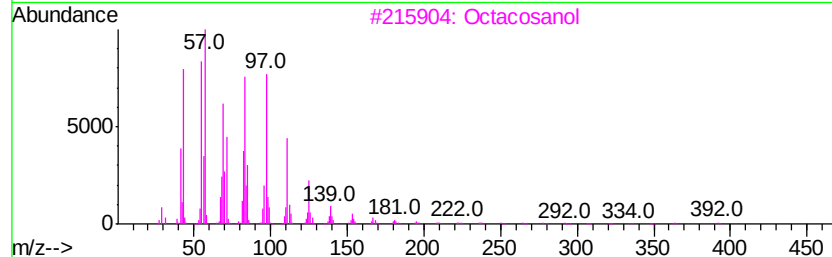
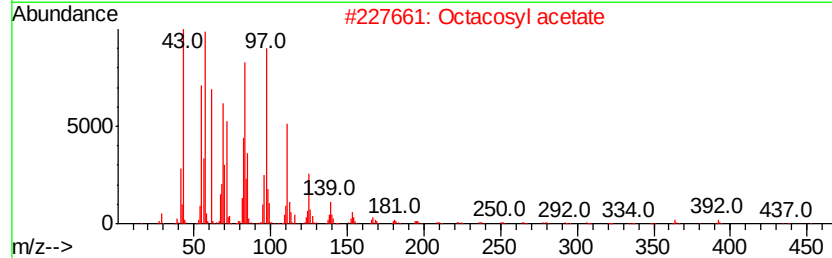
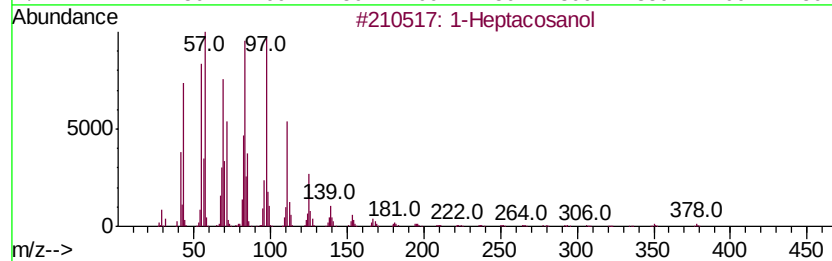
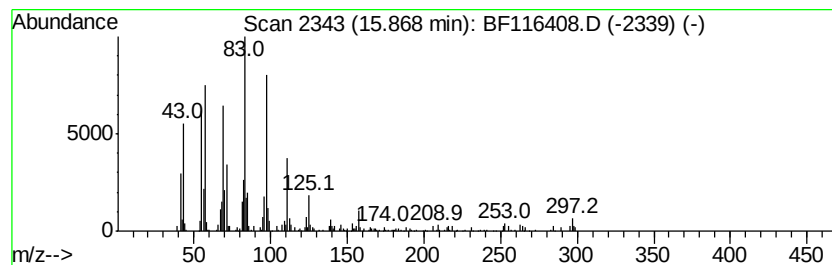
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Heptacosanol Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	6.54 ng	240538	Perylene-d12	15.42

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	60
2			Octacosyl acetate	452	C30H60O2	018206-97-8	60
3			Octacosanol	410	C28H58O	000557-61-9	53
4			1-Heneicosanol	312	C21H44O	015594-90-8	53
5			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	53



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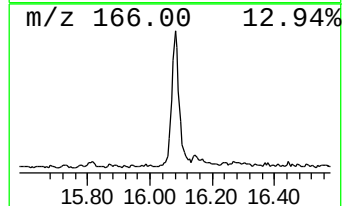
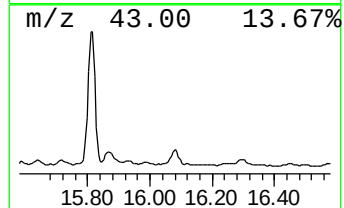
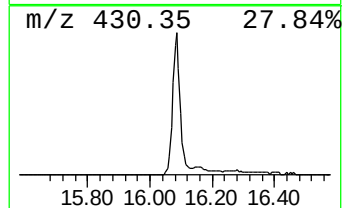
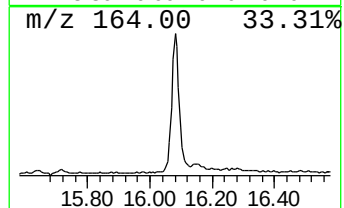
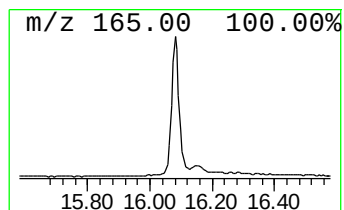
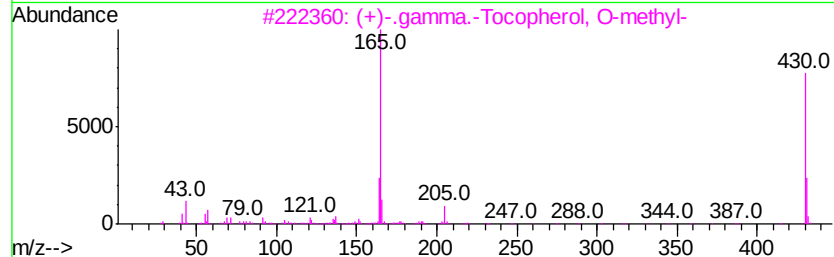
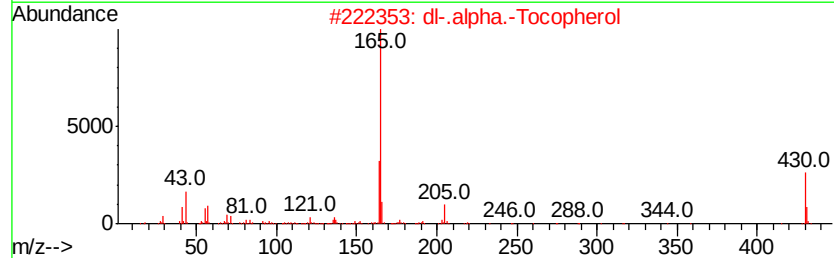
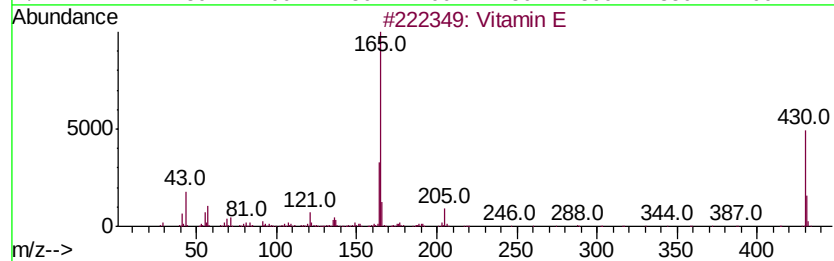
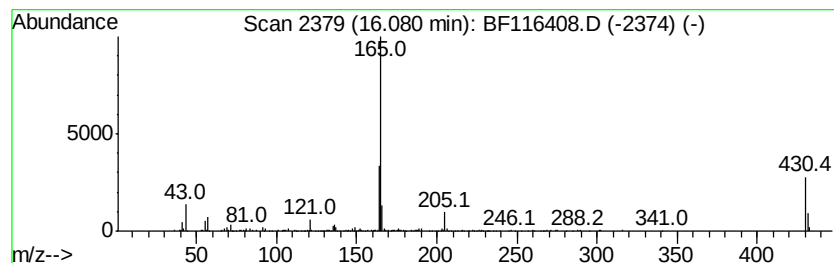
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Vitamin E Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	12.60 ng	463081	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Vitamin E	430	C29H50O2	000059-02-9	96
2		dl-.alpha.-Tocopherol	430	C29H50O2	010191-41-0	95
3		(+)-.gamma.-Tocopherol, O-methyl-	430	C29H50O2	1000374-72-2	94
