

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF073120\
 Data File : BF121152.D
 Acq On : 31 Jul 2020 12:21
 Operator : JU/CG
 Sample : L3453-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-067

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-BF071620.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	5.010	493	497	502	rVB	26466	34293	1.08%	0.131%
2	5.422	562	567	570	rBV	2479920	2560054	80.35%	9.796%
3	6.439	735	740	743	rBV	2484816	2561860	80.41%	9.803%
4	6.627	770	772	778	rBV2	34505	45216	1.42%	0.173%
5	6.798	797	801	804	rBV	928252	748252	23.49%	2.863%
6	7.363	891	897	900	rBV	1757728	1744349	54.75%	6.675%
7	8.080	1015	1019	1022	rBV	1200942	1000096	31.39%	3.827%
8	9.157	1197	1202	1205	rBV	3158682	3138926	98.52%	12.011%
9	9.263	1217	1220	1225	rBV3	29478	48550	1.52%	0.186%
10	9.492	1256	1259	1265	rVB7	33211	41262	1.30%	0.158%
11	9.551	1265	1269	1273	rBV	458524	385145	12.09%	1.474%
12	9.645	1282	1285	1290	rBV3	22669	33109	1.04%	0.127%
13	9.839	1300	1318	1321	rBV	1257587	1459656	45.82%	5.585%
14	9.957	1335	1338	1342	rVB	39536	35605	1.12%	0.136%
15	10.045	1348	1353	1356	rBV5	20730	34261	1.08%	0.131%
16	10.110	1361	1364	1369	rVB2	25931	37809	1.19%	0.145%
17	10.268	1389	1391	1401	rVB5	24443	49251	1.55%	0.188%
18	10.545	1434	1438	1443	rBV3	16762	38453	1.21%	0.147%
19	10.627	1447	1452	1456	rBV	1889986	1938727	60.85%	7.418%
