

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030620\
 Data File : BF119260.D
 Acq On : 6 Mar 2020 20:11
 Operator : CG/JU
 Sample : L1803-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 N38129

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-BF022020.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	5.351	552	555	577	rBV	870846	1120198	30.06%	4.562%
2	6.375	727	729	749	rBV	489801	695049	18.65%	2.831%
3	6.722	785	788	798	rBV	643073	559897	15.02%	2.280%
4	6.881	811	815	833	rBV	2488153	2358441	63.28%	9.605%
5	7.292	880	885	898	rBV	1702434	1776007	47.65%	7.233%
6	8.004	1003	1006	1009	rBV	829109	693308	18.60%	2.823%
7	8.028	1009	1010	1021	rVB2	69305	88647	2.38%	0.361%
8	9.080	1184	1189	1192	rBV	4160538	3711887	99.60%	15.117%
9	9.475	1254	1256	1260	rBV	114165	96999	2.60%	0.395%
10	9.757	1300	1304	1315	rVB	1014860	910388	24.43%	3.708%
11	10.551	1435	1439	1453	rBV	2580706	2619033	70.27%	10.666%
12	10.669	1456	1459	1466	rVB2	43161	54872	1.47%	0.223%
13	11.239	1553	1556	1565	rBV	1052449	961338	25.79%	3.915%
14	11.486	1594	1598	1606	rBV3	25999	47060	1.26%	0.192%
15	11.698	1630	1634	1643	rBV4	54320	76992	2.07%	0.314%
16	11.774	1643	1647	1659	rBV	490810	622440	16.70%	2.535%
17	12.016	1685	1688	1691	rVB	127359	99719	2.68%	0.406%
18	12.474	1760	1766	1776	rBV5	70677	149582	4.01%	0.609%
19	12.557	1776	1780	1794	rVV2	147391	210595	5.65%	0.858%
20	12.821	1821	1825	1829	rBV	3920197	3726937	100.00%	15.178%
