

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031119\
 Data File : BF112969.D
 Acq On : 11 Mar 2019 21:55
 Operator : JU/SJ
 Sample : K1691-01 2X
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CL-02-030819-A

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-BF022719.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	5.334	548	552	562	rBV	1729195	1653680	74.05%	4.521%
2	6.363	723	727	746	rBV	2071280	1831615	82.02%	5.008%
3	6.498	746	750	753	rBV	1945380	1819009	81.46%	4.973%
4	6.728	785	789	796	rBV	1328724	1079077	48.32%	2.950%
5	6.886	812	816	825	rBV	1444845	1324569	59.32%	3.621%
6	7.286	879	884	893	rBV	1173266	1114970	49.93%	3.048%
7	8.010	1003	1007	1015	rBV	1485129	1519831	68.06%	4.155%
8	8.727	1123	1129	1136	rBV	47849	53880	2.41%	0.147%
9	8.822	1141	1145	1152	rVB	42073	48397	2.17%	0.132%
10	9.086	1186	1190	1202	rBV	2323689	2157484	96.61%	5.899%
11	9.180	1204	1206	1209	rVB2	31948	31889	1.43%	0.087%
12	9.351	1231	1235	1243	rBV3	26549	45314	2.03%	0.124%
13	9.422	1244	1247	1250	rVV	38536	39948	1.79%	0.109%
14	9.480	1254	1257	1263	rVV	133022	131246	5.88%	0.359%
15	9.622	1278	1281	1285	rBV	32086	28142	1.26%	0.077%
16	9.710	1293	1296	1300	rVB	26468	25292	1.13%	0.069%
17	9.763	1300	1305	1308	rBV	2164485	1990640	89.14%	5.442%
18	9.792	1308	1310	1315	rVB	170872	148773	6.66%	0.407%
19	9.969	1336	1340	1343	rBV	100880	101255	4.53%	0.277%
20	10.174	1370	1375	1376	rBV3	21462	24567	1.10%	0.067%
21	10.204	1378	1380	1385	rVB2	37617	30755	1.38%	0.084%
22	10.304	1394	1397	1403	rBV	179618	183699	8.23%	0.502%