20	10.774	1474	1477	1482	rVB2	46557	56955	1.79%	0.218%
21	10.974	1507	1511	1518	rBV6	33686	61845	1.94%	0.237%
22	11.327	1566	1571	1574	rBV	1284651	1242781	39.01%	4.755%
23	11.710	1633	1636	1645	rVB	41520	48914	1.54%	0.187%
24	11.857	1657	1661	1668	rBV2	195951	229455	7.20%	0.878%
25	11.998	1682	1685	1690	rBV2	71809	124195	3.90%	0.475%
26	12.133	1706	1708	1714	rVB	22651	31998	1.00%	0.122%
27	12.298	1733	1736	1740	rBV	179811	143337	4.50%	0.548%
28	12.504	1768	1771	1774	rBV	65963	76457	2.40%	0.293%
29	12.574	1781	1783	1787	rVB	49132	48598	1.53%	0.186%
30	12.639	1790	1794	1798	rBV2	74576	102045	3.20%	0.390%
31	12.915	1836	1841	1844	rBV	3130052	3185936	100.00%	12.191%
32	13.127	1874	1877	1884	rVB4	30597	54256	1.70%	0.208%
33	13.356	1906	1916	1918	rBV5	158499	429450	13.48%	1.643%
34	13.809	1989	1993	1998	rBV	600485	956173	30.01%	3.659%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.962	2015	2019	2023	rBV	934084	924640	29.02%	3.538%
36	14.433	2096	2099	2100	rBV	97553	82797	2.60%	0.317%
37	14.733	2148	2150	2155	rVB	72812	74818	2.35%	0.286%
38	14.809	2160	2163	2165	rBV	76145	98008	3.08%	0.375%
39	15.068	2203	2207	2211	rBV	294342	308620	9.69%	1.181%
40	15.421	2262	2267	2276	rVB	649510	944583	29.65%	3.614%
41	15.868	2339	2343	2348	rVB	196045	314914	9.88%	1.205%
42	15.927	2349	2353	2361	rVB2	109909	197269	6.19%	0.755%
43	17.433	2603	2609	2624	rVB6	155983	461093	14.47%	1.764%

