

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031419\
 Data File : BF113050.D
 Acq On : 14 Mar 2019 15:28
 Operator : JU/SJ
 Sample : K1866-09
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MR-MH-15-COMP

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	5.346	549	554	557	rBV	4376771	4675174	84.67%	6.890%
2	6.375	723	729	732	rBV	4249264	4993711	90.44%	7.360%
3	6.498	745	750	753	rBV	4610351	4981162	90.21%	7.341%
4	6.722	785	788	792	rBV	1305520	1232757	22.33%	1.817%
5	6.881	811	815	819	rBV	3790335	3808986	68.98%	5.614%
6	7.287	878	884	887	rBV	2874369	3228626	58.47%	4.758%
7	8.010	1001	1007	1012	rBV	1491067	1527357	27.66%	2.251%
8	8.628	1106	1112	1119	rBV	86329	82649	1.50%	0.122%
9	9.086	1184	1190	1193	rBV	5349408	5304235	96.06%	7.817%
10	9.475	1252	1256	1265	rVB	503799	445380	8.07%	0.656%
11	9.757	1298	1304	1313	rBV2	1975043	1784586	32.32%	2.630%
12	10.545	1432	1438	1441	rBV	3807408	3871445	70.11%	5.706%
13	11.233	1551	1555	1558	rBV	2033146	1967693	35.64%	2.900%
14	11.257	1558	1559	1563	rVB	315047	184225	3.34%	0.272%
15	11.469	1590	1595	1602	rBV5	29075	55556	1.01%	0.082%
16	11.698	1630	1634	1637	rBV4	43974	59842	1.08%	0.088%
17	11.739	1637	1641	1643	rVV	146095	177509	3.21%	0.262%
18	11.780	1643	1648	1656	rVV2	1974542	2260646	40.94%	3.332%
19	11.845	1656	1659	1661	rVV	122256	142124	2.57%	0.209%
20	11.869	1661	1663	1670	rVB2	63400	71782	1.30%	0.106%
21	12.051	1692	1694	1701	rVB3	53482	59813	1.08%	0.088%
22	12.333	1736	1742	1745	rVB3	87938	107792	1.95%	0.159%
23	12.439	1757	1760	1764	rBV	517995	488039	8.84%	0.719%
24	12.475	1764	1766	1774	rVB3	134325	216737	3.93%	0.319%
25	12.557	1774	1780	1793	rBV	1000490	1150003	20.83%	1.695%
26	12.669	1793	1799	1802	rBV	467346	474020	8.58%	0.699%
27	12.822	1820	1825	1828	rBV	5334784	5521708	100.00%	8.138%
28	12.886	1832	1836	1840	rBV2	55605	77956	1.41%	0.115%
29	12.998	1852	1855	1858	rVB	84068	87840	1.59%	0.129%
30	13.039	1858	1862	1863	rBV3	59767	62544	1.13%	0.092%
31	13.057	1863	1865	1869	rVV2	171964	160673	2.91%	0.237%
32	13.098	1869	1872	1876	rVV	70361	65265	1.18%	0.096%
33	13.280	1898	1903	1904	rBV5	44035	58717	1.06%	0.087%
34	13.298	1904	1906	1912	rVB4	49082	60604	1.10%	0.089%

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 Integrator: RTE
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 Sampling : 1
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 Max Peaks: 100
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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35	13.398	1920	1923	1926	rVB	146262	115240	2.09%	0.170%
36	13.504	1933	1941	1946	rBV3	64443	113010	2.05%	0.167%
37	13.610	1955	1959	1961	rBV2	62191	82599	1.50%	0.122%
38	13.722	1972	1978	1986	rBV3	965766	1352060	24.49%	1.993%
39	13.863	1994	2002	2005	rBV	2272598	2477822	44.87%	3.652%
40	13.886	2005	2006	2011	rVV	298142	214925	3.89%	0.317%
41	13.951	2013	2017	2024	rVV5	119796	243017	4.40%	0.358%
42	14.039	2028	2032	2039	rVV	327751	333472	6.04%	0.491%
43	14.251	2063	2068	2072	rBV3	139997	213584	3.87%	0.315%
44	14.345	2077	2084	2090	rBV2	631305	938688	17.00%	1.383%
45	14.439	2097	2100	2103	rBV4	65881	70352	1.27%	0.104%
46	14.551	2115	2119	2125	rVB3	214298	257595	4.67%	0.380%
47	14.610	2126	2129	2132	rBV	614940	677878	12.28%	0.999%
48	14.639	2132	2134	2142	rVB	405836	434862	7.88%	0.641%
49	14.704	2142	2145	2148	rBV	209734	205082	3.71%	0.302%
50	14.768	2153	2156	2162	rVB	245717	260625	4.72%	0.384%
51	14.868	2167	2173	2176	rBV	234362	428267	7.76%	0.631%
52	14.951	2183	2187	2191	rBV	772487	955164	17.30%	1.408%
53	14.980	2191	2192	2198	rVV	180869	206749	3.74%	0.305%
54	15.063	2202	2206	2210	rBV4	75823	109928	1.99%	0.162%
55	15.151	2217	2221	2224	rBV	119846	142484	2.58%	0.210%
56	15.204	2224	2230	2235	rVB	217154	357388	6.47%	0.527%
57	15.268	2236	2241	2245	rBV	1613069	2076904	37.61%	3.061%
58	15.304	2245	2247	2253	rVB2	338837	412950	7.48%	0.609%
59	15.492	2274	2279	2287	rVB	396656	518003	9.38%	0.763%
60	15.710	2311	2316	2321	rBV	610287	869940	15.75%	1.282%
61	15.763	2321	2325	2333	rVV2	257027	517091	9.36%	0.762%
62	16.174	2391	2395	2399	rBV	118646	212593	3.85%	0.313%
63	16.210	2399	2401	2409	rVB	123635	173146	3.14%	0.255%
64	16.445	2435	2441	2449	rBV2	340559	633239	11.47%	0.933%
65	16.621	2467	2471	2474	rBV3	94116	167290	3.03%	0.247%
66	16.721	2484	2488	2496	rVB	141148	275476	4.99%	0.406%
67	16.815	2498	2504	2513	rVB6	145659	412540	7.47%	0.608%
68	17.027	2537	2540	2551	rVB2	82949	178466	3.23%	0.263%
69	17.186	2560	2567	2575	rBV3	250039	621040	11.25%	0.915%
70	17.751	2659	2663	2672	rVB2	153948	353952	6.41%	0.522%
71	18.945	2857	2866	2870	rBV4	257199	791343	14.33%	1.166%

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

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

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

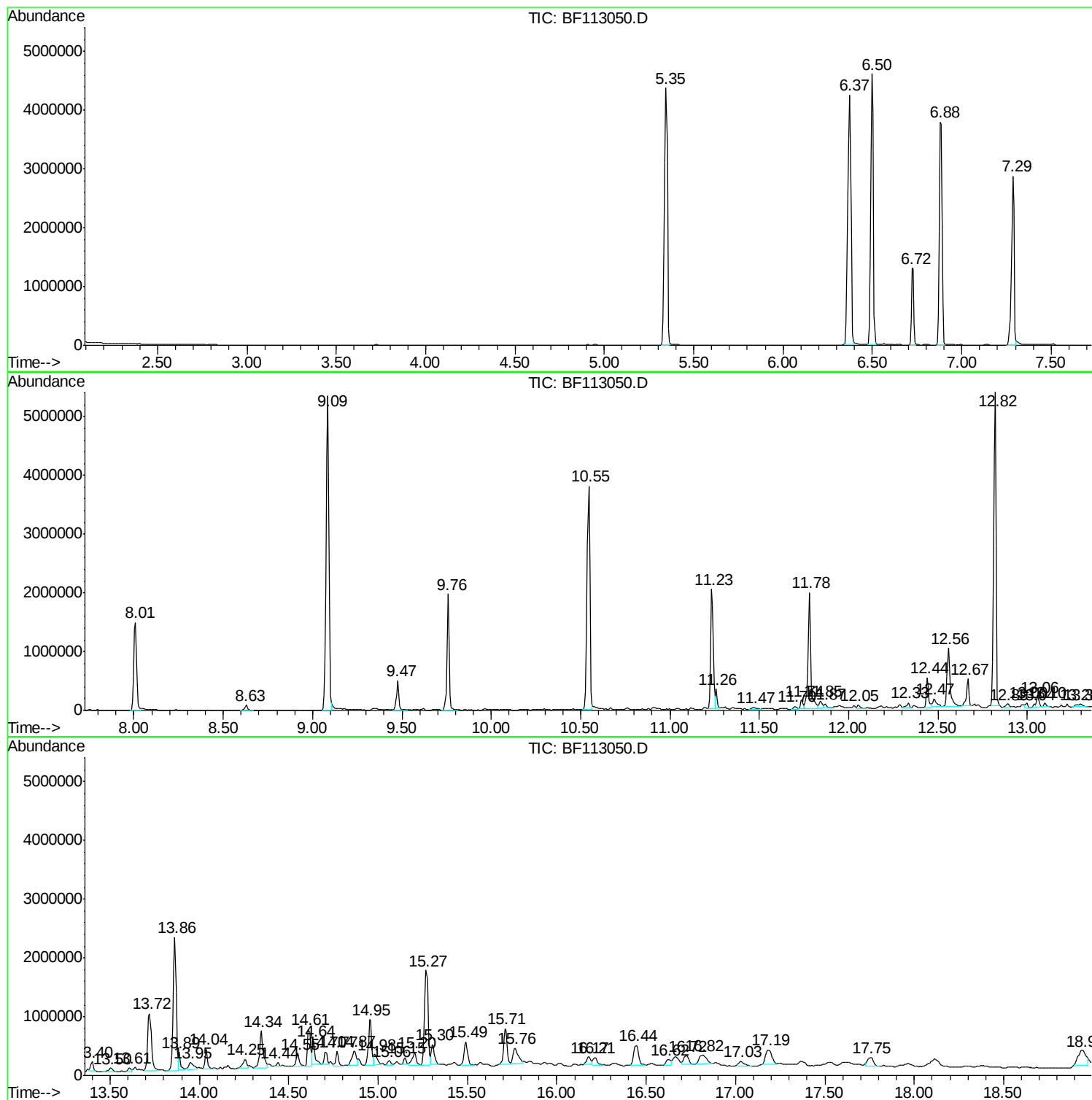
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Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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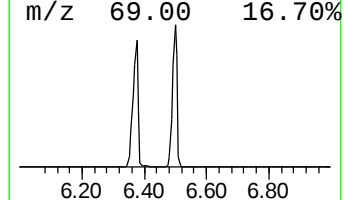
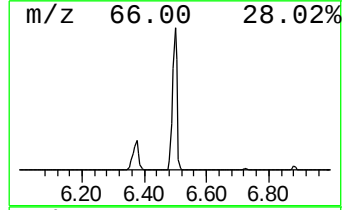
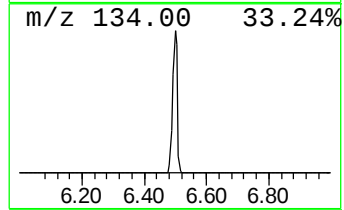
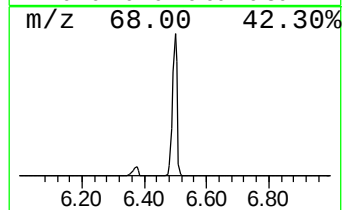
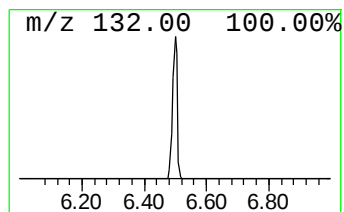
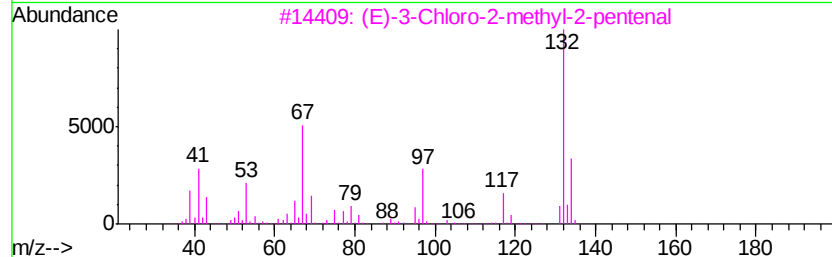
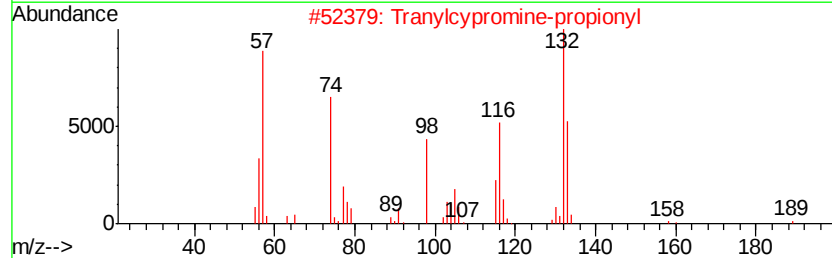
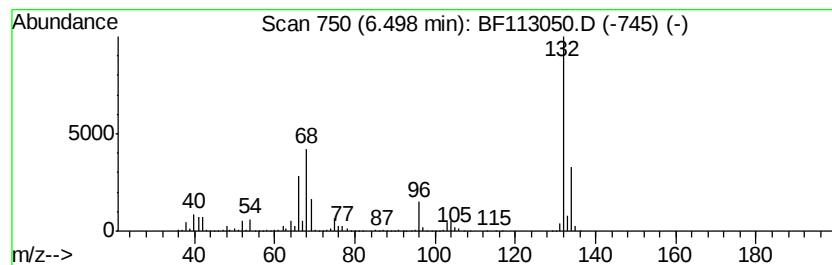
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	80.81 ng	4981160	1,4-Dichlorobenzene-d4	6.73

