

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062220\
 Data File : BF120678.D
 Acq On : 22 Jun 2020 16:04
 Operator : JU/CG
 Sample : L3082-03
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3

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-BF061020.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	5.410	560	565	568	rBV	2998558	3078189	59.08%	7.535%
2	6.440	734	740	743	rBV	3001922	3306143	63.45%	8.093%
3	6.798	797	801	804	rBV	785885	675553	12.97%	1.654%
4	6.951	823	827	831	rBV	2810435	2683889	51.51%	6.570%
5	7.363	891	897	900	rBV	2283256	2214906	42.51%	5.422%
6	8.081	1015	1019	1022	rBV	1075404	948370	18.20%	2.322%
7	9.157	1197	1202	1205	rBV	4808183	4518367	86.72%	11.061%
8	9.545	1265	1268	1272	rBV	188571	160221	3.08%	0.392%
9	9.769	1302	1306	1313	rVB2	25470	52462	1.01%	0.128%
10	9.833	1313	1317	1320	rBV	1419055	1109236	21.29%	2.715%
11	10.628	1446	1452	1455	rBV	2602303	2524332	48.45%	6.179%
12	11.322	1566	1570	1573	rBV	1209426	1074798	20.63%	2.631%
13	11.851	1655	1660	1662	rBV2	91909	106399	2.04%	0.260%
14	12.433	1739	1759	1772	rBV	477011	1931090	37.06%	4.727%
15	12.916	1835	1841	1844	rBV	4757312	5210352	100.00%	12.755%
16	13.063	1863	1866	1871	rBV	46397	60220	1.16%	0.147%
17	13.121	1873	1876	1887	rVB4	56847	137608	2.64%	0.337%
18	13.510	1931	1942	1953	rVB	831297	1932647	37.09%	4.731%
19	13.751	1979	1983	1986	rVB	55876	63979	1.23%	0.157%
20	13.821	1986	1995	2002	rBV2	562594	992490	19.05%	2.430%
21	13.963	2015	2019	2022	rBV	1369401	1168953	22.44%	2.862%
22	14.045	2030	2033	2040	rVB4	54775	85005	1.63%	0.208%
23	14.121	2043	2046	2054	rVB2	53163	83758	1.61%	0.205%
24	14.227	2056	2064	2069	rBV	1056555	1694699	32.53%	4.149%
25	14.280	2069	2073	2082	rVB6	53131	145313	2.79%	0.356%
26	14.574	2116	2123	2128	rBV3	367798	753089	14.45%	1.844%
27	14.615	2128	2130	2136	rVB2	127934	160039	3.07%	0.392%
28	14.733	2146	2150	2153	rBV	85078	88477	1.70%	0.217%
29	14.804	2155	2162	2171	rVB	636523	1137230	21.83%	2.784%
30	15.057	2202	2205	2210	rVB	72236	84640	1.62%	0.207%
31	15.210	2223	2231	2233	rBV5	60612	117550	2.26%	0.288%
32	15.410	2259	2265	2268	rBV	1094856	1550397	29.76%	3.795%
33	15.527	2283	2285	2294	rVB7	32329	69128	1.33%	0.169%
34	15.821	2329	2335	2344	rBV4	155731	486250	9.33%	1.190%

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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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35	15.921	2347	2352	2358	rVB6	100490	233296	4.48%	0.571%
36	16.157	2386	2392	2399	rVB	78310	154383	2.96%	0.378%
37	16.339	2421	2423	2427	rVB	56336	57062	1.10%	0.140%