21	13.051	1860	1864	1870	rBV2	34428	41855	1.12%	0.170%
22	13.392	1914	1922	1924	rBV3	41460	50937	1.37%	0.207%
23	13.721	1974	1978	1992	rVB	263511	457291	12.27%	1.862%
24	13.880	2002	2005	2015	rVB	874157	844569	22.66%	3.439%
25	14.033	2027	2031	2034	rBV	81189	74443	2.00%	0.303%
26	14.339	2079	2083	2086	rBV	111985	104502	2.80%	0.426%
27	14.633	2130	2133	2136	rVB	130782	116684	3.13%	0.475%
28	14.704	2141	2145	2149	rVB	1096526	1090786	29.27%	4.442%
29	14.945	2182	2186	2191	rBV	115717	134627	3.61%	0.548%
30	15.186	2222	2227	2230	rBV	92450	111580	2.99%	0.454%
31	15.304	2241	2247	2256	rBV	619827	859156	23.05%	3.499%
32	15.704	2310	2315	2319	rBV	63447	89255	2.39%	0.363%

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Misc :
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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

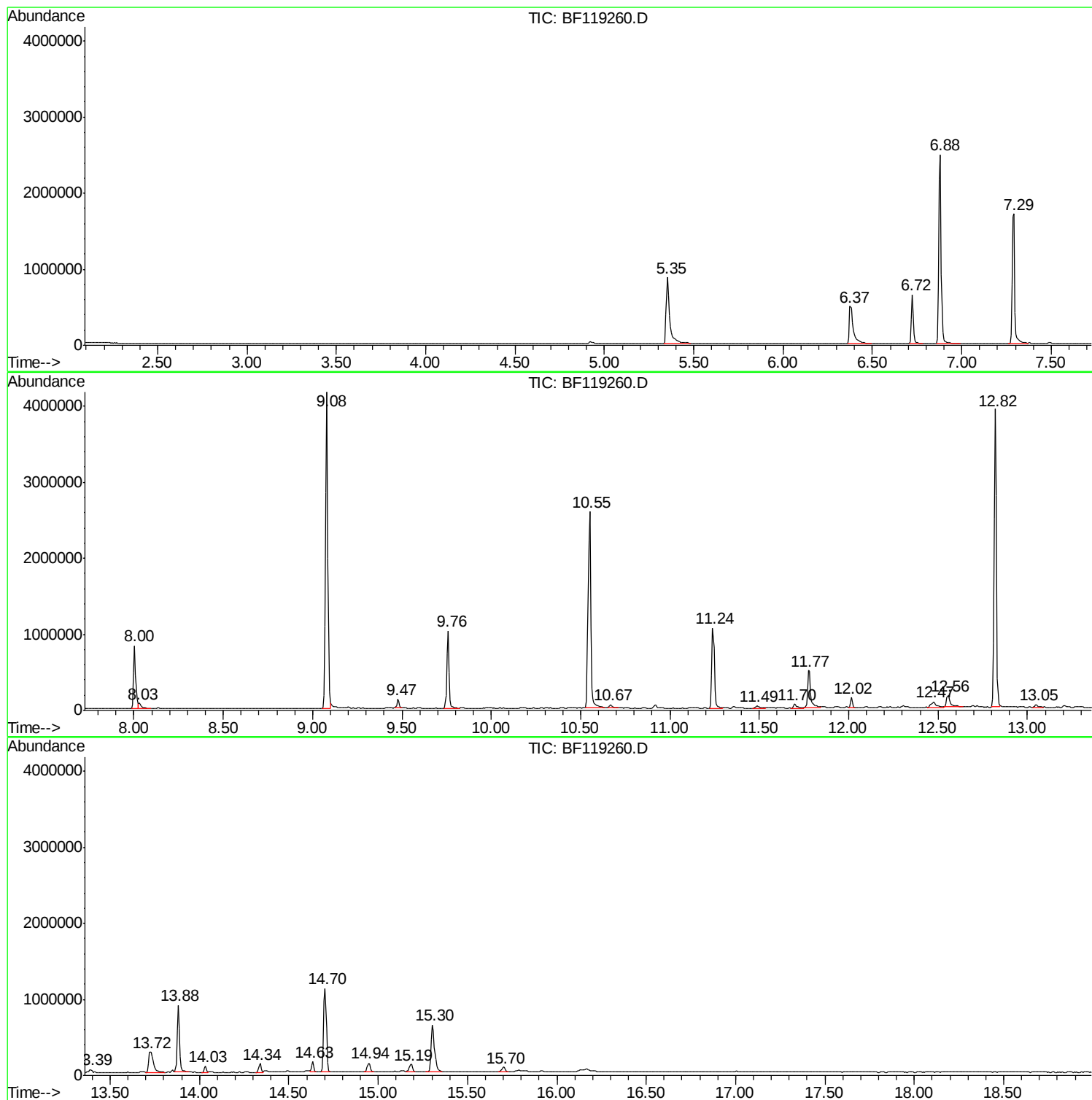
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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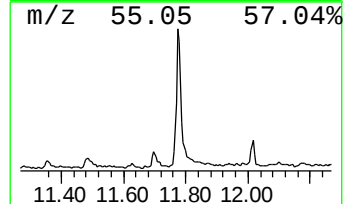
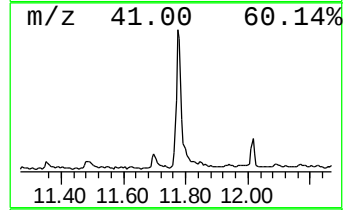
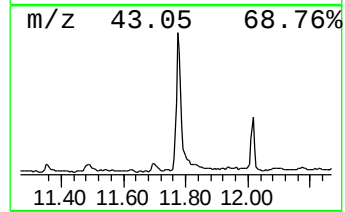
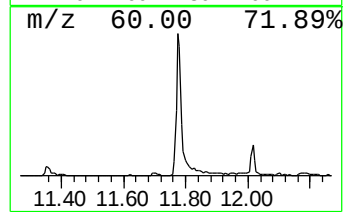
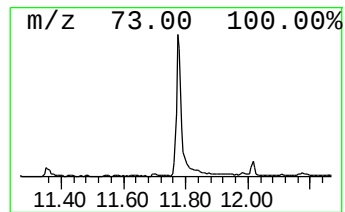
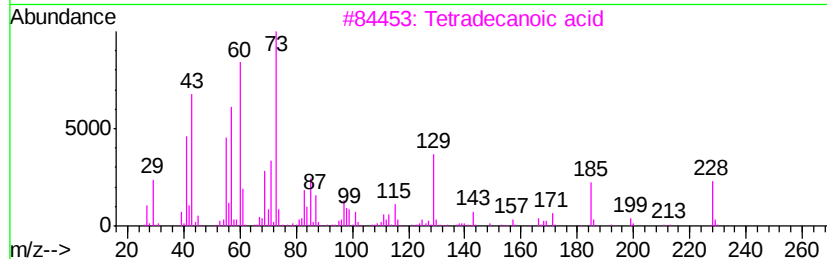
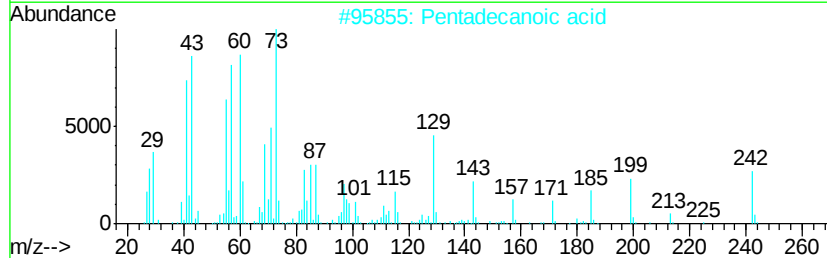
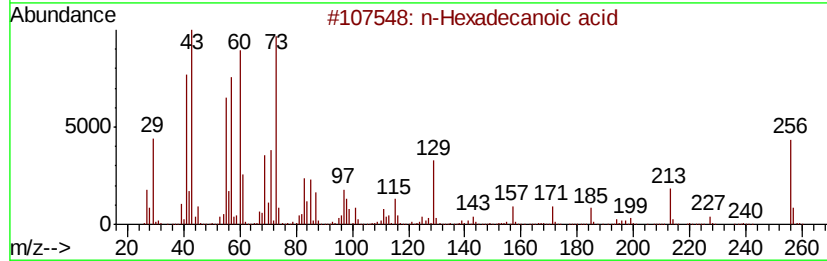
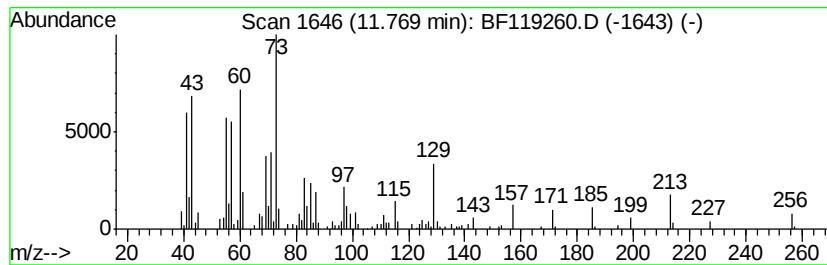