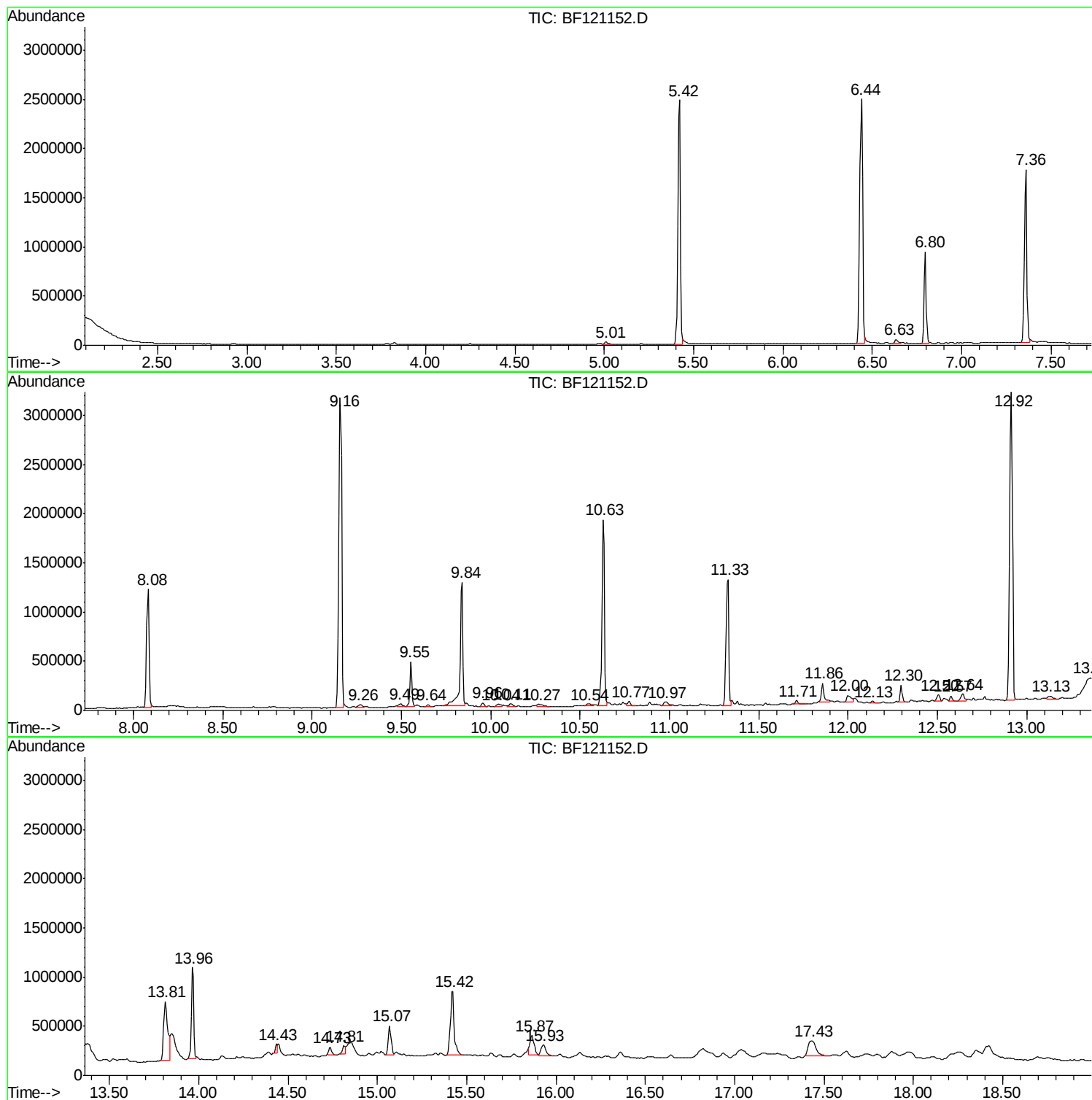
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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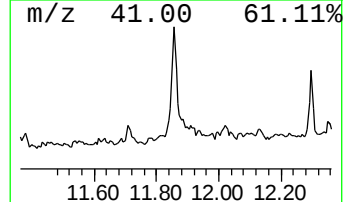
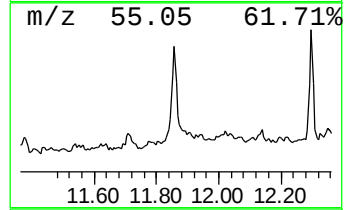
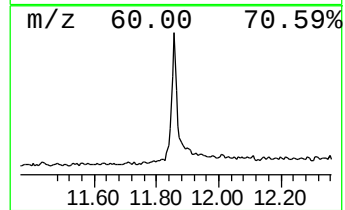
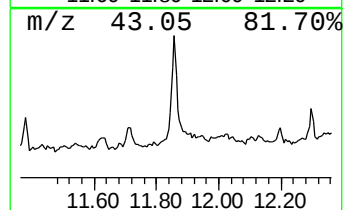
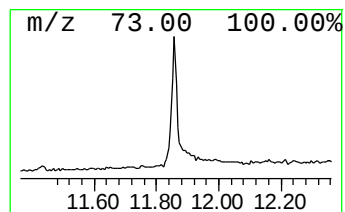
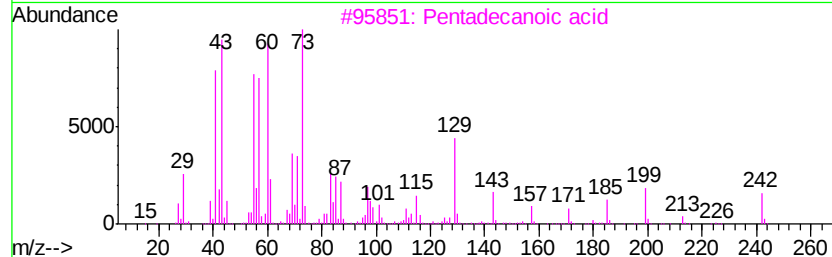
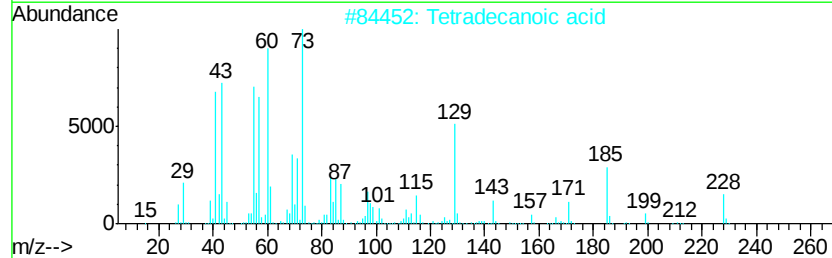
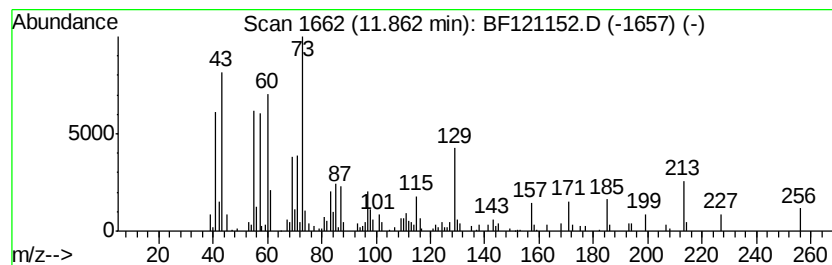
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.86	3.69 ng	229455	Phenanthrene-d10		11.33
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76



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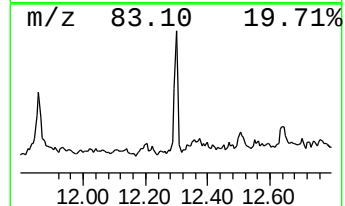
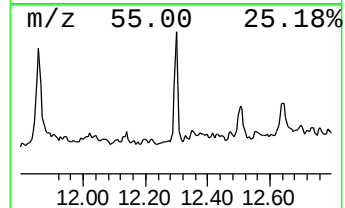
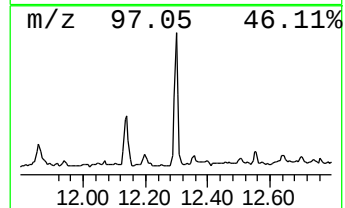
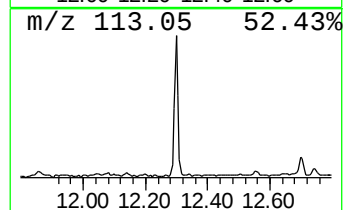
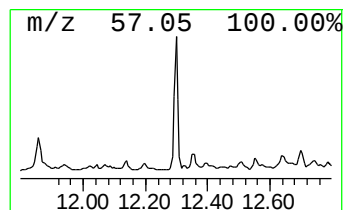
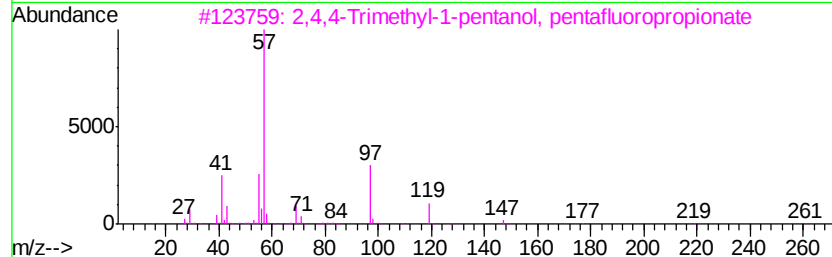
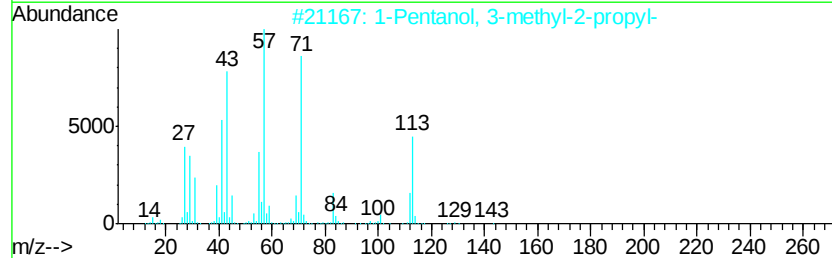
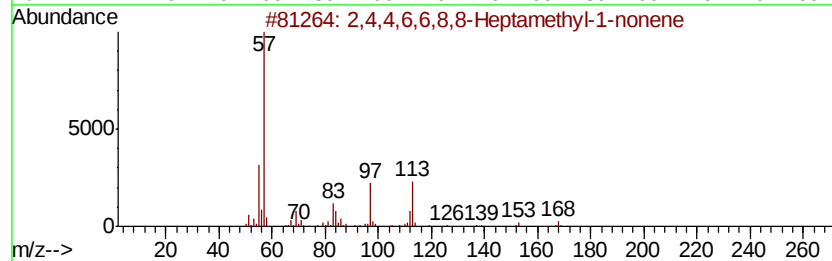
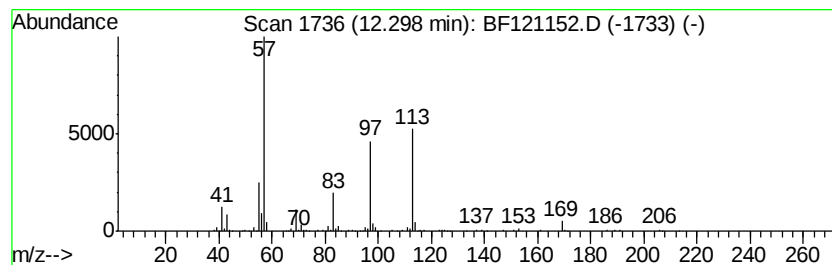
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	2.31 ng	143337	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	64
2		1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	38
3		2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32
4		Pvrazole, 3-nitro-	113	C3H3N3O2	026621-44-3	17