4		.alpha.-Tocopherol-.beta.-D-mann...	592	C35H60O7	1000156-68-2	53
5		Benzenamine, 3-methoxy-2,4,6-tri...	165	C10H15NO	034874-88-9	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116408.D
Acq On : 20 Aug 2019 00:38
Operator : HP/JU
Sample : K4223-15
Misc :
ALS Vial : 17 Sample Multiplier: 1

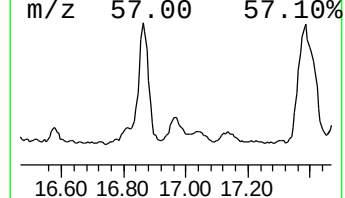
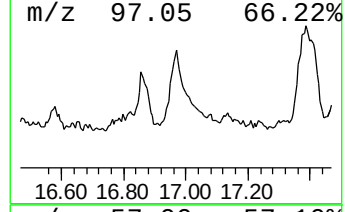
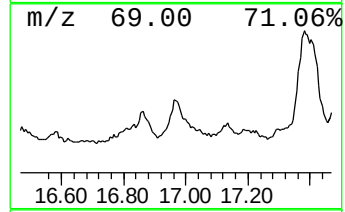
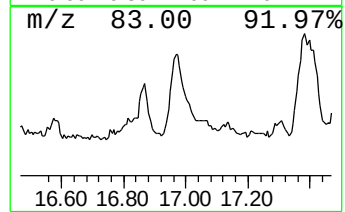
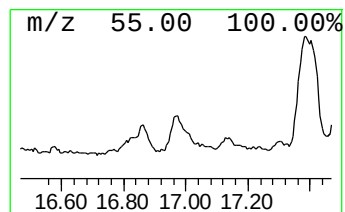
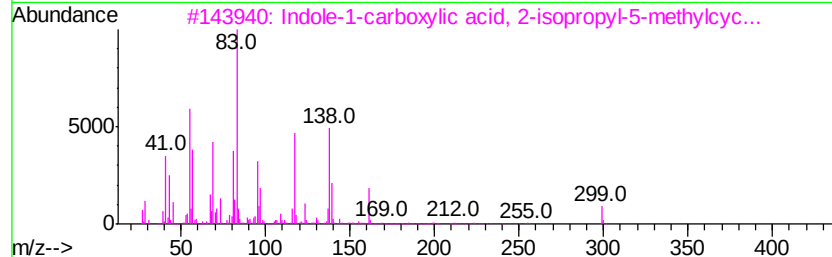
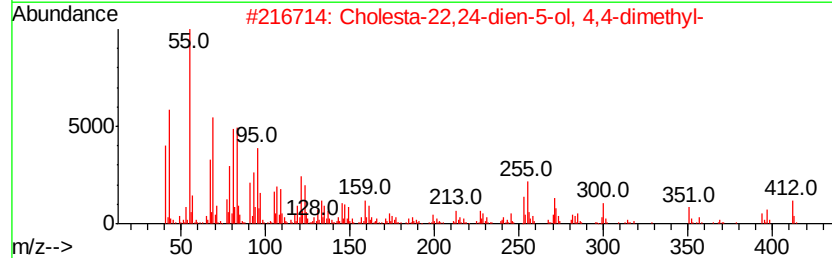
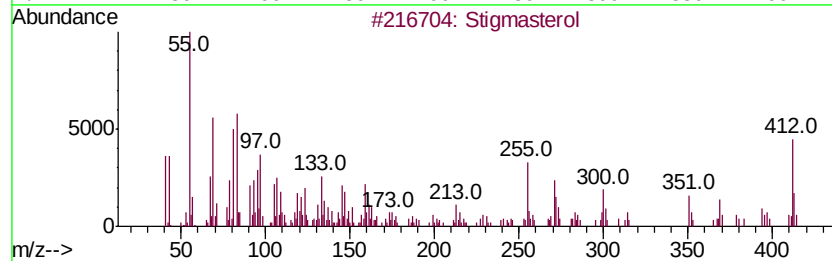
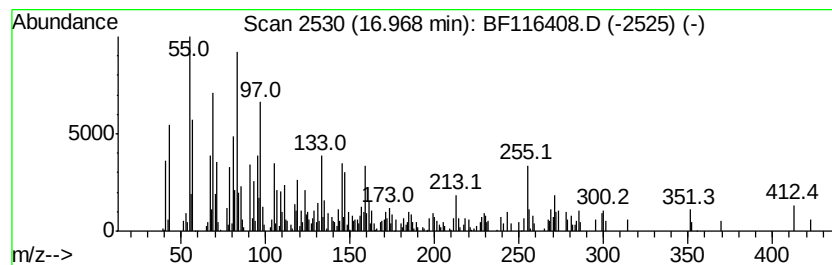
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Stigmasterol Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.97	10.18 ng	374204	Perylene-d12	15.42
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Stigmasterol	412 C29H48O	000083-48-7 80
2		Cholesta-22,24-dien-5-ol, 4,4-di...	412 C29H48O	1000128-66-1 46
3		Indole-1-carboxylic acid, 2-isop...	299 C19H25NO2	1000210-71-4 38
4		10-Chlorodecanol, dimethylpenta...	416 C18H26ClF5OSi	1000368-75-4 32
5		Ergosta-5,22-dien-3-ol, 24-methy...	412 C29H48O	053755-22-9 27



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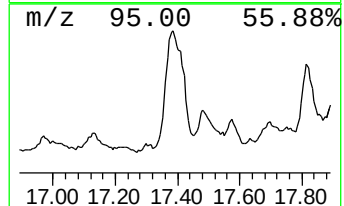
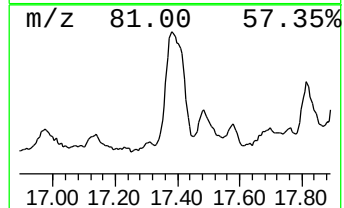