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.77	12.95 ng	622440	Phenanthrene-d10	11.24		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4		Tridecanoic acid	214	C13H26O2	000638-53-9	64
5		n-Decanoic acid	172	C10H20O2	000334-48-5	64



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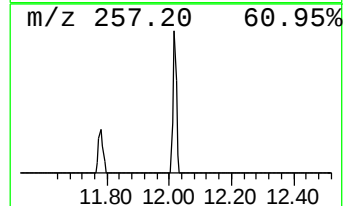
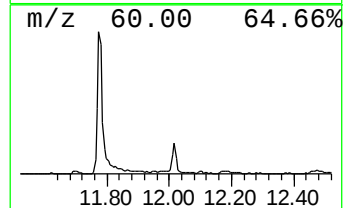
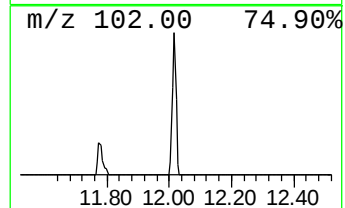
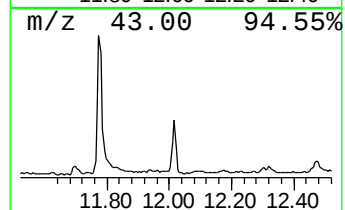
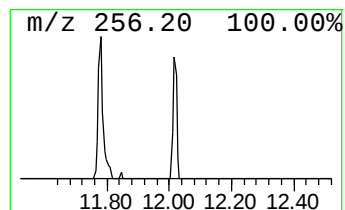
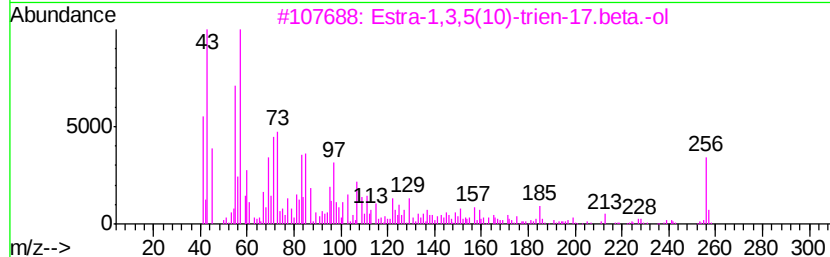
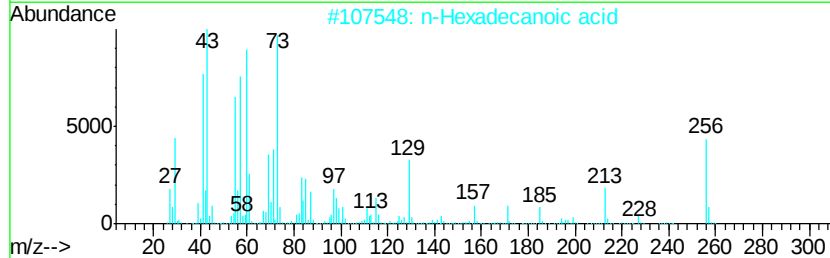
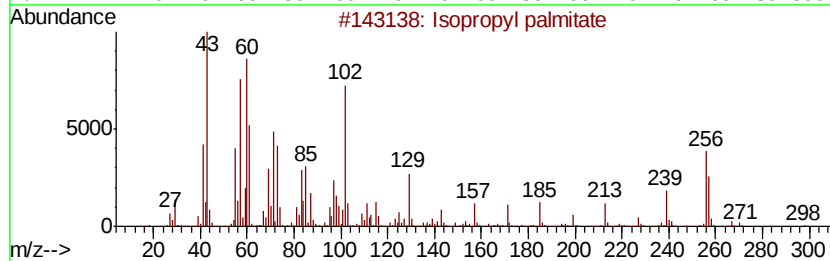
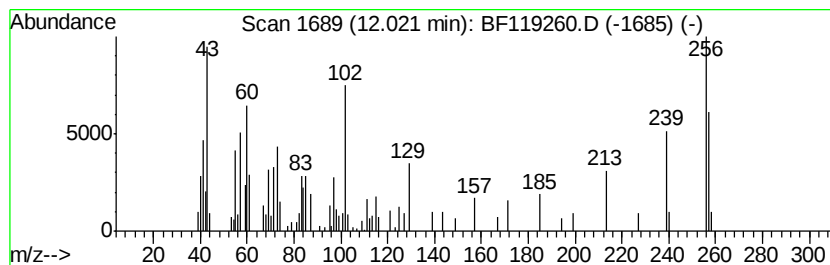
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Isopropyl palmitate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	2.07 ng	99719	Phenanthrene-d10	11.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl palmitate	298	C19H38O2	000142-91-6	52
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	42
3		Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	42
4		Isopropyl myristate	270	C17H34O2	000110-27-0	16
5		Methanone, (2-amino-6,7-dihydro-...	257	C14H15N3O2	1000338-27-1	14



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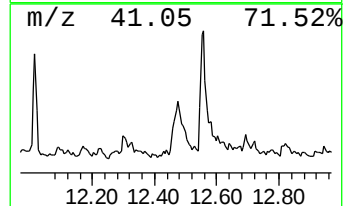
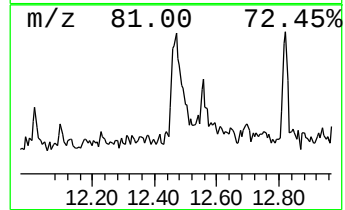
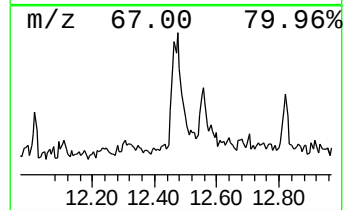
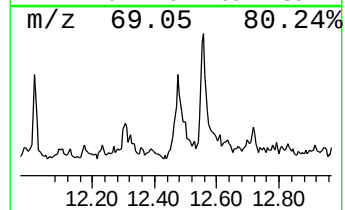
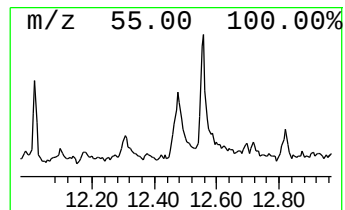