5		2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	16



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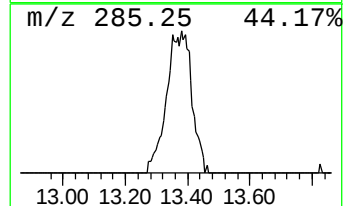
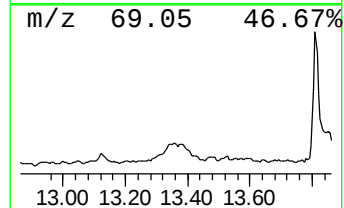
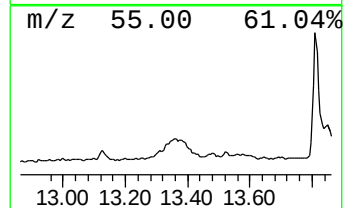
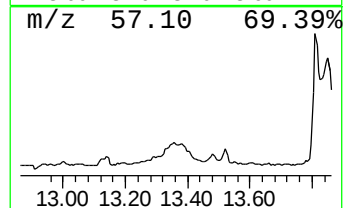
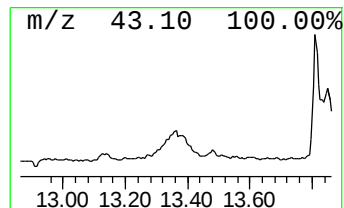
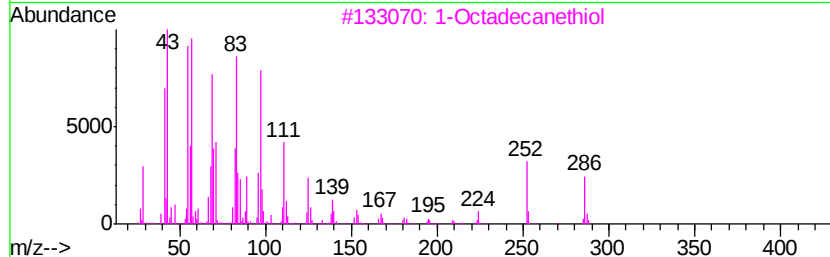
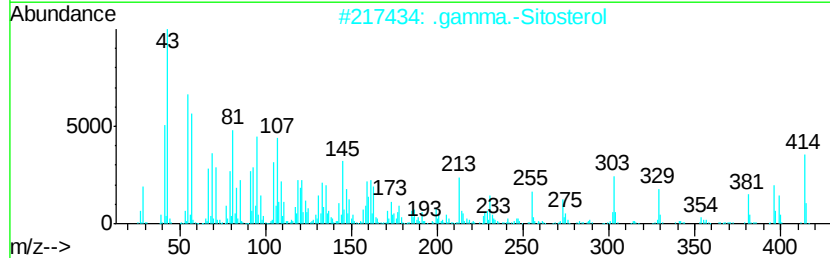
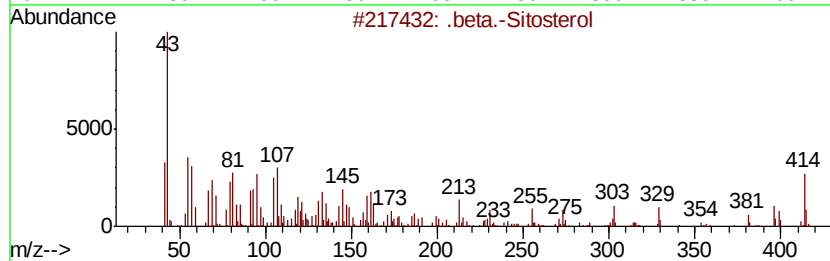
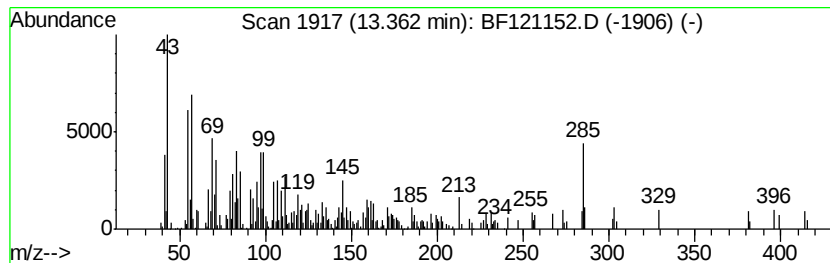
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 .beta.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.36	9.29 ng	429450	Chrysene-d12	13.96		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Sitosterol	414	C29H50O	000083-46-5	91
2		.gamma.-Sitosterol	414	C29H50O	000083-47-6	56
3		1-Octadecanethiol	286	C18H38S	002885-00-9	43
4		Fumaric acid, but-3-yn-2-yl dode...	336	C20H32O4	1000345-28-8	27
5		Cyclopentanone, oxime	99	C5H9NO	001192-28-5	11



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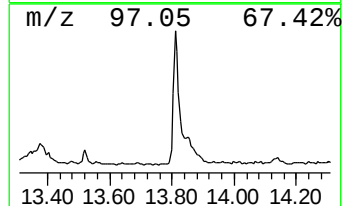
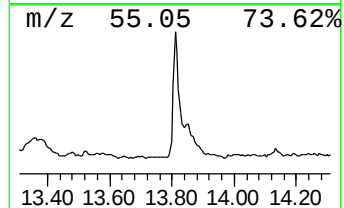
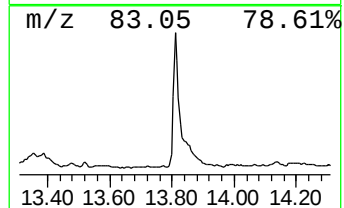
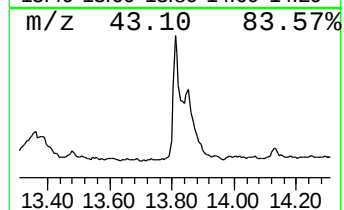
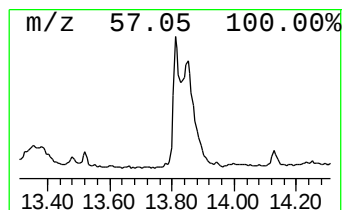
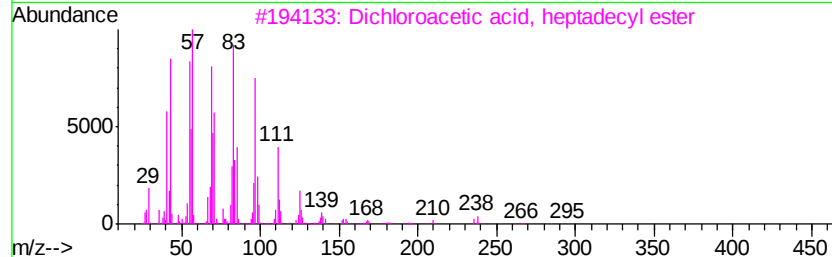
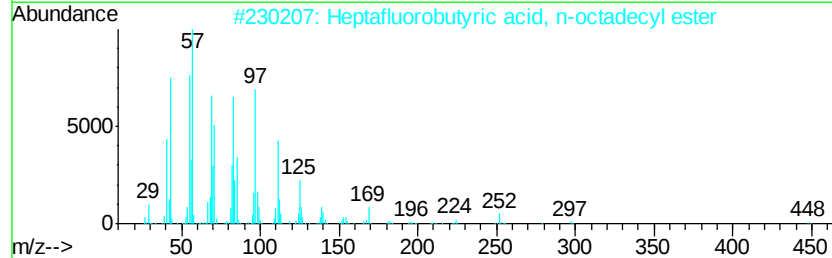
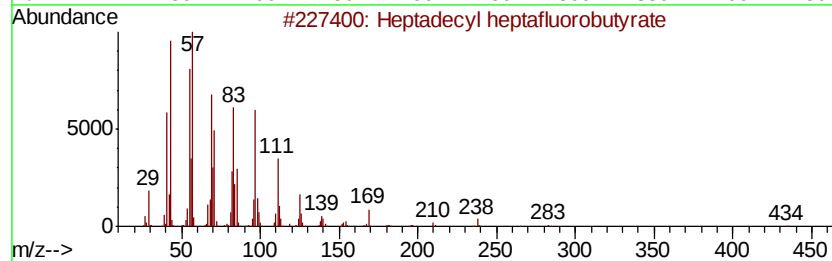
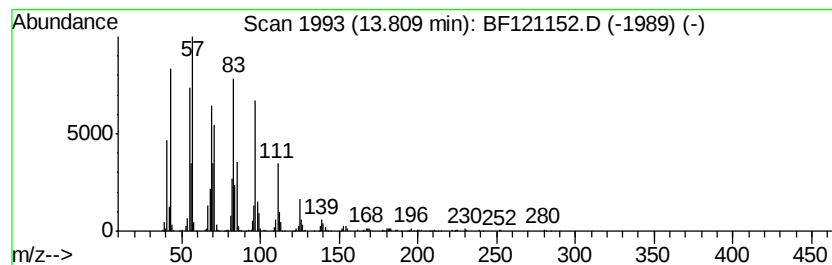