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



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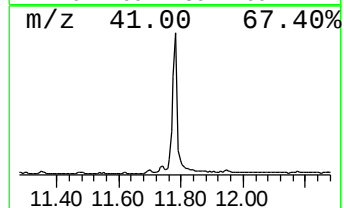
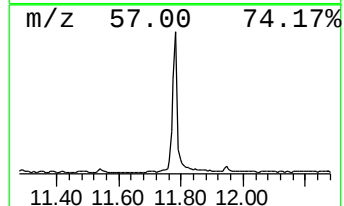
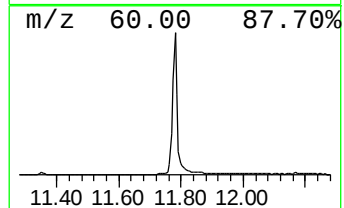
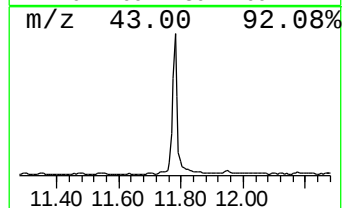
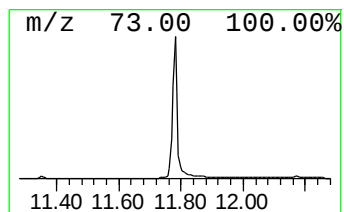
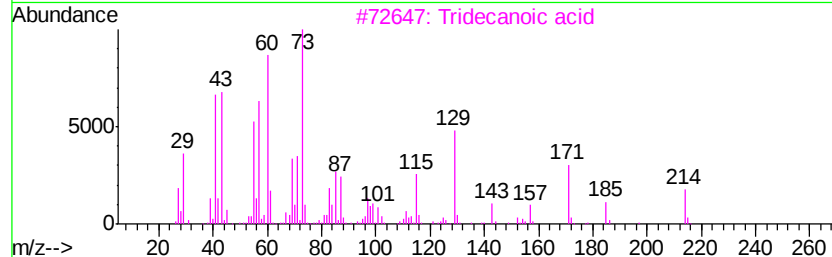
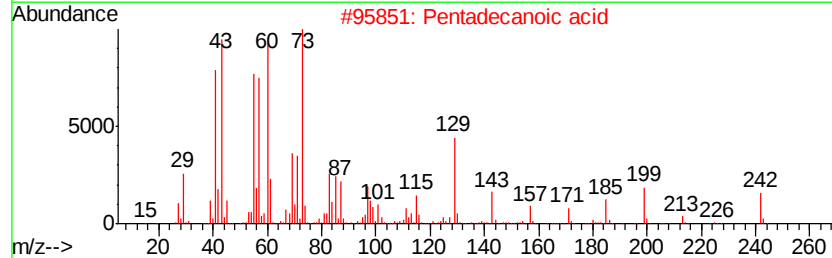
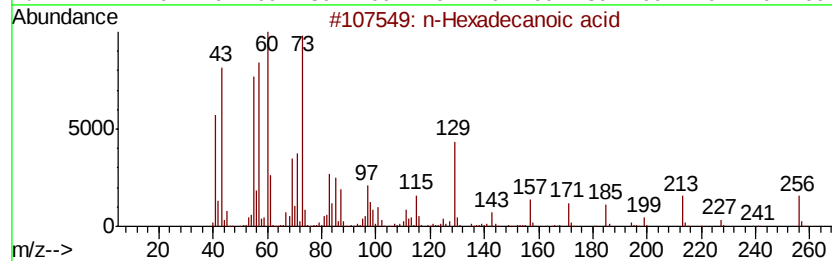
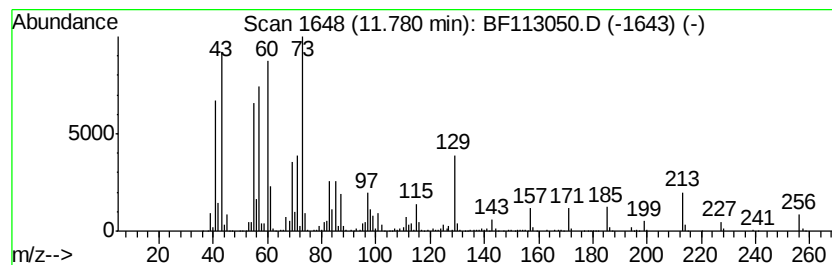
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	22.98 ng	2260650	Phenanthrene-d10	11.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		Tridecanoic acid	214	C13H26O2	000638-53-9	92
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5		Dodecanoic acid	200	C12H24O2	000143-07-7	72



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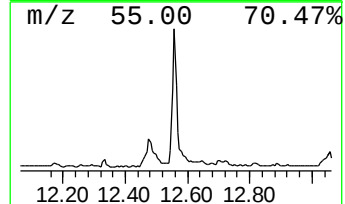
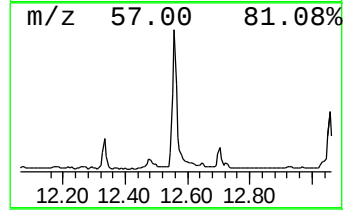
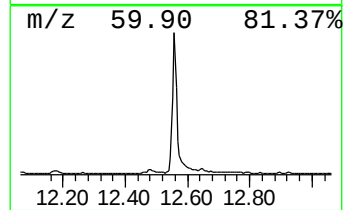
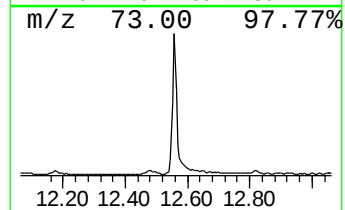
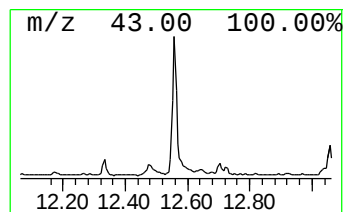
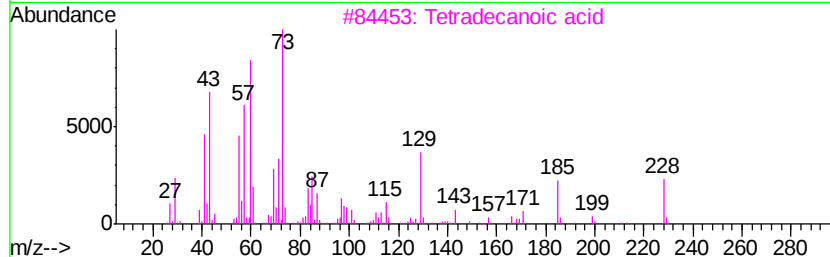
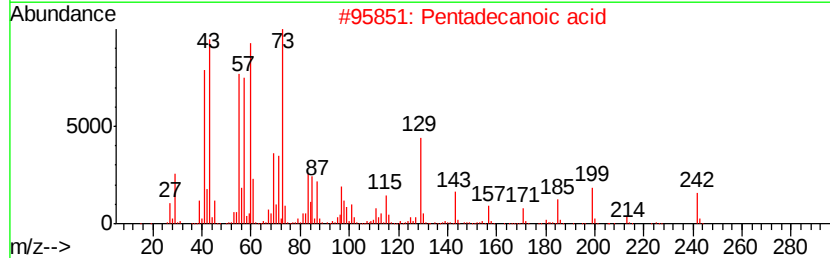
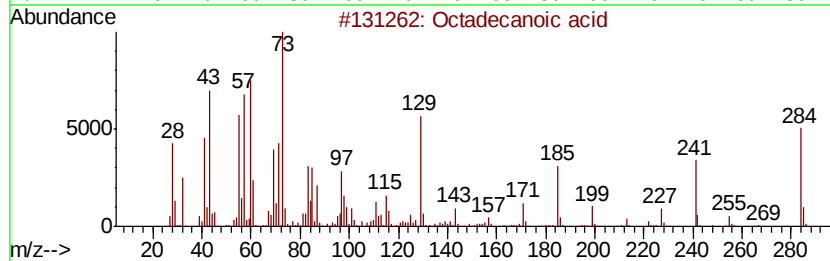
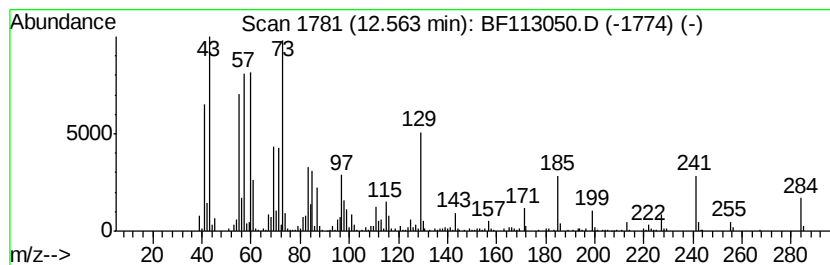
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.56	9.28 ng	1150000	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68