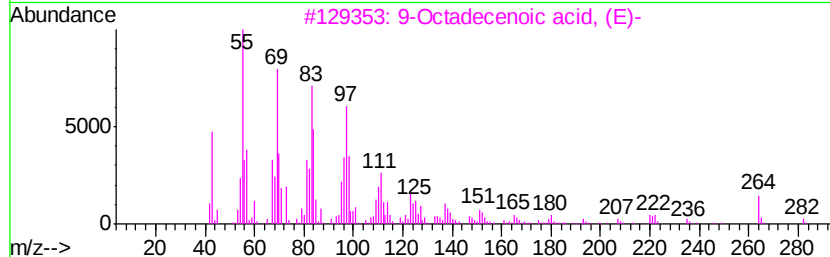
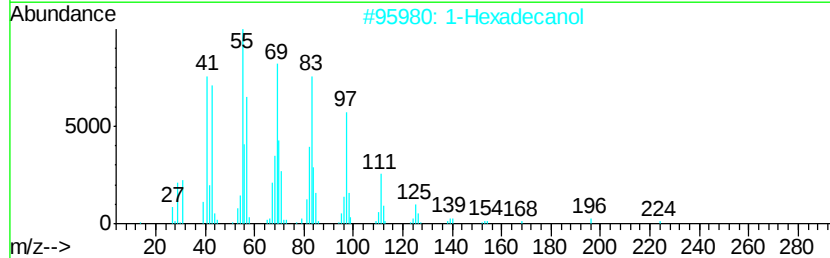
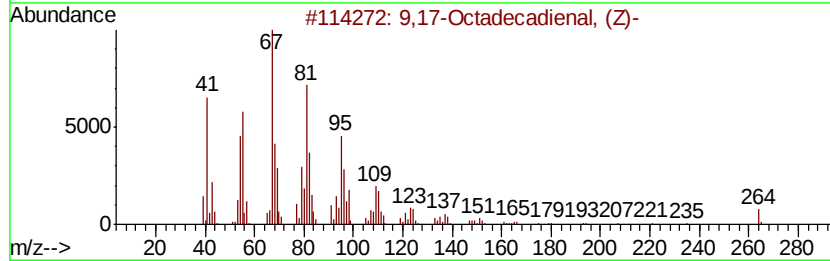
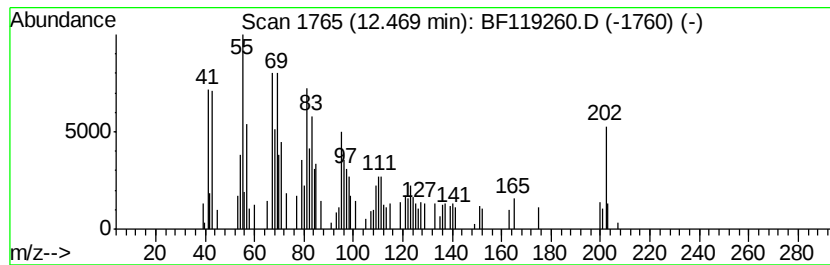
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9,17-Octadecadienal, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.47	3.11 ng	149582	Phenanthrene-d10	11.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,17-Octadecadienal, (Z)-	264	C18H32O	056554-35-9	55
2	1-Hexadecanol	242	C16H34O	036653-82-4	55
3	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	45
4	Oleic Acid	282	C18H34O2	000112-80-1	41
5	cis-Vaccenic acid	282	C18H34O2	000506-17-2	41



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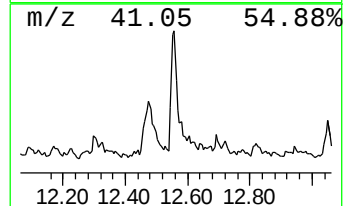
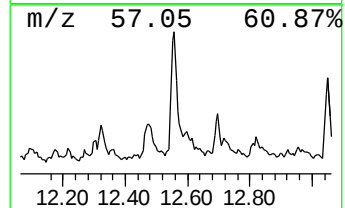
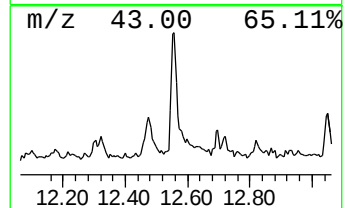
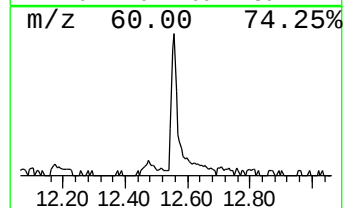
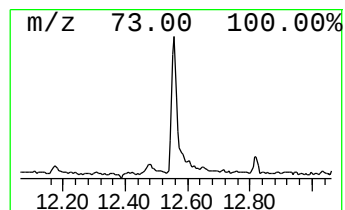
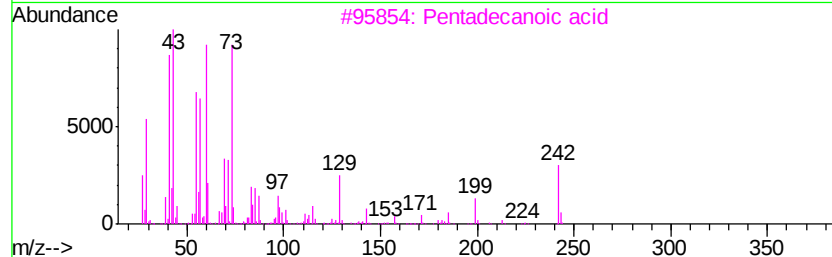
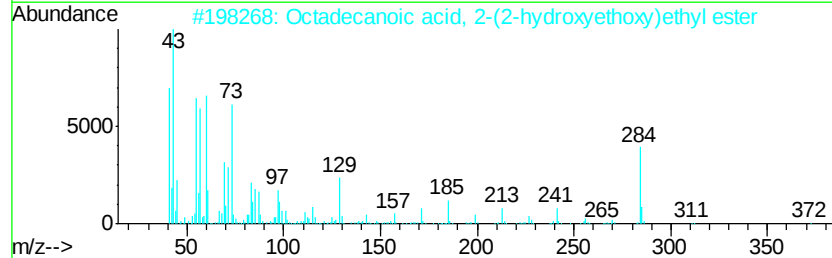
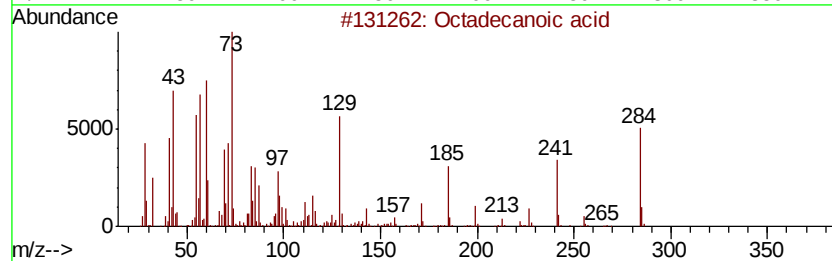
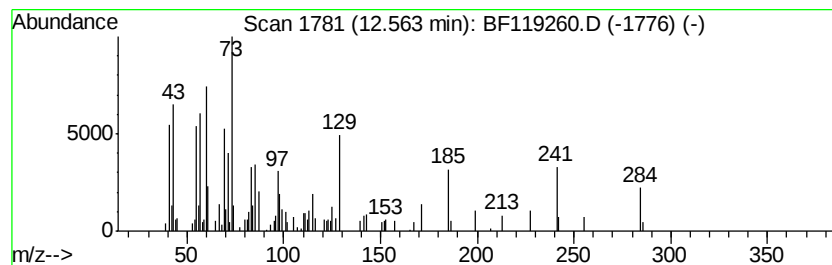
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	4.38 ng	210595	Phenanthrene-d10	11.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	72
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5		n-Decanoic acid	172	C10H20O2	000334-48-5	50



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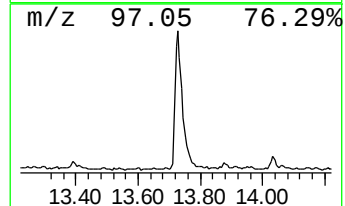
