

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042319\
 Data File : BF113922.D
 Acq On : 23 Apr 2019 16:07
 Operator : JU/SJ
 Sample : K2201-09 5X
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PL-01-041819-E

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-BF042219.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	5.516	579	583	600	rVB	1678765	1558682	43.42%	3.955%
2	6.522	749	754	758	rBV	1810808	1632898	45.49%	4.144%
3	6.551	758	759	769	rVB	48607	43603	1.21%	0.111%
4	6.669	774	779	789	rBV	1784783	1753045	48.83%	4.448%
5	6.840	803	808	811	rBV	65856	54458	1.52%	0.138%
6	6.898	814	818	828	rVB	2522990	2180526	60.74%	5.533%
7	7.057	841	845	852	rVV	1584212	1416299	39.45%	3.594%
8	7.140	856	859	862	rVV	53380	54013	1.50%	0.137%
9	7.169	862	864	875	rVB3	35955	53525	1.49%	0.136%
10	7.298	882	886	890	rBV	153872	148029	4.12%	0.376%
11	7.416	902	906	908	rBV	43611	39045	1.09%	0.099%
12	7.451	908	912	915	rBV	1199123	1040863	29.00%	2.641%
13	7.710	952	956	959	rVB	78535	64633	1.80%	0.164%
14	7.828	973	976	980	rBV	53990	53088	1.48%	0.135%
15	7.922	989	992	996	rVB	50899	43427	1.21%	0.110%
16	8.034	1008	1011	1018	rBV2	33432	38134	1.06%	0.097%
17	8.122	1023	1026	1029	rBV	73596	59186	1.65%	0.150%
18	8.181	1032	1036	1039	rBV	3083031	2607893	72.65%	6.618%