23	10.421	1414	1417	1422	rVV4	20081	27152	1.22%	0.074%
24	10.463	1422	1424	1429	rVB	44038	40958	1.83%	0.112%
25	10.545	1434	1438	1453	rVV	1982046	1928418	86.36%	5.272%
26	10.674	1457	1460	1465	rVB3	55519	58872	2.64%	0.161%
27	11.004	1514	1516	1520	rBV3	21495	25345	1.13%	0.069%
28	11.045	1520	1523	1528	rVB2	38449	53322	2.39%	0.146%
29	11.133	1534	1538	1545	rVB3	86297	156246	7.00%	0.427%
30	11.239	1552	1556	1558	rBV	2393749	2148780	96.22%	5.875%
31	11.263	1558	1560	1564	rVV	1220093	988255	44.26%	2.702%
32	11.316	1565	1569	1573	rVB	294671	332442	14.89%	0.909%
33	11.468	1592	1595	1598	rBV	80574	76492	3.43%	0.209%
34	11.545	1604	1608	1610	rBV3	36347	46944	2.10%	0.128%

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Integrator: RTE

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35	11.568	1610	1612	1615	rVB2	29490	24888	1.11%	0.068%
36	11.645	1621	1625	1631	rVB	235593	228687	10.24%	0.625%
37	11.739	1638	1641	1643	rBV	115468	104524	4.68%	0.286%
38	11.774	1643	1647	1651	rVV2	384700	454932	20.37%	1.244%
39	11.816	1651	1654	1657	rVV2	84624	107012	4.79%	0.293%
40	11.851	1657	1660	1662	rVV	268135	269929	12.09%	0.738%
41	11.868	1662	1663	1669	rVB	85874	78308	3.51%	0.214%
42	12.033	1688	1691	1693	rBV	89955	75599	3.39%	0.207%
43	12.215	1719	1722	1723	rBV	34437	31472	1.41%	0.086%
44	12.286	1731	1734	1737	rBV	90348	108737	4.87%	0.297%
45	12.321	1737	1740	1742	rVV	893884	806625	36.12%	2.205%
46	12.345	1742	1744	1747	rVV	762396	639224	28.63%	1.748%
47	12.368	1747	1748	1753	rVB3	87901	52042	2.33%	0.142%