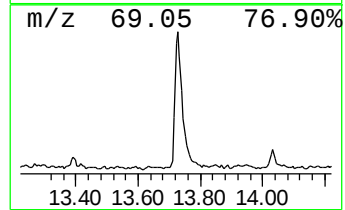
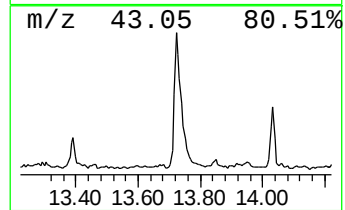
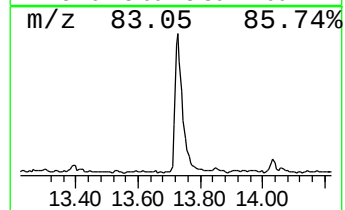
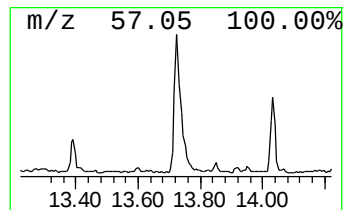
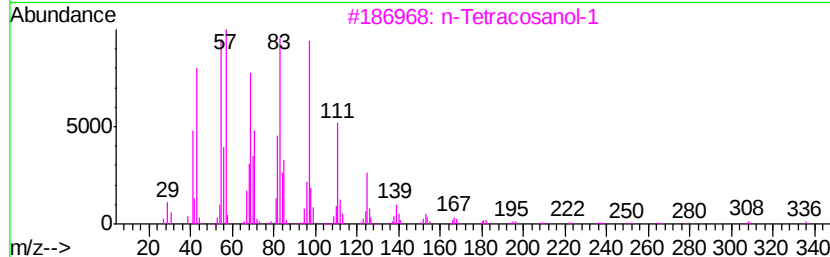
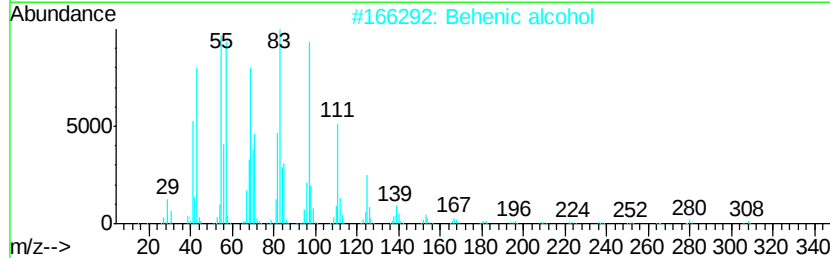
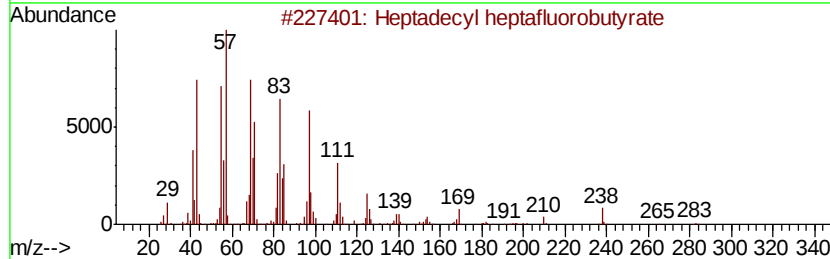
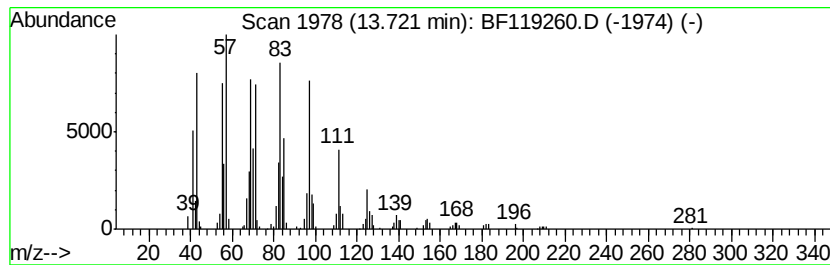
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	10.83 ng	457291	Chrysene-d12	13.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	94
2		Behenic alcohol	326	C22H46O	000661-19-8	93
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



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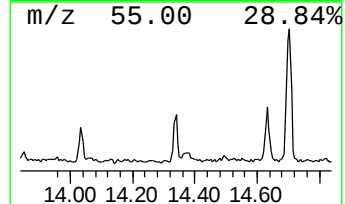
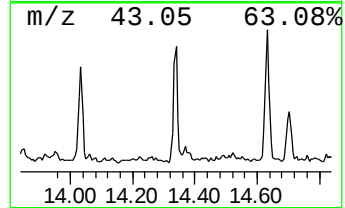
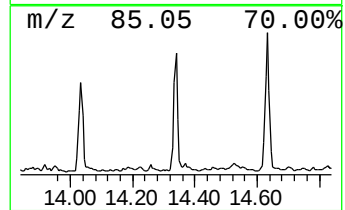
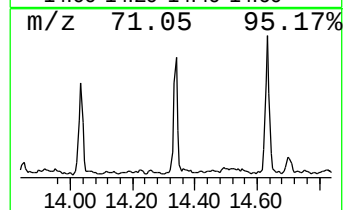
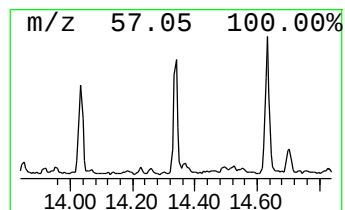
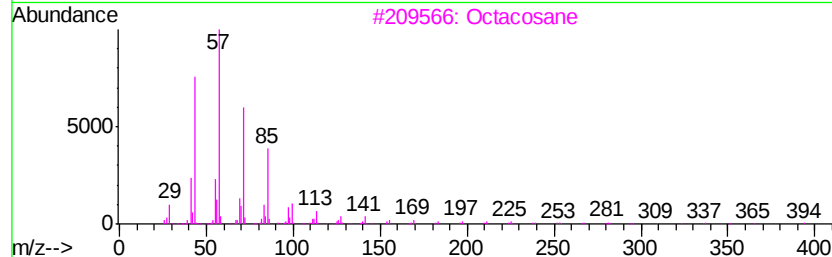
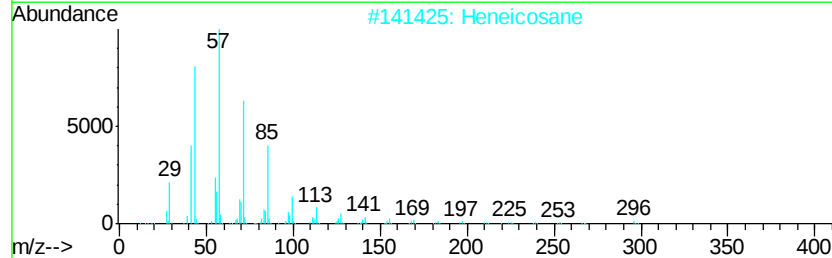
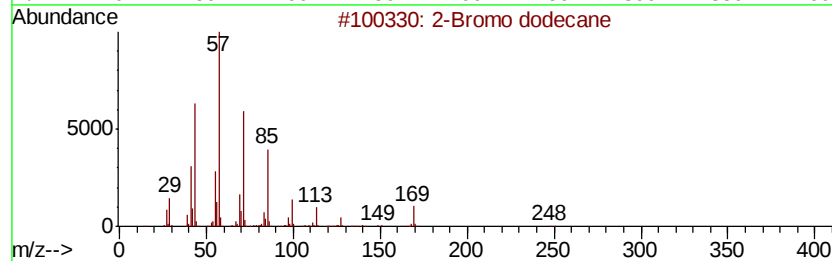
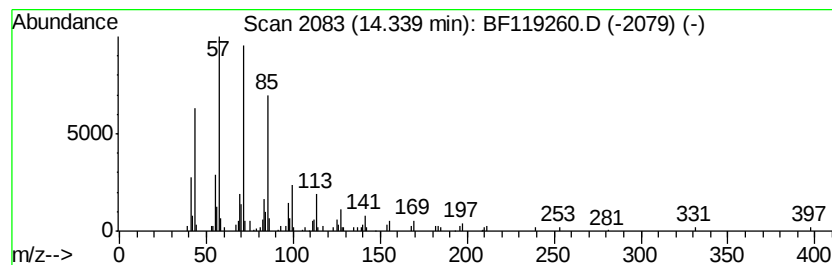
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Bromo dodecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.47 ng	104502	Chrysene-d12	13.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Bromo dodecane	248	C12H25Br	013187-99-0	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		Octacosane	394	C28H58	000630-02-4	87
4		Eicosane	282	C20H42	000112-95-8	87
5		Triacontane	422	C30H62	000638-68-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030620\