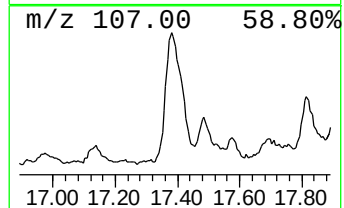
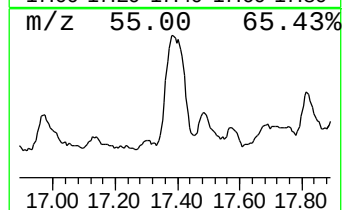
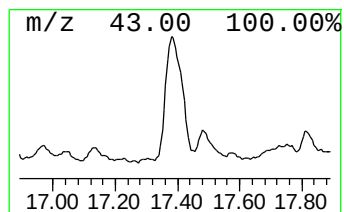
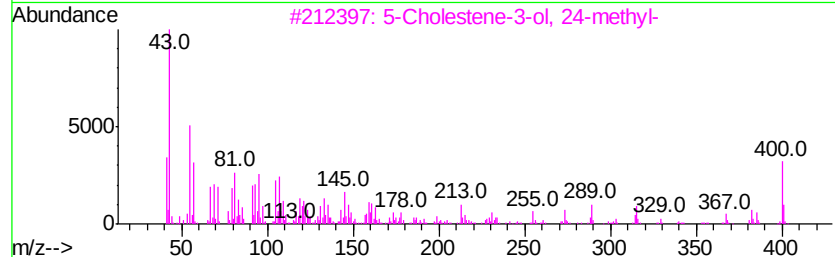
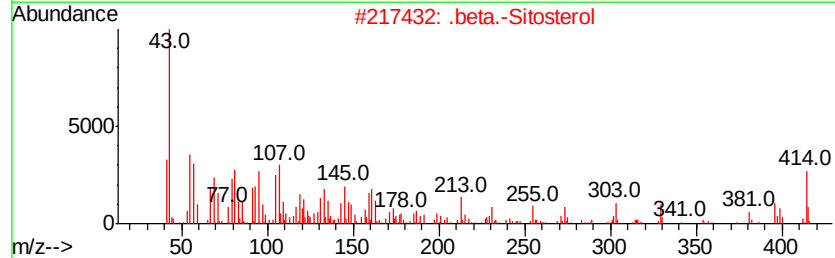
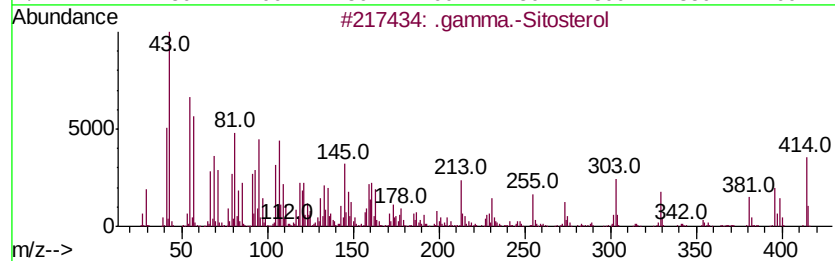
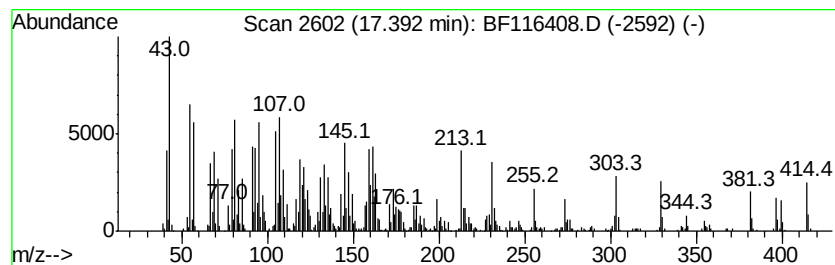
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 .gamma.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.39	98.73 ng	3629620	Perylene-d12	15.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	99
3	5-Cholestene-3-ol, 24-methyl-	400	C28H48O	1000214-17-4	68
4	Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	49
5	Isocholesteryl methyl ether	400	C28H48O	029944-53-4	38



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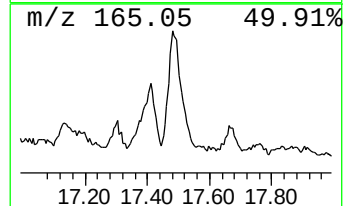
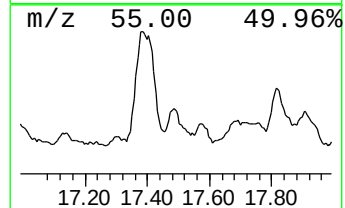
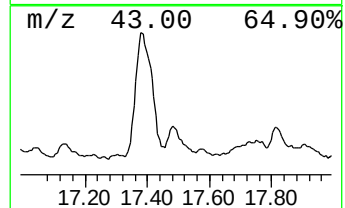
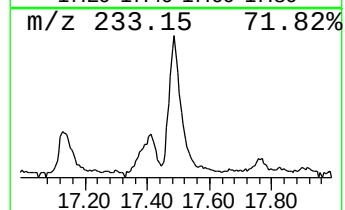
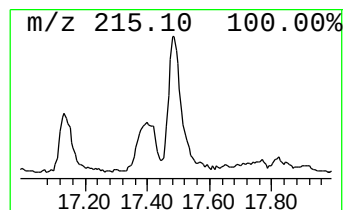
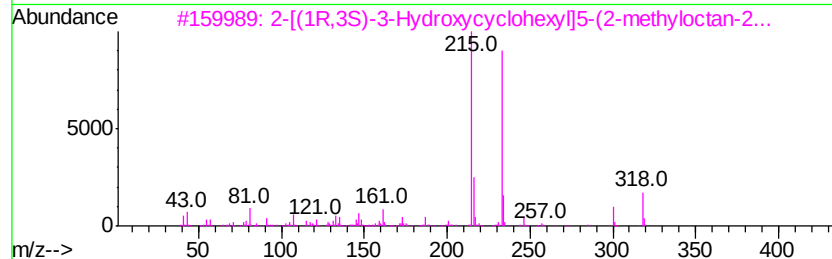
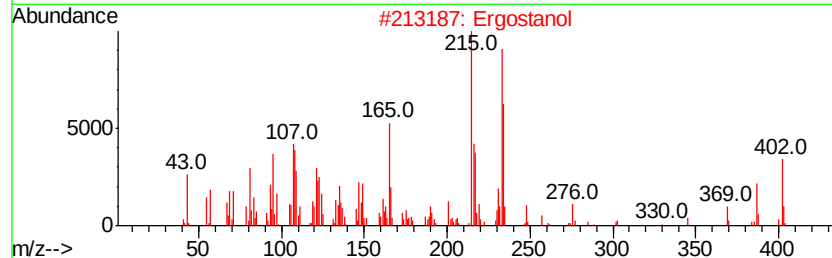
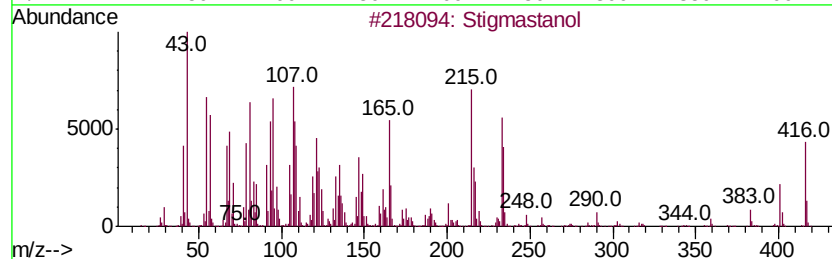
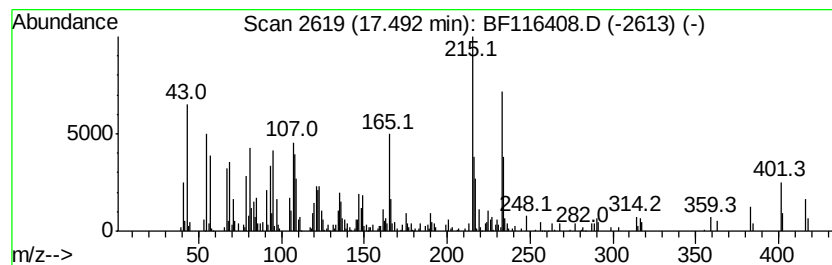
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Ergostanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.49	15.79 ng	580348	Perylene-d12	15.42
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Stigmastanol	416 C29H52O	019466-47-8 83