48	12.445	1756	1761	1765	rBV	1549775	1458320	65.31%	3.987%
49	12.557	1778	1780	1783	rBV2	89178	94758	4.24%	0.259%
50	12.668	1794	1799	1803	rBV	1167373	1298496	58.15%	3.550%
51	12.792	1817	1820	1821	rBV	82124	74707	3.35%	0.204%
52	12.815	1821	1824	1831	rVB	2382149	2203476	98.67%	6.024%
53	12.974	1849	1851	1852	rBV	55379	45922	2.06%	0.126%
54	12.998	1853	1855	1858	rVB2	191593	176475	7.90%	0.482%
55	13.062	1863	1866	1869	rBV	184298	169742	7.60%	0.464%
56	13.104	1870	1873	1876	rBV	101708	99167	4.44%	0.271%
57	13.192	1886	1888	1891	rBV	53437	45099	2.02%	0.123%
58	13.227	1891	1894	1896	rBV	56872	67344	3.02%	0.184%
59	13.721	1975	1978	1986	rVB4	217050	299411	13.41%	0.819%
60	13.862	1997	2002	2005	rBV2	1923429	2233090	100.00%	6.105%
61	13.886	2005	2006	2013	rVB	476218	383827	17.19%	1.049%
62	13.968	2018	2020	2024	rVB	102142	87955	3.94%	0.240%
63	14.045	2031	2033	2036	rBV3	97472	82775	3.71%	0.226%
64	14.345	2082	2084	2087	rVB	140657	121300	5.43%	0.332%
65	14.874	2170	2174	2177	rBV	400340	635318	28.45%	1.737%
66	14.962	2186	2189	2196	rVB3	275642	407567	18.25%	1.114%
67	15.151	2218	2221	2227	rBV	248716	322657	14.45%	0.882%
68	15.209	2228	2231	2234	rBV	313671	378877	16.97%	1.036%
69	15.274	2237	2242	2245	rVV	1133134	1399408	62.67%	3.826%
70	15.721	2315	2318	2322	rVB	190231	241377	10.81%	0.660%

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

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Peak separation: 5

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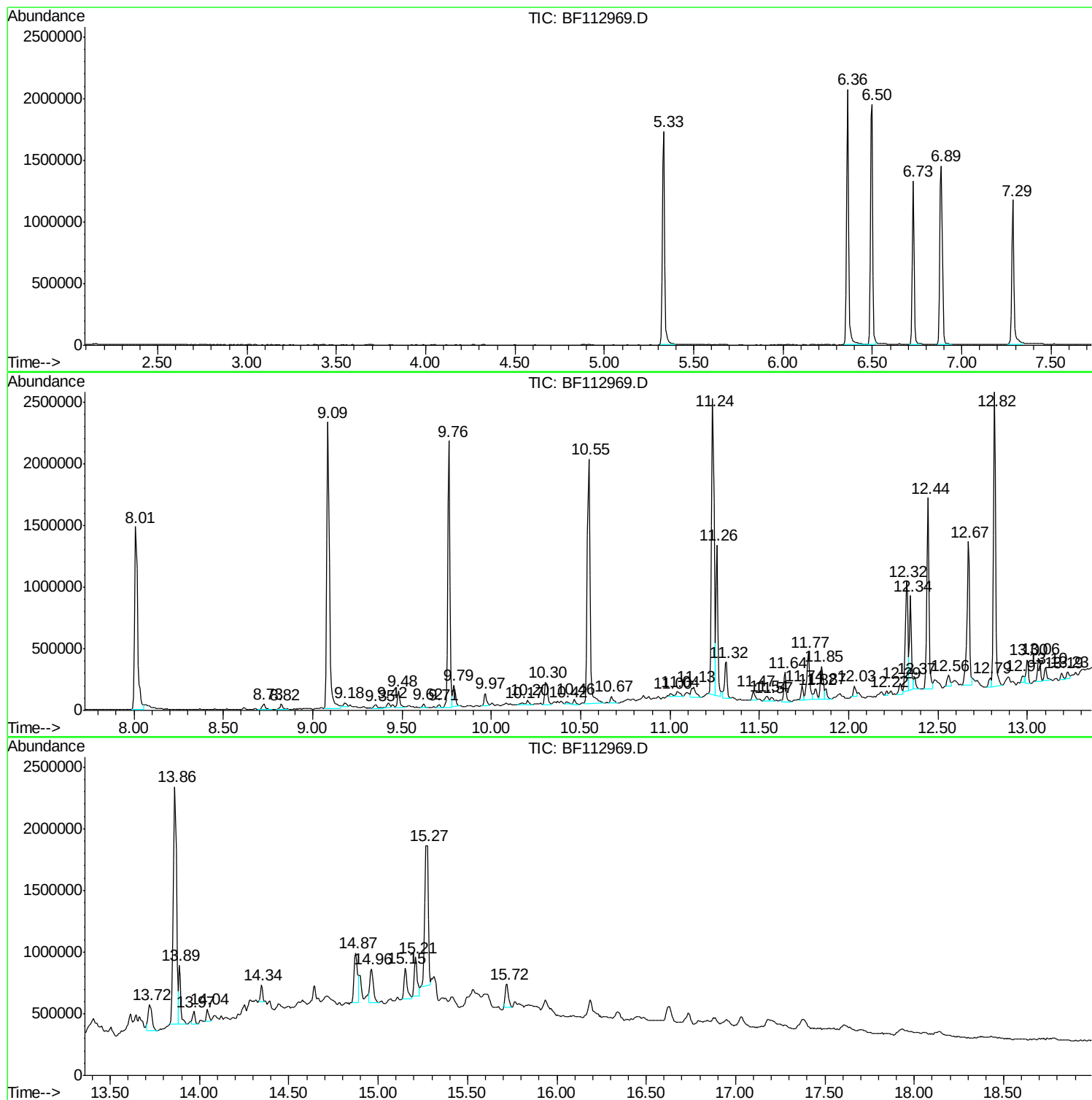
