

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031920\
 Data File : BF119462.D
 Acq On : 20 Mar 2020 2:44
 Operator : CG/JU
 Sample : L1965-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 80564952

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-BF031820.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	2.140	5	9	16	rVB	307264	435861	5.89%	0.667%
2	5.075	500	508	515	rBV	101309	125473	1.70%	0.192%
3	5.463	569	574	577	rBV	7331826	7402360	100.00%	11.322%
4	6.475	740	746	748	rBV	6191470	7151926	96.62%	10.939%
5	6.669	776	779	786	rBV	149896	137222	1.85%	0.210%
6	6.851	806	810	813	rBV	2654944	2154199	29.10%	3.295%
7	7.010	832	837	840	rVB	6214255	5823608	78.67%	8.907%
8	7.410	900	905	908	rBV	4473791	4660193	62.96%	7.128%
9	8.133	1023	1028	1032	rBV	3007116	2697586	36.44%	4.126%
10	9.216	1206	1212	1215	rBV	7806532	7363970	99.48%	11.263%
11	9.604	1274	1278	1282	rBV	742842	602567	8.14%	0.922%
12	9.892	1321	1327	1331	rBV	2985190	2631894	35.55%	4.025%
13	10.680	1456	1461	1464	rBV	4002171	3609539	48.76%	5.521%