2		Ergostanol	402 C28H50O	006538-02-9 52
3		2-[(1R,3S)-3-Hydroxycyclohexyl]5...	318 C21H34O2	070434-82-1 35
4		5-(2-Methyloctan-2-yl)-3-(1R,3R-...	332 C22H36O2	070434-92-3 22
5		4-Aminodiphenylsulfone	233 C12H11NO2S	007019-01-4 18



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116408.D
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Misc :
ALS Vial : 17 Sample Multiplier: 1

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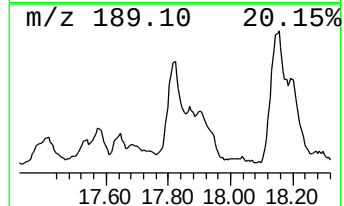
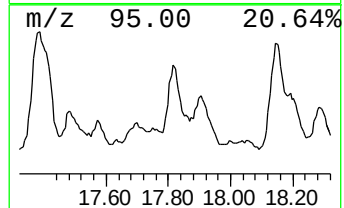
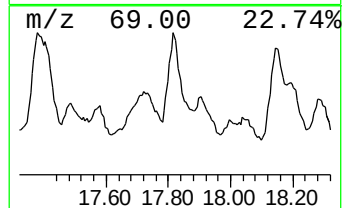
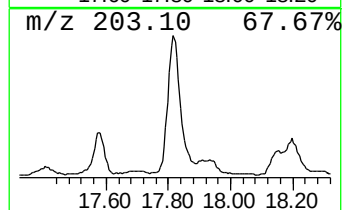
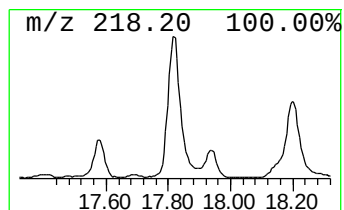
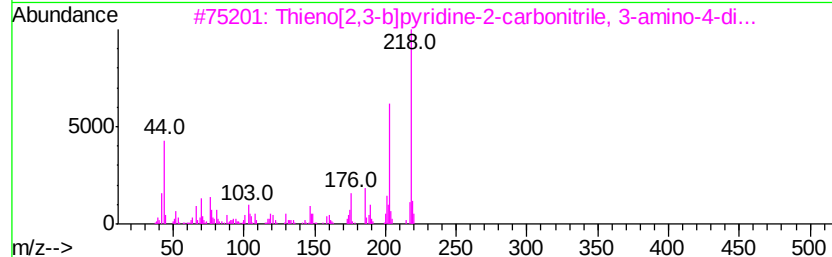
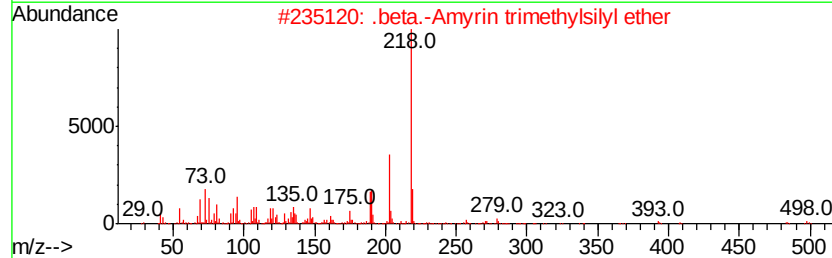
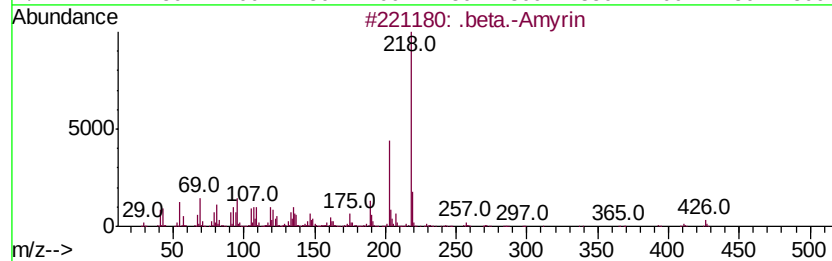
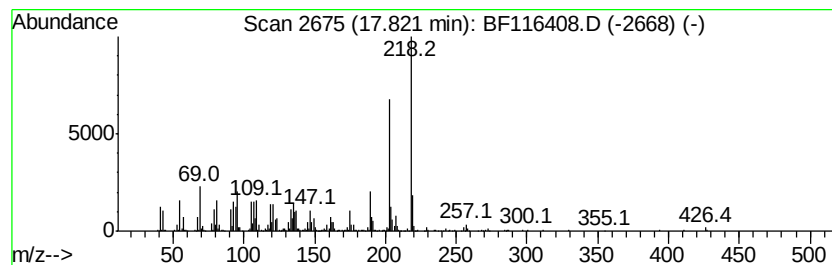
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 .beta.-Amyrin Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.82	32.73 ng	1203110	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Amyrin	426	C30H50O	000559-70-6	91
2		.beta.-Amyrin trimethylsilyl ether	498	C33H58OSi	001721-67-1	72
3		Thieno[2,3-b]pyridine-2-carbonit...	218	C10H10N4S	147992-88-9	64
4		3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	58
5		5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116408.D