 Data File : BF119260.D
 Acq On : 6 Mar 2020 20:11
 Operator : CG/JU
 Sample : L1803-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

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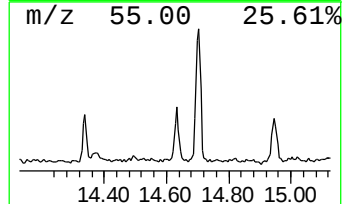
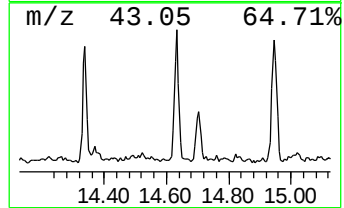
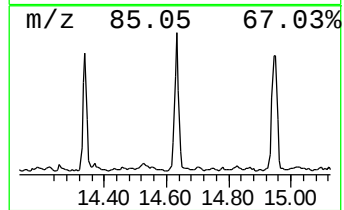
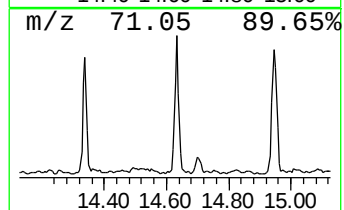
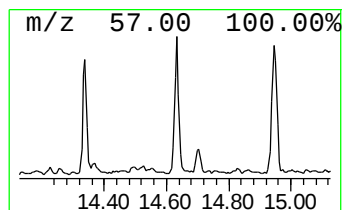
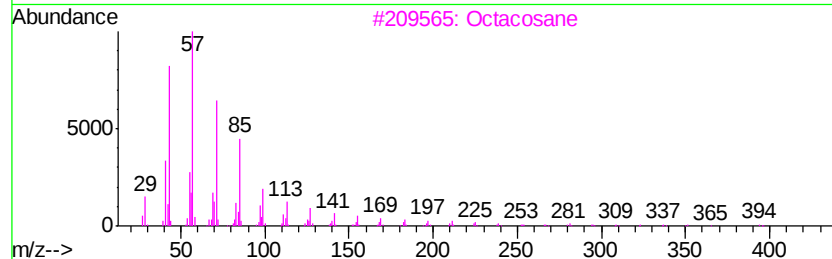
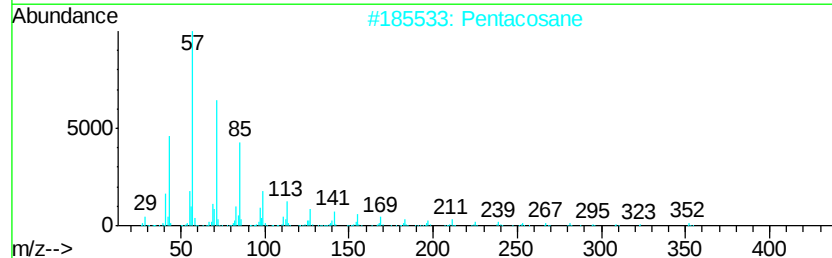
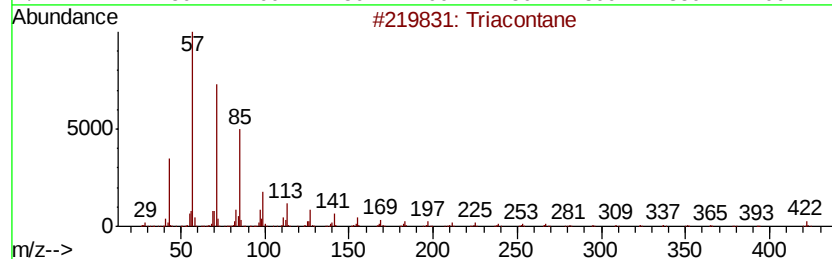
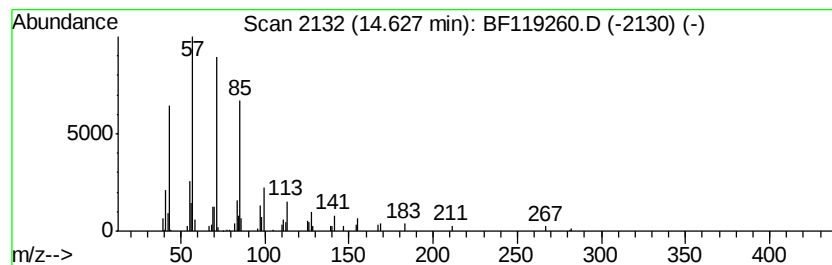
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	2.72 ng	116684	Perylene-d12	15.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triacontane	422	C30H62	000638-68-6	91
2		Pentacosane	352	C25H52	000629-99-2	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030620\
Data File : BF119260.D
Acq On : 6 Mar 2020 20:11
Operator : CG/JU
Sample : L1803-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
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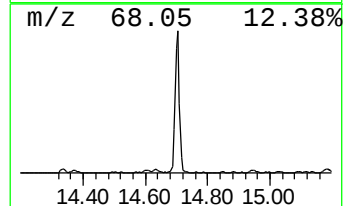
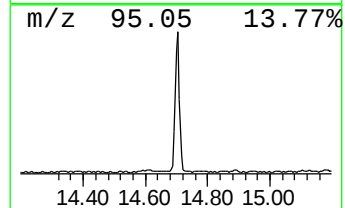
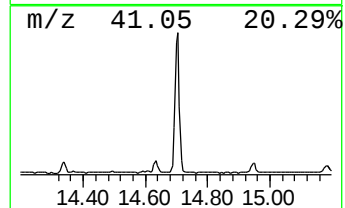
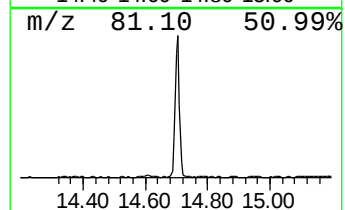
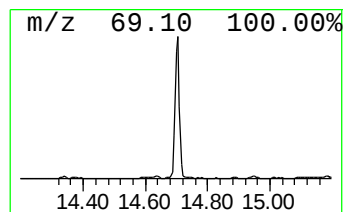
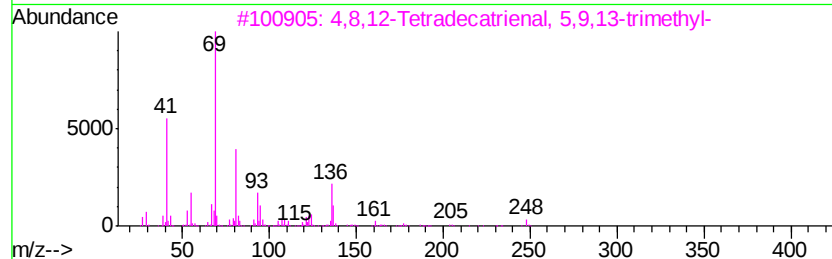
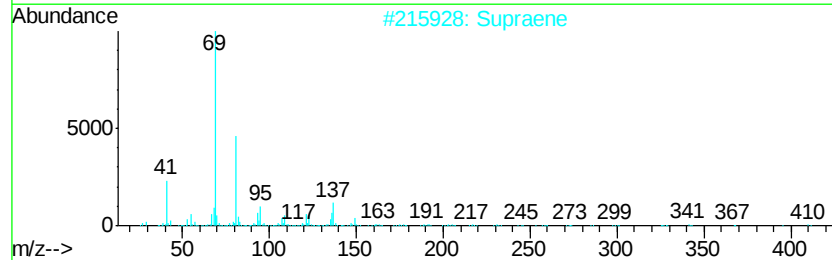
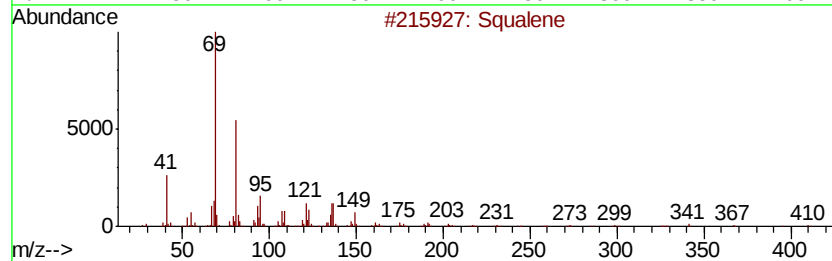