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	20.68 ng	956173	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	94
3		Dichloroacetic acid, heptadecyl ester	366	C19H36Cl2O2	1000282-98-2	91
4		Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	91
5		Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	91



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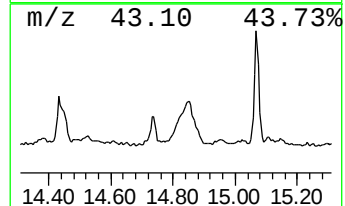
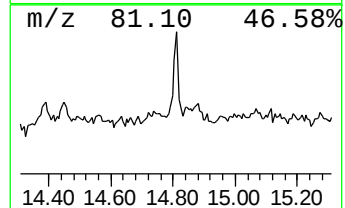
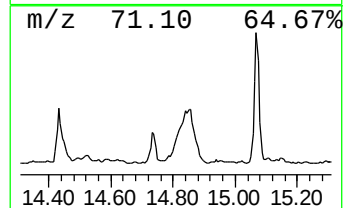
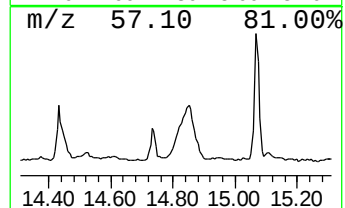
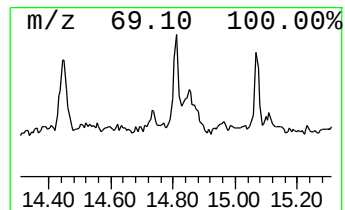
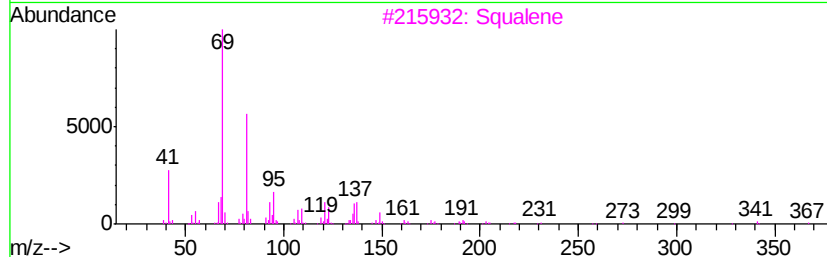
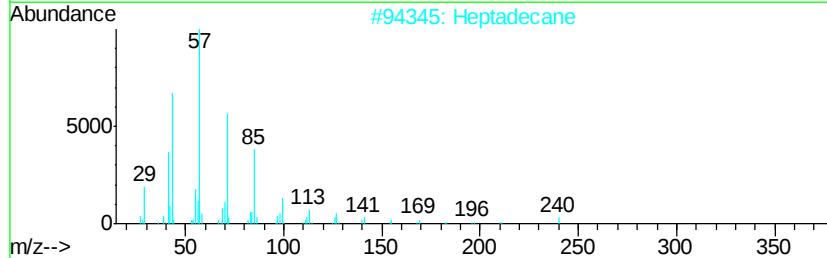
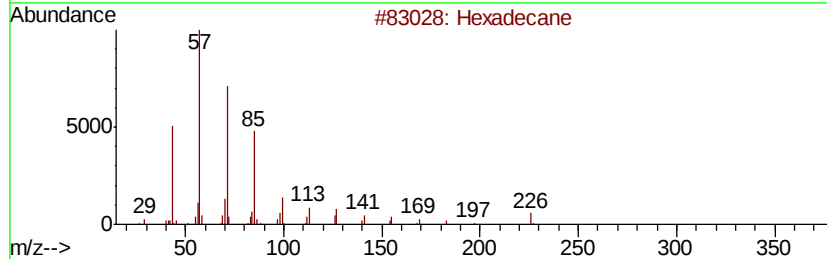
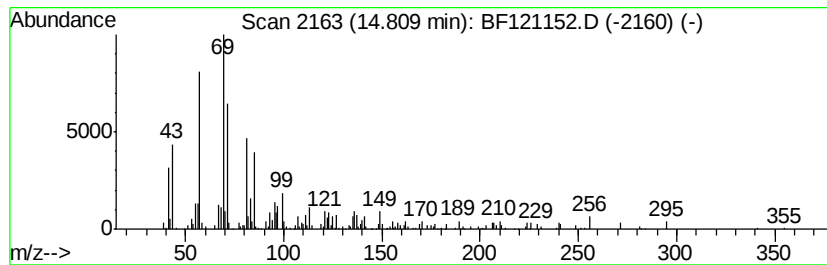
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Peak Number 5 unknown14.81 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	2.08 ng	98008	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	42
2		Heptadecane	240	C17H36	000629-78-7	42
3		Squalene	410	C30H50	000111-02-4	41
4		Docosane, 11-butyl-	366	C26H54	013475-76-8	41
5		Docosane, 11-decyl-	451	C32H66	055401-55-3	38



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Acq On : 31 Jul 2020 12:21
Operator : JU/CG
Sample : L3453-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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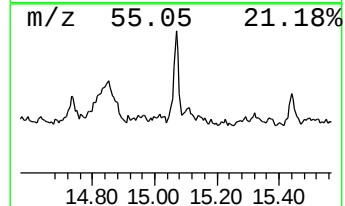