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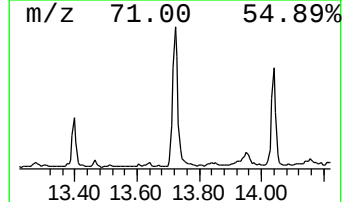
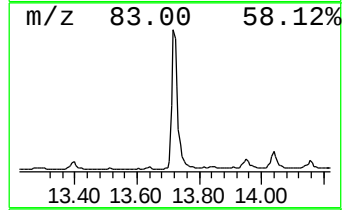
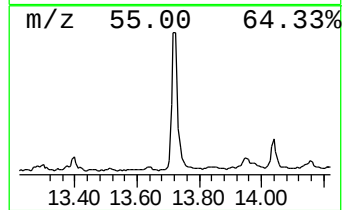
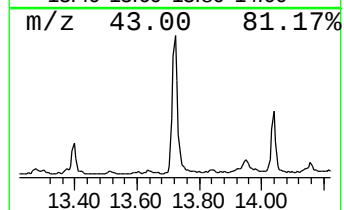
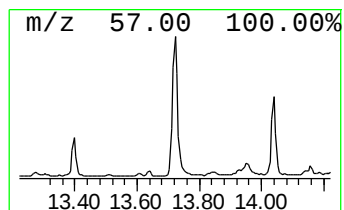
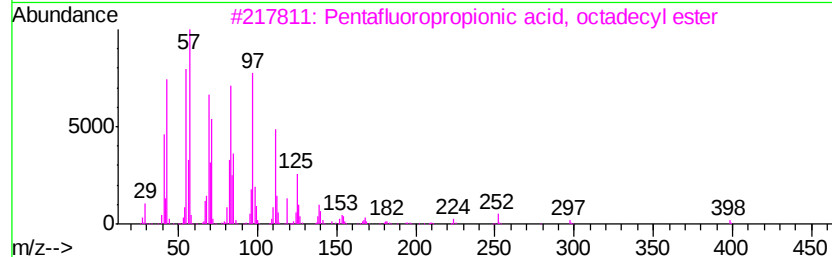
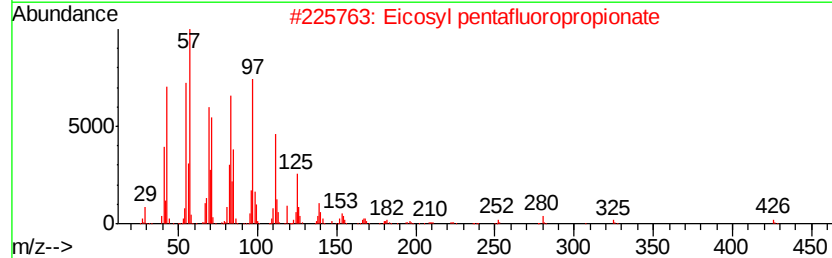
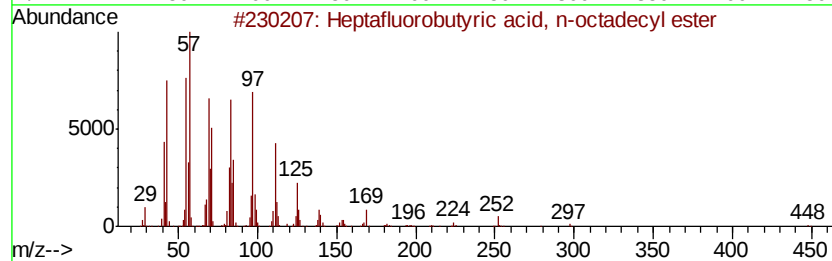
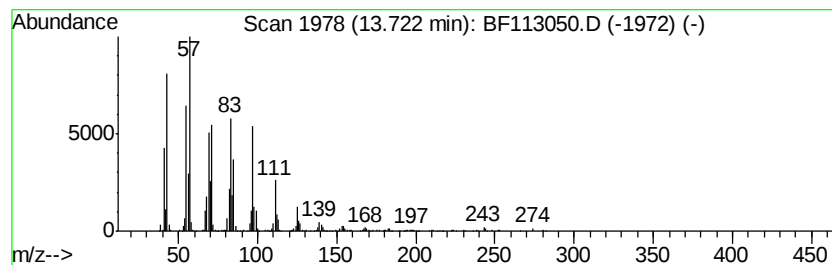
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptafluorobutyric acid, n-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	10.91 ng	1352060	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
2		Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
3		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113050.D
Acq On : 14 Mar 2019 15:28
Operator : JU/SJ
Sample : K1866-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

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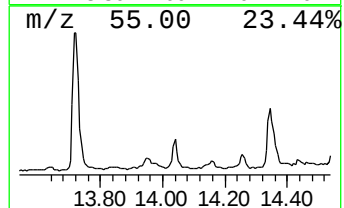
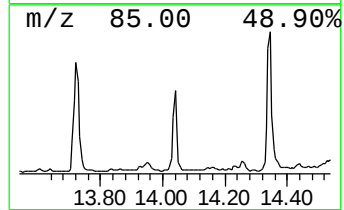
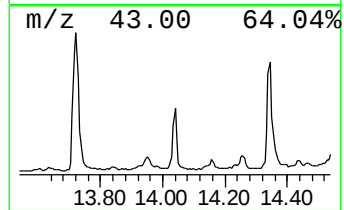
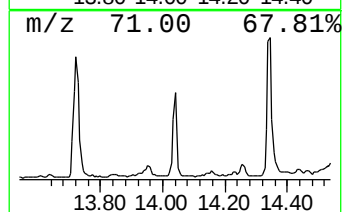
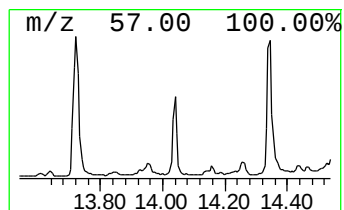
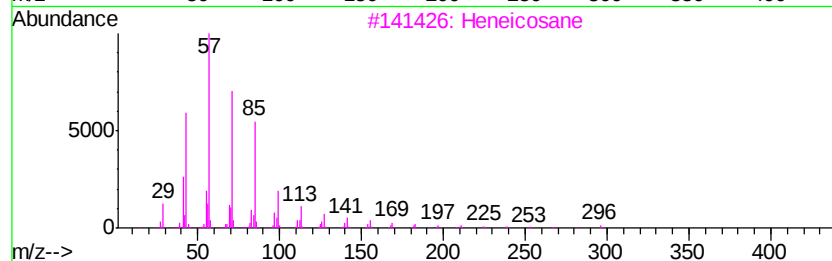
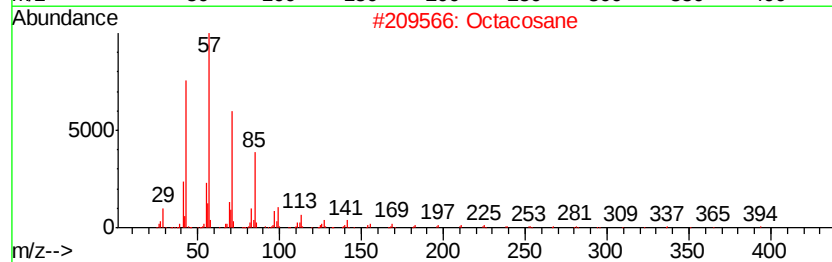
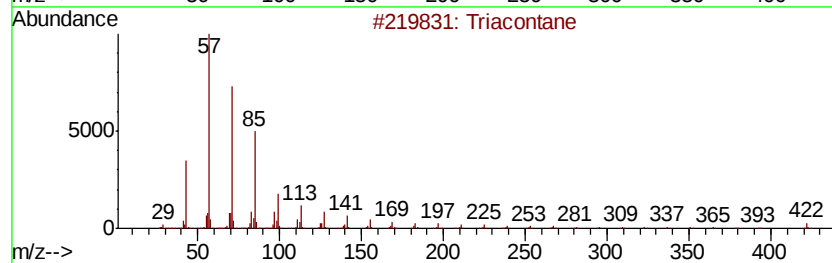
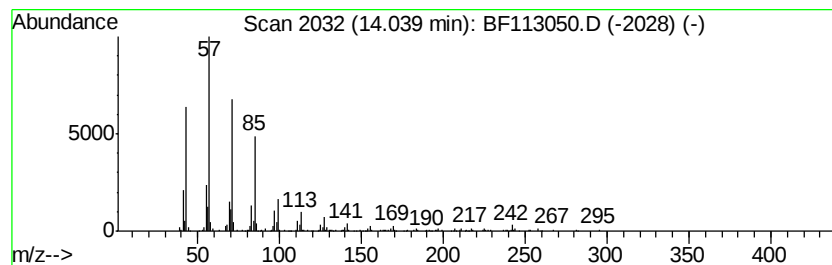
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triacontane Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	2.69 ng	333472	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Tetratetracontane	619	C44H90	007098-22-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
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Sample : K1866-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

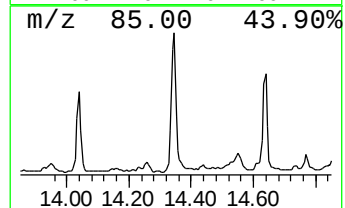
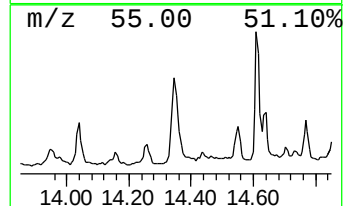
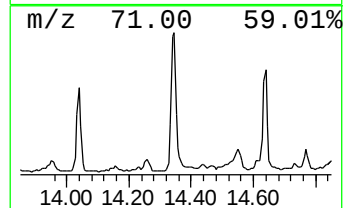
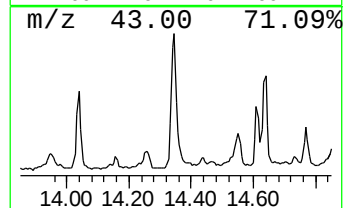
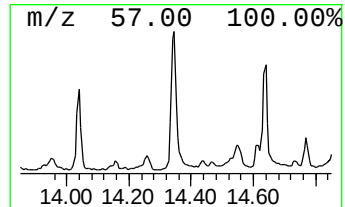
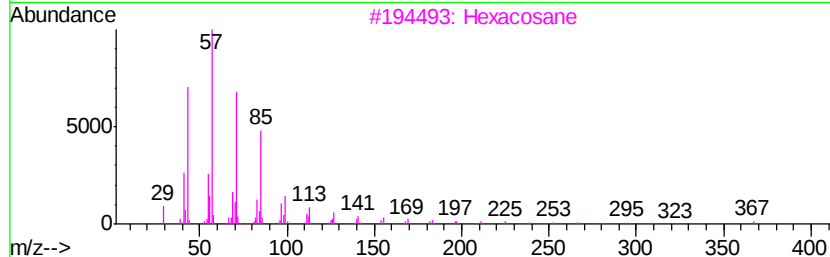
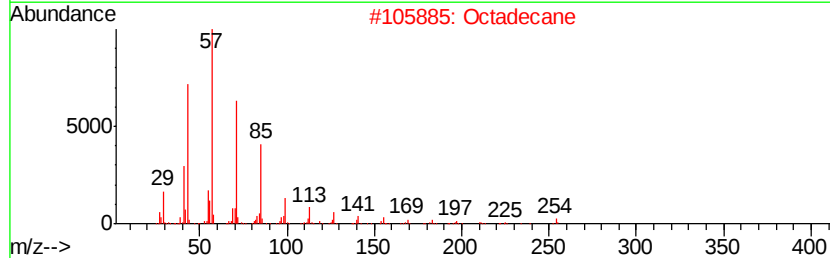
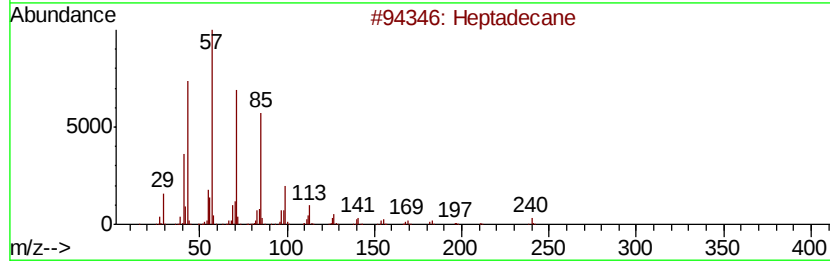
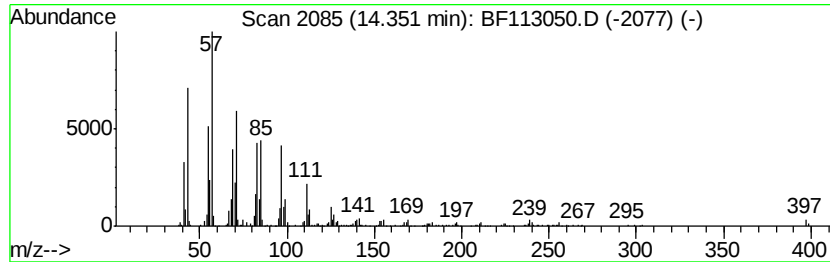
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	7.58 ng	938688	Chrysene-d12	13.86
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	97
2	Octadecane	254 C18H38	000593-45-3	95
3	Hexacosane	366 C26H54	000630-01-3	90
4	Tetracosane	338 C24H50	000646-31-1	90
5	2-methyloctacosane	408 C29H60	1000376-72-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113050.D
Acq On : 14 Mar 2019 15:28
Operator : JU/SJ
Sample : K1866-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