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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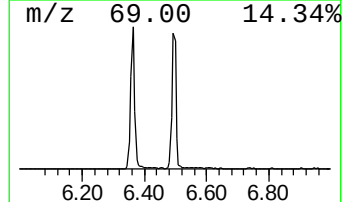
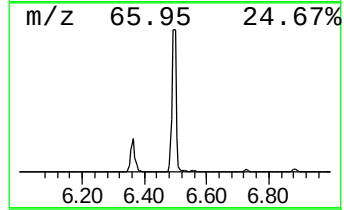
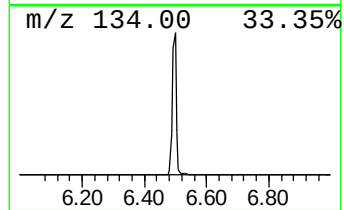
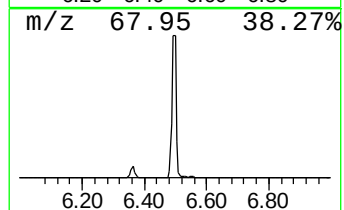
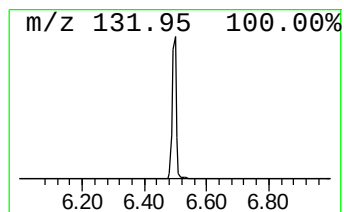
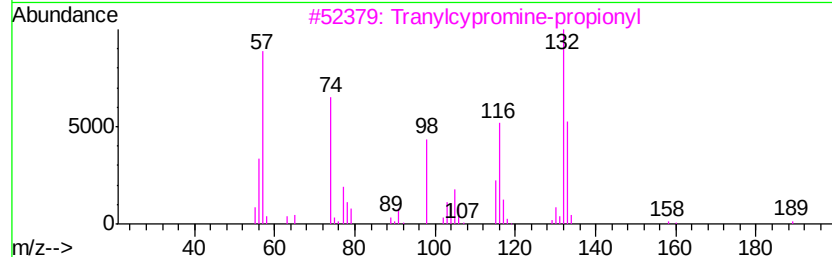
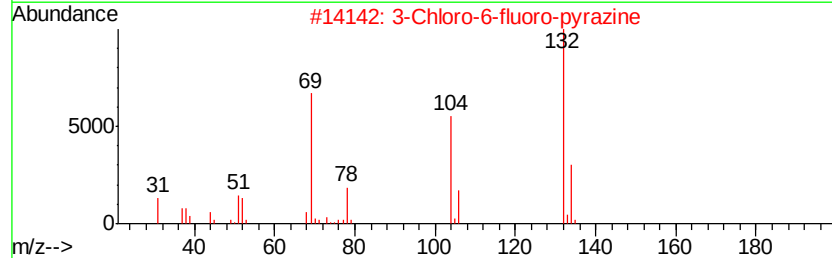
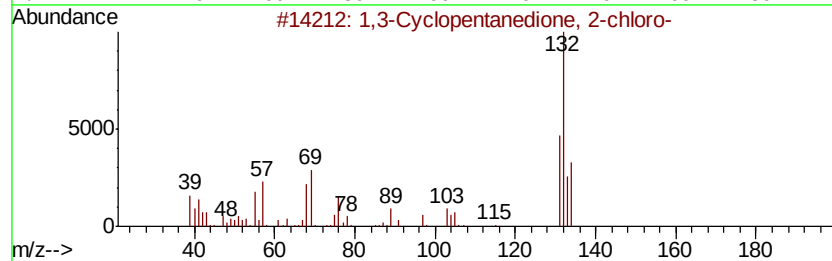
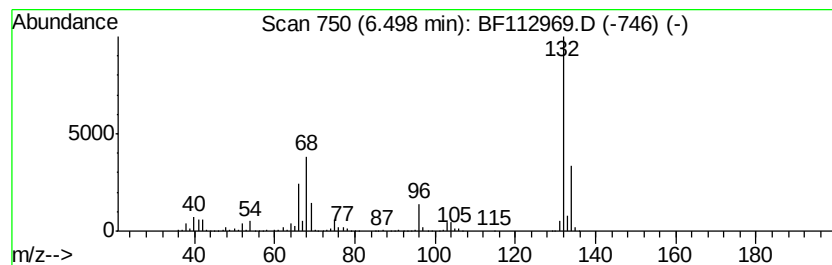
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	33.71 ng	1819010	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	37
2			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3			Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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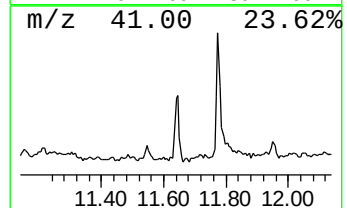
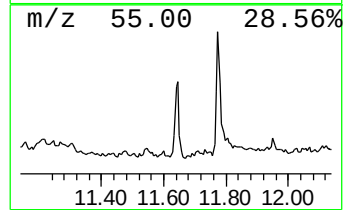
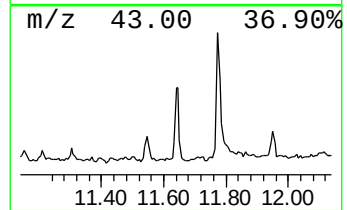
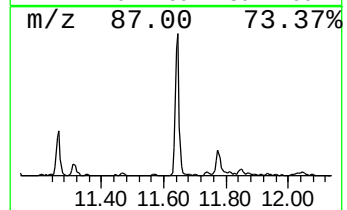
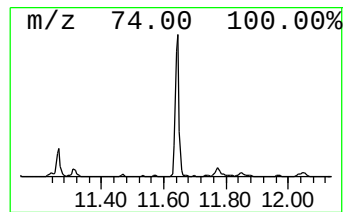
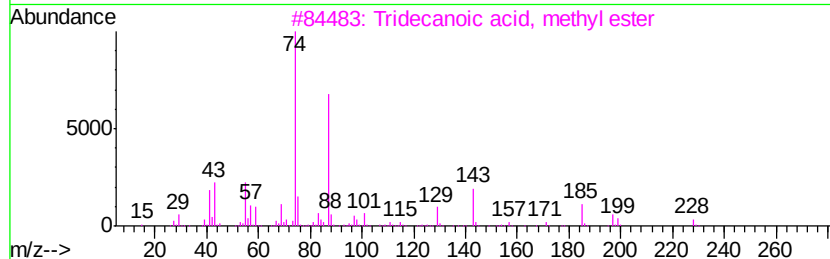
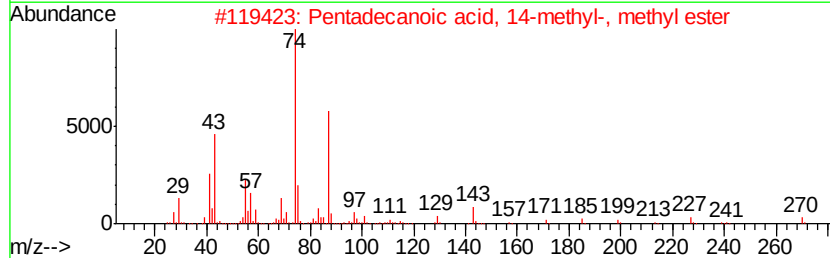
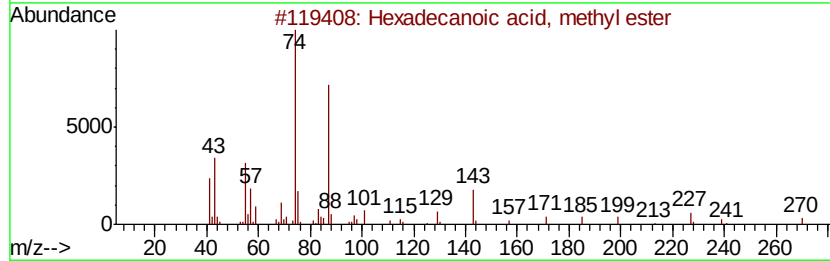
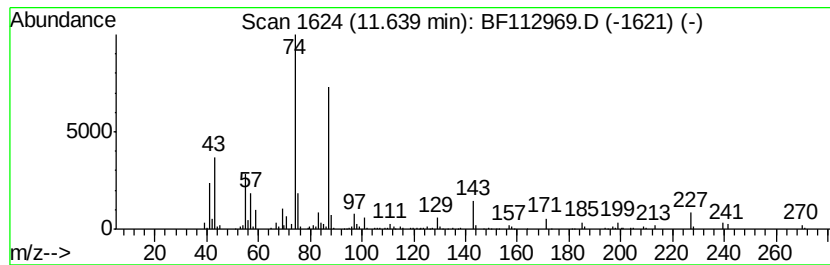
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.64	2.13 ng	228687	Phenanthrene-d10	11.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	72



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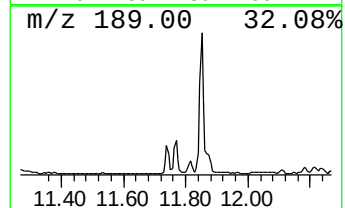
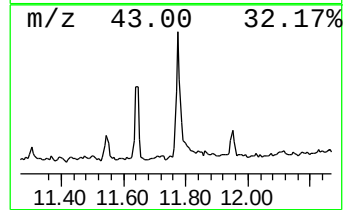
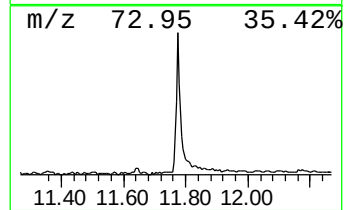
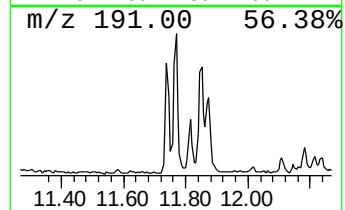
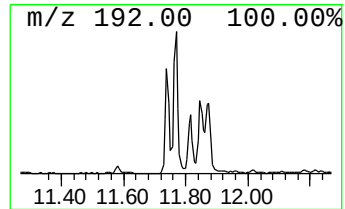
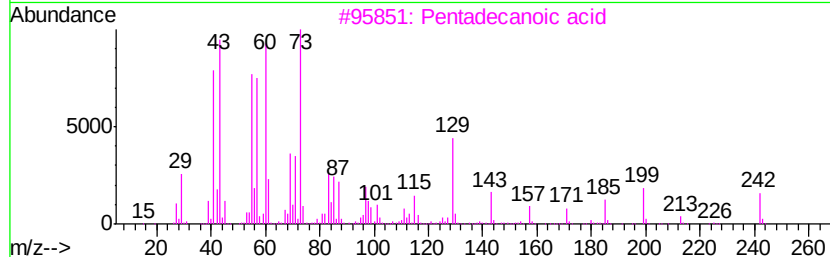