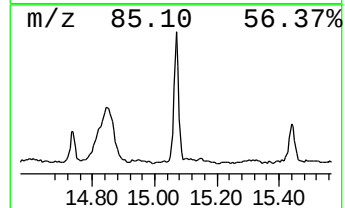
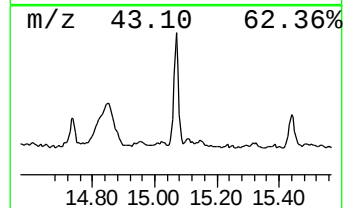
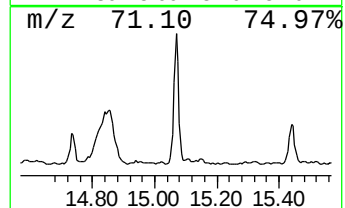
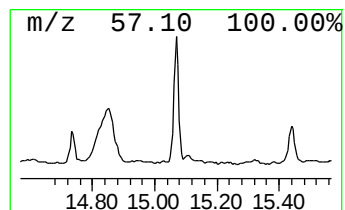
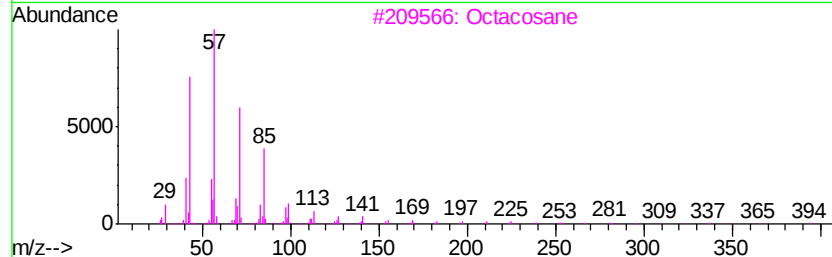
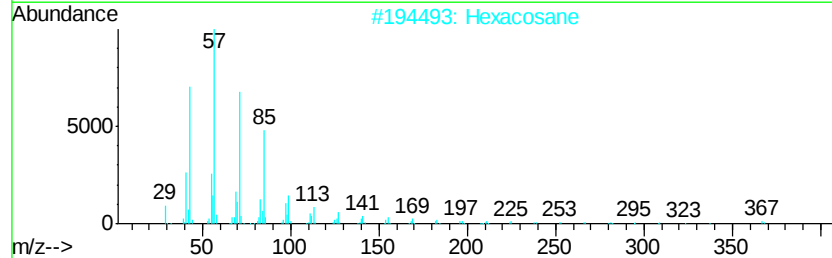
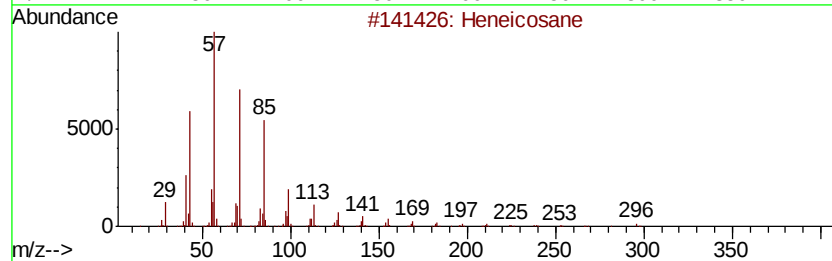
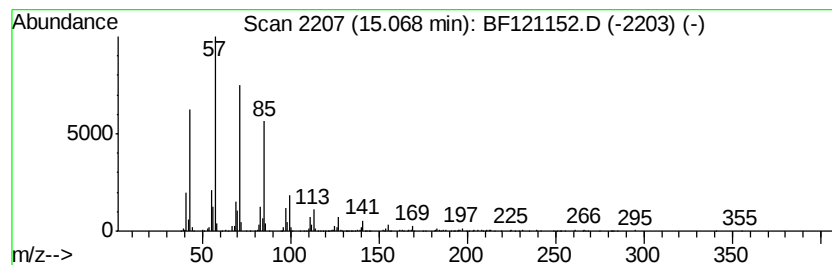
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	6.53 ng	308620	Perylene-d12	15.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	Octacosane		394	C28H58	000630-02-4	91
4	Pentacosane		352	C25H52	000629-99-2	90
5	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF073120\
Data File : BF121152.D
Acq On : 31 Jul 2020 12:21
Operator : JU/CG
Sample : L3453-01
Misc :
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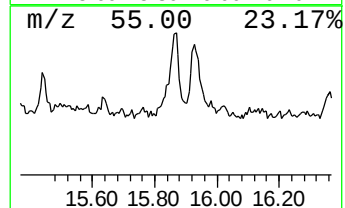
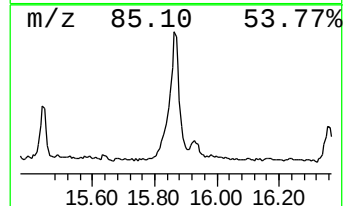
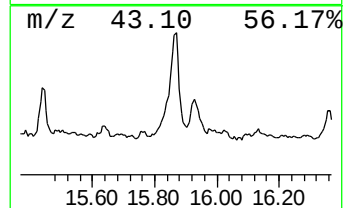
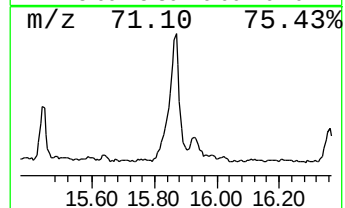
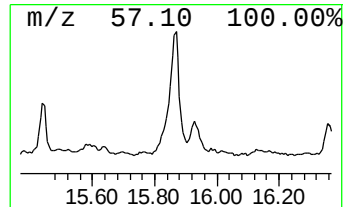
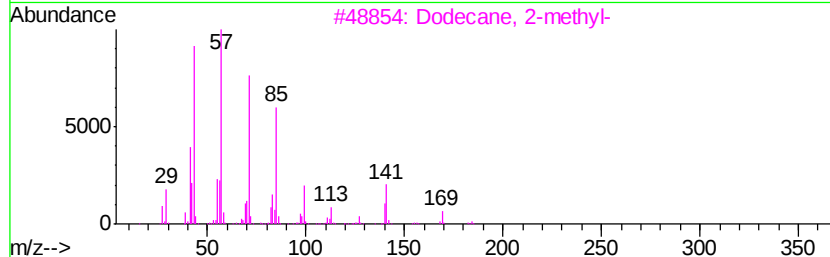
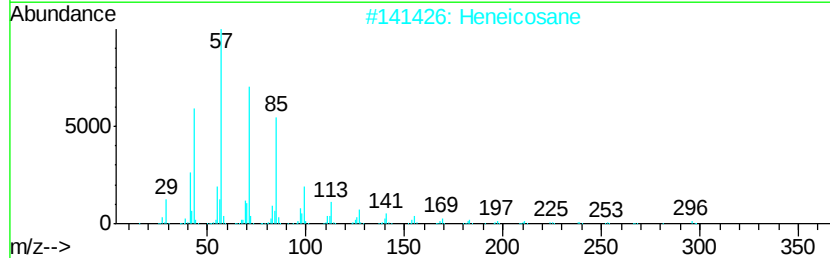
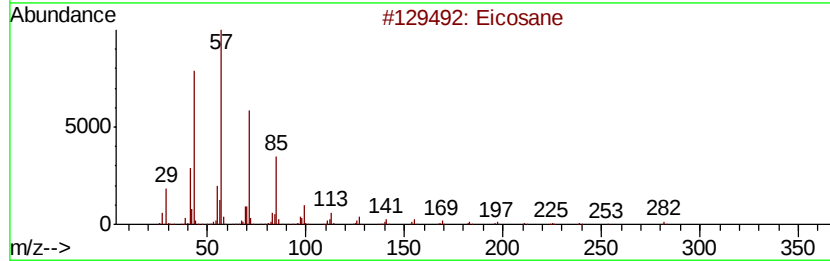
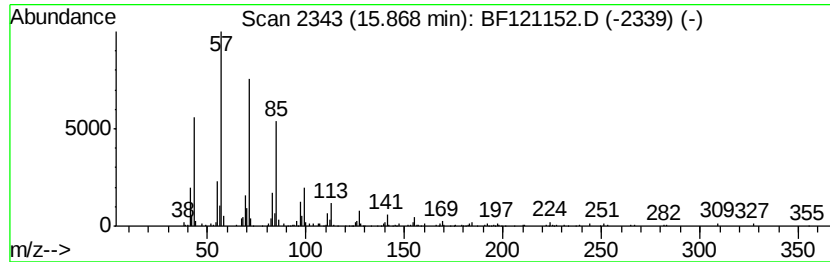
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	6.67 ng	314914	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5		2-methyloctacosane	408	C29H60	1000376-72-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF073120\