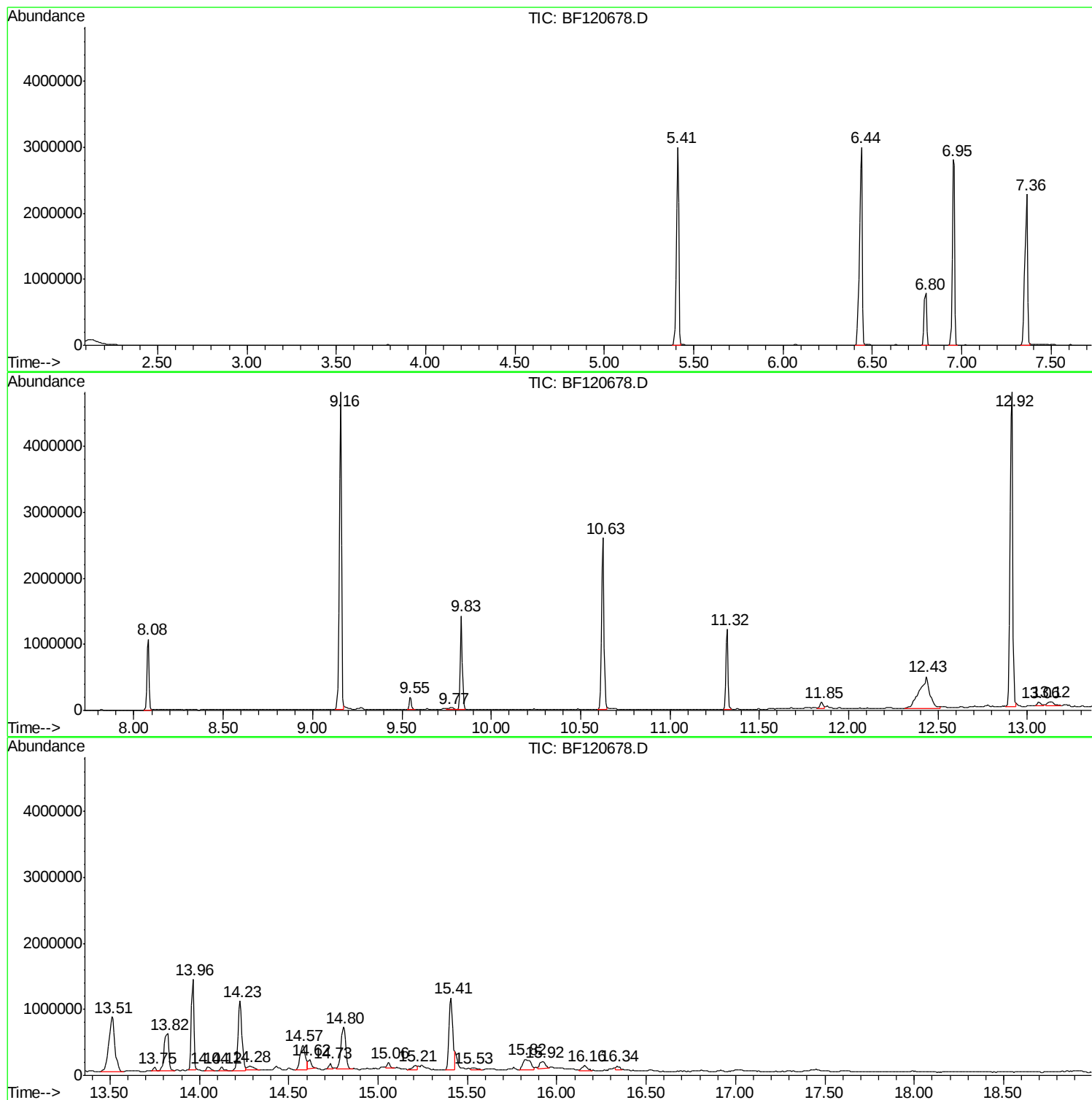
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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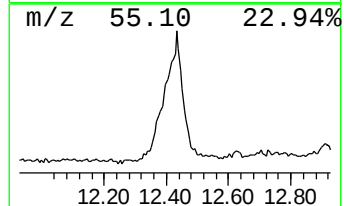
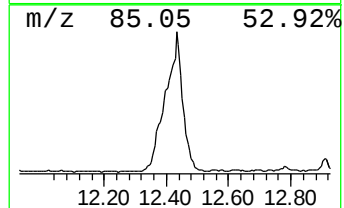
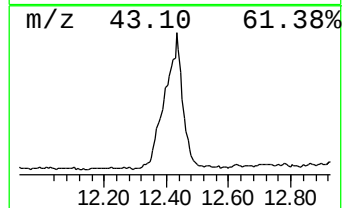
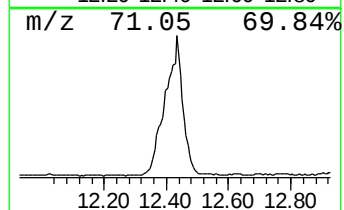
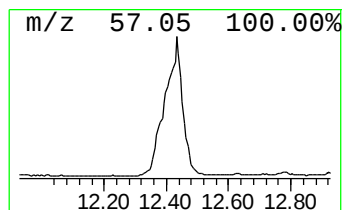
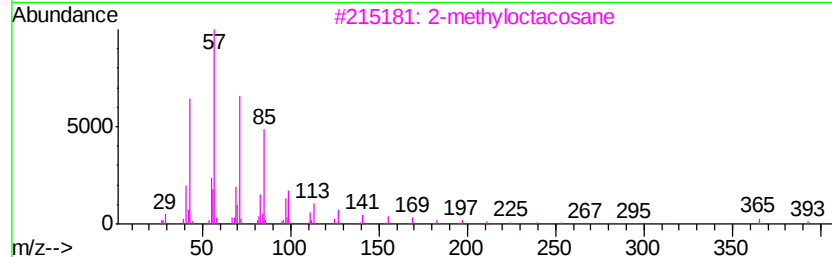
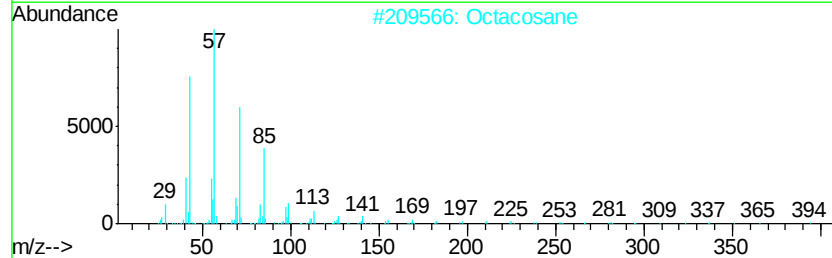
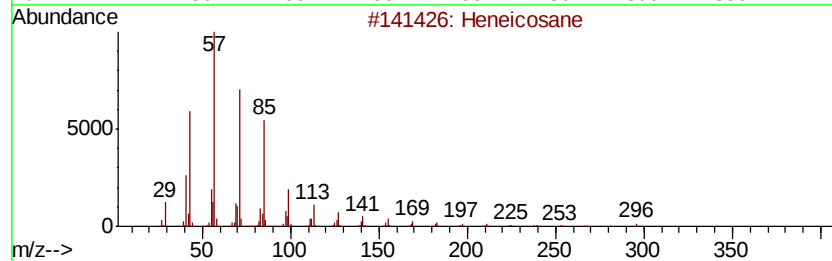
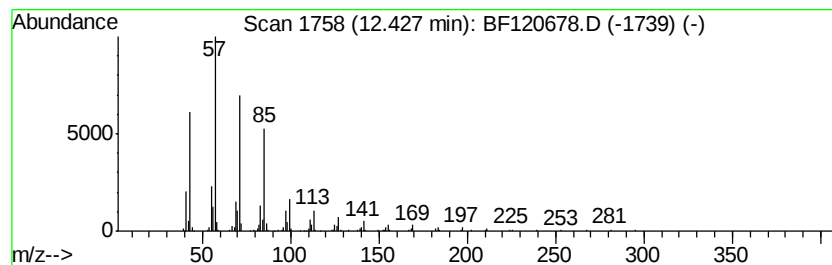
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	35.93 ng	1931090	Phenanthrene-d10	11.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octacosane		394	C28H58	000630-02-4	91
3	2-methyloctacosane		408	C29H60	1000376-72-8	91
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
5	Heptacosane		380	C27H56	000593-49-7	91



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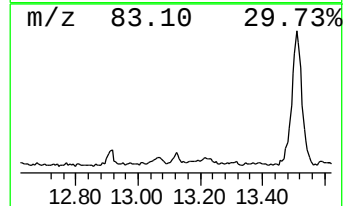
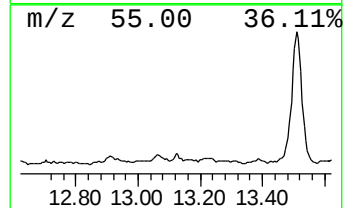
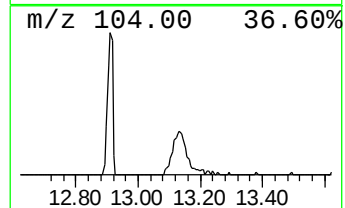
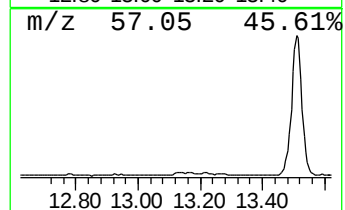
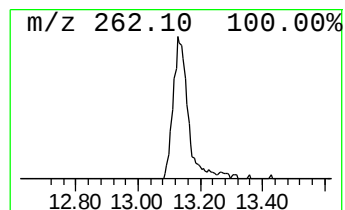
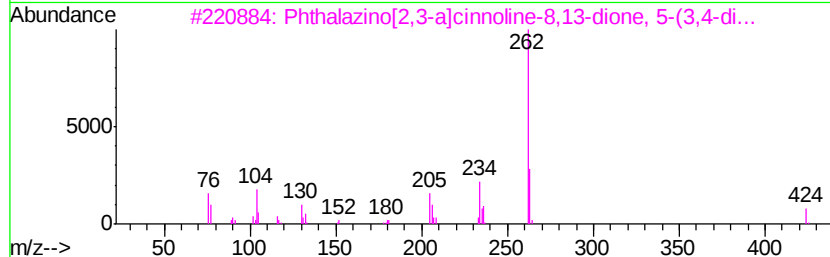
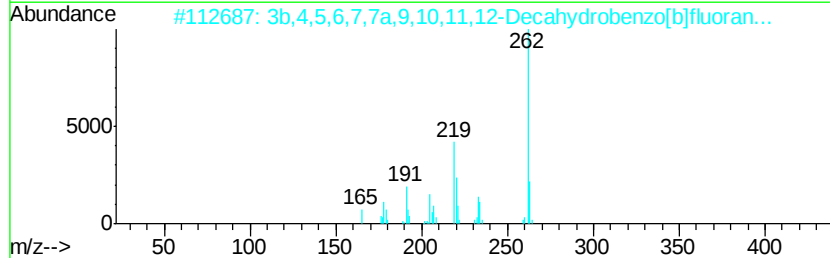
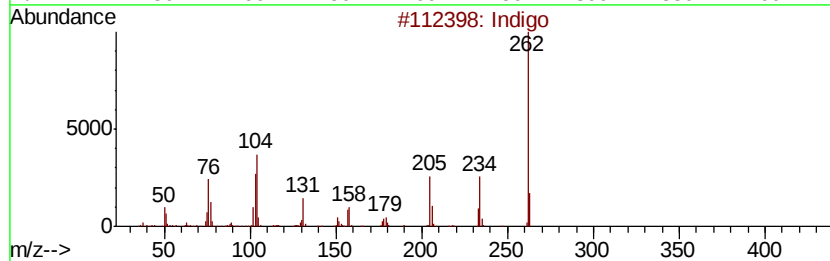
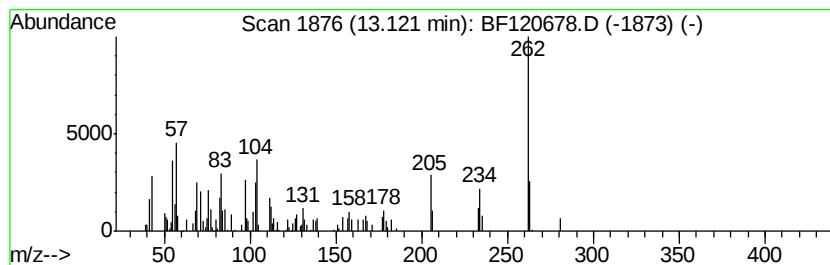
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Indigo Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.12	2.35 ng	137608	Chrysene-d12	13.96		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indigo		262	C16H10N2O2	000482-89-3	98
2	3b,4,5,6,7,7a,9,10,11,12-Decahyd...		262	C20H22	1000080-20-7	72
3	Phthalazino[2,3-a]cinnoline-8,13...		426	C24H18N4O4	074966-82-8	58
4	Perylene, 1,2,3,3a,4,5,6,7,8,9-d...		262	C20H22	068913-00-8	52
5	Anthracene, 1,2,3,4,5,6,7,8-octa...		262	C20H22	125379-29-5	49