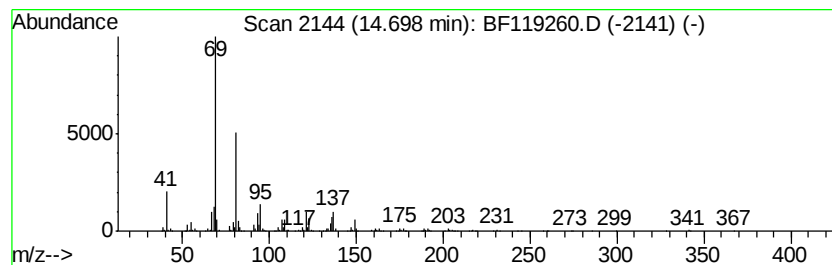
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	25.39 ng	1090790	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	99
2		Supraene	410	C30H50	007683-64-9	90
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030620\
Data File : BF119260.D
Acq On : 6 Mar 2020 20:11
Operator : CG/JU
Sample : L1803-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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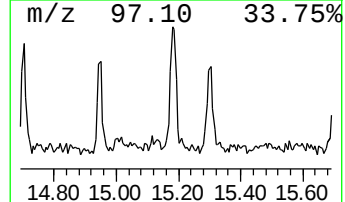
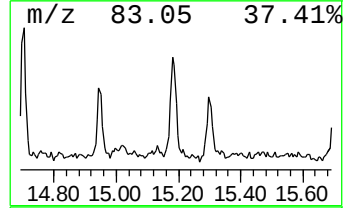
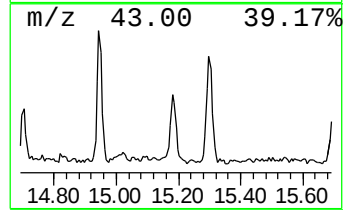
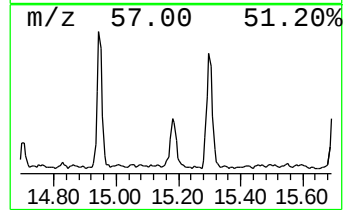
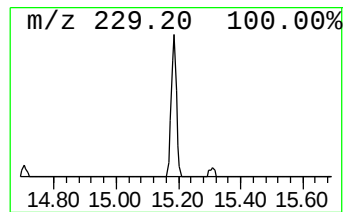
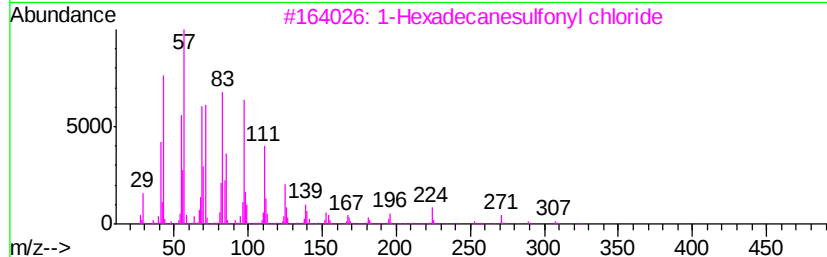
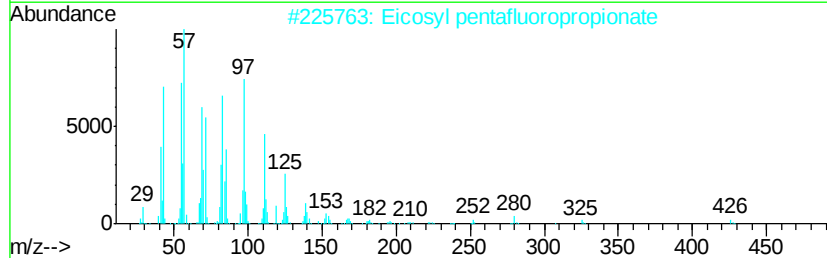
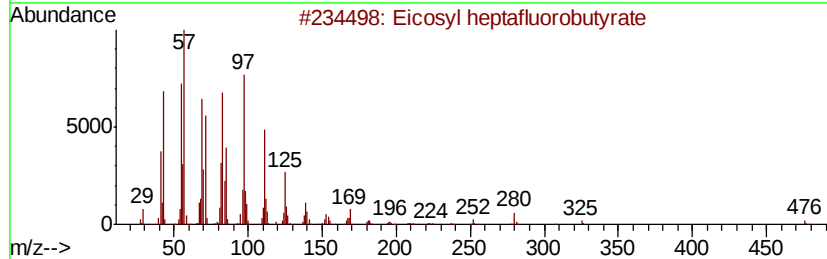
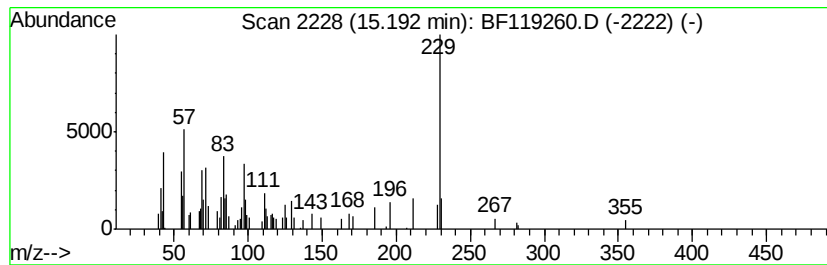
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown15.19 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	2.60 ng	111580	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosyl heptafluorobutyrte	494	C24H41F7O2	1000351-83-5	46
2		Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	46
3		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	46
4		Tetracosyl heptafluorobutyrte	550	C28H49F7O2	1000351-83-7	46
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030620\
Data File : BF119260.D
Acq On : 6 Mar 2020 20:11
Operator : CG/JU