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Misc :
ALS Vial : 17 Sample Multiplier: 1

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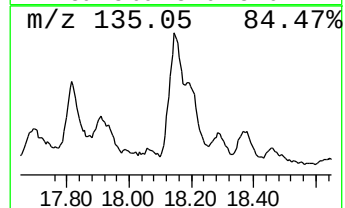
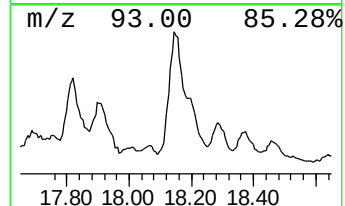
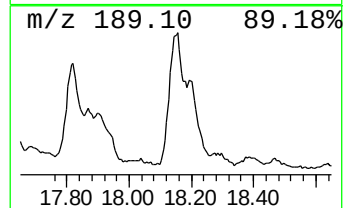
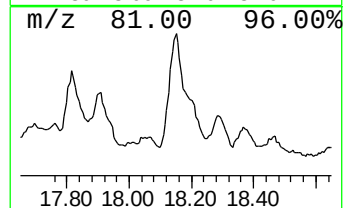
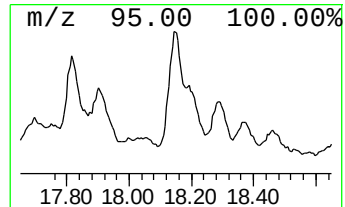
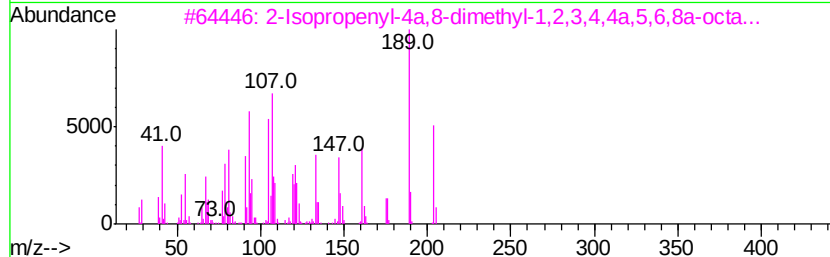
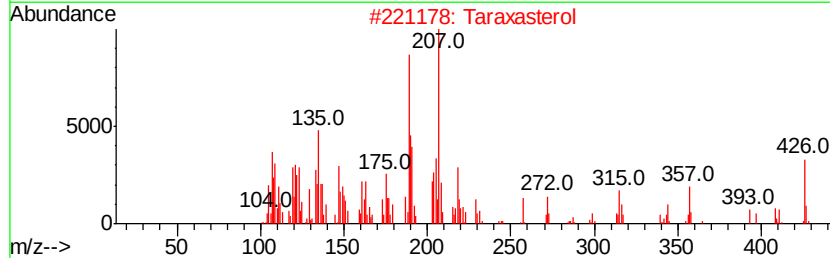
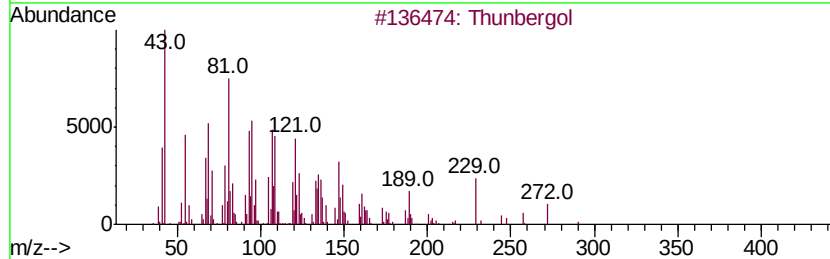
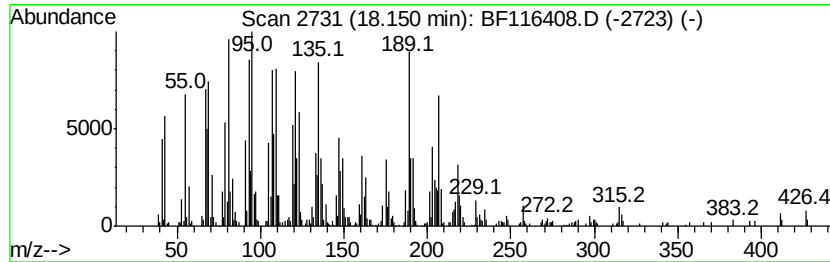
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Thunbergol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.15	44.83 ng	1648170	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thunbergol	290	C20H34O	025269-17-4	86
2		Taraxasterol	426	C30H50O	001059-14-9	78
3		2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0	70
4		Lupeol	426	C30H50O	000545-47-1	52
5		Silane, chlorodiethyl(dodec-9-yn...	302	C16H31ClOSi	1000363-59-2	50



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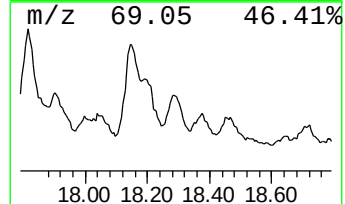
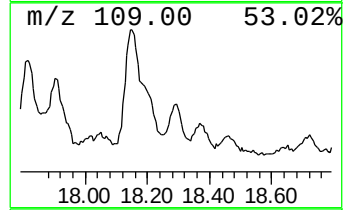
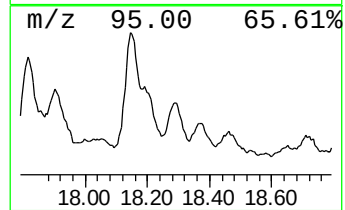
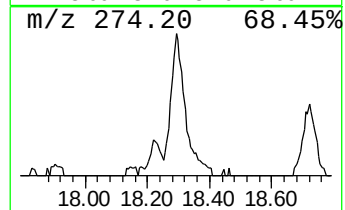
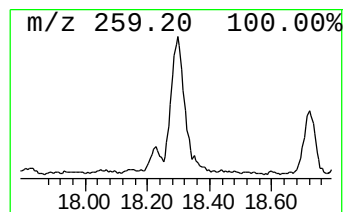
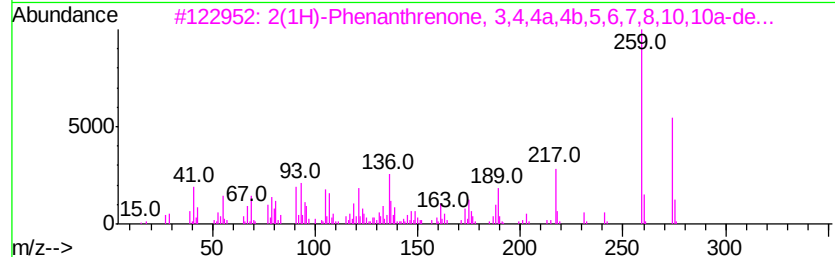
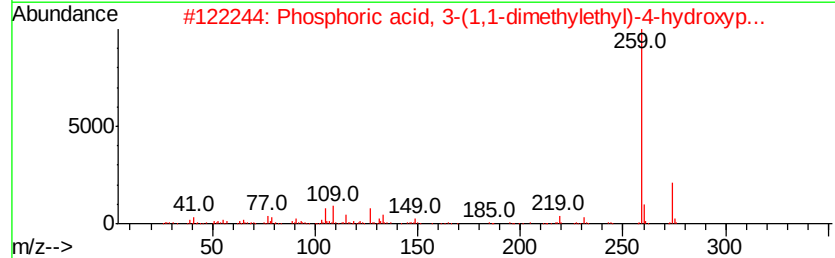
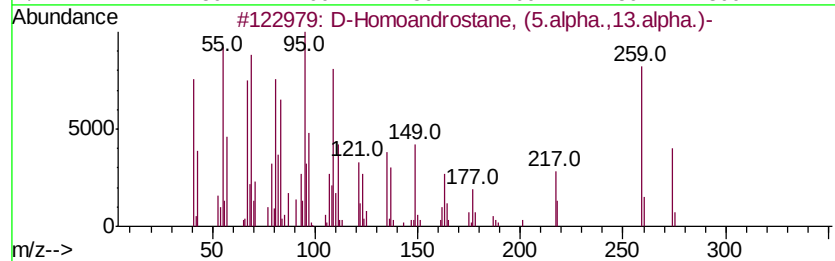