19	8.239	1044	1046	1050	rVB	44443	46655	1.30%	0.118%
20	8.322	1058	1060	1063	rBV	64709	48799	1.36%	0.124%
21	8.563	1098	1101	1106	rBV3	34849	37363	1.04%	0.095%
22	8.722	1125	1128	1133	rBV2	51494	62283	1.74%	0.158%
23	8.892	1154	1157	1162	rVB	102194	84842	2.36%	0.215%
24	8.992	1171	1174	1181	rBV	102747	99011	2.76%	0.251%
25	9.057	1182	1185	1189	rBV	75633	67722	1.89%	0.172%
26	9.169	1201	1204	1208	rBV2	48990	51077	1.42%	0.130%
27	9.210	1208	1211	1214	rBV3	51591	57455	1.60%	0.146%
28	9.251	1214	1218	1221	rBV	2427810	1920515	53.50%	4.873%
29	9.351	1230	1235	1237	rBV2	127194	140666	3.92%	0.357%
30	9.375	1237	1239	1242	rVB	77290	69014	1.92%	0.175%
31	9.463	1250	1254	1258	rBV2	41542	41585	1.16%	0.106%
32	9.598	1267	1277	1279	rBV4	40421	74327	2.07%	0.189%
33	9.639	1282	1284	1289	rVV	304504	308466	8.59%	0.783%
34	9.704	1293	1295	1301	rVB3	62288	64760	1.80%	0.164%

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35	9.792	1307	1310	1315	rBV	139849	125494	3.50%	0.318%
36	9.869	1315	1323	1328	rVV3	84599	99087	2.76%	0.251%
37	9.939	1330	1335	1338	rVV	2768866	2734504	76.18%	6.939%
38	9.969	1338	1340	1342	rVB	133406	106646	2.97%	0.271%
39	10.039	1349	1352	1356	rBV3	36585	44033	1.23%	0.112%
40	10.104	1360	1363	1366	rVV2	40334	53185	1.48%	0.135%
41	10.133	1366	1368	1372	rVB	114013	109841	3.06%	0.279%