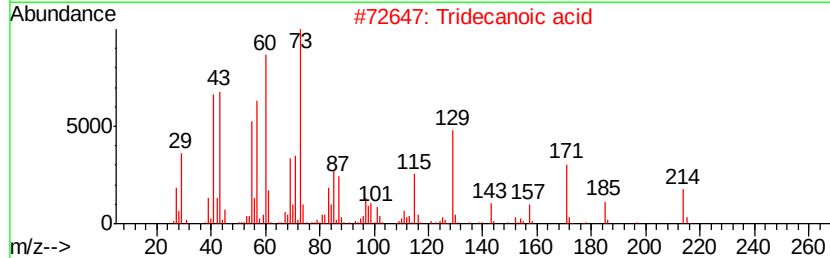
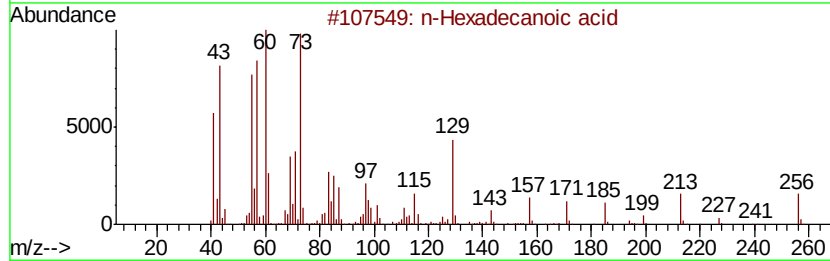
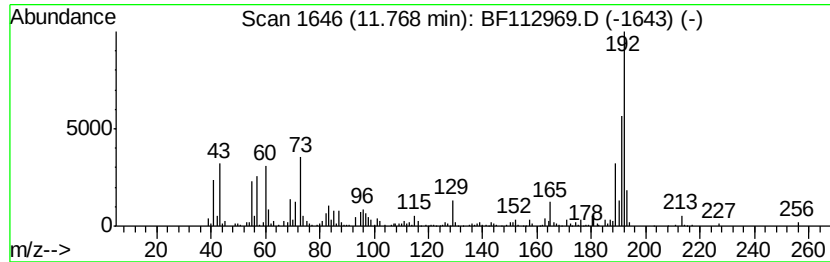
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.77	4.23 ng	454932	Phenanthrene-d10	11.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	59



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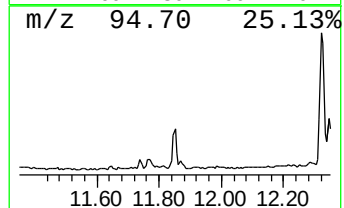
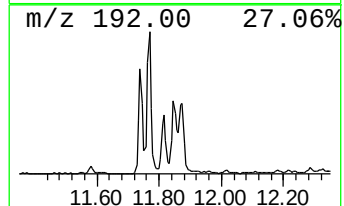
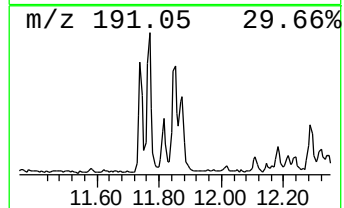
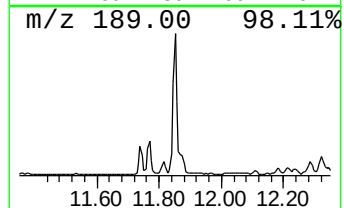
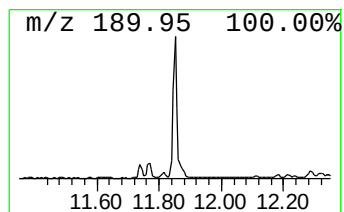
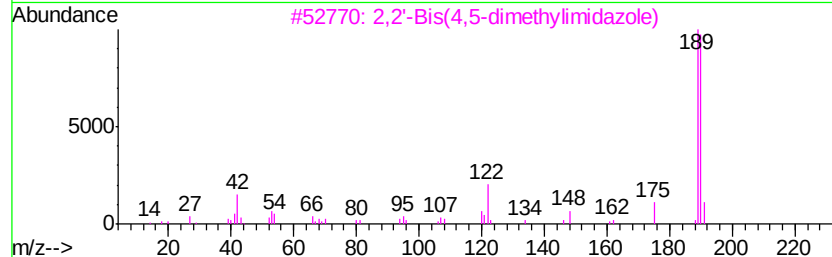
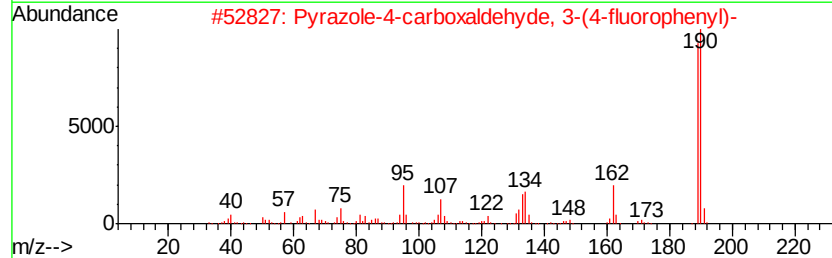
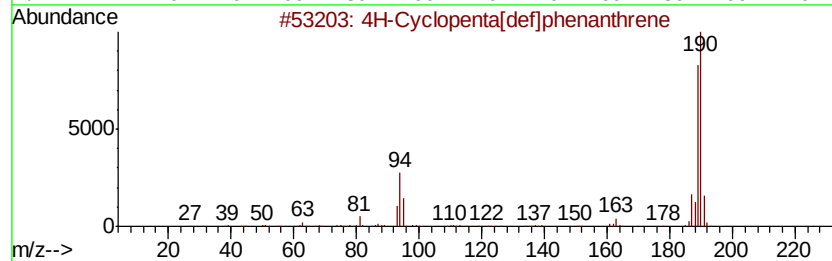
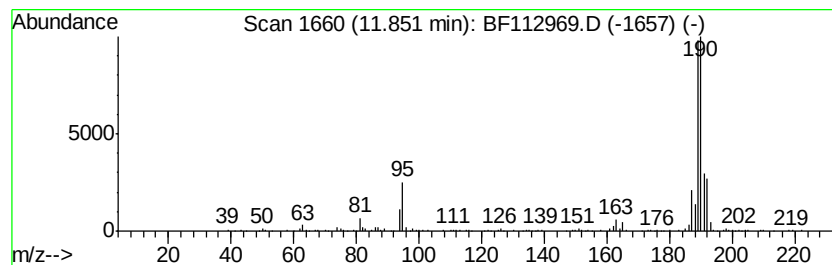
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.85	2.51 ng	269929	Phenanthrene-d10	11.24		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2		Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	58
3		2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
4		Methyl diselenide	190	C2H6Se2	007101-31-7	35
5		1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112969.D
Acq On : 11 Mar 2019 21:55
Operator : JU/SJ
Sample : K1691-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-030819-A

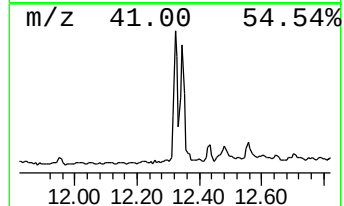
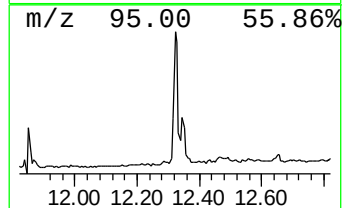
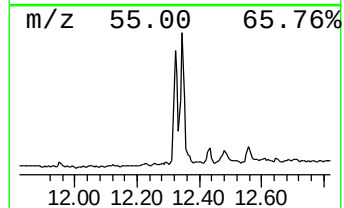
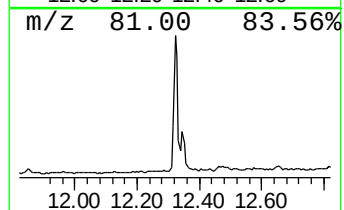
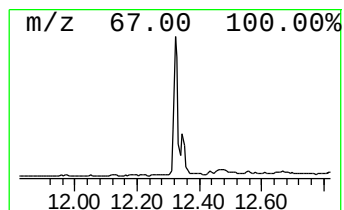
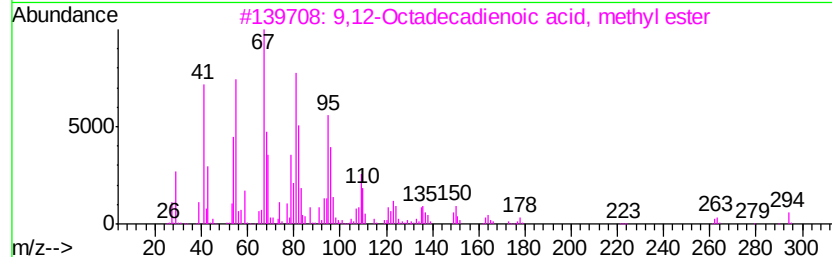
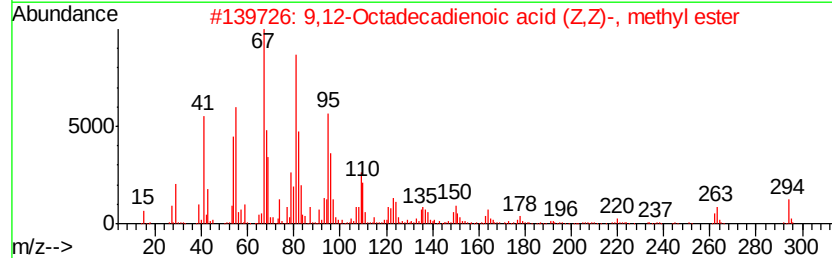
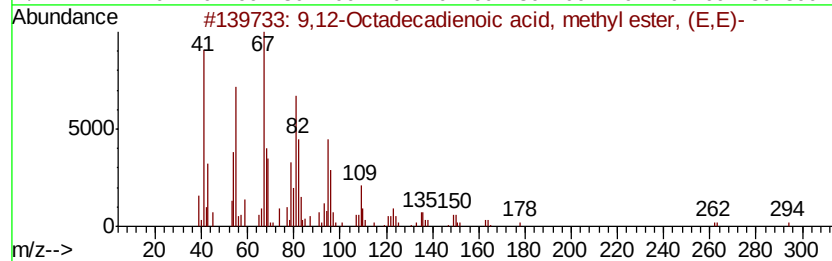