14	10.804	1479	1482	1491	rVB3	85460	131643	1.78%	0.201%
15	11.380	1576	1580	1583	rBV	2715304	2262241	30.56%	3.460%
16	11.839	1654	1658	1661	rBV	364533	426653	5.76%	0.653%
17	11.868	1661	1663	1667	rVV2	171473	207921	2.81%	0.318%
18	11.910	1667	1670	1677	rVV	998759	909468	12.29%	1.391%
19	12.086	1697	1700	1703	rBV2	80294	77160	1.04%	0.118%
20	12.592	1783	1786	1789	rBV	321685	298304	4.03%	0.456%
21	12.698	1800	1804	1811	rBV2	471125	510563	6.90%	0.781%
22	12.821	1822	1825	1828	rVB	299166	251659	3.40%	0.385%
23	12.974	1846	1851	1854	rBV	6277575	5802451	78.39%	8.875%
24	13.210	1889	1891	1894	rVB3	69601	76407	1.03%	0.117%
25	13.868	2000	2003	2011	rBV	852426	890287	12.03%	1.362%
26	14.021	2025	2029	2032	rBV	2233583	2306511	31.16%	3.528%
27	14.045	2032	2033	2038	rVB	167833	122014	1.65%	0.187%
28	14.198	2056	2059	2062	rBV	173295	155266	2.10%	0.237%
29	14.504	2108	2111	2115	rBV	559388	572948	7.74%	0.876%
30	14.815	2161	2164	2173	rVB	266314	345451	4.67%	0.528%