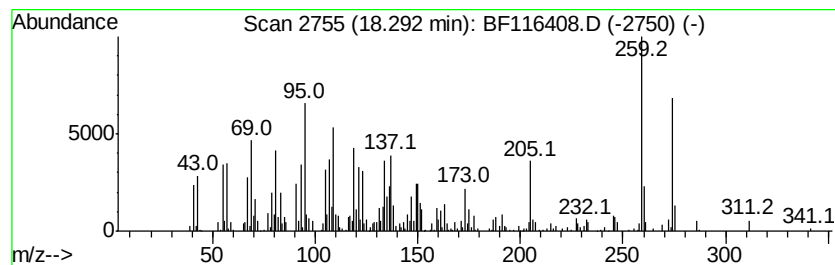
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 D-Homoandrostande, (5.alpha.... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	10.64 ng	391115	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	D-Homoandrostande, (5.alpha.,13.a...	274	C20H34	054482-31-4	50
2		Phosphoric acid, 3-(1,1-dimethyl...	274	C12H19O5P	094420-61-8	38
3		2(1H)-Phenanthrenone, 3,4,4a,4b,...	274	C19H30O	007715-44-8	38
4		1,3-DIETHYL-2-HYDROXYBENZOTHAZO...	274	C14H14N2O2S	1000227-15-3	35
5		10H-Phenoxaphosphine, 2-ethyl-10...	274	C15H15O3P	036360-91-5	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
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Acq On : 20 Aug 2019 00:38
Operator : HP/JU
Sample : K4223-15
Misc :
ALS Vial : 17 Sample Multiplier: 1

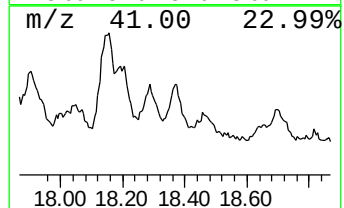
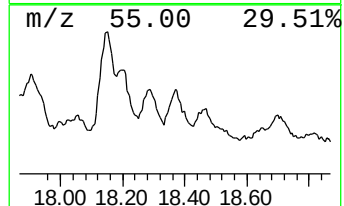
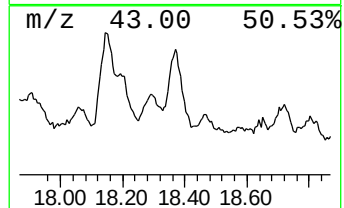
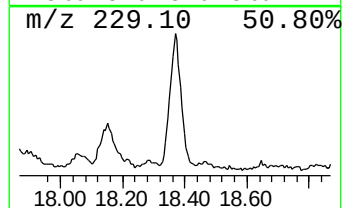
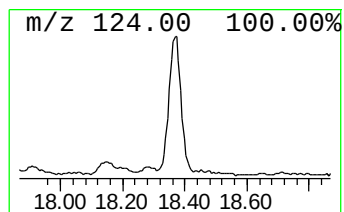
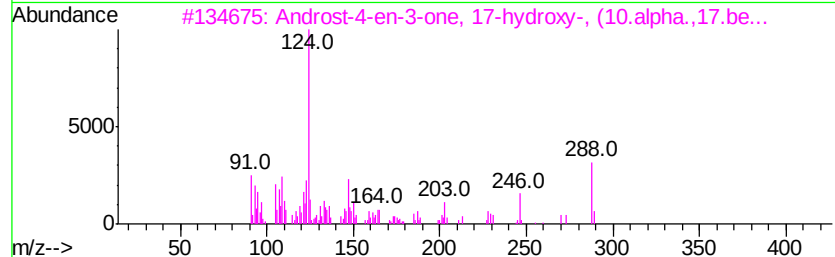
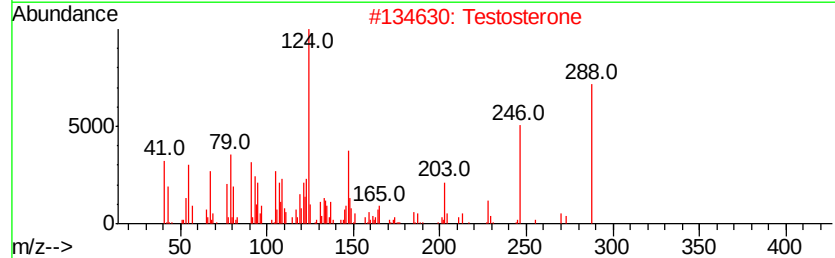
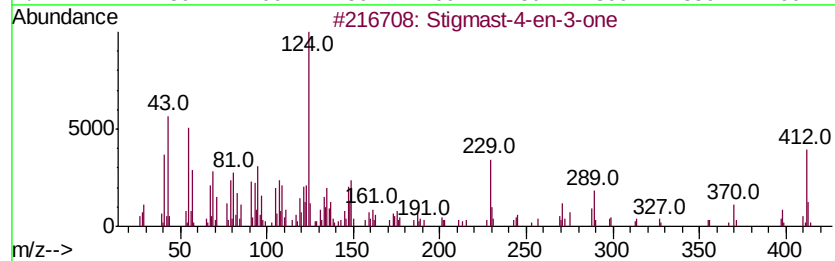
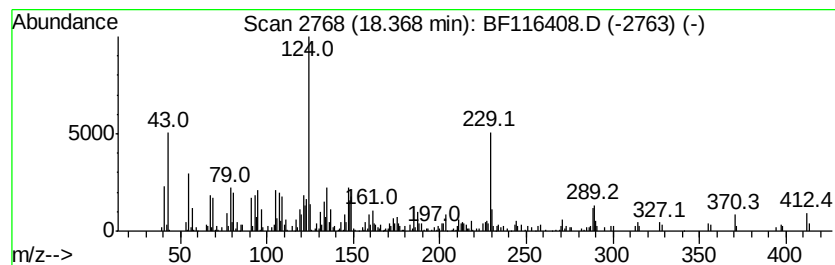
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Stigmast-4-en-3-one Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	14.96 ng	550118	Perylene-d12	15.42