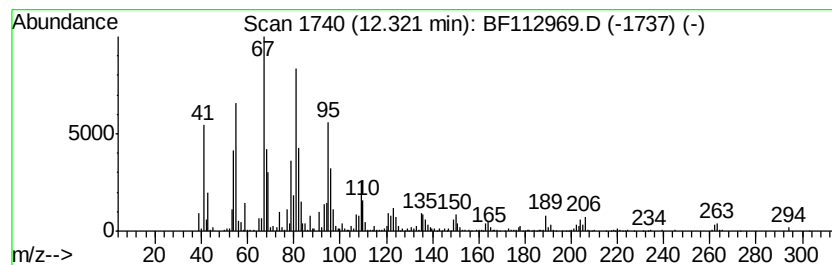
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	7.51 ng	806625	Phenanthrene-d10	11.24

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
4			9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98
5			9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
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Acq On : 11 Mar 2019 21:55
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Misc :
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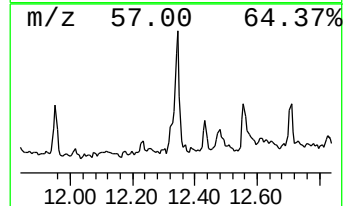
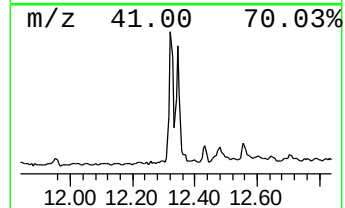
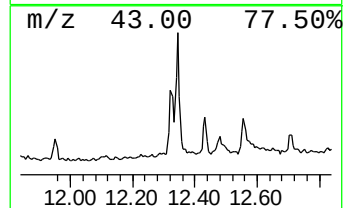
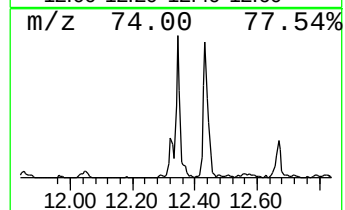
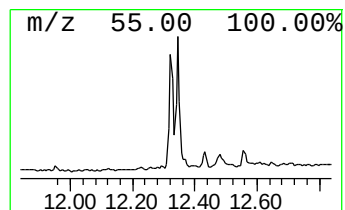
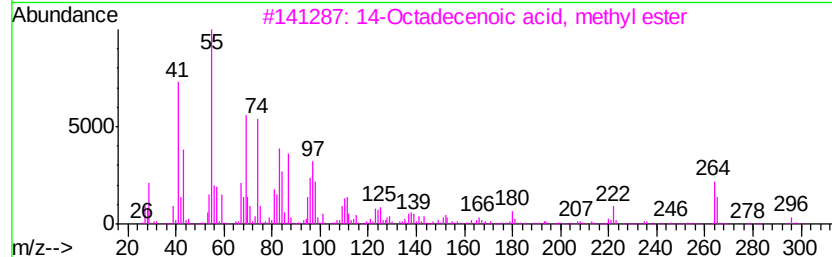
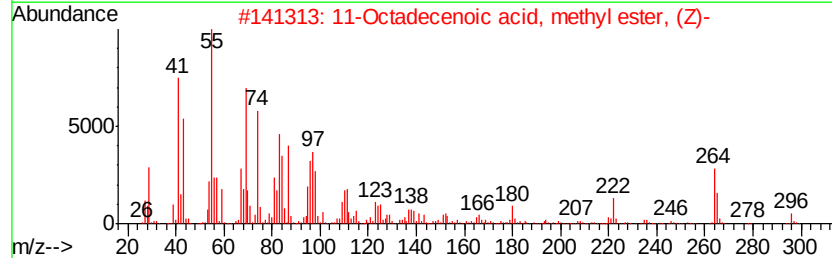
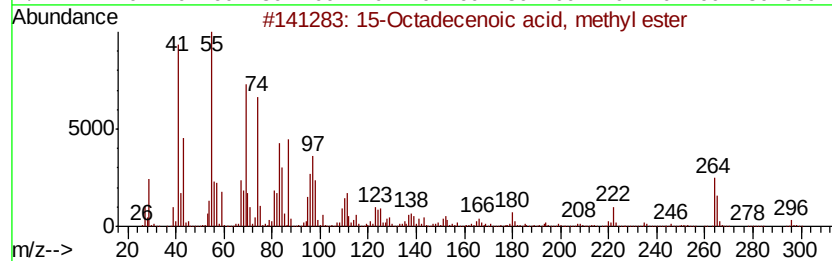
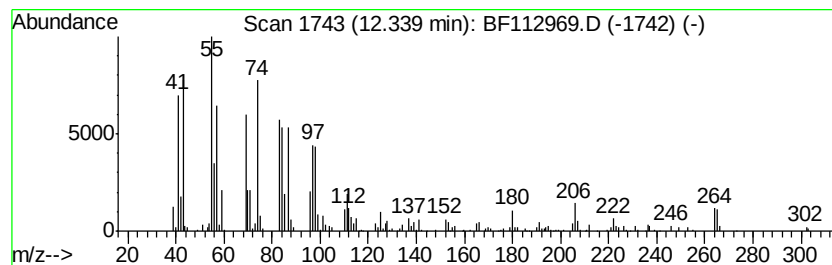
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 15-Octadecenoic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.34	5.95 ng	639224	Phenanthrene-d10	11.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	94
2	11-Octadecenoic acid, methyl ester	296	C19H36O2	001937-63-9	94
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	93
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
5	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
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Sample : K1691-01 2X
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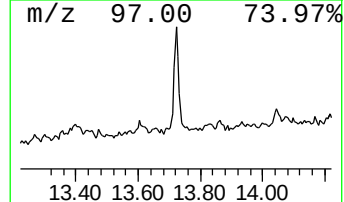
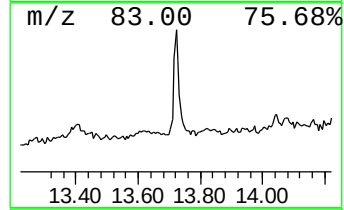
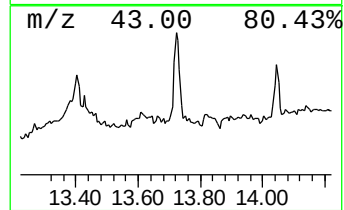