31	14.956	2186	2188	2193	rVB4	182656	190024	2.57%	0.291%
32	15.156	2218	2222	2230	rBV	794565	1120833	15.14%	1.714%
33	15.498	2275	2280	2283	rBV	1386043	1633127	22.06%	2.498%
34	15.745	2320	2322	2327	rVB	215911	250751	3.39%	0.384%

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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	15.986	2359	2363	2368	rBV	530534	805489	10.88%	1.232%
36	16.033	2368	2371	2381	rVB3	263049	498001	6.73%	0.762%
37	17.809	2668	2673	2686	rVB3	306779	739912	10.00%	1.132%

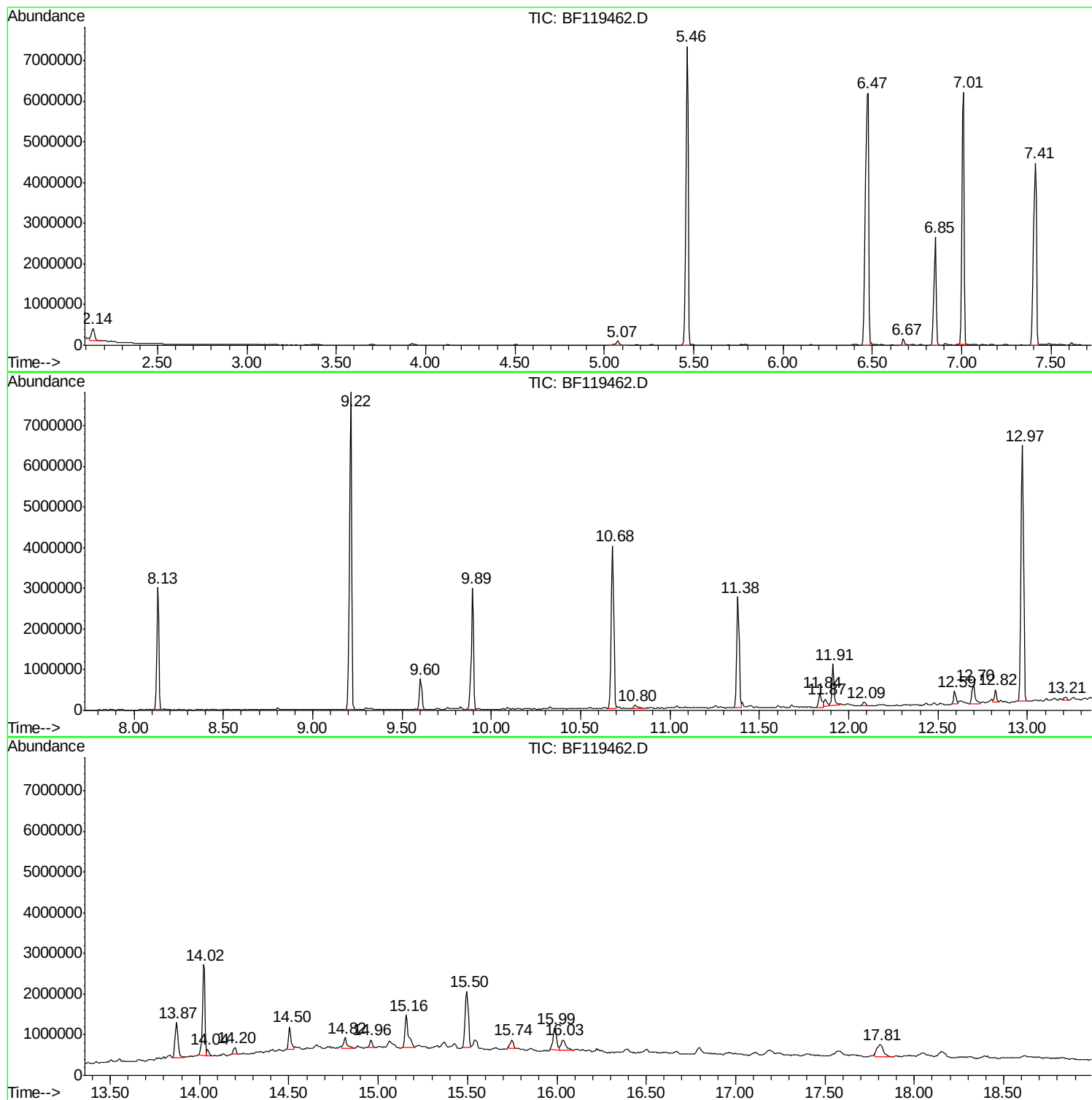
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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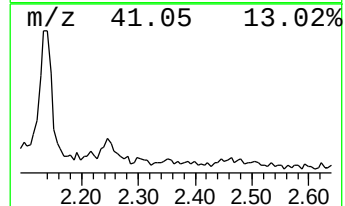
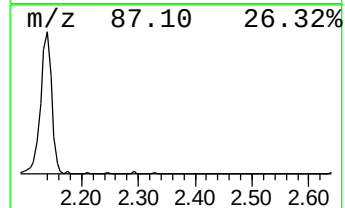
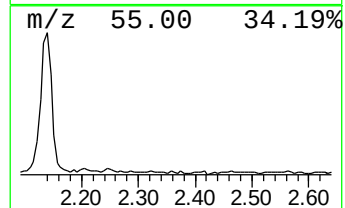
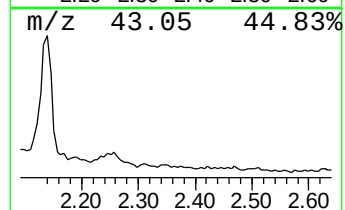
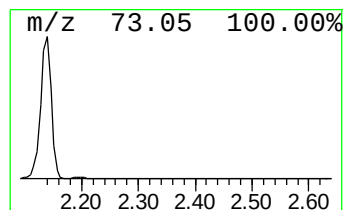
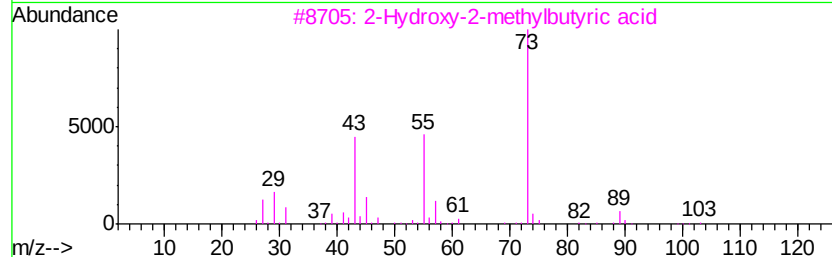
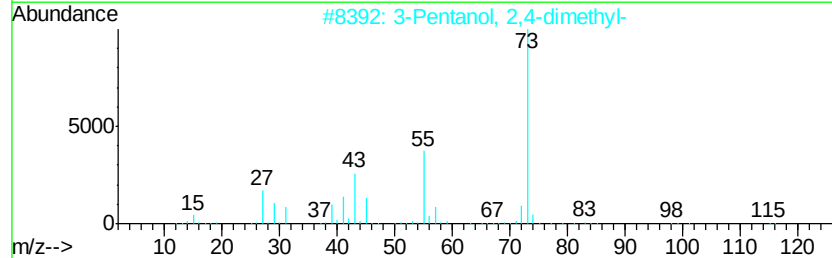
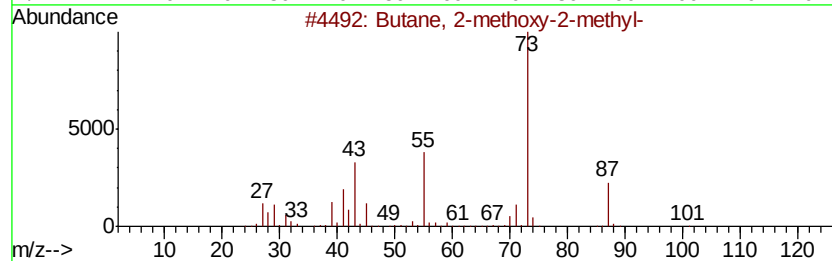
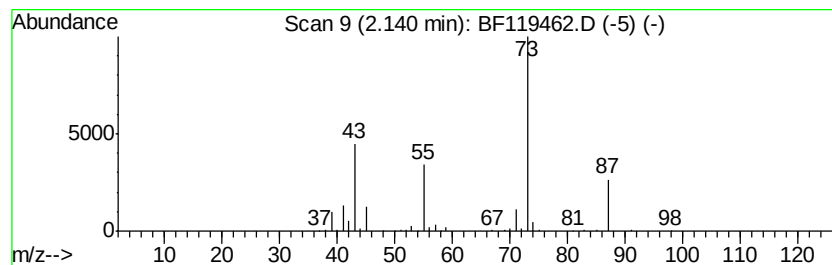