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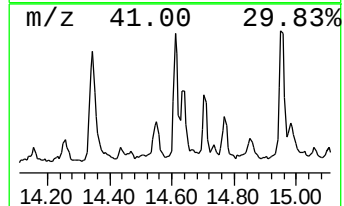
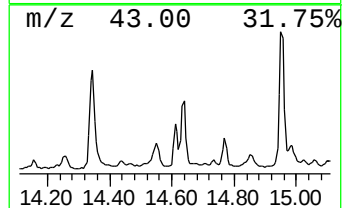
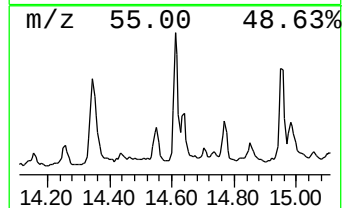
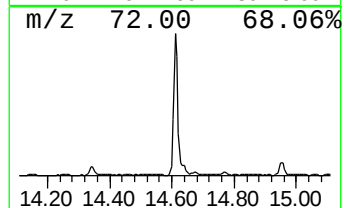
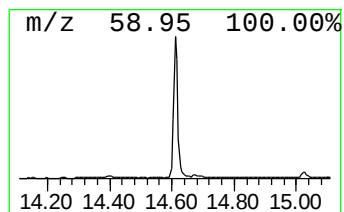
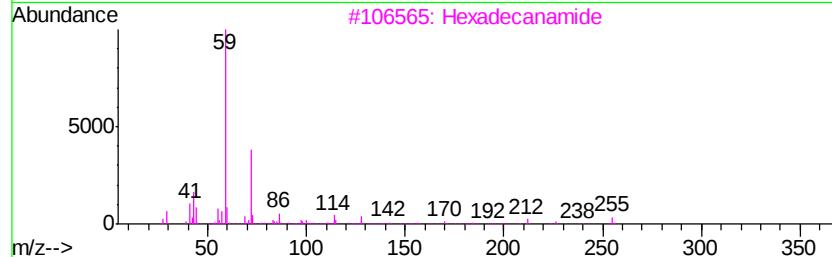
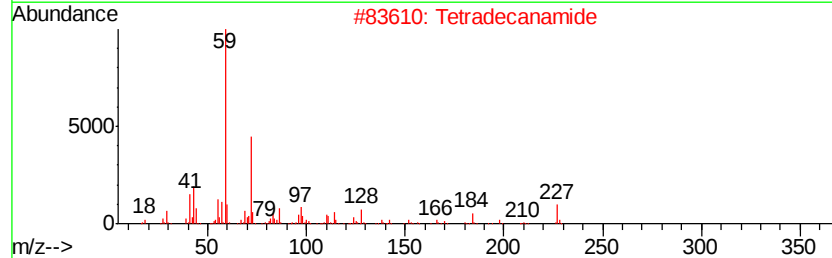
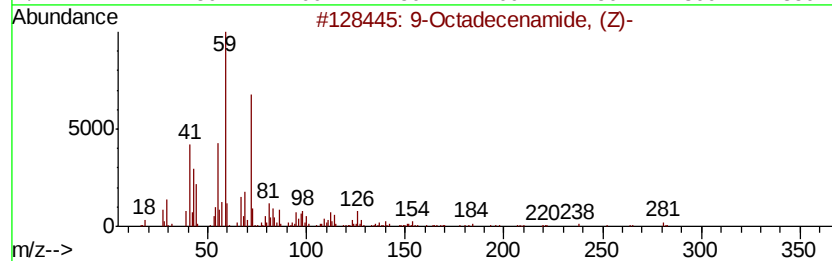
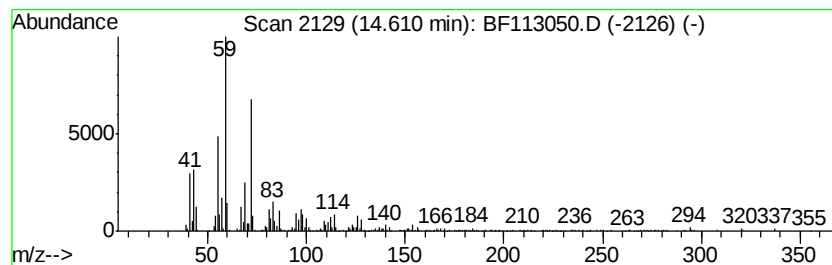
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	6.53 ng	677878	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		Tetradecanamide	227	C14H29NO	000638-58-4	59
3		Hexadecanamide	255	C16H33NO	000629-54-9	56
4		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	56
5		Octadecanamide	283	C18H37NO	000124-26-5	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
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Acq On : 14 Mar 2019 15:28
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ALS Vial : 4 Sample Multiplier: 1