42	10.216	1379	1382	1385	rVB2	36701	42820	1.19%	0.109%
43	10.251	1385	1388	1391	rBV2	58773	64085	1.79%	0.163%
44	10.345	1400	1404	1406	rBV	100133	97877	2.73%	0.248%
45	10.363	1406	1407	1410	rVB	66506	49953	1.39%	0.127%
46	10.475	1423	1426	1430	rBV2	184588	209103	5.83%	0.531%
47	10.586	1440	1445	1448	rBV	127748	138236	3.85%	0.351%
48	10.628	1449	1452	1457	rVB3	83172	99324	2.77%	0.252%
49	10.716	1463	1467	1473	rBV	1156451	1095882	30.53%	2.781%
50	10.839	1485	1488	1489	rBV	91980	77920	2.17%	0.198%
51	10.957	1506	1508	1512	rBV2	64813	58907	1.64%	0.149%
52	11.033	1518	1521	1523	rBV2	86074	71109	1.98%	0.180%
53	11.104	1530	1533	1538	rVB3	72571	64097	1.79%	0.163%
54	11.222	1551	1553	1557	rBV3	35045	42642	1.19%	0.108%
55	11.286	1561	1564	1567	rVV2	91269	96872	2.70%	0.246%
56	11.316	1567	1569	1574	rVB	86622	90694	2.53%	0.230%
57	11.422	1583	1587	1589	rBV	3209601	2782140	77.50%	7.060%
58	11.439	1589	1590	1593	rVV	488431	378800	10.55%	0.961%
59	11.492	1596	1599	1602	rVB	249277	196226	5.47%	0.498%
60	11.639	1621	1624	1627	rBV	117906	111460	3.10%	0.283%
61	11.710	1634	1636	1639	rBV	75436	59346	1.65%	0.151%
62	11.810	1648	1653	1655	rBV	209062	180137	5.02%	0.457%
63	11.922	1669	1672	1673	rBV	85859	81543	2.27%	0.207%
64	11.945	1673	1676	1679	rVV2	355602	356613	9.93%	0.905%