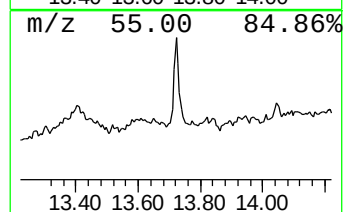
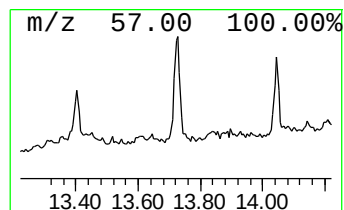
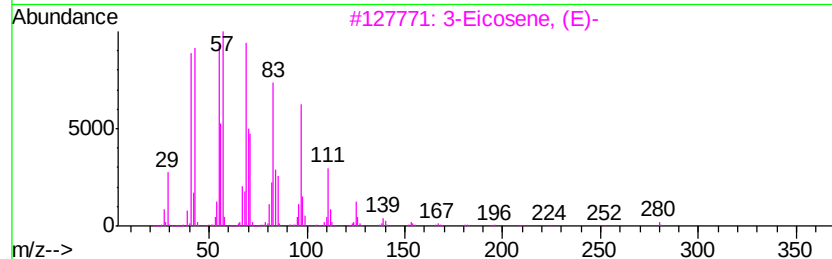
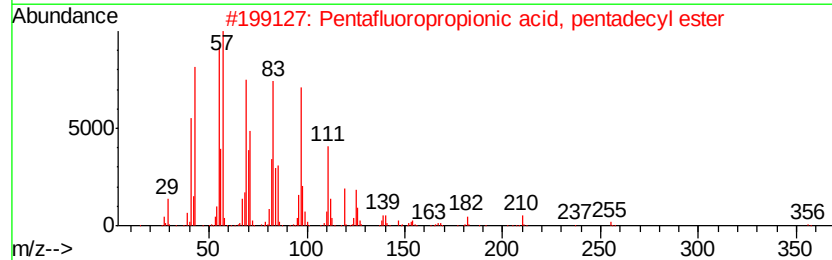
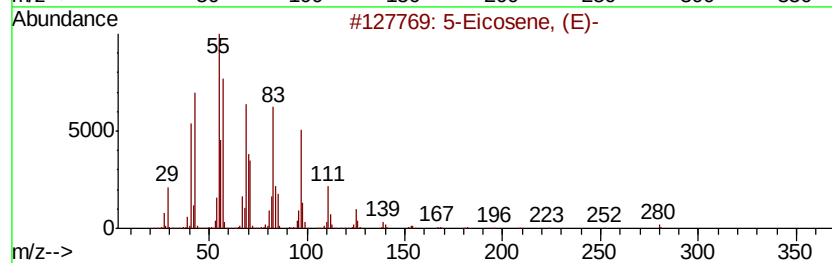
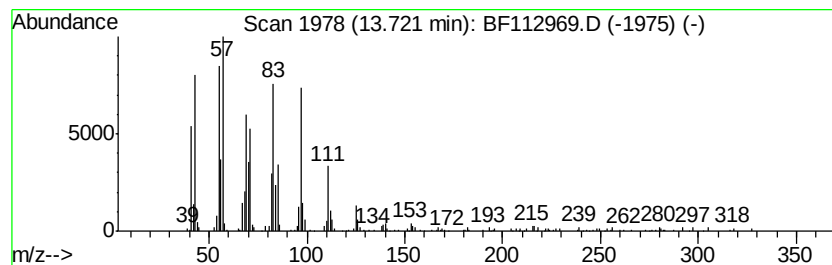
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 5-Eicosene, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.72	2.68 ng	299411	Chrysene-d12		13.86		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3			3-Eicosene, (E)-	280	C20H40	074685-33-9	93
4			9-Eicosene, (E)-	280	C20H40	074685-29-3	93
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



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Sample : K1691-01 2X
Misc :
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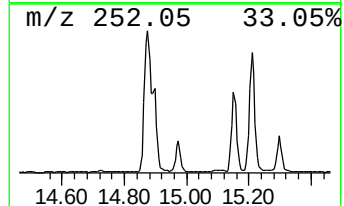
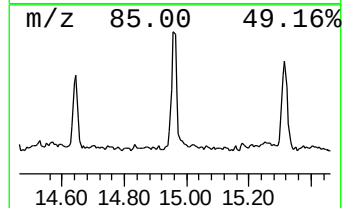
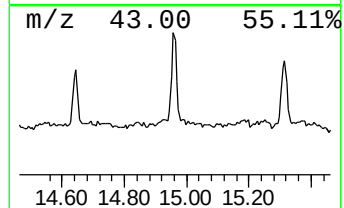
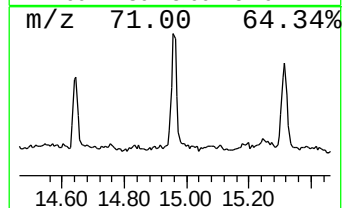
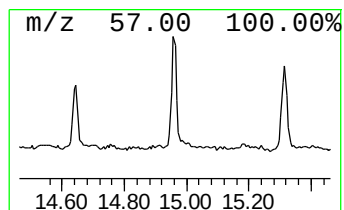
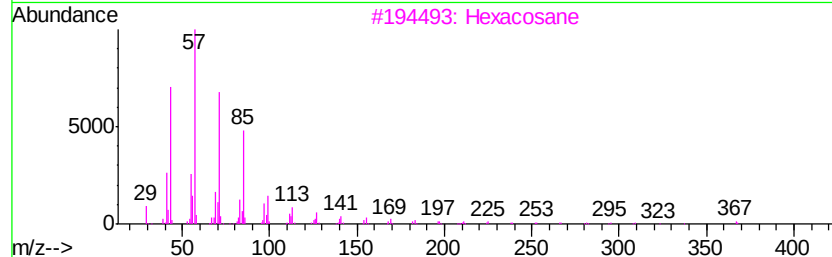
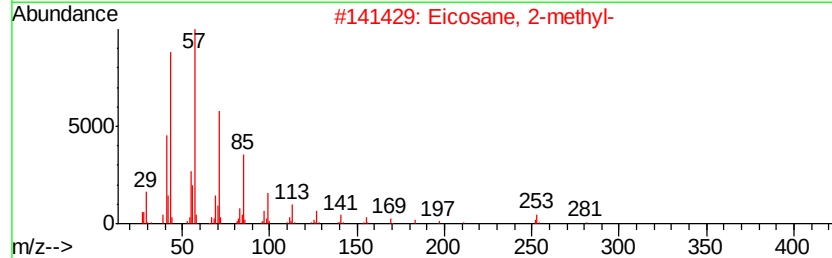
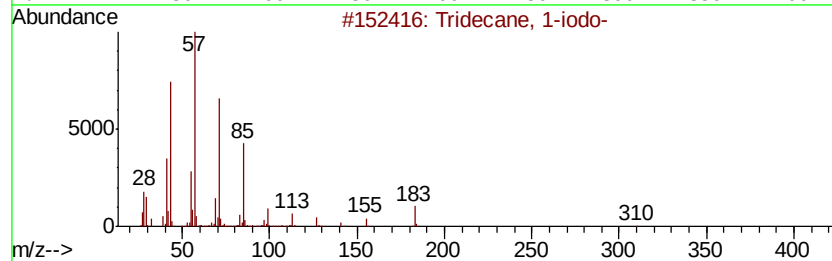
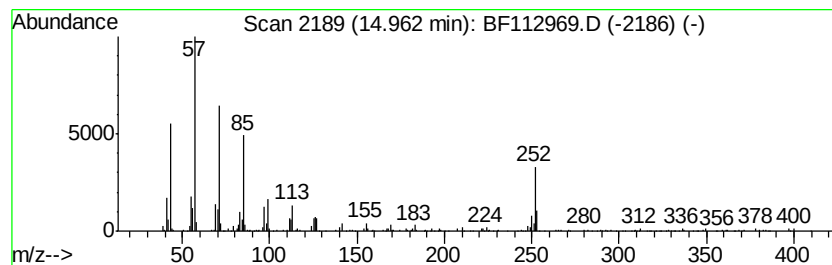
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tridecane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.96	5.82 ng	407567	Perylene-d12	15.27	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83
2	Eicosane, 2-methyl-	296	C21H44	001560-84-5	64
3	Hexacosane	366	C26H54	000630-01-3	64
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	64
5	Heneicosane	296	C21H44	000629-94-7	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