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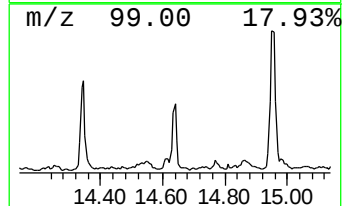
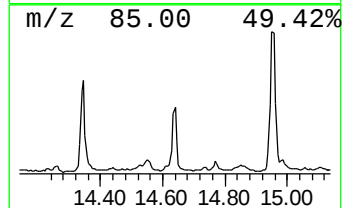
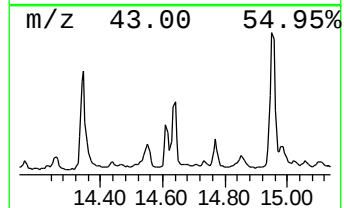
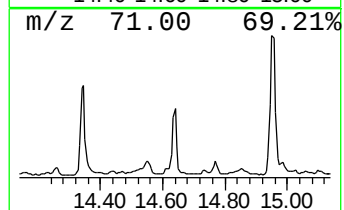
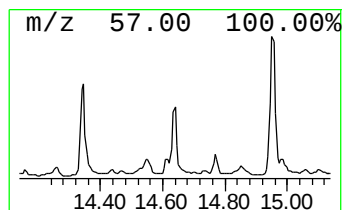
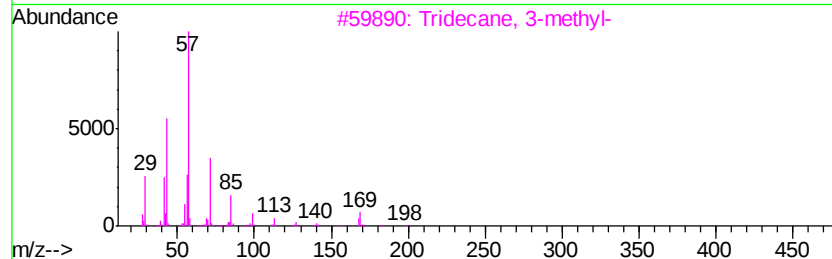
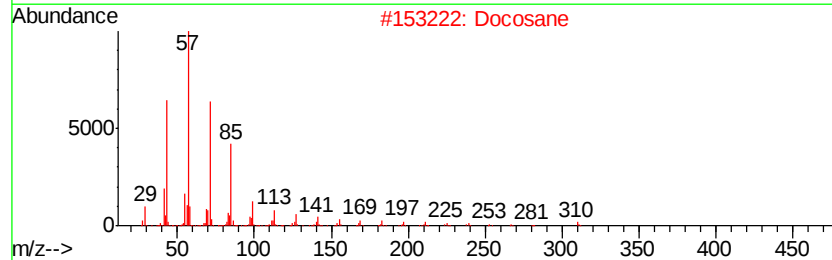
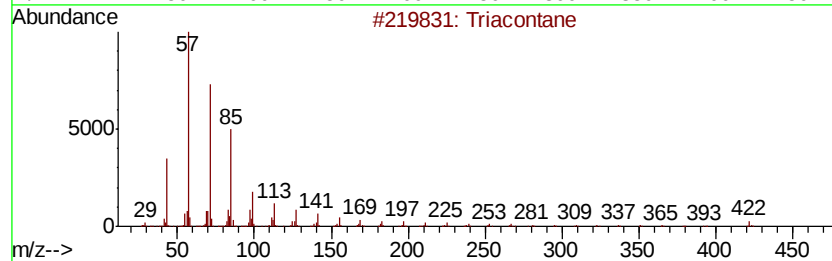
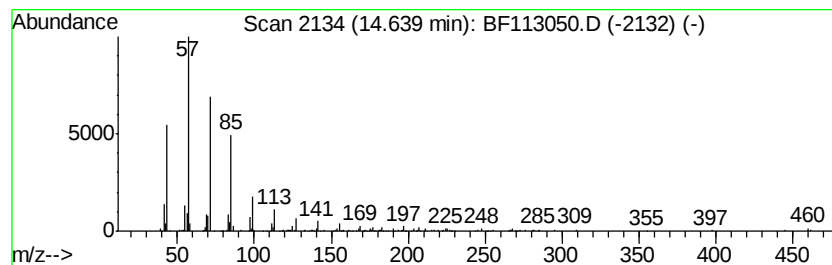
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Docosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	4.19 ng	434862	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	86
2		Docosane	310	C22H46	000629-97-0	86
3		Tridecane, 3-methyl-	198	C14H30	006418-41-3	86
4		2-Bromotetradecane	276	C14H29Br	074036-95-6	86
5		Octadecane	254	C18H38	000593-45-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
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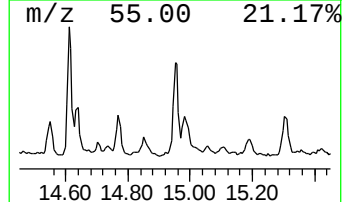
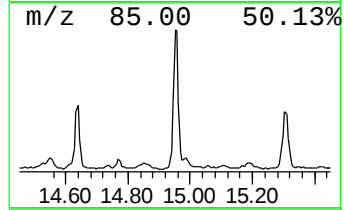
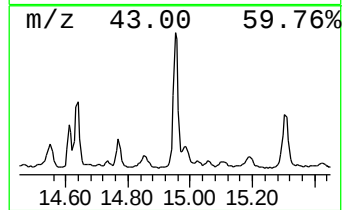
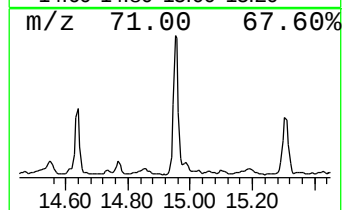
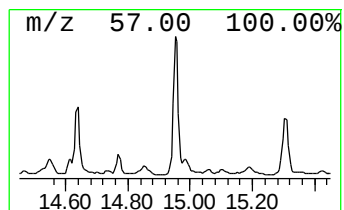
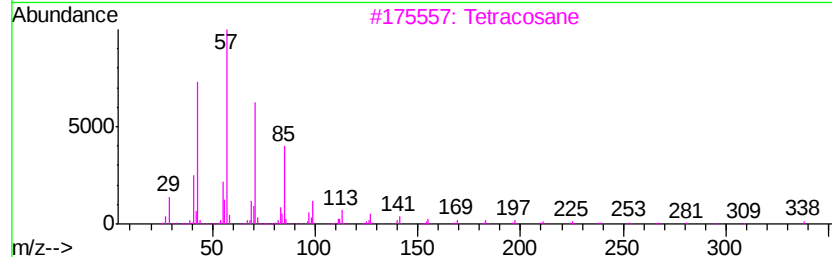
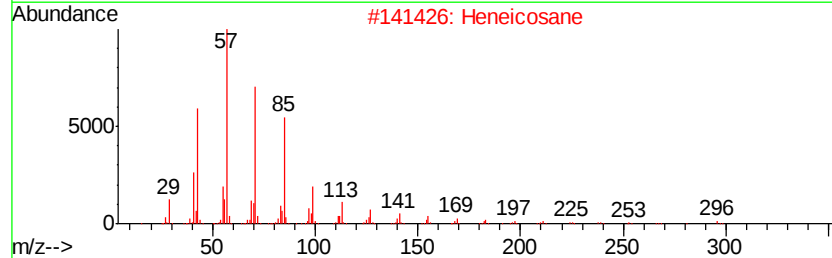
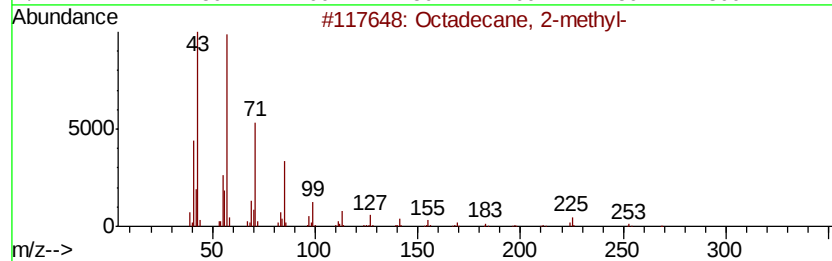
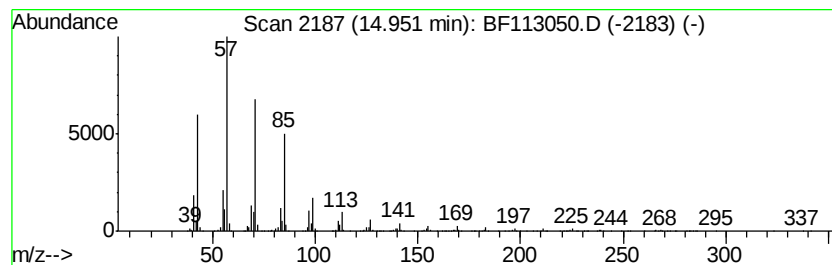
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	9.20 ng	955164	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2		Heneicosane	296	C21H44	000629-94-7	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		Hexadecane	226	C16H34	000544-76-3	87
5		Octacosane	394	C28H58	000630-02-4	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
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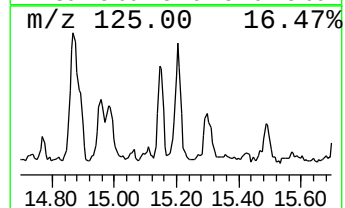
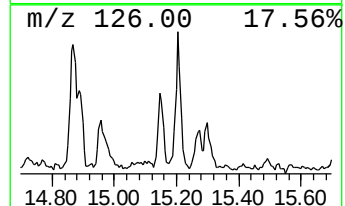
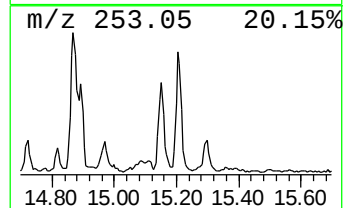
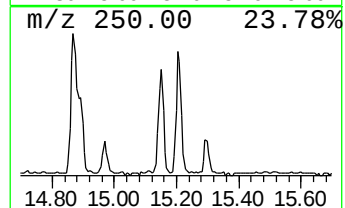
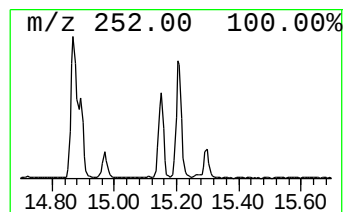
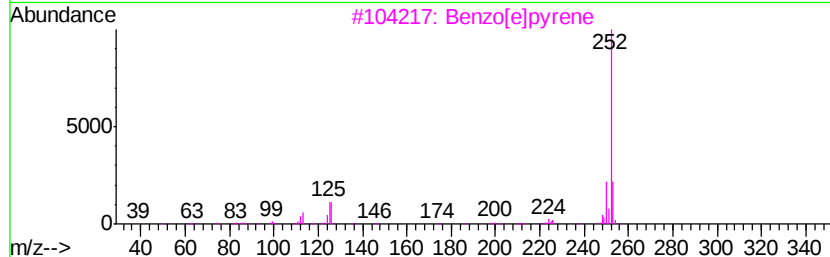
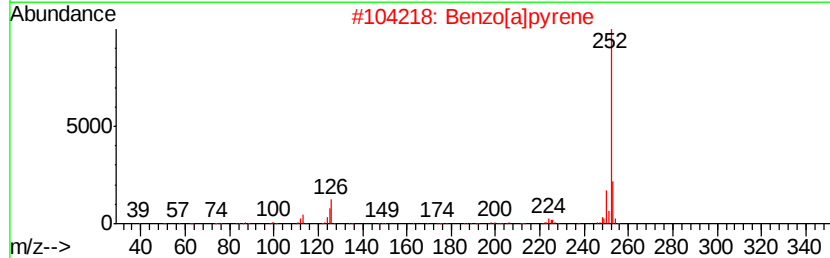
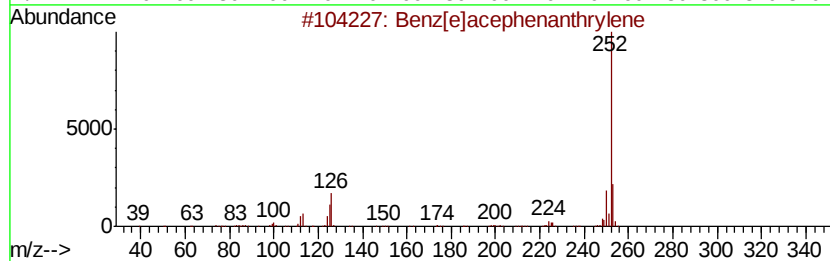
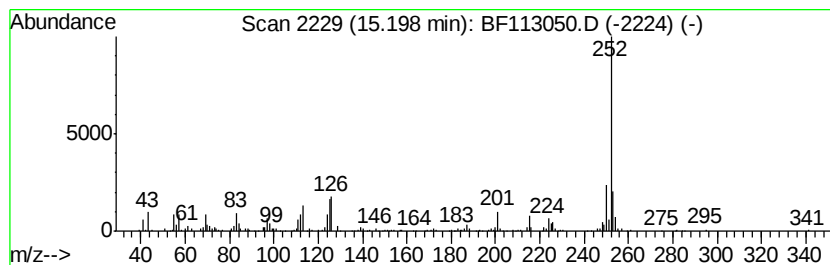
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benz[e]acephenanthrylene Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.20	3.44 ng	357388	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
2		Benzo[a]pyrene	252	C20H12	000050-32-8	95
3		Benzo[e]pyrene	252	C20H12	000192-97-2	95
4		Perylene	252	C20H12	000198-55-0	94
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113050.D
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ClientSampleId :
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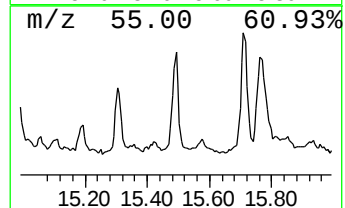
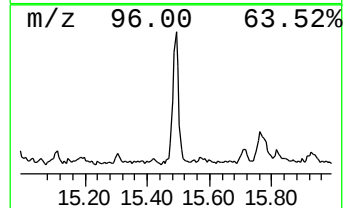
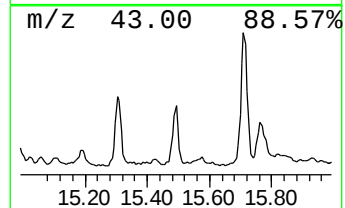
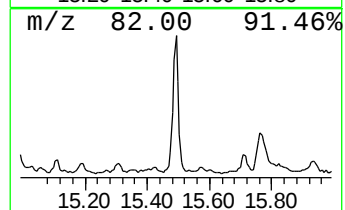
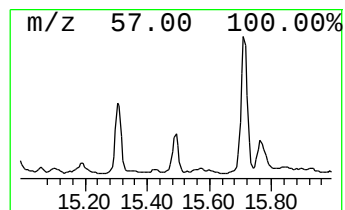
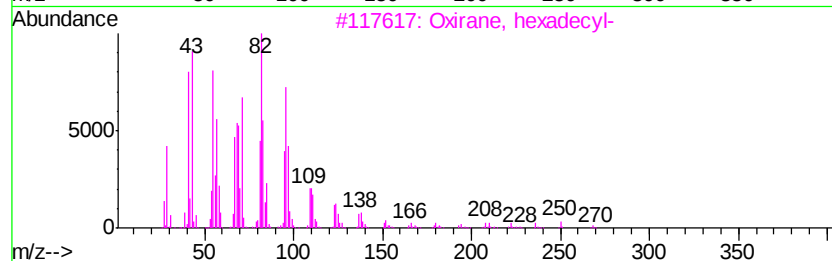
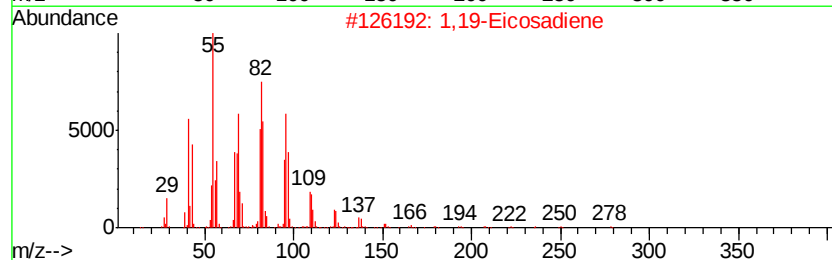
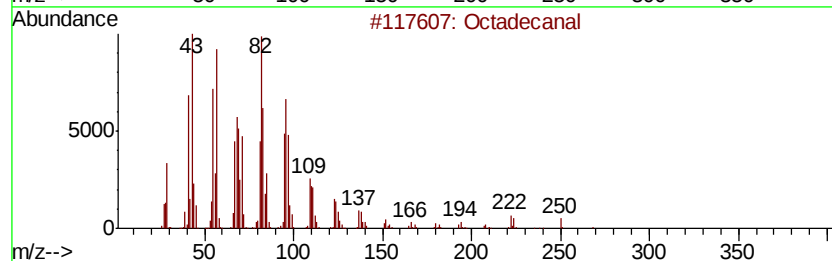
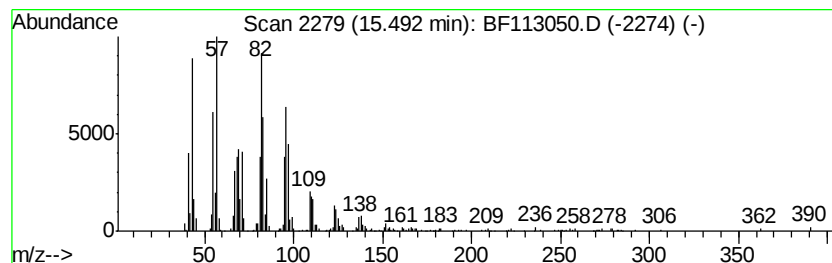
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecanal Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.49	4.99 ng	518003	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanal	268	C18H36O	000638-66-4	91
2		1,19-Eicosadiene	278	C20H38	014811-95-1	91
3		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4		15-Octadecenal	266	C18H34O	056554-93-9	90
5		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113050.D
Acq On : 14 Mar 2019 15:28
Operator : JU/SJ
Sample : K1866-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-MH-15-COMP