65	11.975	1679	1681	1683	rVV	82687	60295	1.68%	0.153%
66	12.027	1687	1690	1693	rBV2	128871	145270	4.05%	0.369%
67	12.122	1703	1706	1709	rVB	85730	69560	1.94%	0.177%
68	12.210	1719	1721	1723	rBV	58101	52580	1.46%	0.133%
69	12.233	1723	1725	1730	rVB3	46981	56688	1.58%	0.144%
70	12.345	1741	1744	1746	rBV	41806	46177	1.29%	0.117%
71	12.398	1750	1753	1755	rBV2	53142	64423	1.79%	0.163%

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72	12.469	1762	1765	1767	rBV	105668	101924	2.84%	0.259%
73	12.498	1767	1770	1771	rVV	539176	499543	13.92%	1.268%
74	12.516	1771	1773	1778	rVB2	738481	611231	17.03%	1.551%
75	12.598	1784	1787	1789	rBV2	112317	113676	3.17%	0.288%
76	12.627	1789	1792	1798	rVV	888396	874168	24.35%	2.218%
77	12.727	1806	1809	1811	rBV2	180088	180075	5.02%	0.457%
78	12.786	1816	1819	1822	rBV2	47028	57167	1.59%	0.145%
79	12.857	1826	1831	1834	rBV	847730	896525	24.97%	2.275%
80	12.998	1852	1855	1859	rBV	2214316	2043618	56.93%	5.186%
81	13.163	1881	1883	1884	rBV2	62568	53668	1.50%	0.136%
82	13.186	1885	1887	1890	rVB	149865	119918	3.34%	0.304%
83	13.233	1893	1895	1897	rBV	110111	112541	3.14%	0.286%
84	13.292	1902	1905	1908	rBV2	120413	144436	4.02%	0.367%
85	13.416	1924	1926	1928	rBV	66105	48433	1.35%	0.123%
86	13.539	1945	1947	1950	rBV	103210	88687	2.47%	0.225%