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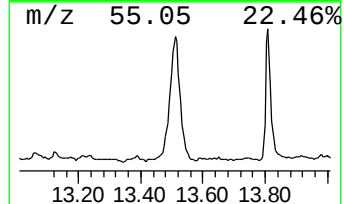
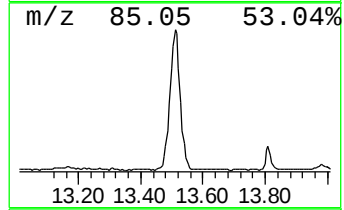
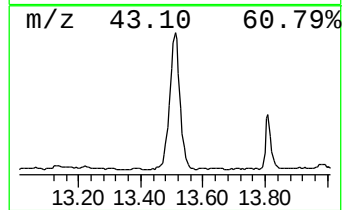
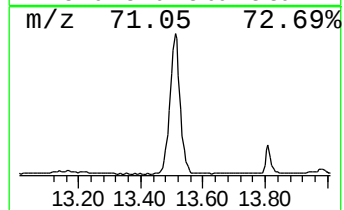
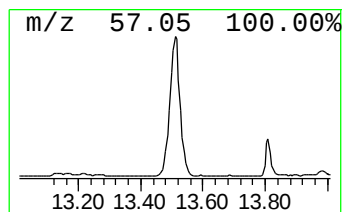
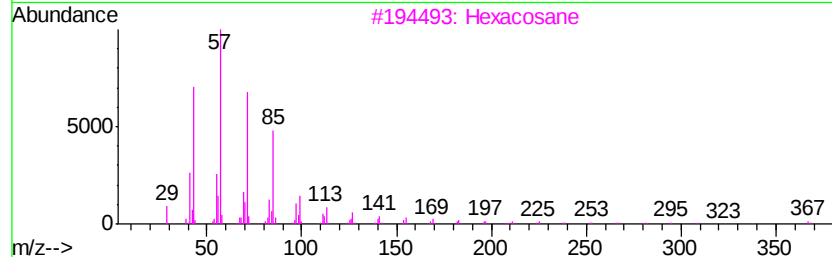
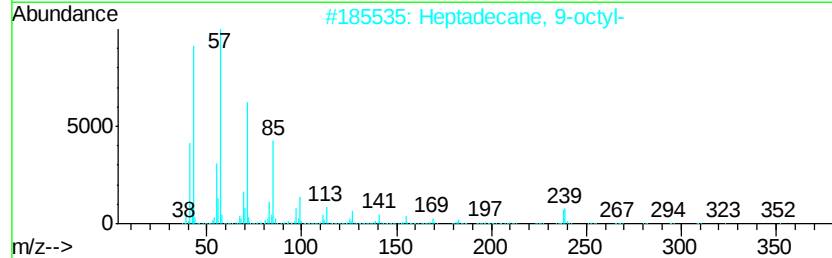
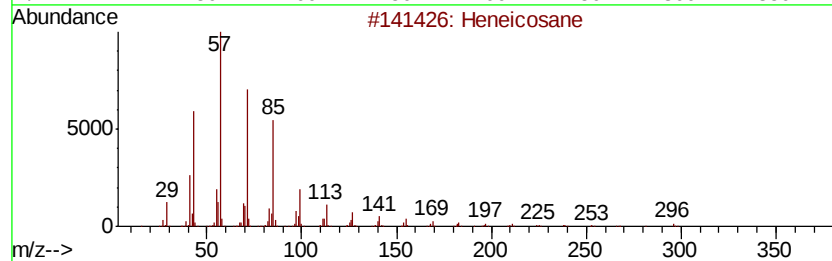
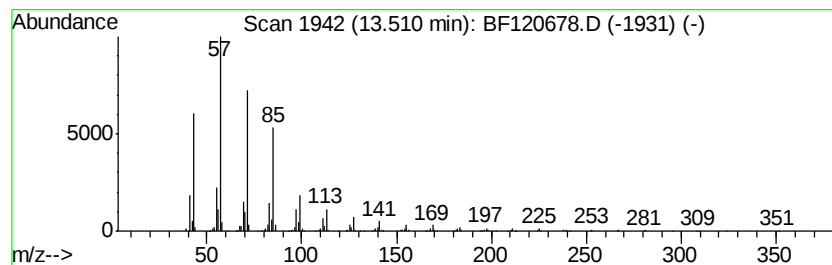
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Heptadecane, 9-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	33.07 ng	1932650	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		Hexacosane	366	C26H54	000630-01-3	90
4		Eicosane, 2-methyl-	296	C21H44	001560-84-5	90
5		Octadecane	254	C18H38	000593-45-3	87