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.14	4.05 ng	435861	1,4-Dichlorobenzene-d4	6.85	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	28
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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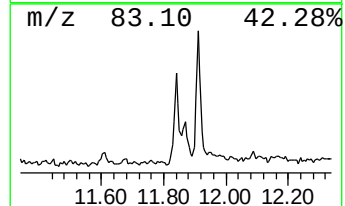
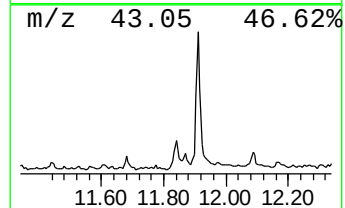
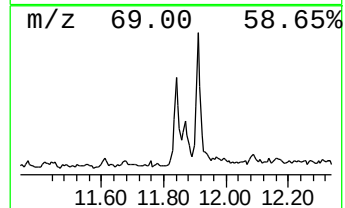
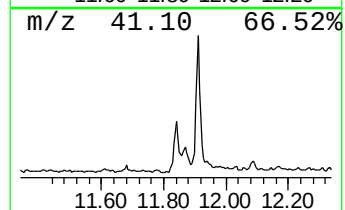
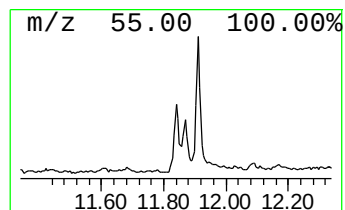
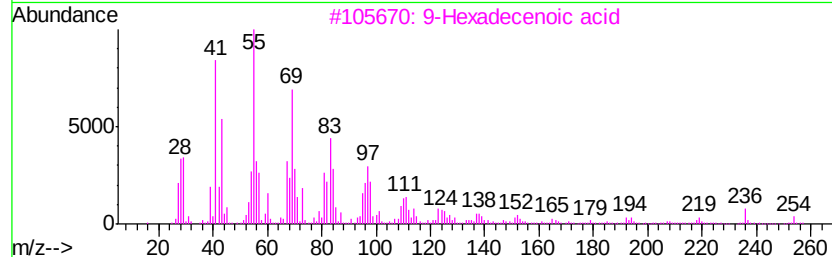
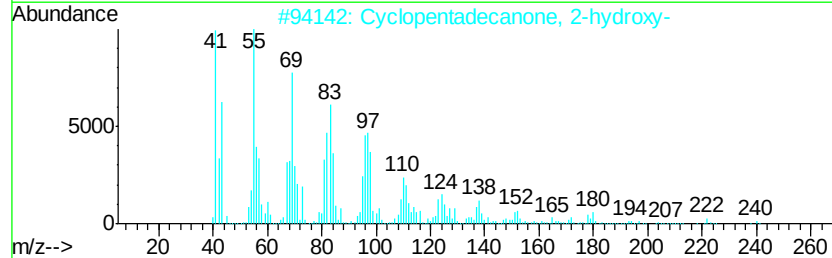
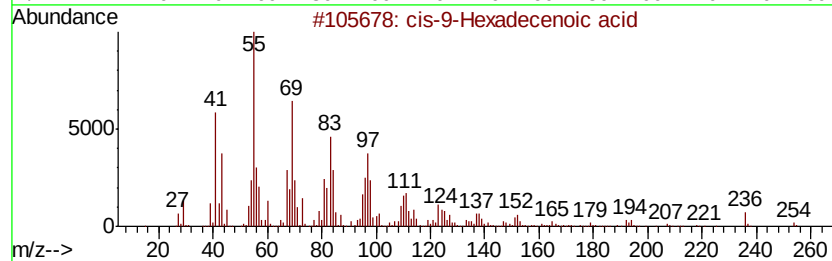
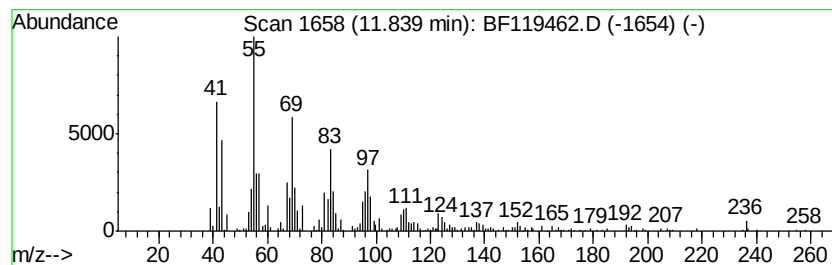
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 cis-9-Hexadecenoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.84	3.77 ng	426653	Phenanthrene-d10	11.38	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	91
2	Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	91
3	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	90
4	13-Borabicyclo[7.3.0]tridecane, ...	236	C15H29BO	1000156-41-7	87