87	13.580	1951	1954	1957	rVV2	121926	122633	3.42%	0.311%
88	13.910	2007	2010	2013	rVB2	145800	149337	4.16%	0.379%
89	14.063	2030	2036	2039	rBV	2937491	3589748	100.00%	9.109%
90	14.086	2039	2040	2043	rVB	507034	277793	7.74%	0.705%
91	14.227	2062	2064	2071	rVB3	208696	206263	5.75%	0.523%
92	14.545	2115	2118	2121	rVB2	184683	183283	5.11%	0.465%
93	14.857	2168	2171	2174	rBV2	245768	245516	6.84%	0.623%
94	15.121	2213	2216	2218	rBV	301323	370192	10.31%	0.939%
95	15.563	2286	2291	2294	rBV	1546629	2088634	58.18%	5.300%

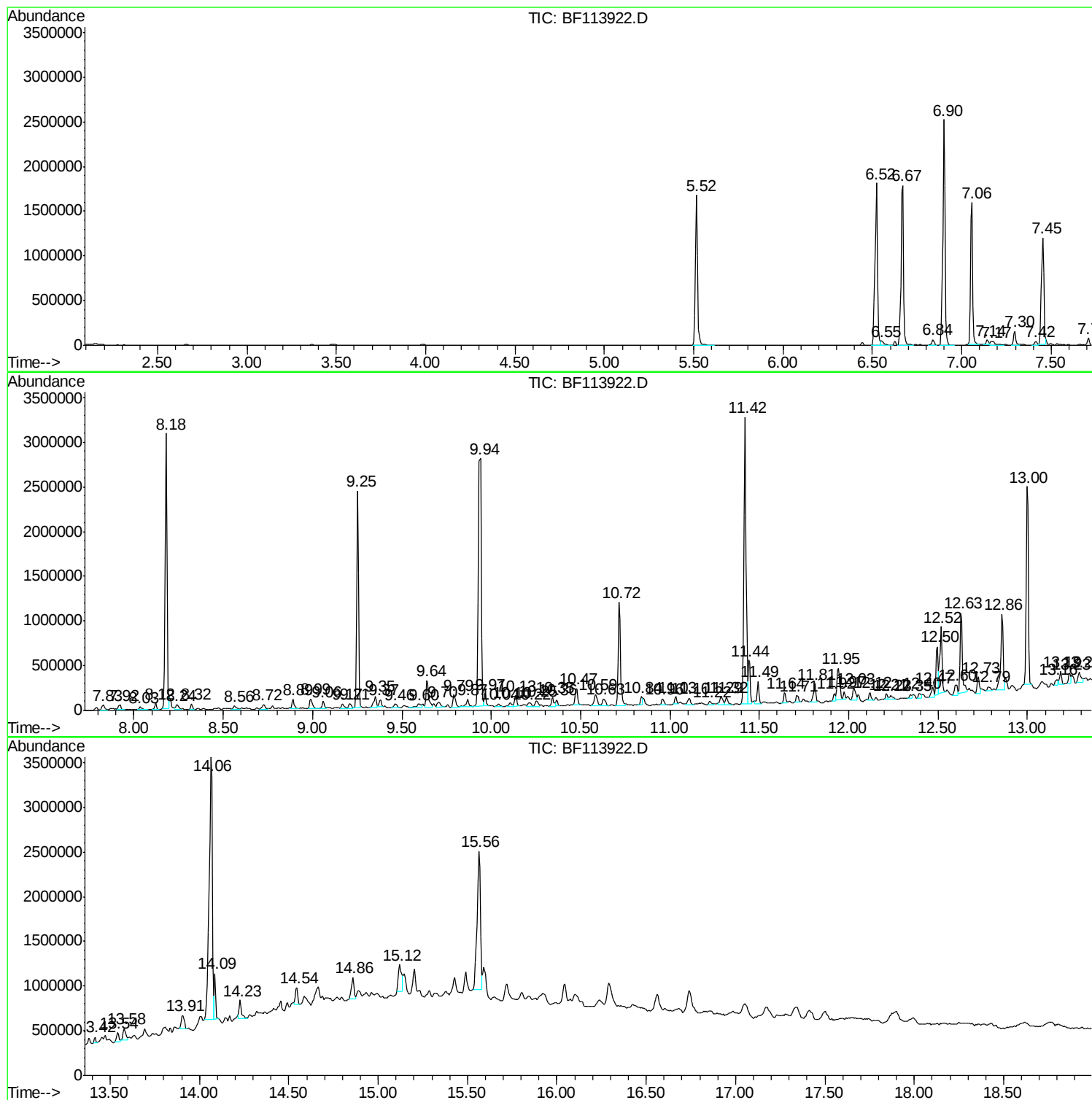
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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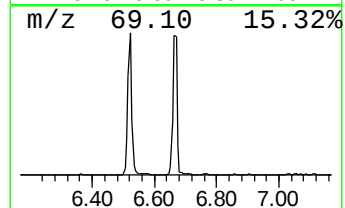
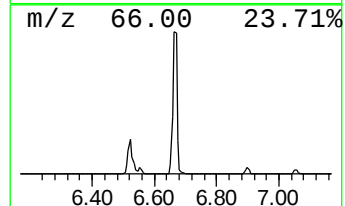
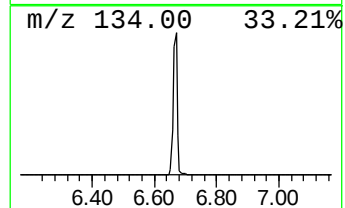
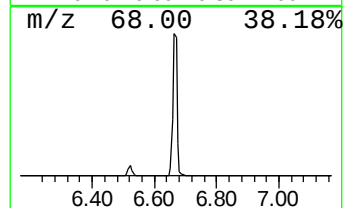
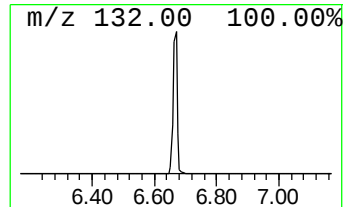
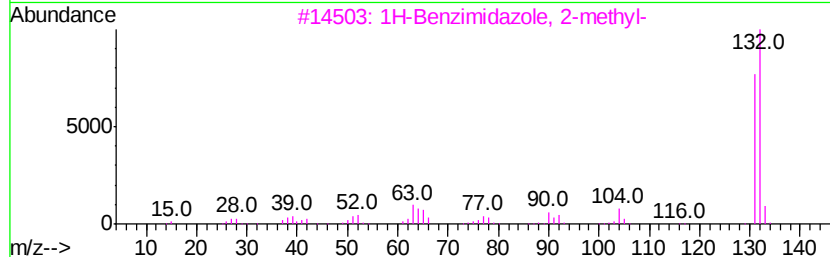
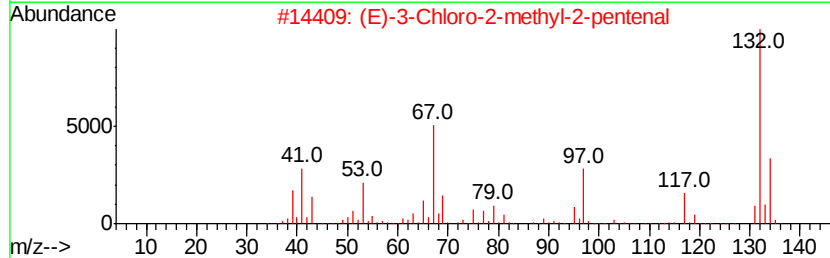
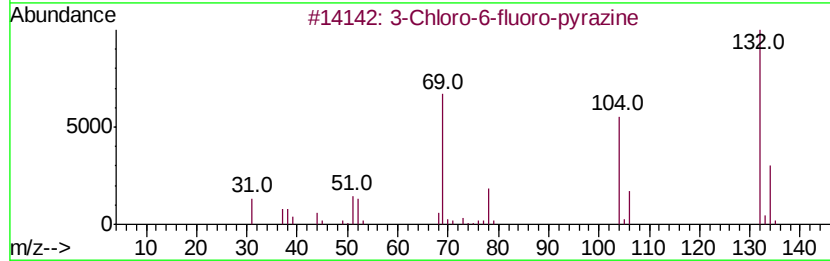
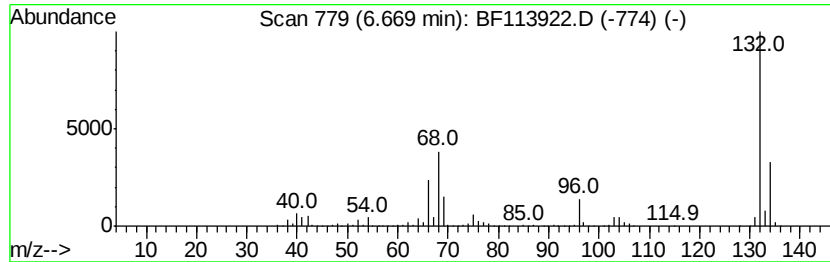
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	16.08 ng	1753050	1,4-Dichlorobenzene-d4	6.90

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		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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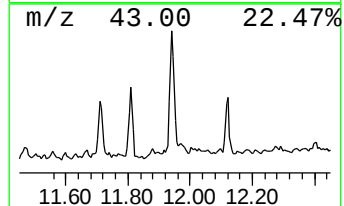