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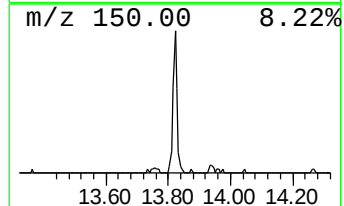
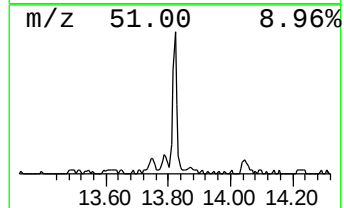
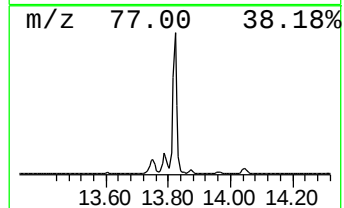
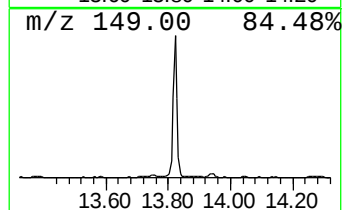
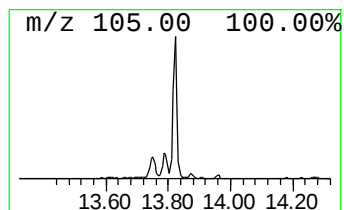
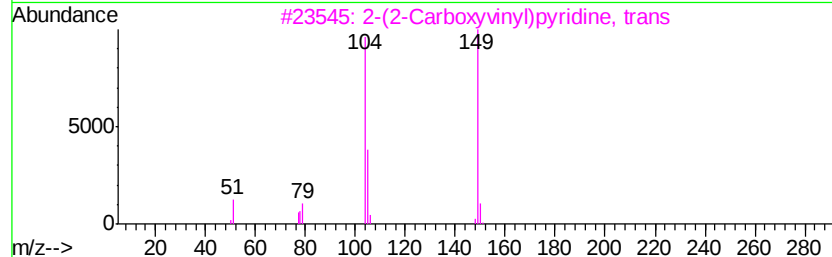
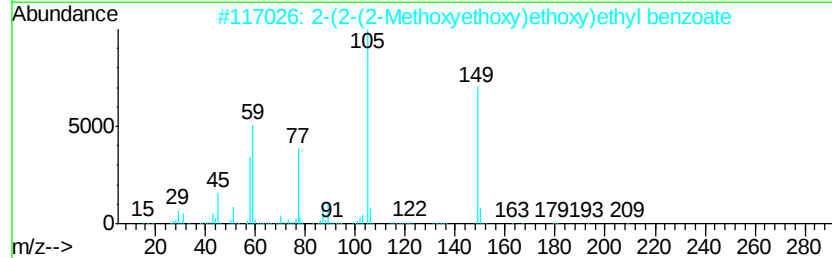
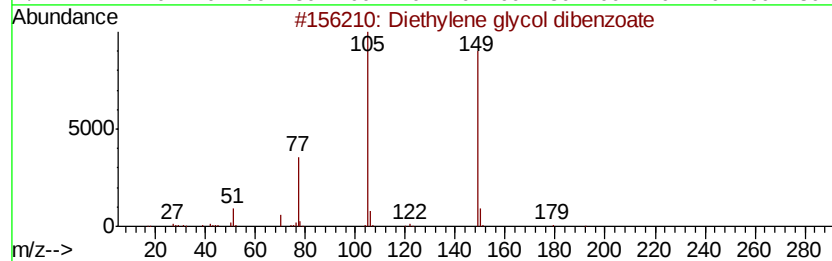
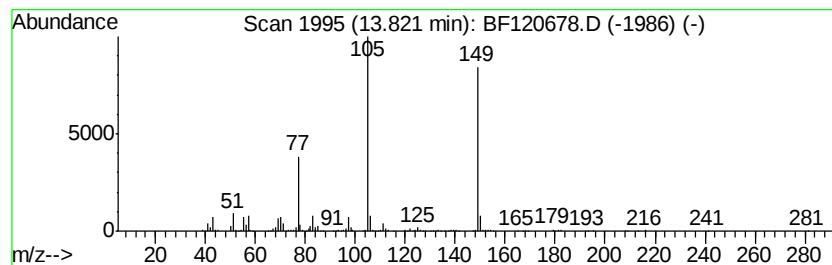
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	16.98 ng	992490	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	87
2		2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	78
3		2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	49
4		1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-18-9	43
5		Phthalic acid, 2-methoxyethyl te...	420	C25H40O5	1000315-80-9	43



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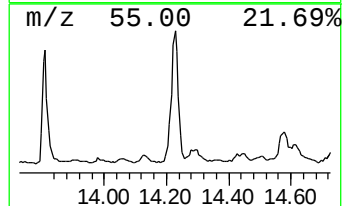
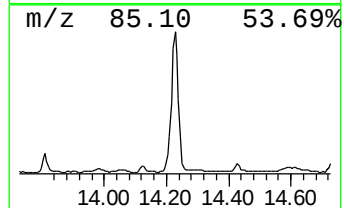
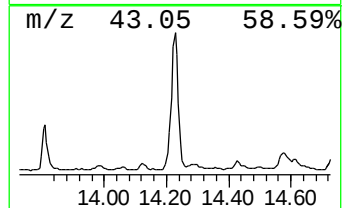
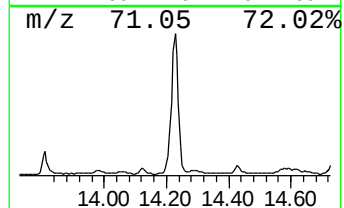
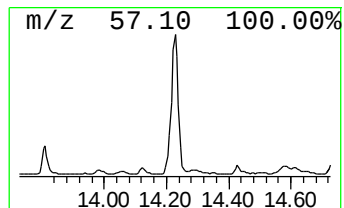
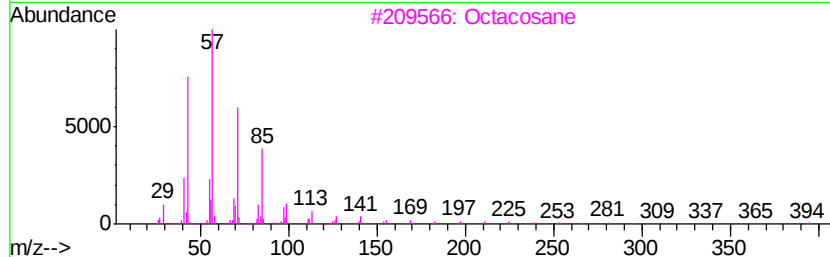
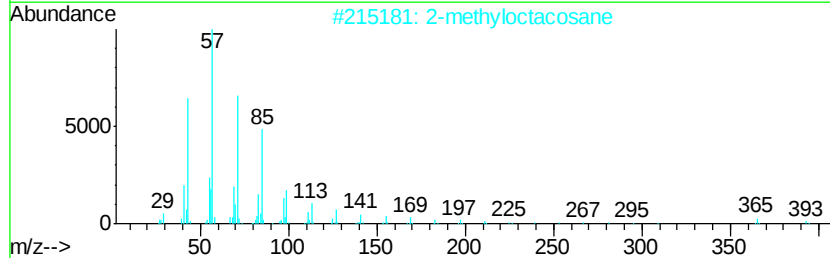
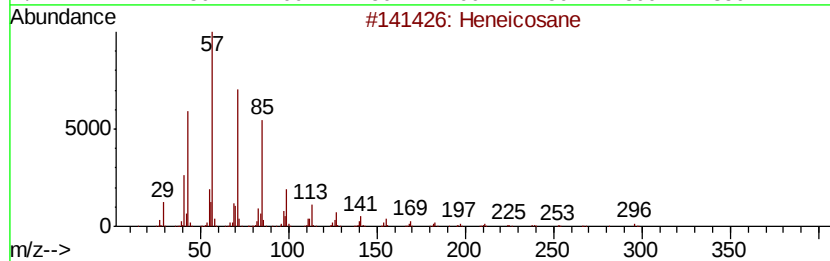
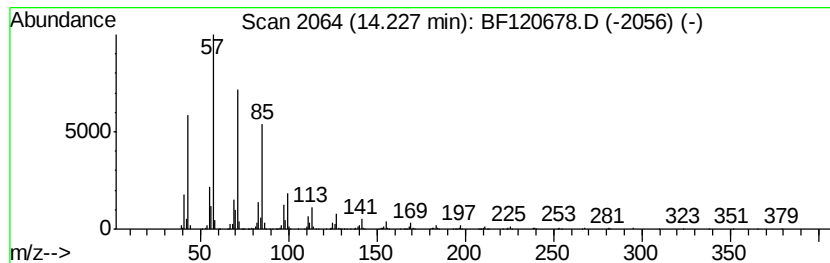
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Peak Number 6 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	29.00 ng	1694700	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062220\
Data File : BF120678.D
Acq On : 22 Jun 2020 16:04
Operator : JU/CG
Sample : L3082-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3