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Stigmast-4-en-3-one	412 C29H48O	001058-61-3 98
2		Testosterone	288 C19H28O2	000058-22-0 81
3		Androst-4-en-3-one, 17-hydroxy-,...	288 C19H28O2	000604-39-7 46
4		Androst-4-en-3-one, 17-hydroxy-,...	288 C19H28O2	000481-30-1 42
5		Isonicotinic acid, dodecyl ester	291 C18H29NO2	1000299-88-7 38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116408.D
Acq On : 20 Aug 2019 00:38
Operator : HP/JU
Sample : K4223-15
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-8

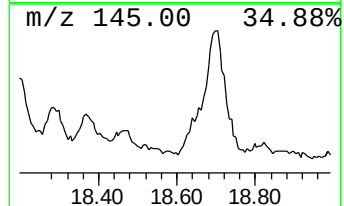
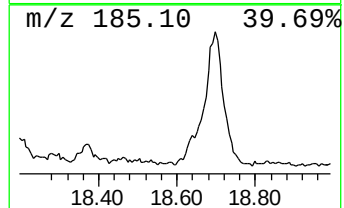
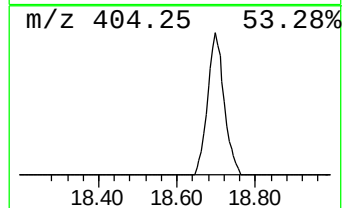
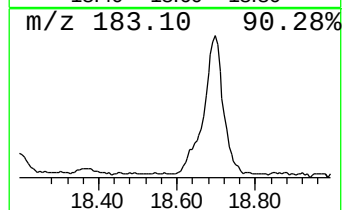
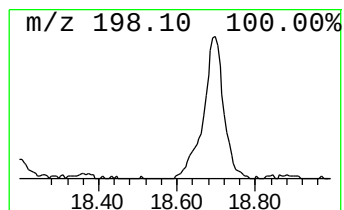
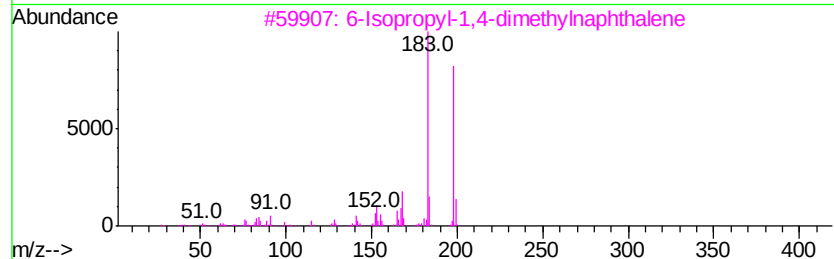
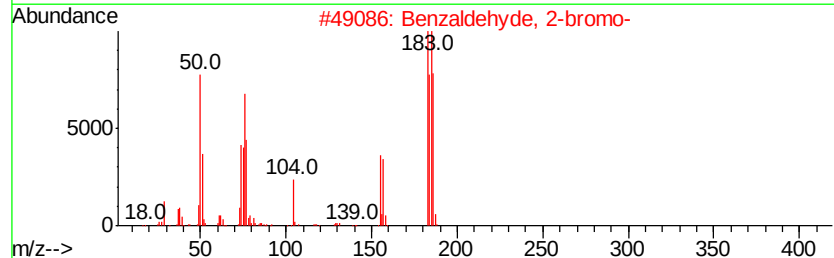
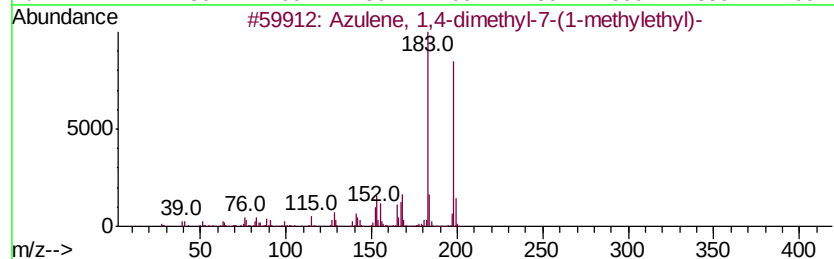
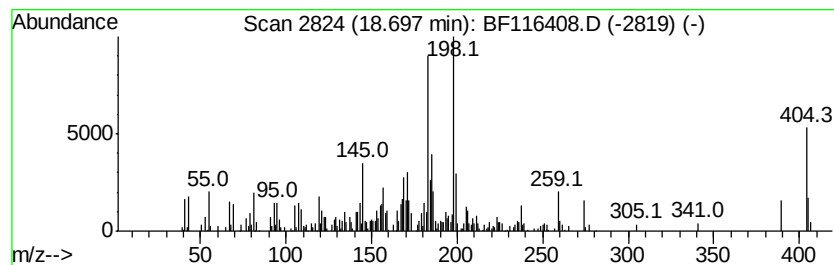
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Azulene, 1,4-dimethyl-7-(1-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.70	19.30 ng	709659	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	64
2		Benzaldehyde, 2-bromo-	184	C7H5BrO	006630-33-7	50
3		6-Isopropyl-1,4-dimethylnaphthalene	198	C15H18	000489-77-0	43
4		Naphthalene, 1,6-dimethyl-4-(1-methyl-...	198	C15H18	000483-78-3	43