Sample : L1803-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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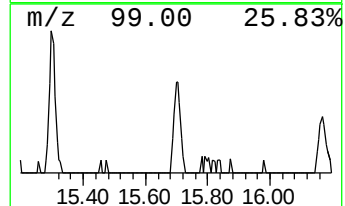
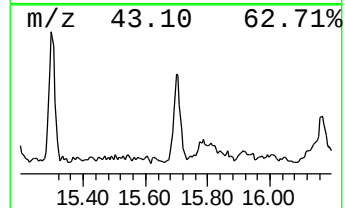
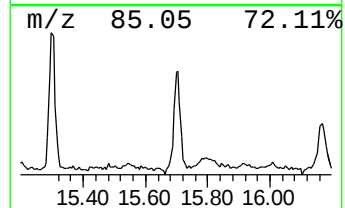
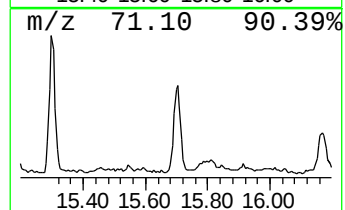
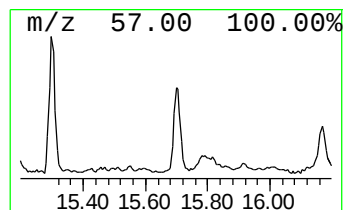
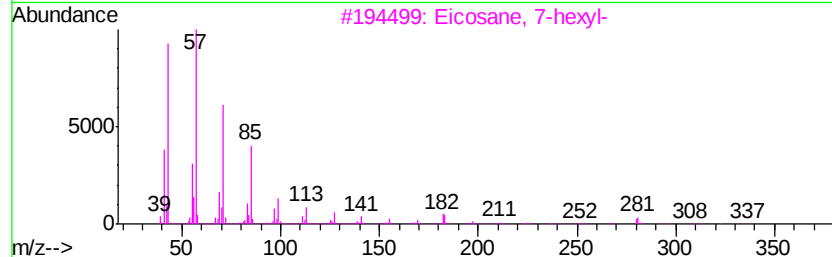
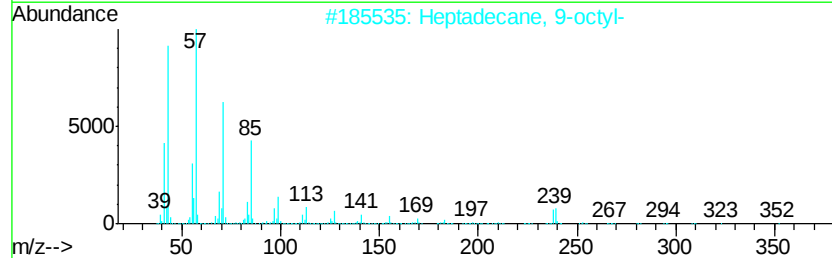
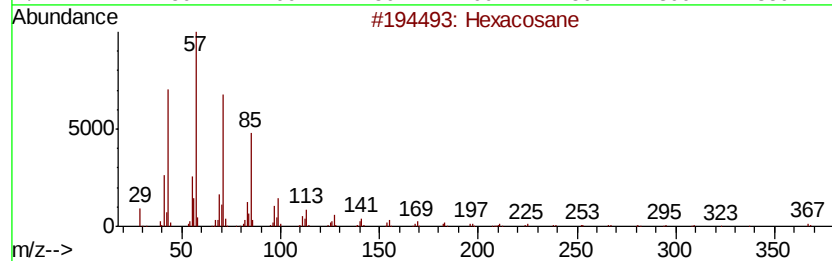
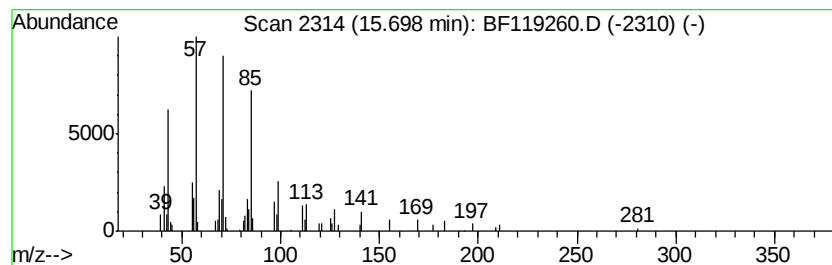
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	2.08 ng	89255	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
4		Hentriacontane	437	C31H64	000630-04-6	90
5		Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030620\
Data File : BF119260.D
Acq On : 6 Mar 2020 20:11
Operator : CG/JU
Sample : L1803-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.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	11.77	12.9	ng	622440	4	11.24	961338	20.0
Isopropyl palmitate	12.02	2.1	ng	99719	4	11.24	961338	20.0
9,17-Octadecadien...	12.47	3.1	ng	149582	4	11.24	961338	20.0
Octadecanoic acid	12.56	4.4	ng	210595	4	11.24	961338	20.0
Heptadecyl heptaf...	13.72	10.8	ng	457291	5	13.88	844569	20.0
2-Bromo dodecane	14.34	2.5	ng	104502	5	13.88	844569	20.0
triacontane	14.63	2.7	ng	116684	6	15.30	859156	20.0
Squalene	14.70	25.4	ng	1090790	6	15.30	859156	20.0
unknown15.19	15.19	2.6	ng	111580	6	15.30	859156	20.0
Hexacosane	15.70	2.1	ng	89255	6	15.30	859156	20.0