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Sample : K1691-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

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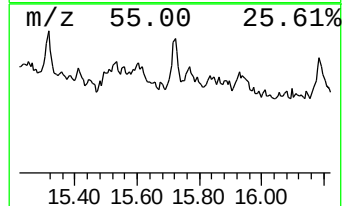
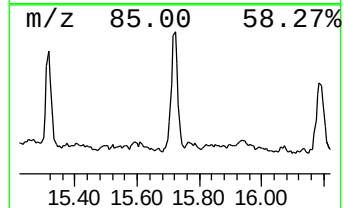
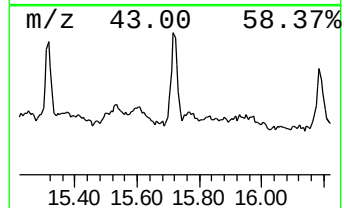
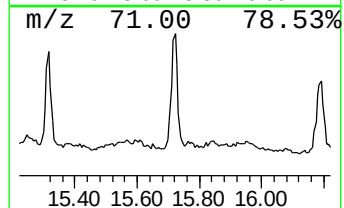
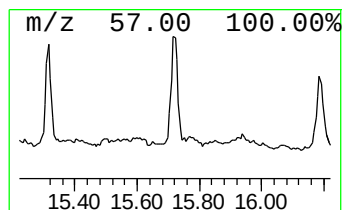
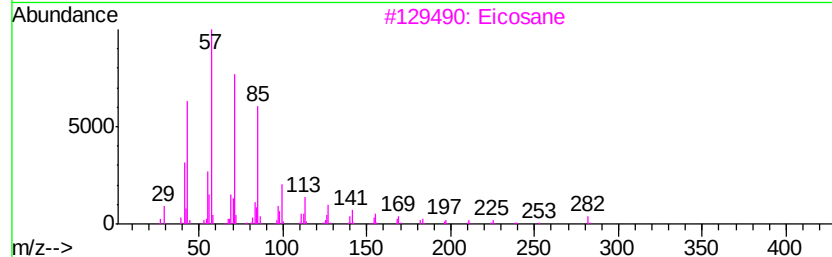
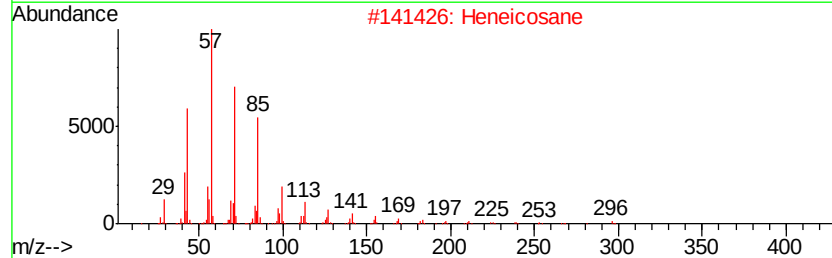
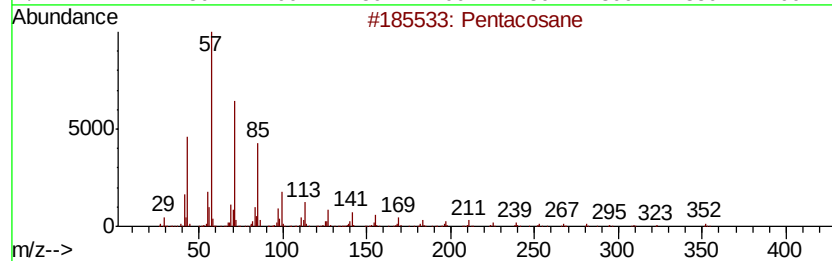
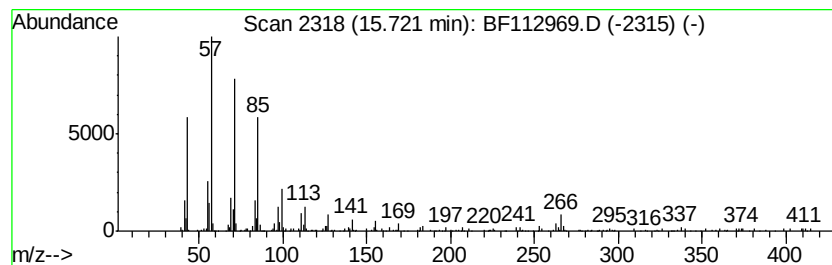
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	3.45 ng	241377	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	93
2		Heneicosane	296	C21H44	000629-94-7	92
3		Eicosane	282	C20H42	000112-95-8	90
4		2-methyloctacosane	408	C29H60	1000376-72-8	87
5		Octacosane	394	C28H58	000630-02-4	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031119\
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ALS Vial : 17 Sample Multiplier: 1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Hexadecanoic acid...	11.64	2.1	ng	228687	4	11.24	2148780	20.0
n-Hexadecanoic acid	11.77	4.2	ng	454932	4	11.24	2148780	20.0
4H-Cyclopenta[def...	11.85	2.5	ng	269929	4	11.24	2148780	20.0
9,12-Octadecadien...	12.32	7.5	ng	806625	4	11.24	2148780	20.0
15-Octadecenoic a...	12.34	6.0	ng	639224	4	11.24	2148780	20.0
5-Eicosene, (E)-	13.72	2.7	ng	299411	5	13.86	2233090	20.0
Tridecane, 1-iodo-	14.96	5.8	ng	407567	6	15.27	1399410	20.0
Pentacosane	15.72	3.5	ng	241377	6	15.27	1399410	20.0