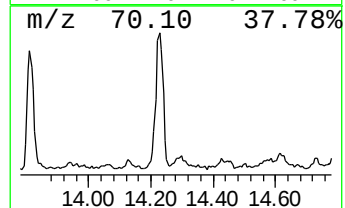
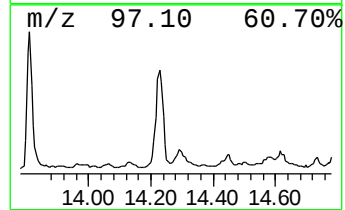
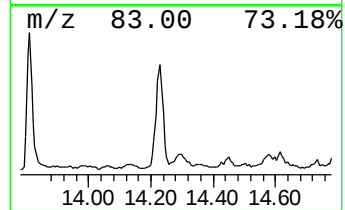
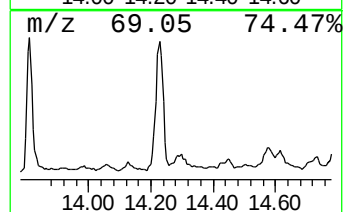
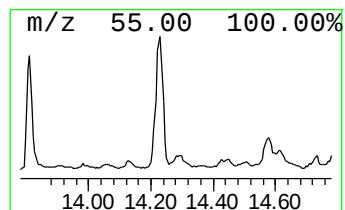
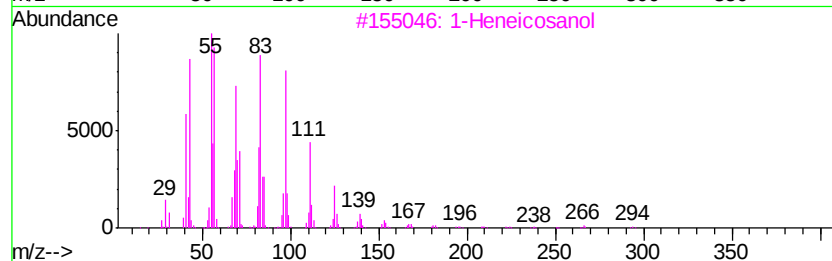
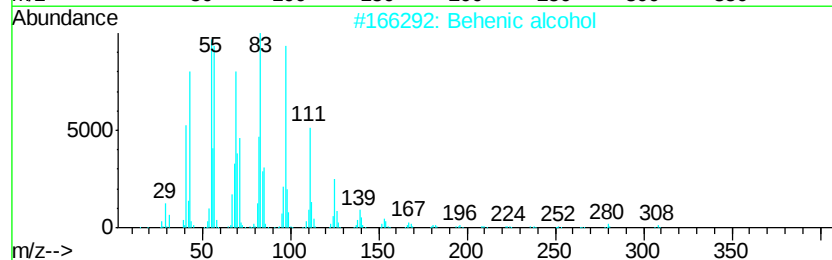
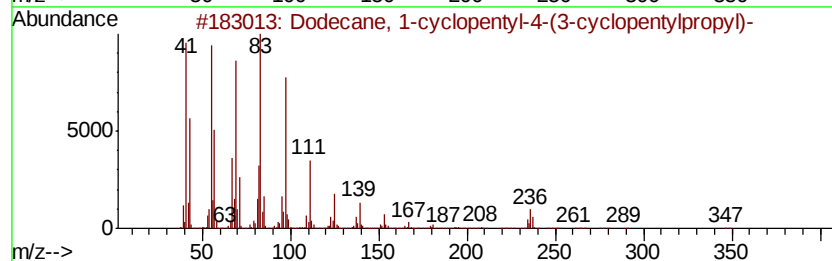
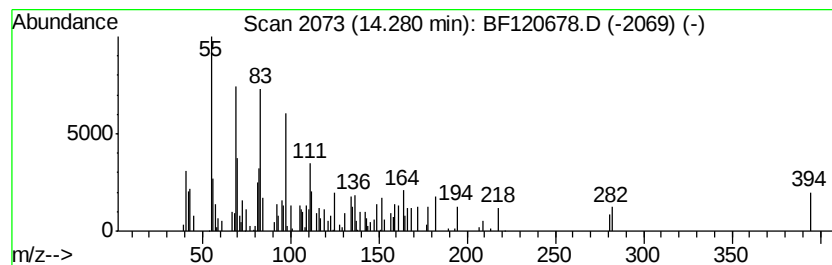
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dodecane, 1-cyclopentyl-4-(... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.28	2.49 ng	145313	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 1-cvclopentvl-4-(3-cvc...	348	C25H48	007225-68-5	52
2		Behenic alcohol	326	C22H46O	000661-19-8	43
3		1-Heneicosanol	312	C21H44O	015594-90-8	43
4		4-Undecene, 6-methyl-	168	C12H24	1000061-85-4	35
5		3-Hexene, 2,2-dimethyl-, (E)-	112	C8H16	000690-93-7	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062220\
Data File : BF120678.D
Acq On : 22 Jun 2020 16:04
Operator : JU/CG
Sample : L3082-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