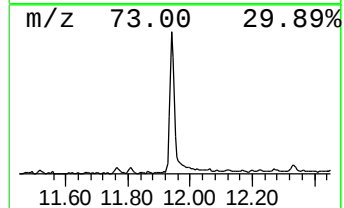
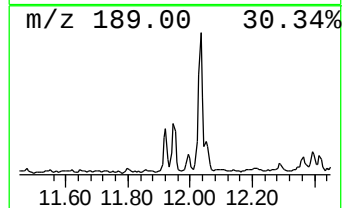
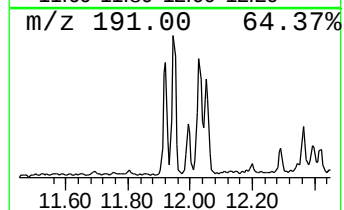
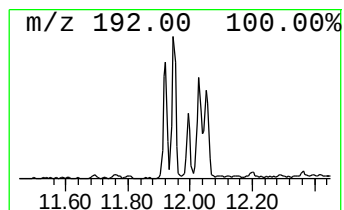
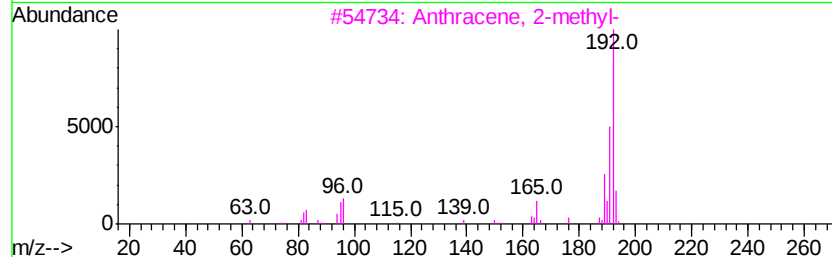
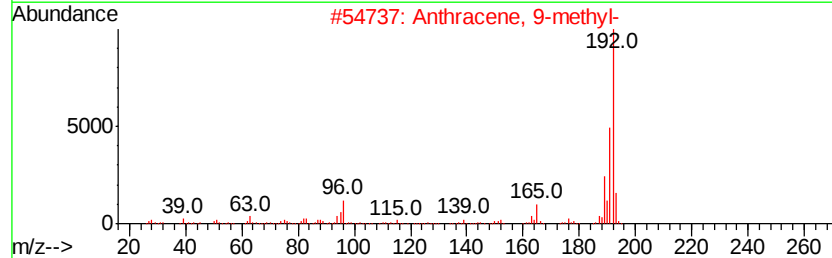
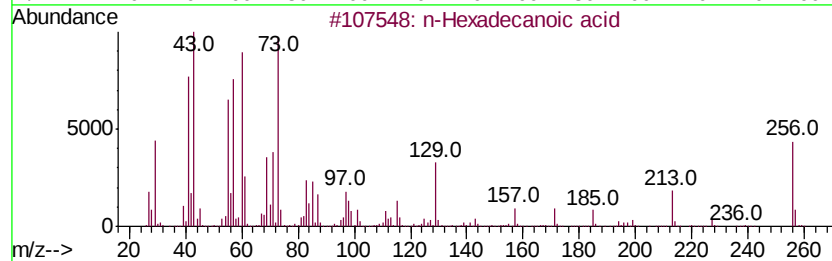
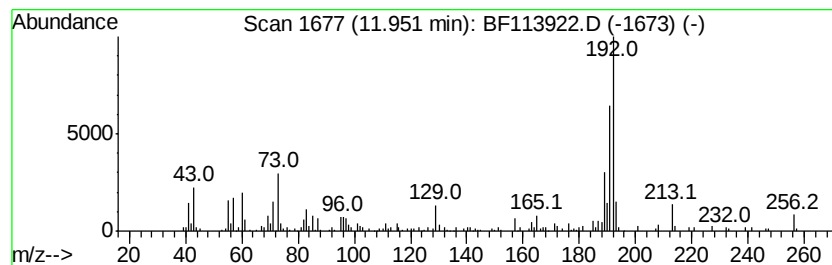
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.95	2.56 ng	356613	Phenanthrene-d10	11.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	89
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	86
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	86



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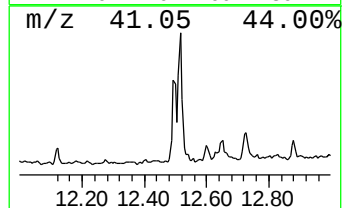
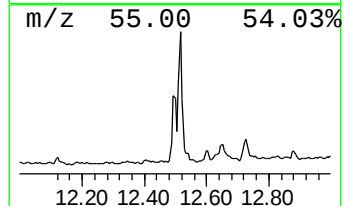
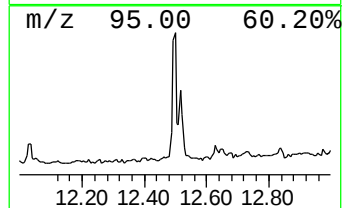
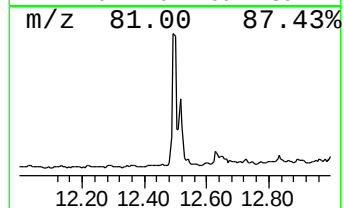
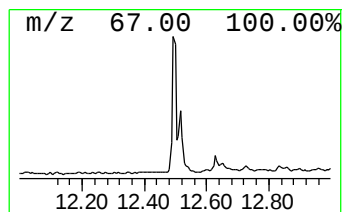
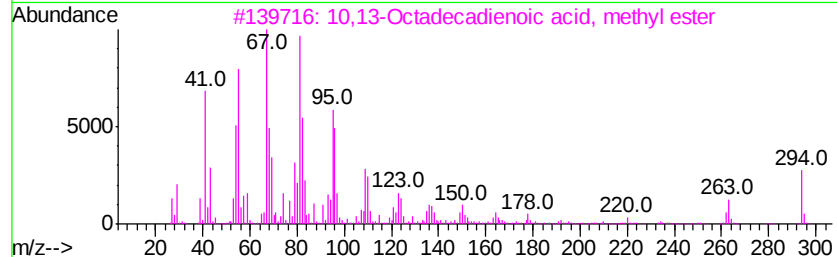
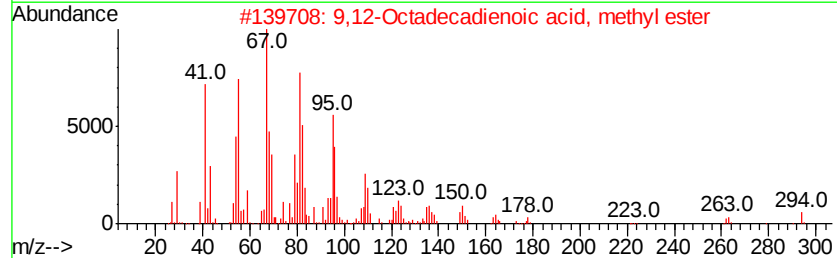
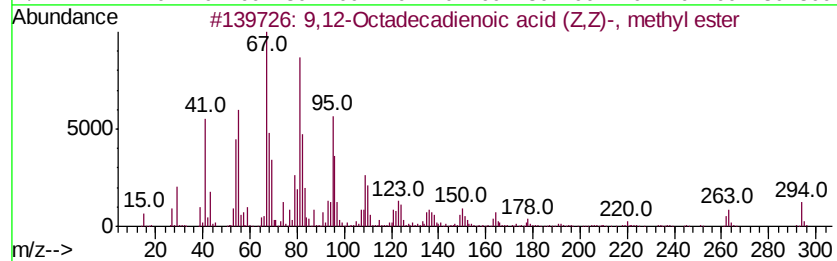
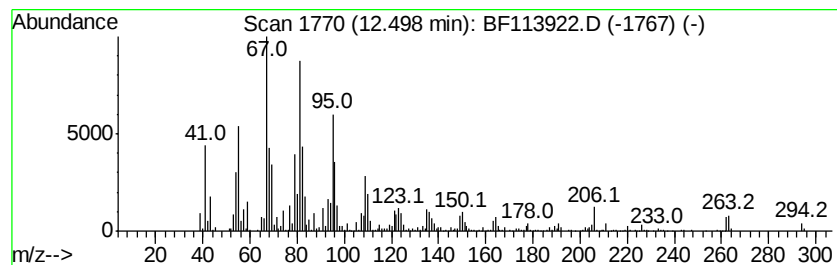
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Peak Number 4 9,12-Octadecadienoic acid (... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.50	3.59 ng	499543	Phenanthrene-d10	11.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