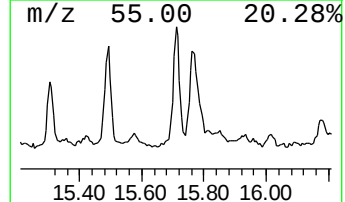
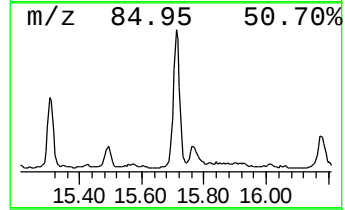
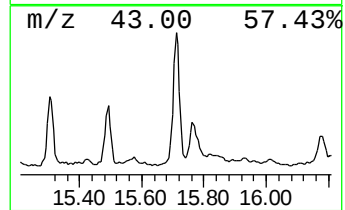
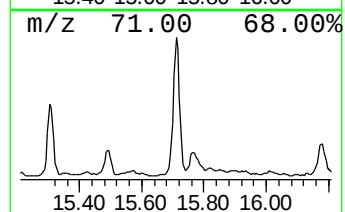
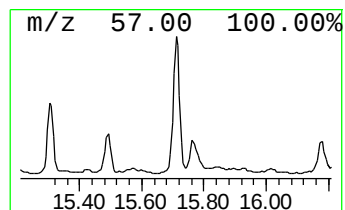
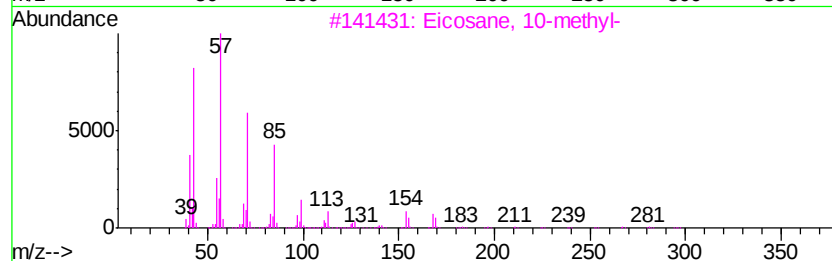
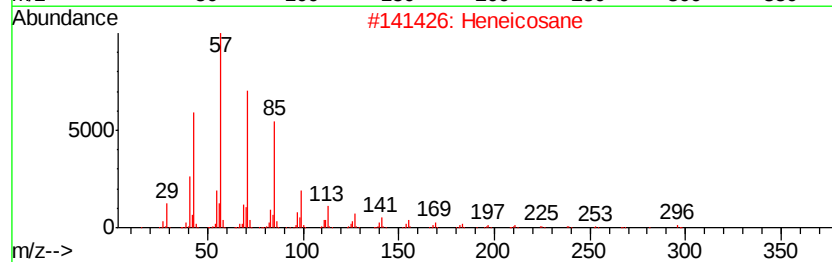
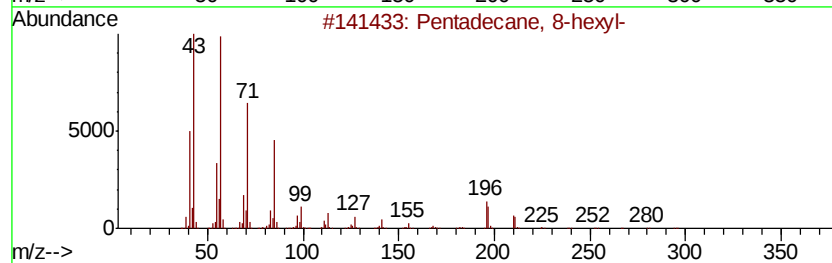
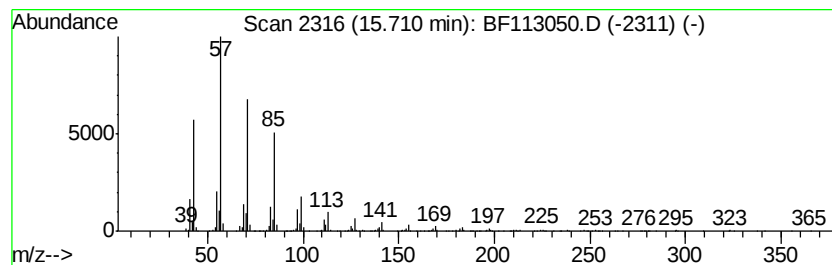
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Pentadecane, 8-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	8.38 ng	869940	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5		Tetracosane	338	C24H50	000646-31-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
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ClientSampleId :
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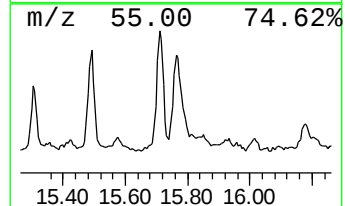
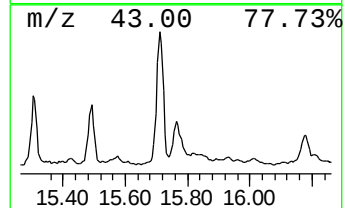
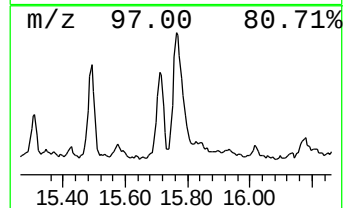
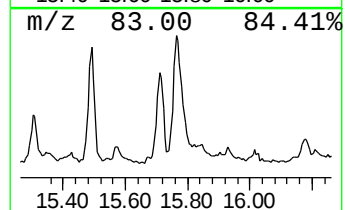
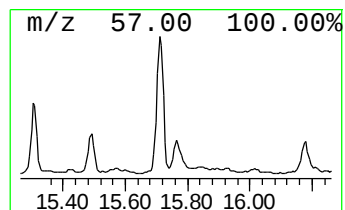
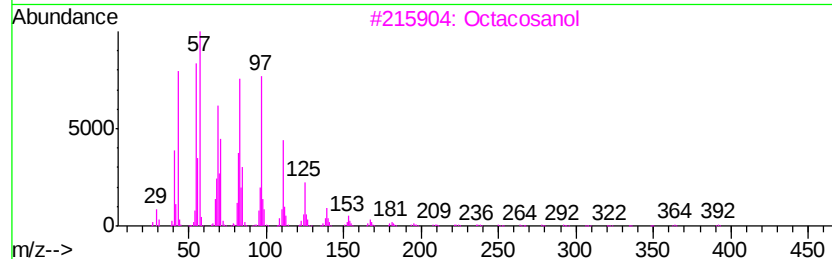
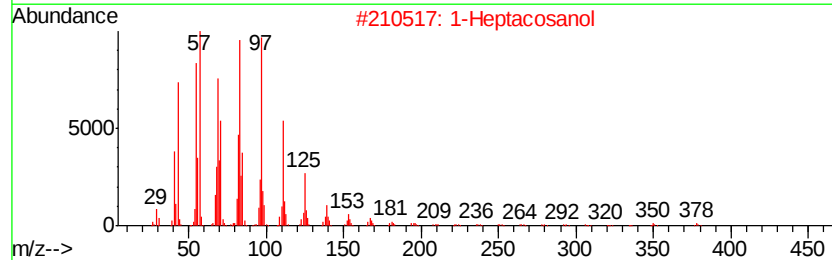
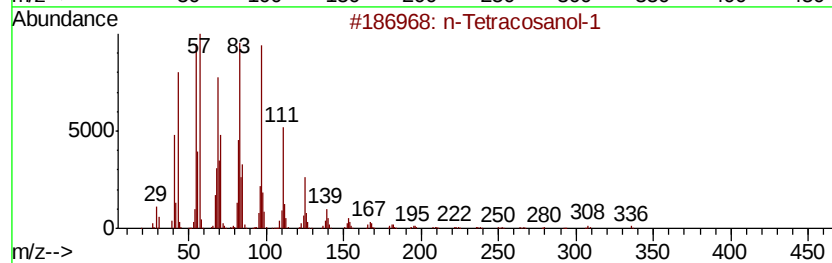
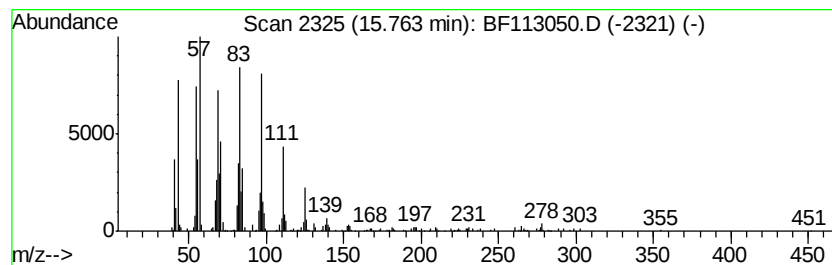
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 n-Tetracosanol-1 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.76	4.98 ng	517091	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2		1-Heptacosanol	396	C27H56O	002004-39-9	95
3		Octacosanol	410	C28H58O	000557-61-9	94
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		1-Docosene	308	C22H44	001599-67-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113050.D
Acq On : 14 Mar 2019 15:28
Operator : JU/SJ
Sample : K1866-09
Misc :
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Instrument :
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ClientSampleId :
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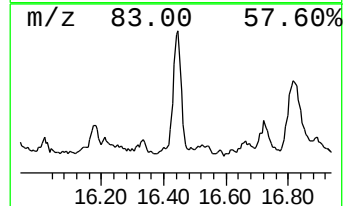
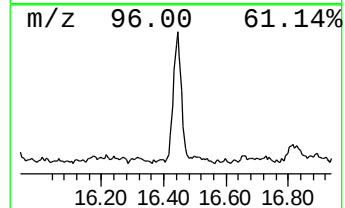
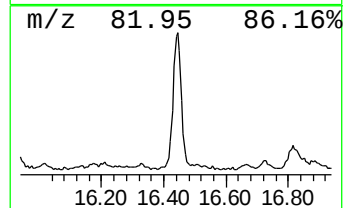
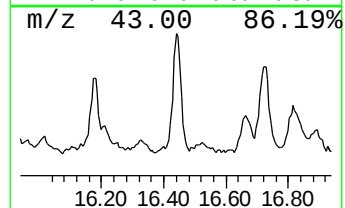
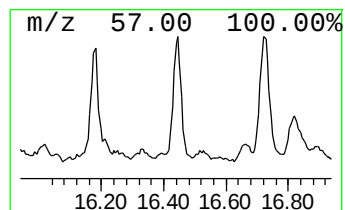
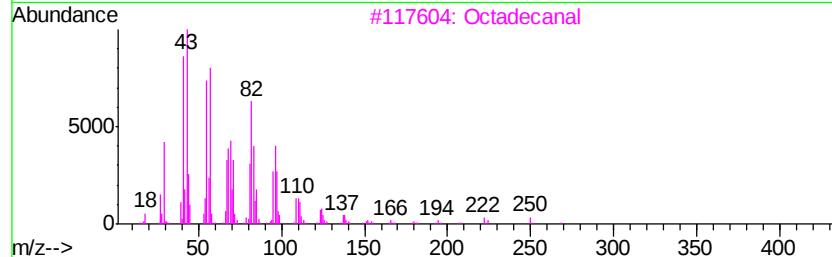
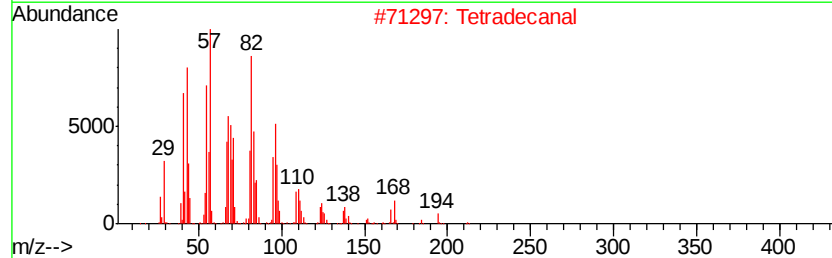
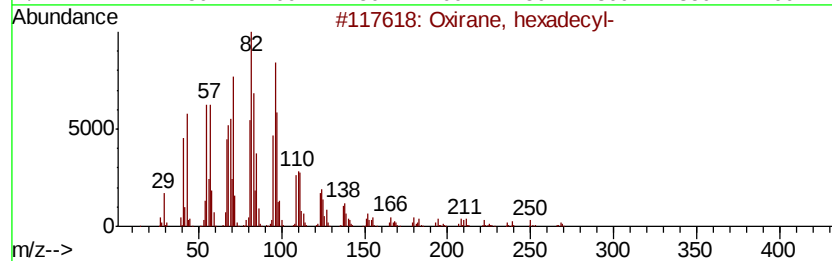
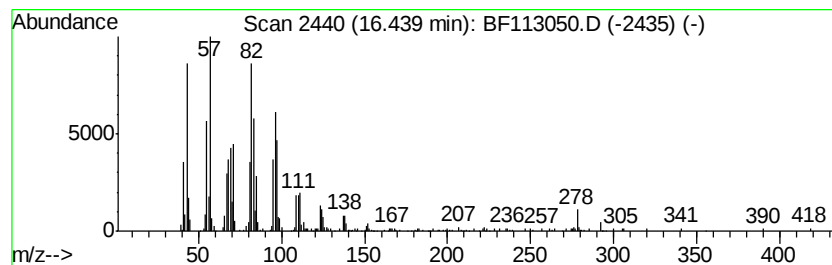
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Oxirane, hexadecyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.44	6.10 ng	633239	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2		Tetradecanal	212	C14H28O	000124-25-4	91
3		Octadecanal	268	C18H36O	000638-66-4	90
4		1,22-Docosanediol	342	C22H46O2	022513-81-1	68
5		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	60