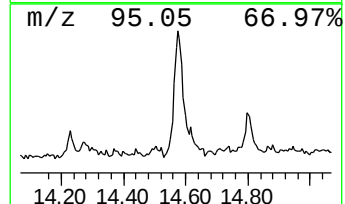
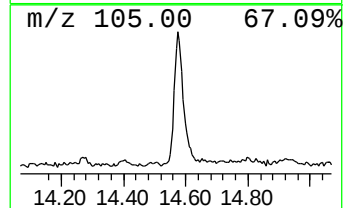
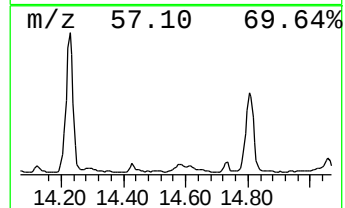
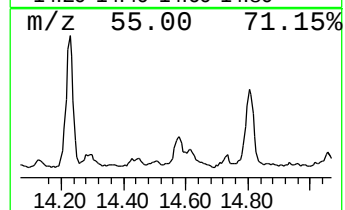
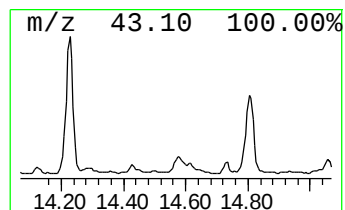
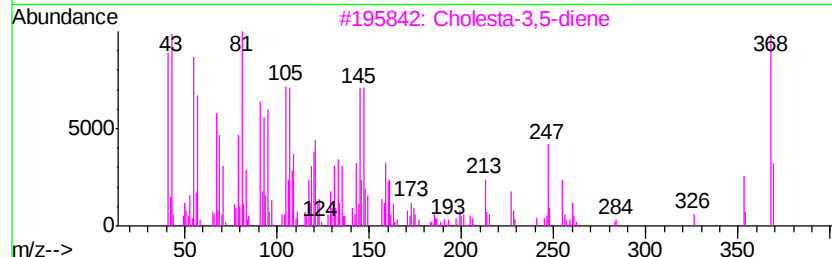
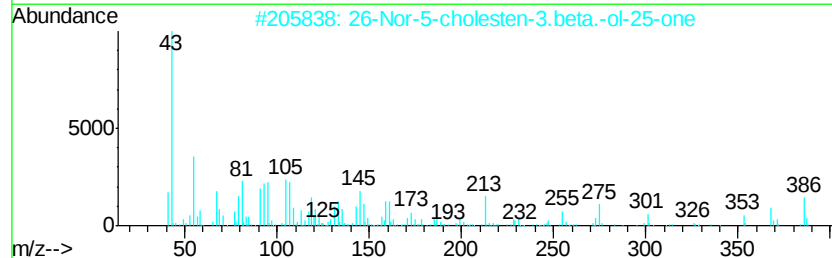
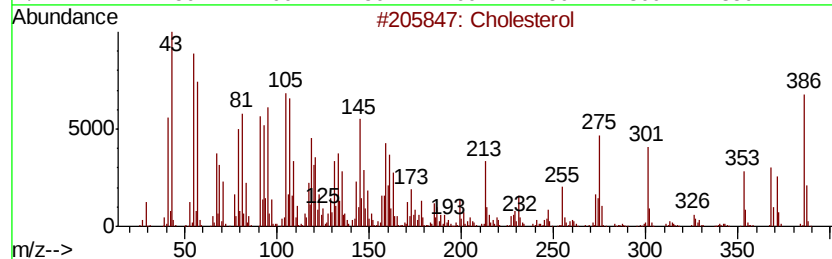
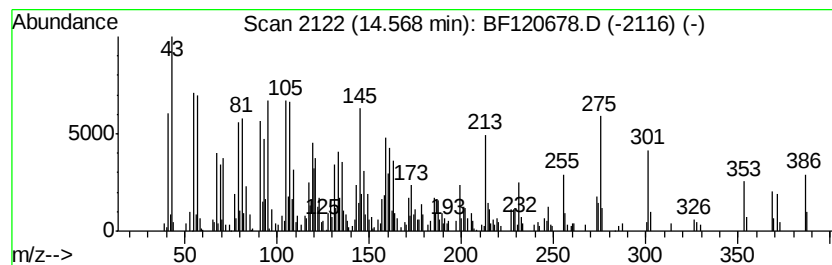
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cholesterol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.57	12.88 ng	753089	Chrysene-d12	13.96		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cholesterol	386	C27H46O	000057-88-5	99
2		26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	99
3		Cholesta-3,5-diene	368	C27H44	000747-90-0	35
4		21-Acetoxypregnenolone	374	C23H34O4	000566-78-9	12
5		Cholest-5-en-3-ol (3.beta.)-, ac...	428	C29H48O2	000604-35-3	11



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062220\
Data File : BF120678.D
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Operator : JU/CG
Sample : L3082-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

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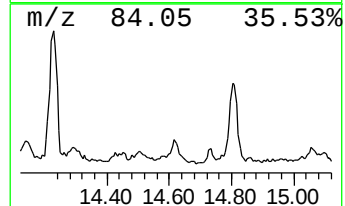
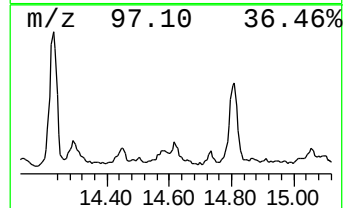
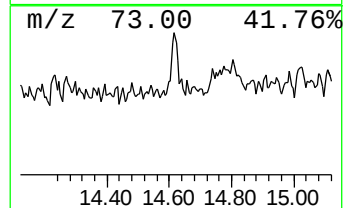
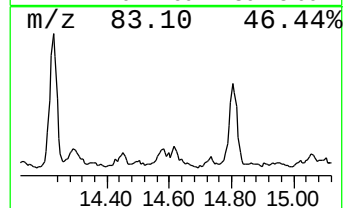
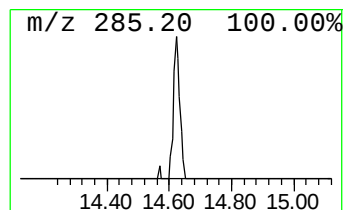
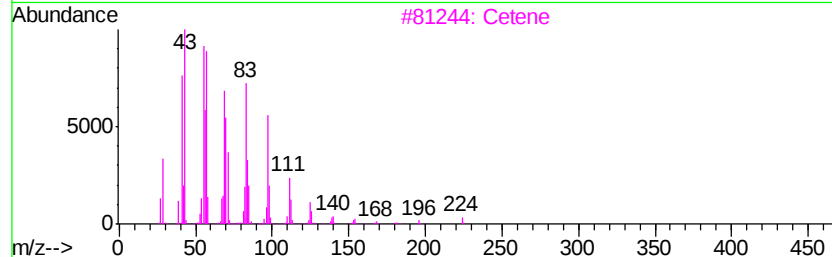
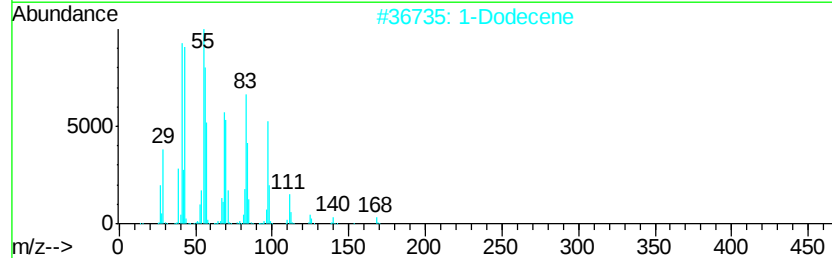
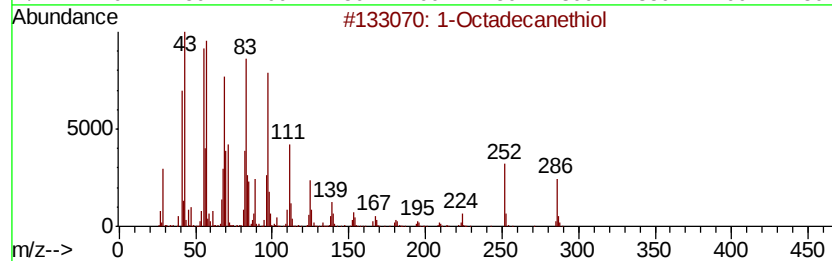
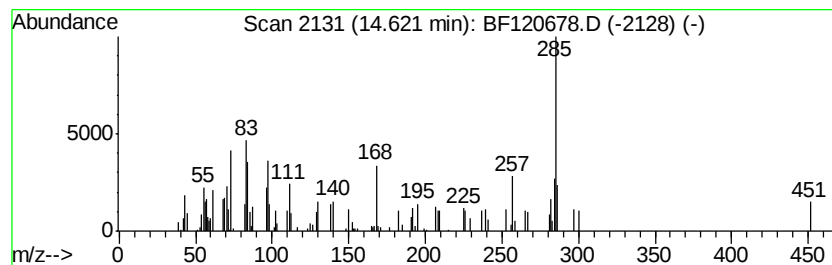
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Octadecanethiol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.74 ng	160039	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Octadecanethiol	286	C18H38S	002885-00-9	58
2		1-Dodecene	168	C12H24	000112-41-4	46
3		Cetene	224	C16H32	000629-73-2	38
4		1-Tridecene	182	C13H26	002437-56-1	38
5		Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062220\
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Sample : L3082-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