4	9,15-Octadecadienoic acid, methv...	294	C19H34O2	017309-05-6	99
5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	98



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042319\
Data File : BF113922.D
Acq On : 23 Apr 2019 16:07
Operator : JU/SJ
Sample : K2201-09 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

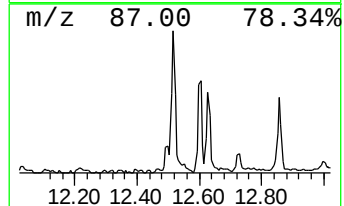
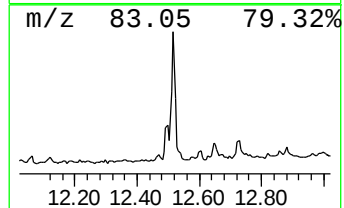
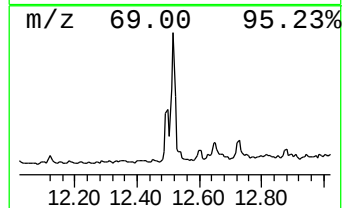
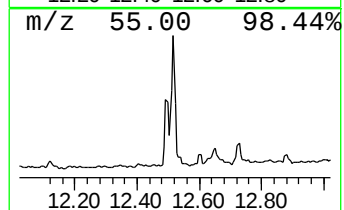
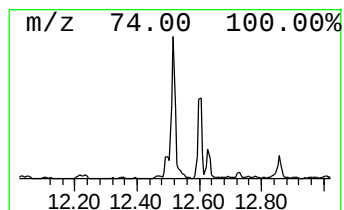
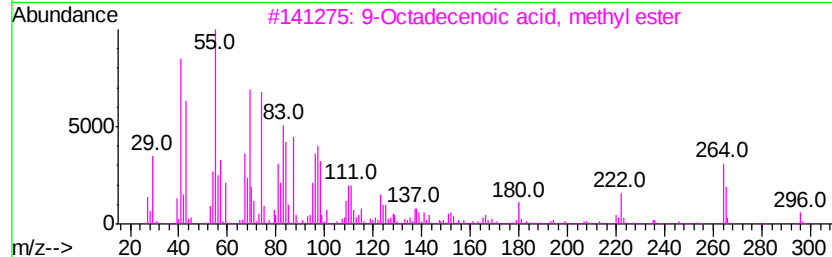
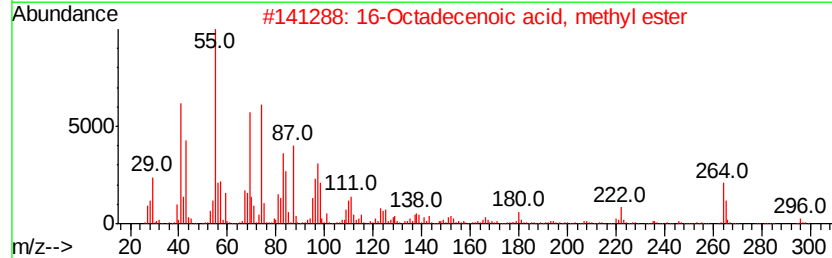
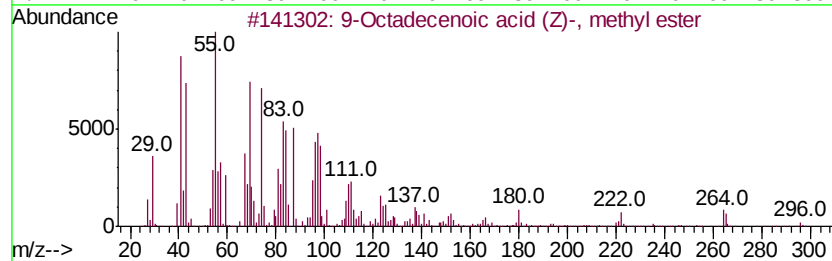
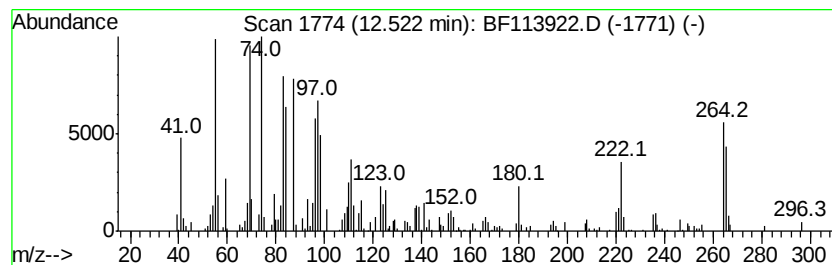
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BNA_F
ClientSampleId :
PL-01-041819-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.52	4.39 ng	611231	Phenanthrene-d10	11.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
3	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	96
5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	96



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042319\
Data File : BF113922.D
Acq On : 23 Apr 2019 16:07
Operator : JU/SJ
Sample : K2201-09 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PL-01-041819-E