Data File : BF121152.D
Acq On : 31 Jul 2020 12:21
Operator : JU/CG
Sample : L3453-01
Misc :
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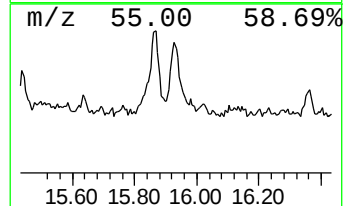
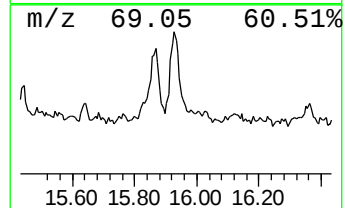
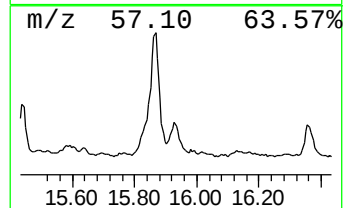
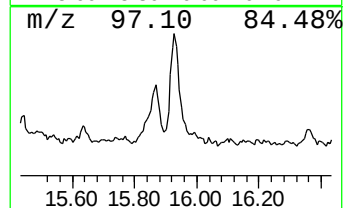
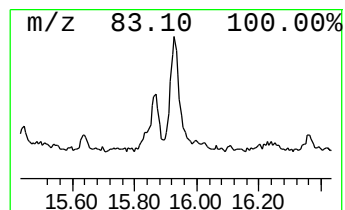
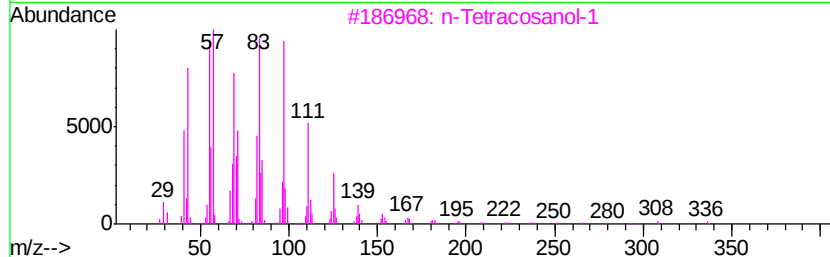
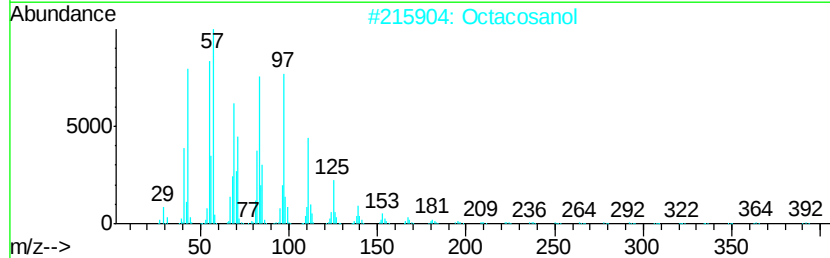
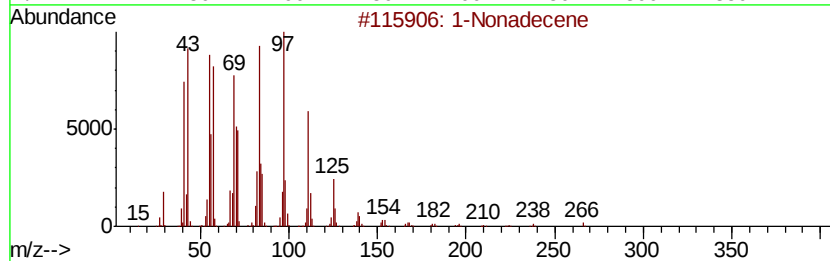
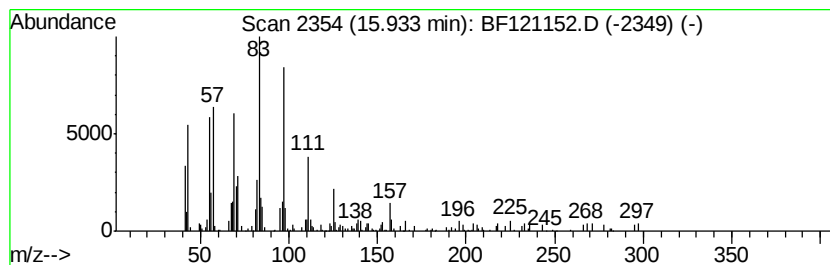
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Nonadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.93	4.18 ng	197269	Perylene-d12	15.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	62
2	Octacosanol	410	C28H58O	000557-61-9	50
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	45
4	1-Octadecene	252	C18H36	000112-88-9	45
5	2-Thiopheneacetic acid, 2-ethylc...	252	C14H20O2S	1000278-96-1	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF073120\
Data File : BF121152.D
Acq On : 31 Jul 2020 12:21
Operator : JU/CG
Sample : L3453-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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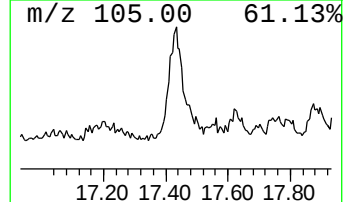
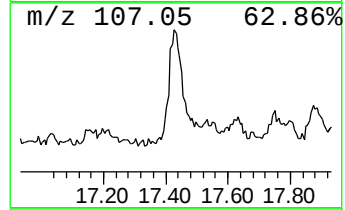
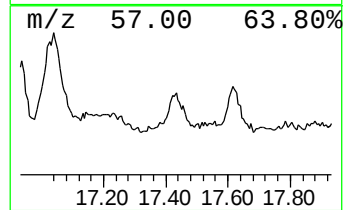
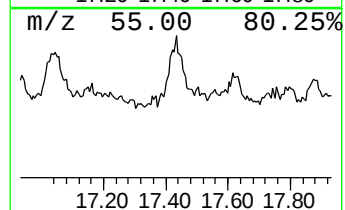
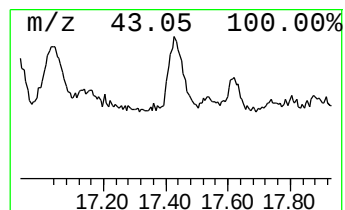