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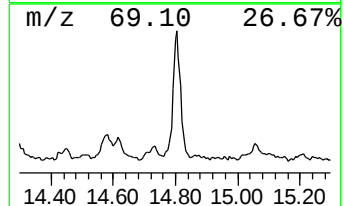
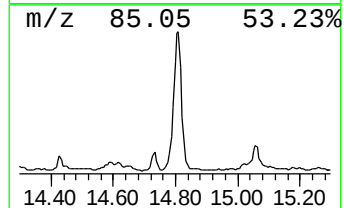
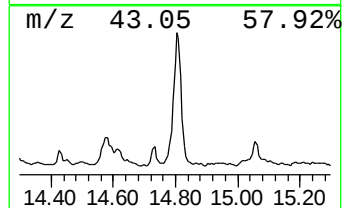
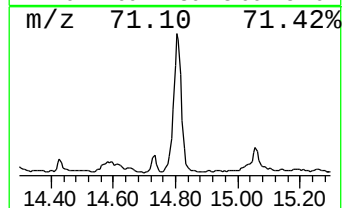
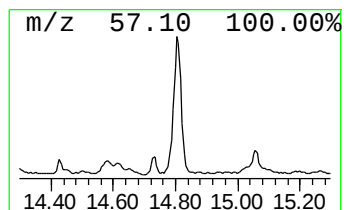
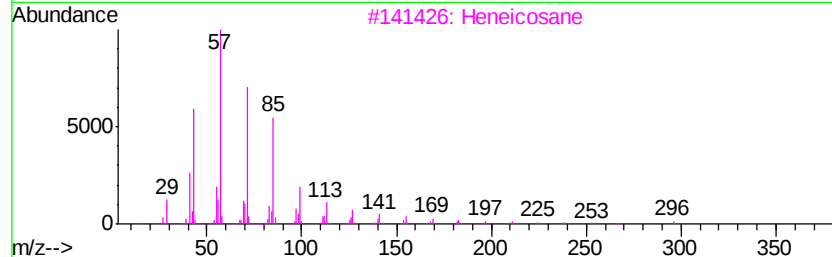
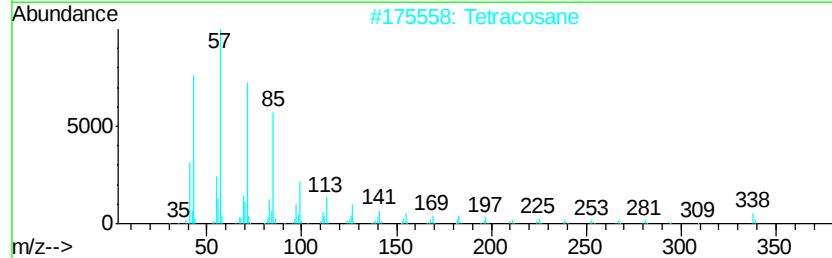
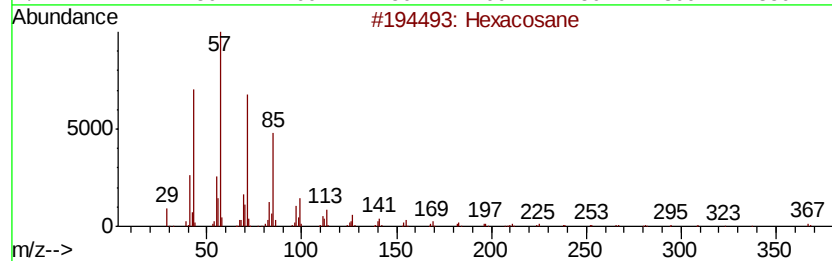
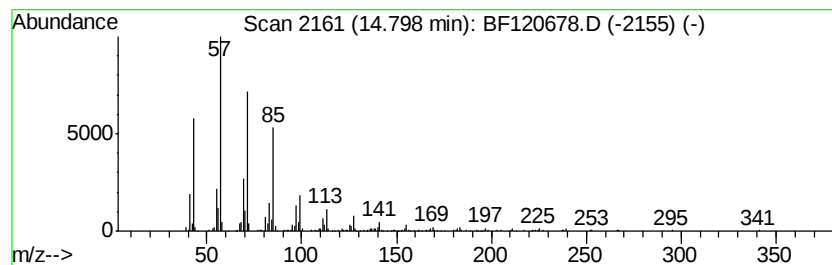
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	14.67 ng	1137230	Perylene-d12	15.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Tetracosane		338	C24H50	000646-31-1	91
3	Heneicosane		296	C21H44	000629-94-7	91
4	Octacosane		394	C28H58	000630-02-4	91
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062220\
Data File : BF120678.D
Acq On : 22 Jun 2020 16:04
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ClientSampleId :
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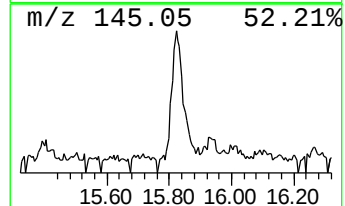
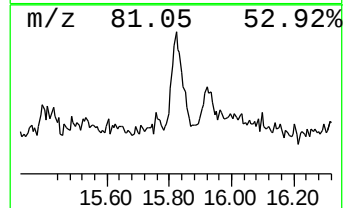
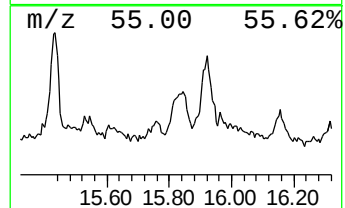
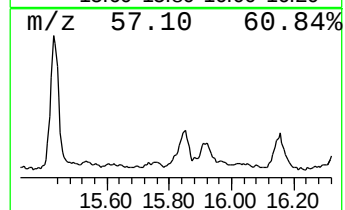
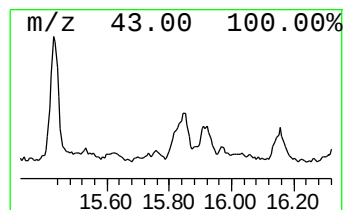
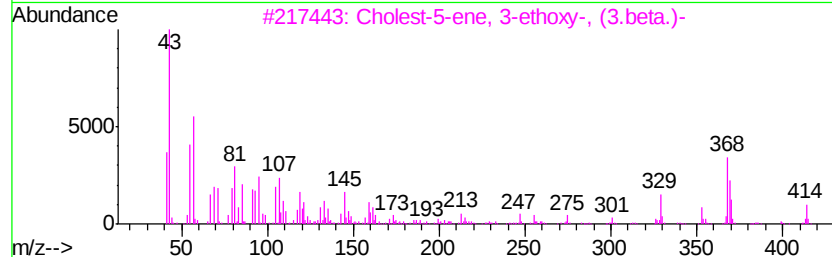
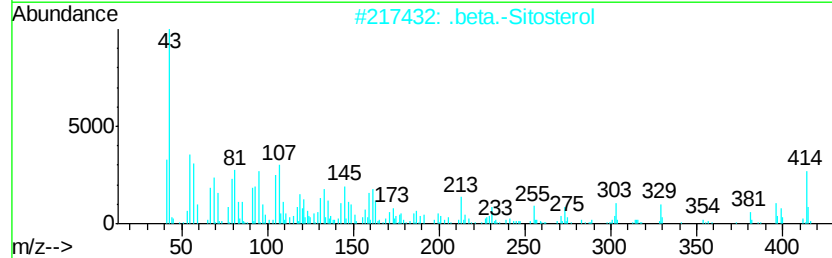
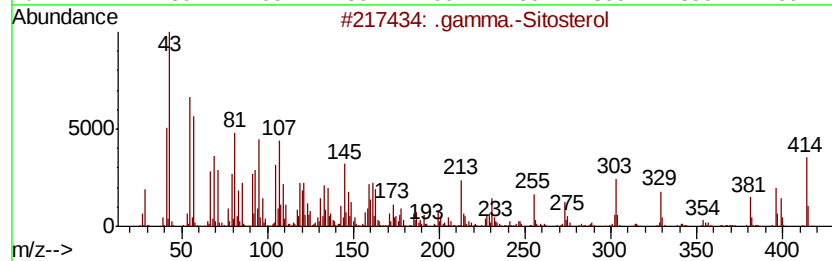
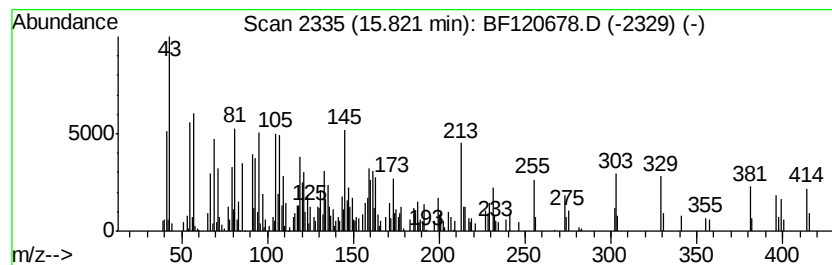
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 .gamma.-Sitosterol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.82	6.27 ng	486250	Perylene-d12	15.41