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
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Misc :
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ClientSampleId :
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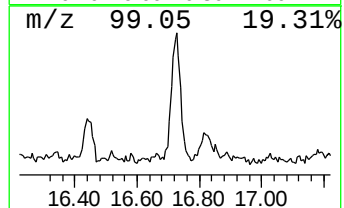
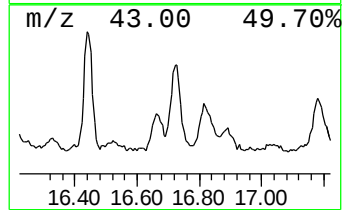
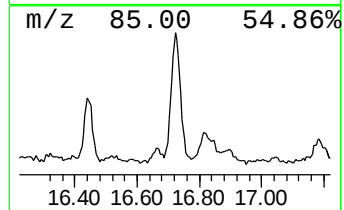
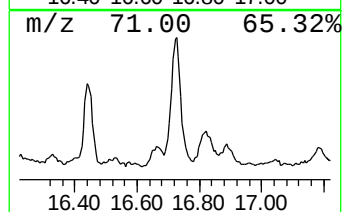
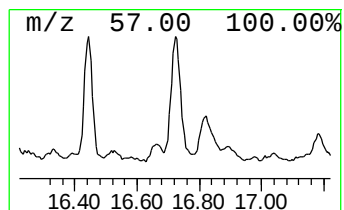
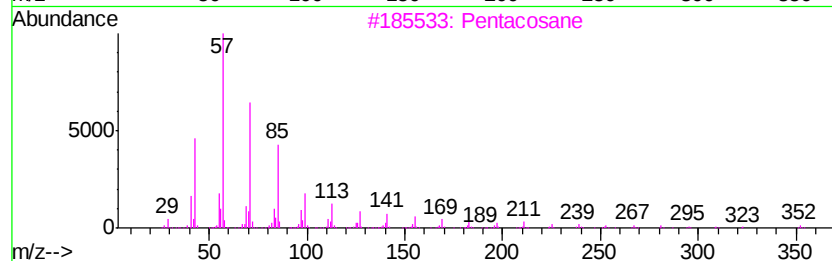
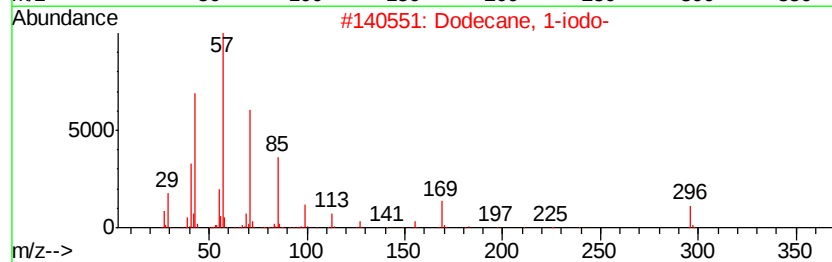
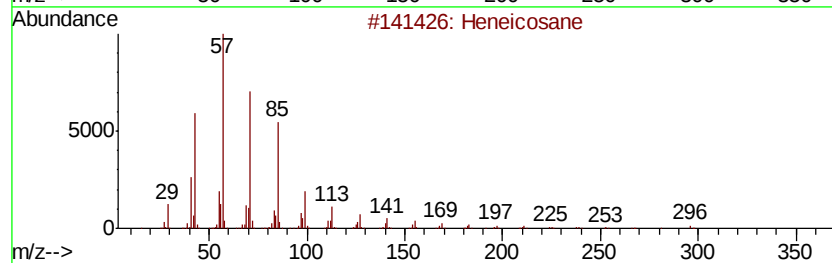
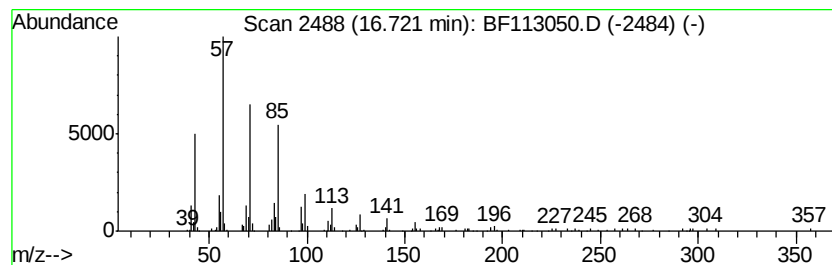
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Heneicosane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	2.65 ng	275476	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	98
2		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	91
3		Pentacosane	352	C25H52	000629-99-2	90
4		Tetracosane, 11-decyl-	479	C34H70	055429-84-0	86
5		Docosane, 11-butyl-	366	C26H54	013475-76-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113050.D
Acq On : 14 Mar 2019 15:28
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Misc :
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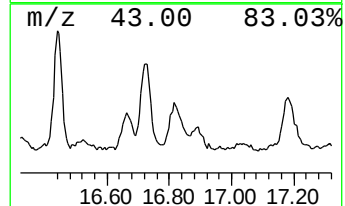
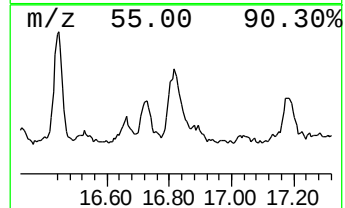
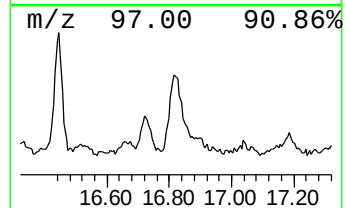
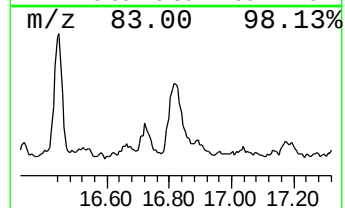
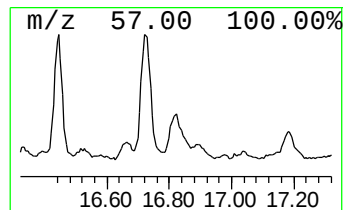
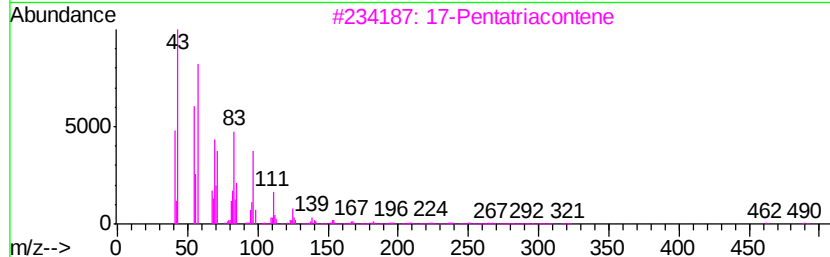
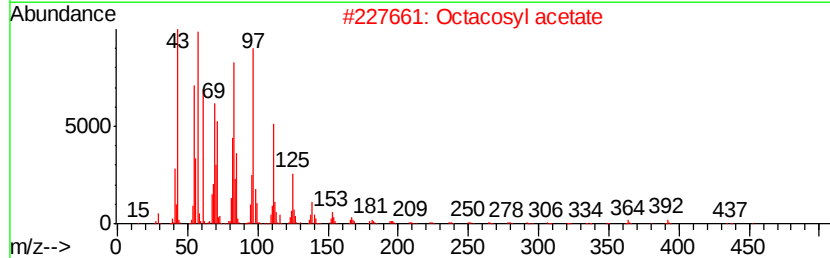
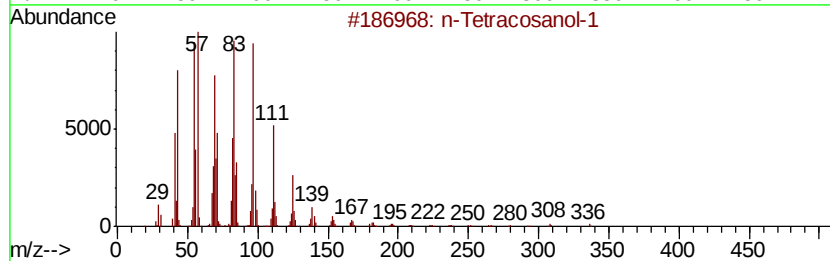
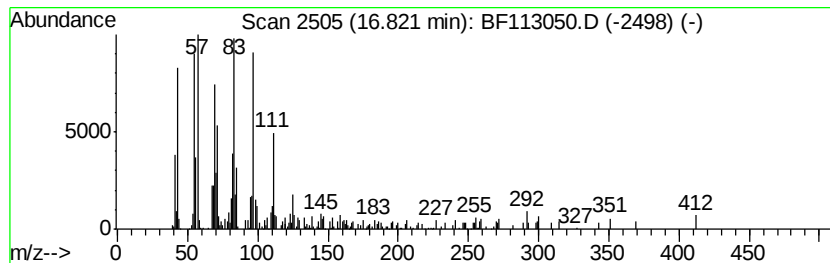
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Octacosyl acetate Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.82	3.97 ng	412540	Perylene-d12	15.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	86
2			Octacosyl acetate	452	C30H60O2	018206-97-8	78
3			17-Pentatriacontene	491	C35H70	006971-40-0	76
4			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	74
5			1-Heptacosanol	396	C27H56O	002004-39-9	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
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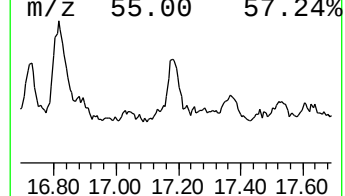
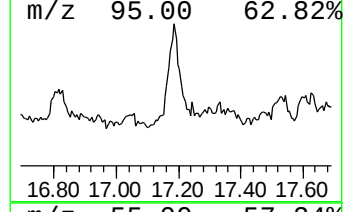
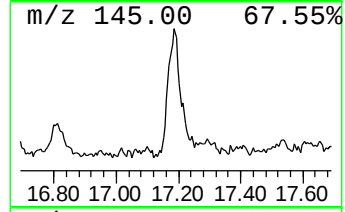
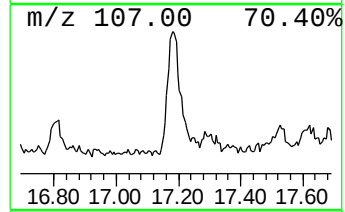
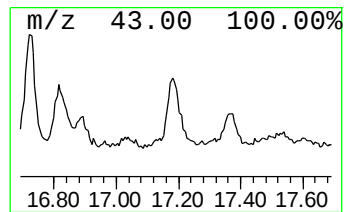
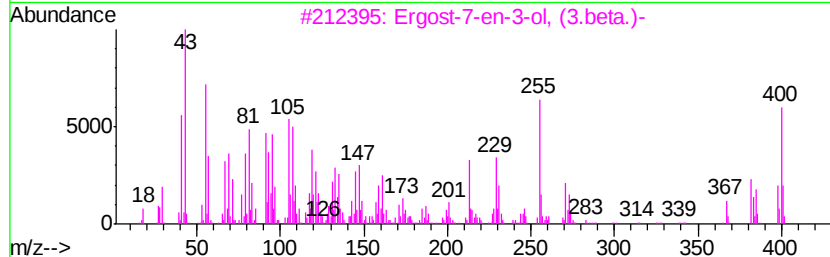
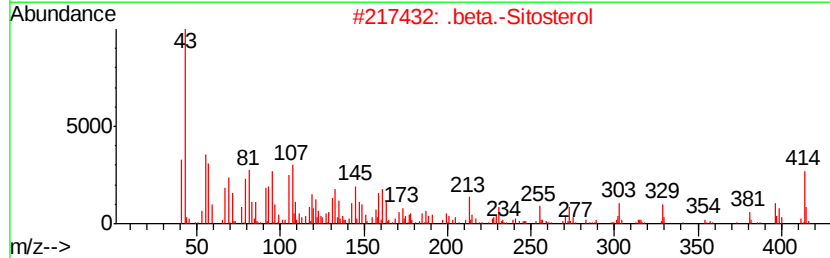
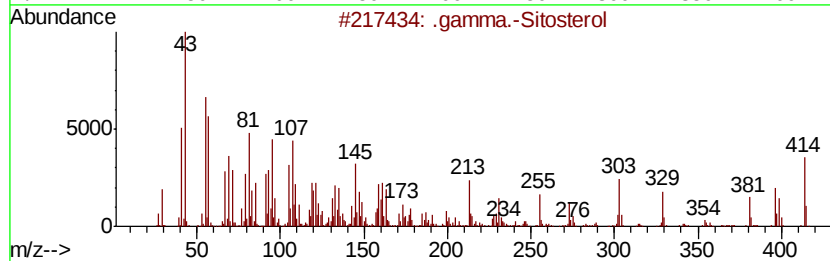
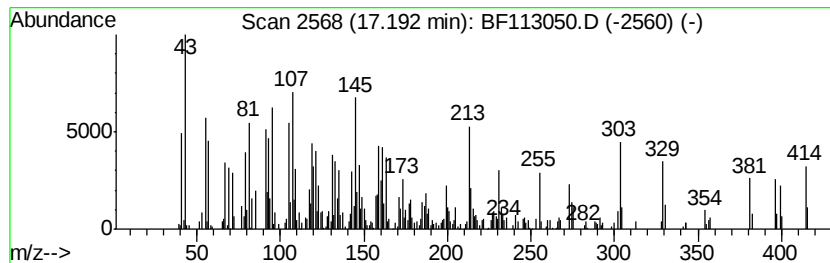
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 .gamma.-Sitosterol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.19	5.98 ng	621040	Perylene-d12	15.27	
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	98
3	Ergost-7-en-3-ol, (3.beta.)-	400	C28H48O	026047-31-4	35
4	5-Cholestene-3-ol, 24-methyl-	400	C28H48O	1000214-17-4	25
5	Stigmastan-3-en-6-ol	414	C29H50O	1000214-19-7	11