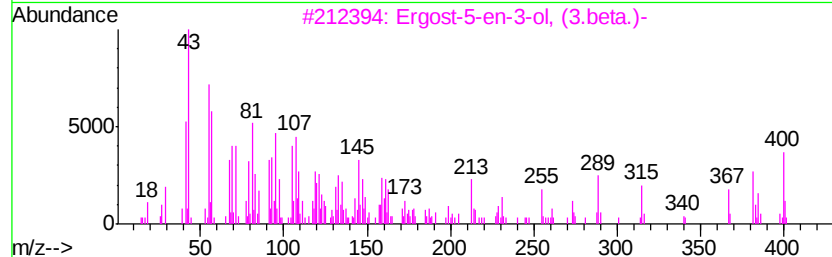
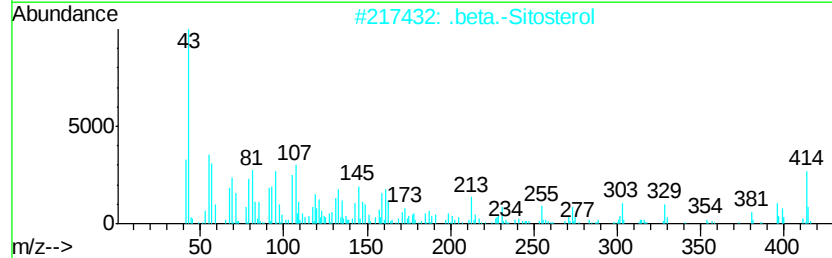
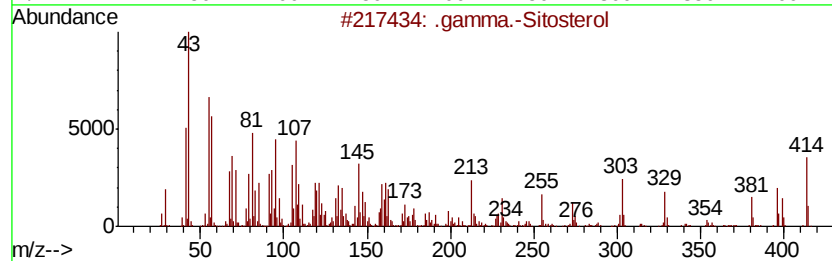
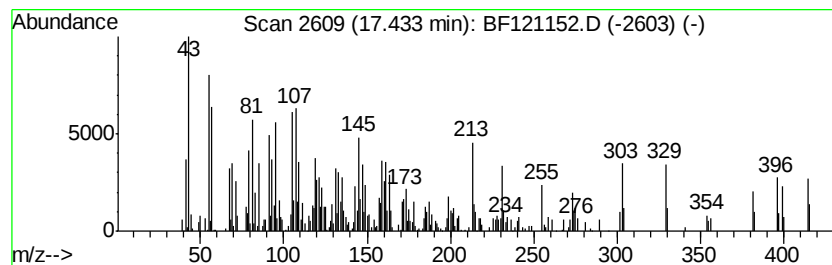
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 .gamma.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.43	9.76 ng	461093	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2		.beta.-Sitosterol	414	C29H50O	000083-46-5	97
3		Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	18
4		22,26-Oxido-4,17-cholestadien-3....	414	C27H42O3	1000252-80-4	15
5		Campesterol	400	C28H48O	000474-62-4	14



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF073120\
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Acq On : 31 Jul 2020 12:21
Operator : JU/CG
Sample : L3453-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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
n-Hexadecanoic acid	11.86	3.7	ng	229455	4	11.33	1242780	20.0
2,4,4,6,6,8,8-Hep...	12.30	2.3	ng	143337	4	11.33	1242780	20.0
.beta.-Sitosterol	13.36	9.3	ng	429450	5	13.96	924640	20.0
Heptadecyl heptaf...	13.81	20.7	ng	956173	5	13.96	924640	20.0
unknown14.81	14.81	2.1	ng	98008	6	15.42	944583	20.0
Heneicosane	15.07	6.5	ng	308620	6	15.42	944583	20.0
Eicosane	15.87	6.7	ng	314914	6	15.42	944583	20.0
1-Nonadecene	15.93	4.2	ng	197269	6	15.42	944583	20.0
.gamma.-Sitosterol	17.43	9.8	ng	461093	6	15.42	944583	20.0