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	96
3		Cholest-5-ene, 3-ethoxy-, (3.beta...	414	C29H50O	000986-19-6	83
4		Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	49
5		Isocholesteryl methyl ether	400	C28H48O	029944-53-4	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062220\
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Sample : L3082-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

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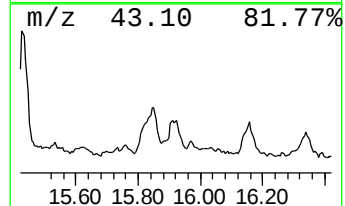
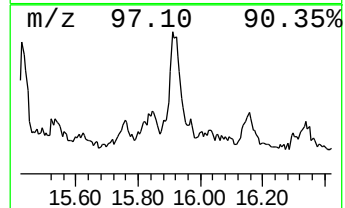
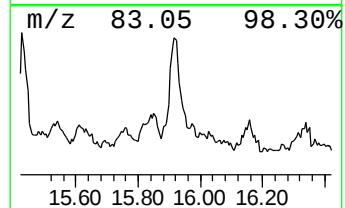
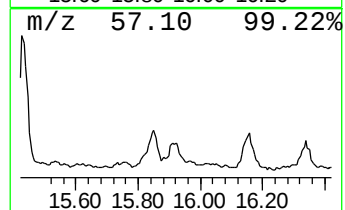
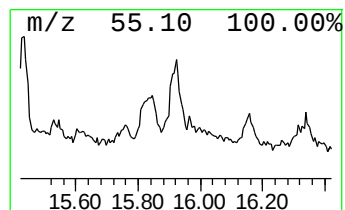
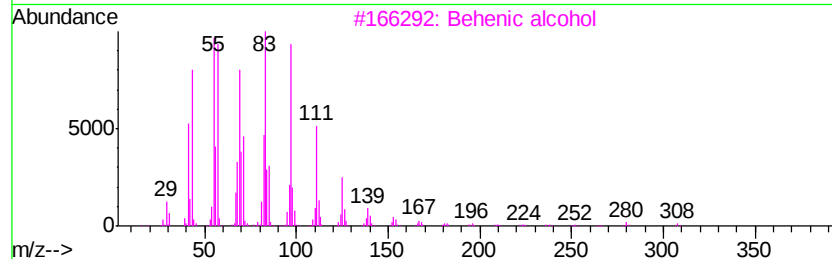
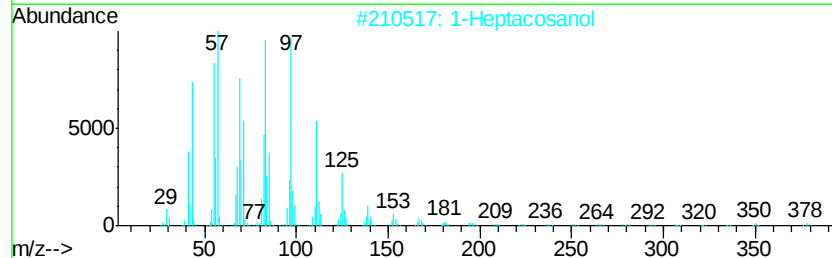
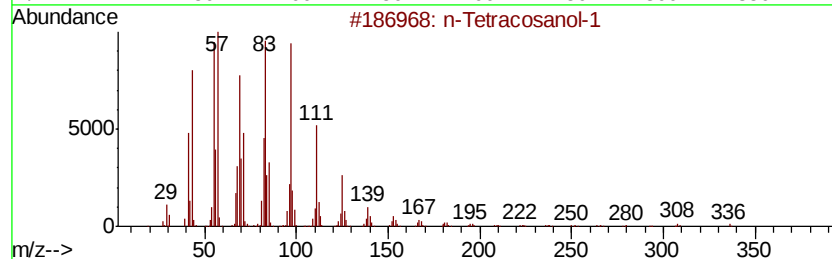
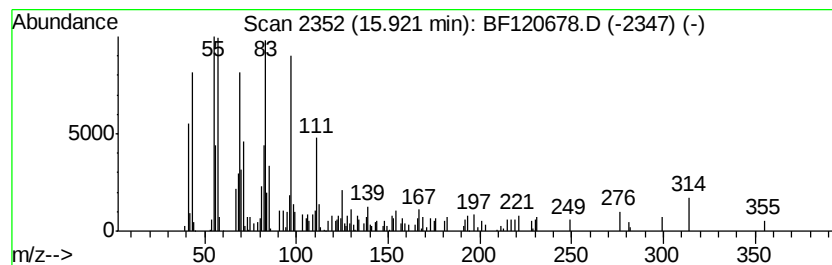
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 n-Tetracosanol-1 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	3.01 ng	233296	Perylene-d12	15.41

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		Behenic alcohol	326	C22H46O	000661-19-8	91
4		Octacosyl acetate	452	C30H60O2	018206-97-8	91
5		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062220\
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ClientSampleId :
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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
Heneicosane	12.43	35.9	ng	1931090	4	11.32	1074800	20.0
Indigo	13.12	2.4	ng	137608	5	13.96	1168950	20.0
Heptadecane, 9-oc...	13.51	33.1	ng	1932650	5	13.96	1168950	20.0
Diethylene glycol...	13.82	17.0	ng	992490	5	13.96	1168950	20.0
2-methyloctacosane	14.23	29.0	ng	1694700	5	13.96	1168950	20.0
Dodecane, 1-cyclo...	14.28	2.5	ng	145313	5	13.96	1168950	20.0
Cholesterol	14.57	12.9	ng	753089	5	13.96	1168950	20.0
1-Octadecanethiol	14.62	2.7	ng	160039	5	13.96	1168950	20.0
Hexacosane	14.80	14.7	ng	1137230	6	15.41	1550400	20.0
.gamma.-Sitosterol	15.82	6.3	ng	486250	6	15.41	1550400	20.0
n-Tetracosanol-1	15.92	3.0	ng	233296	6	15.41	1550400	20.0