5		4-Bromobenzoic acid, 2-tridecyl ...	382	C20H31BrO2	1000282-08-7	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081919\
 Data File : BF116408.D
 Acq On : 20 Aug 2019 00:38
 Operator : HP/JU
 Sample : K4223-15
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-8

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	84.3	ng	2446650	1	6.80	580343	20.0
n-Hexadecanoic acid	11.85	27.7	ng	1520590	4	11.32	1097430	20.0
n-Heptadecanol-1	12.35	14.1	ng	771906	4	11.32	1097430	20.0
Phytol	12.45	8.7	ng	479179	4	11.32	1097430	20.0
Octadecanoic acid	12.63	8.0	ng	436312	4	11.32	1097430	20.0
Ethanol, 2-(tetra...	13.79	19.0	ng	754251	5	13.96	793174	20.0
Tritetracontane	14.41	19.9	ng	788908	5	13.96	793174	20.0
Squalene	14.78	7.4	ng	272562	6	15.42	735228	20.0
2-methyloctacosane	15.82	36.4	ng	1339380	6	15.42	735228	20.0
1-Heptacosanol	15.87	6.5	ng	240538	6	15.42	735228	20.0
Vitamin E	16.08	12.6	ng	463081	6	15.42	735228	20.0
Stigmasterol	16.97	10.2	ng	374204	6	15.42	735228	20.0
.gamma.-Sitosterol	17.39	98.7	ng	3629620	6	15.42	735228	20.0
Ergosterol	17.49	15.8	ng	580348	6	15.42	735228	20.0
.beta.-Amyrin	17.82	32.7	ng	1203110	6	15.42	735228	20.0
Thunbergol	18.15	44.8	ng	1648170	6	15.42	735228	20.0
D-Homoandrostande,...	18.29	10.6	ng	391115	6	15.42	735228	20.0
Stigmast-4-en-3-one	18.37	15.0	ng	550118	6	15.42	735228	20.0
Azulene, 1,4-dime...	18.70	19.3	ng	709659	6	15.42	735228	20.0