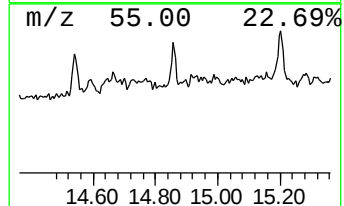
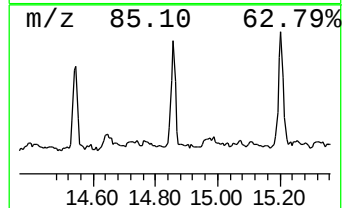
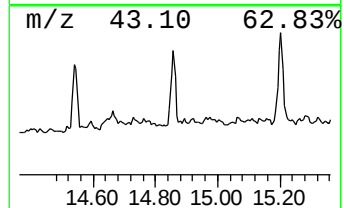
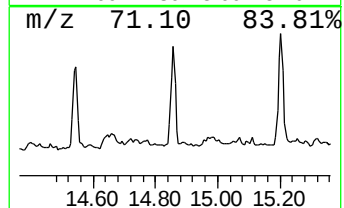
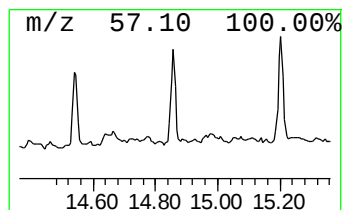
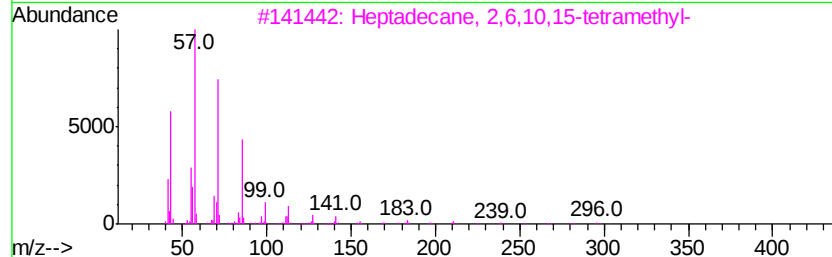
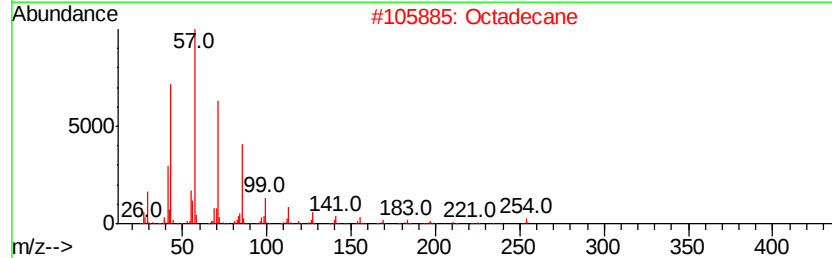
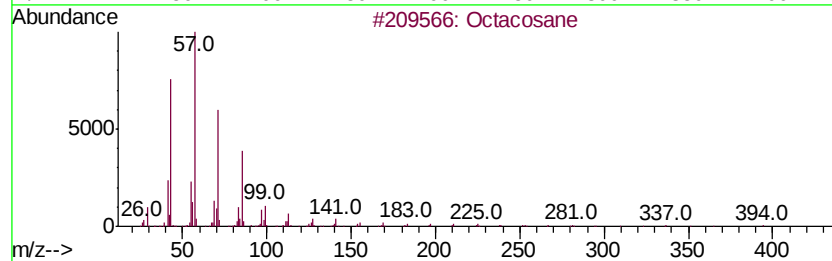
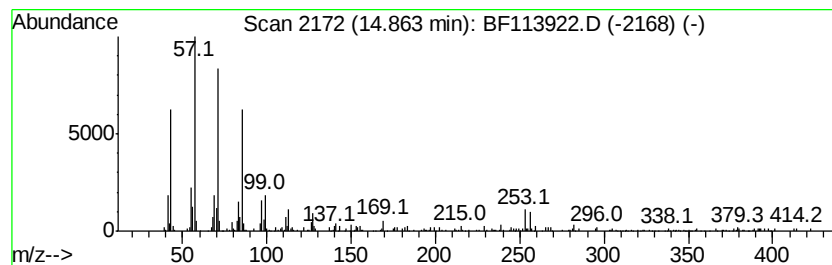
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	2.35 ng	245516	Perylene-d12	15.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	94
2		Octadecane	254	C18H38	000593-45-3	93
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
4		Nonadecane	268	C19H40	000629-92-5	93
5		Docosane, 11-butyl-	366	C26H54	013475-76-8	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042319\
Data File : BF113922.D
Acq On : 23 Apr 2019 16:07
Operator : JU/SJ
Sample : K2201-09 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PL-01-041819-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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
unknown6.67	6.67	16.1	ng	1753050	1	6.90	2180530	20.0
n-Hexadecanoic acid	11.95	2.6	ng	356613	4	11.42	2782140	20.0
9,12-Octadecadien...	12.50	3.6	ng	499543	4	11.42	2782140	20.0
9-Octadecenoic ac...	12.52	4.4	ng	611231	4	11.42	2782140	20.0
Octacosane	14.86	2.4	ng	245516	6	15.56	2088630	20.0