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113050.D
Acq On : 14 Mar 2019 15:28
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Misc :
ALS Vial : 4 Sample Multiplier: 1

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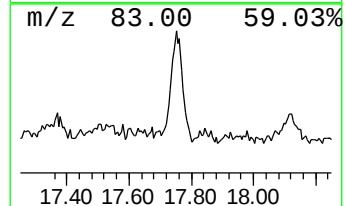
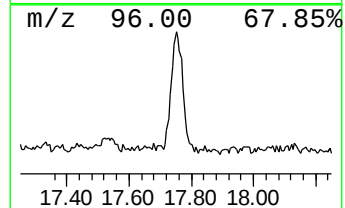
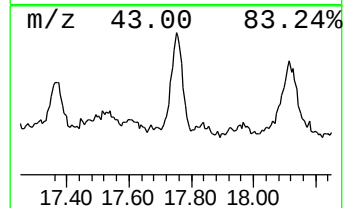
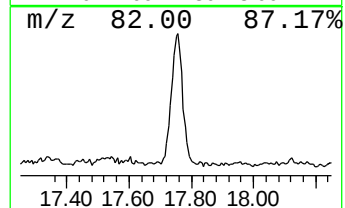
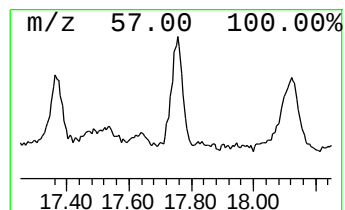
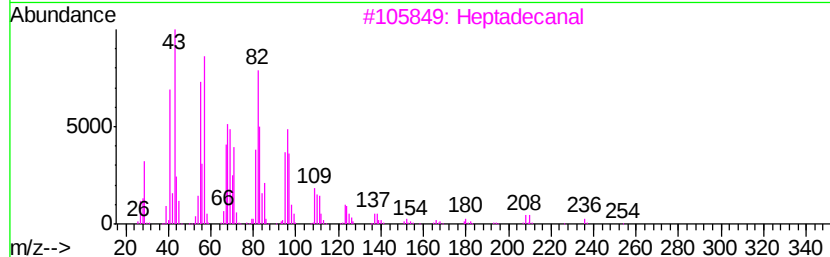
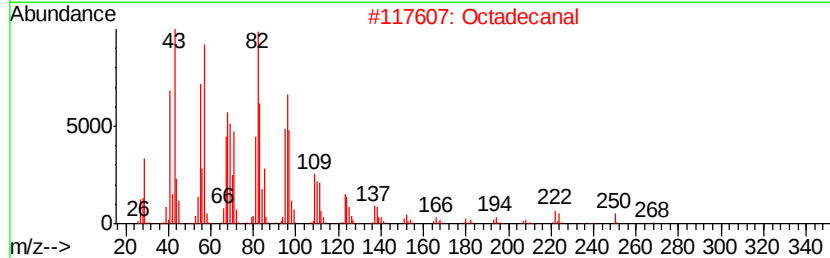
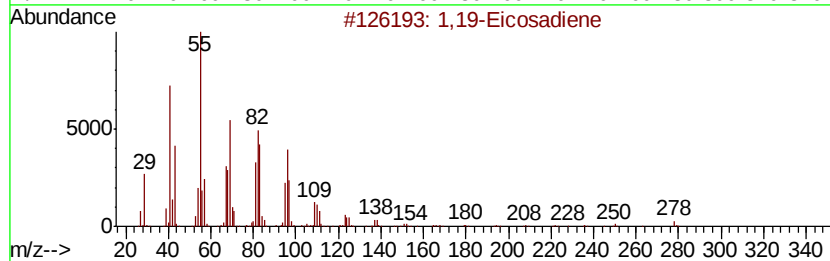
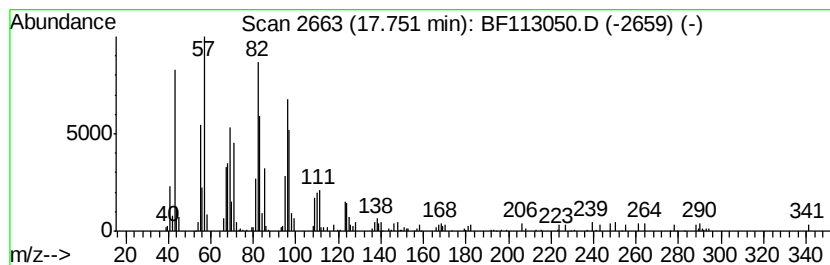
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 1,19-Eicosadiene Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.75	3.41 ng	353952	Perylene-d12	15.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,19-Eicosadiene	278	C20H38	014811-95-1	92
2			Octadecanal	268	C18H36O	000638-66-4	86
3			Heptadecanal	254	C17H34O	1000376-70-0	86
4			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	81
5			Hexadecanal	240	C16H32O	000629-80-1	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113050.D
Acq On : 14 Mar 2019 15:28
Operator : JU/SJ
Sample : K1866-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-MH-15-COMP

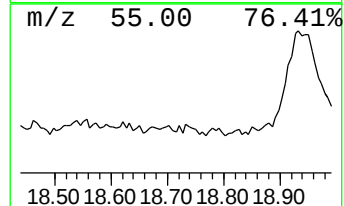
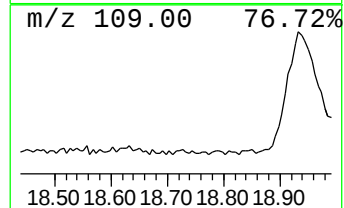
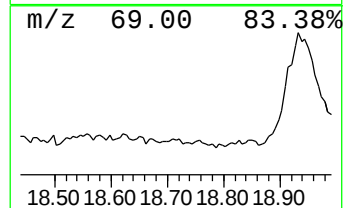
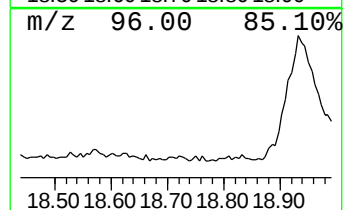
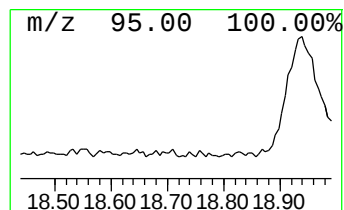
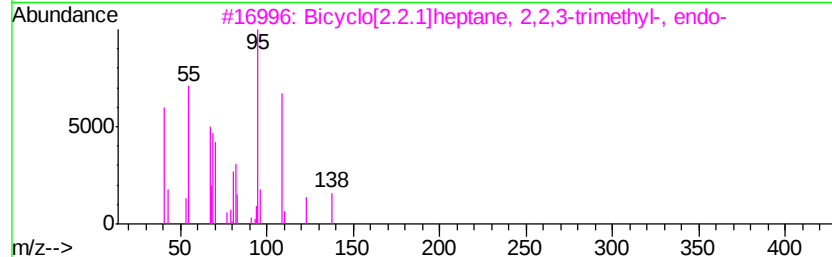
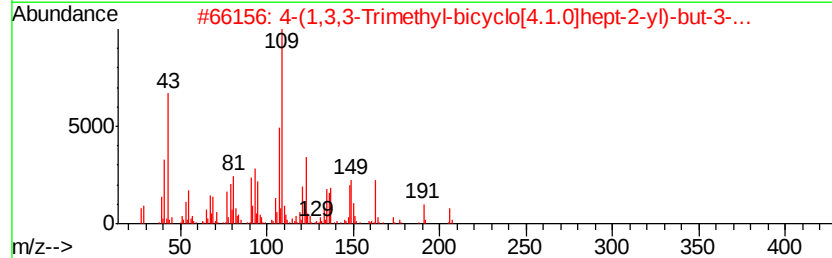
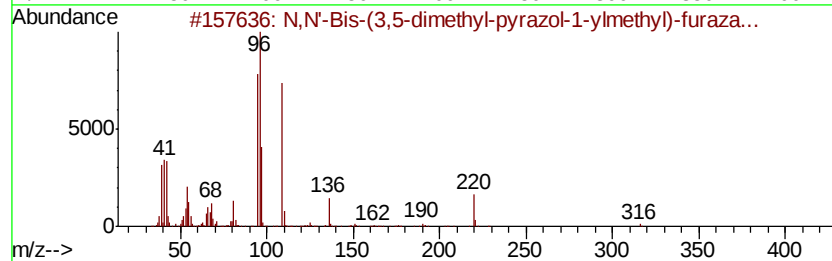
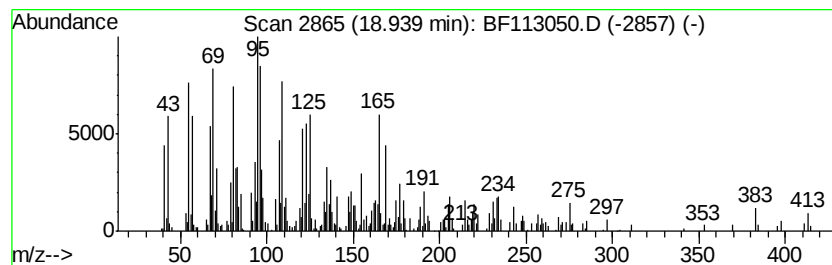
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown18.94 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.94	7.62 ng	791343	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	N,N'-Bis-(3,5-dimethyl-pyrazol-1...	316	C14H20N8O	1000294-70-9	43
2		4-(1,3,3-Trimethyl-bicyclo[4.1.0...	206	C14H22O	077143-31-8	40
3		Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	38
4		Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	30
5		1-Chloro-1-ethyl-3-methyl-1-germ...	206	C7H13ClGe	026311-76-2	15



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031419\
 Data File : BF113050.D
 Acq On : 14 Mar 2019 15:28
 Operator : JU/SJ
 Sample : K1866-09
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MR-MH-15-COMP

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.50	6.50	80.8	ng	4981160	1	6.73	1232760	20.0
n-Hexadecanoic acid	11.78	23.0	ng	2260650	4	11.23	1967690	20.0
Octadecanoic acid	12.56	9.3	ng	1150000	5	13.86	2477820	20.0
Heptafluorobutyri...	13.72	10.9	ng	1352060	5	13.86	2477820	20.0
triacontane	14.04	2.7	ng	333472	5	13.86	2477820	20.0
Heptadecane	14.35	7.6	ng	938688	5	13.86	2477820	20.0
9-Octadecenamide, ...	14.61	6.5	ng	677878	6	15.27	2076900	20.0
Docosane	14.64	4.2	ng	434862	6	15.27	2076900	20.0
Octadecane, 2-met...	14.95	9.2	ng	955164	6	15.27	2076900	20.0
Benz[e]acephenant...	15.20	3.4	ng	357388	6	15.27	2076900	20.0
Octadecanal	15.49	5.0	ng	518003	6	15.27	2076900	20.0
Pentadecane, 8-he...	15.71	8.4	ng	869940	6	15.27	2076900	20.0
n-Tetracosanol-1	15.76	5.0	ng	517091	6	15.27	2076900	20.0
Oxirane, hexadecyl-	16.44	6.1	ng	633239	6	15.27	2076900	20.0
Heneicosane	16.72	2.6	ng	275476	6	15.27	2076900	20.0
Octacosyl acetate	16.82	4.0	ng	412540	6	15.27	2076900	20.0
.gamma.-Sitosterol	17.19	6.0	ng	621040	6	15.27	2076900	20.0
1,19-Eicosadiene	17.75	3.4	ng	353952	6	15.27	2076900	20.0
unknown18.94	18.94	7.6	ng	791343	6	15.27	2076900	20.0