5	cis-5-Dodecenoic acid	198	C12H22O2	002430-94-6	78



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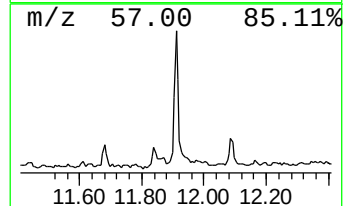
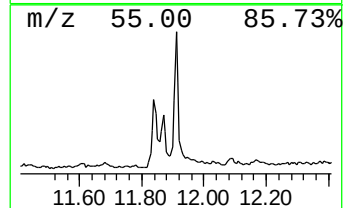
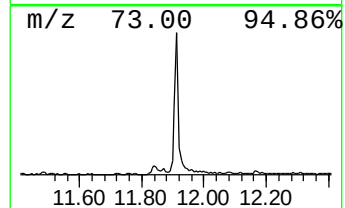
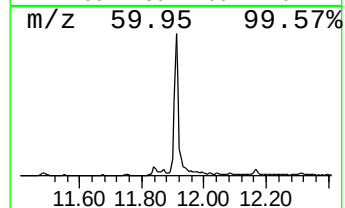
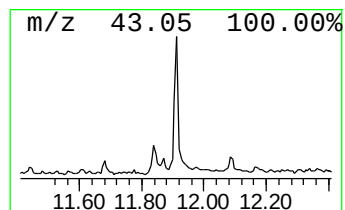
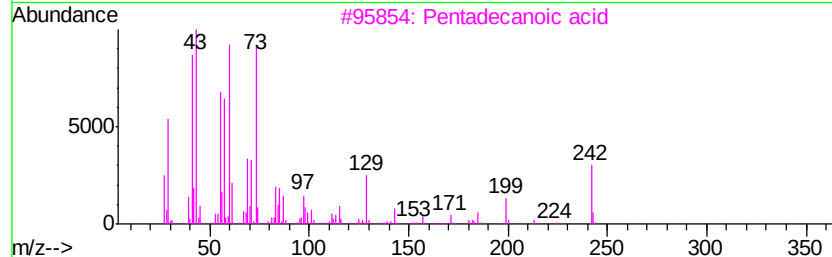
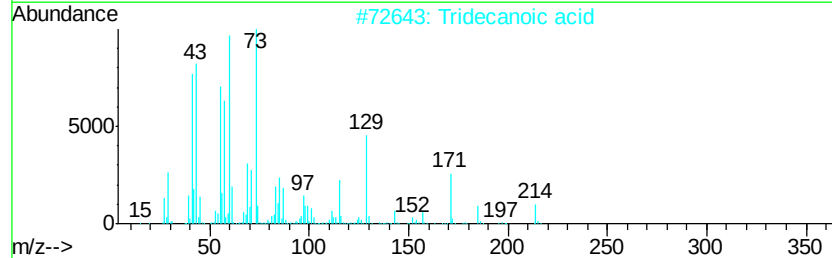
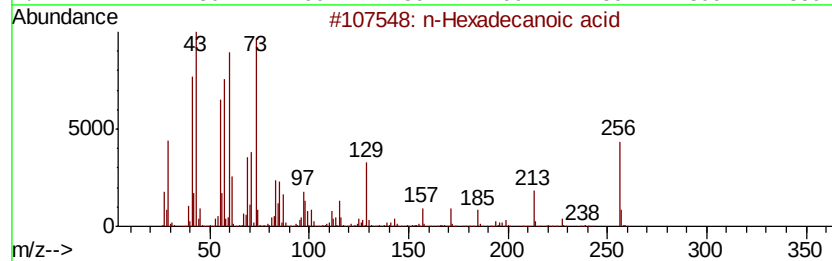
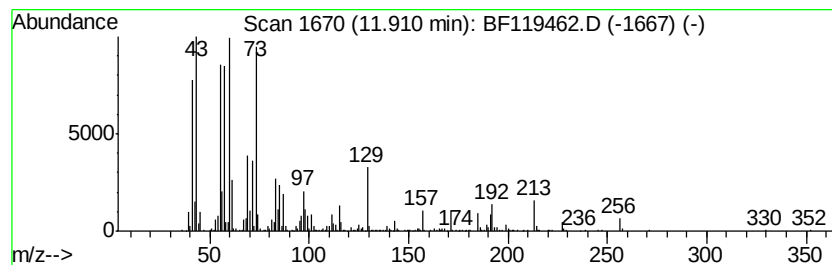
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	8.04 ng	909468	Phenanthrene-d10	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		Octadecanoic acid	284	C18H36O2	000057-11-4	81
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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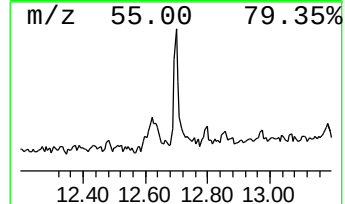
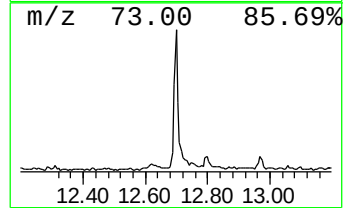
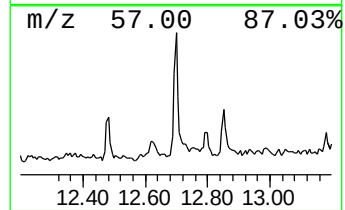
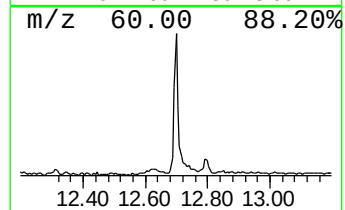
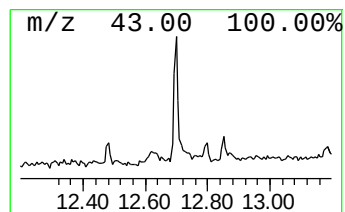
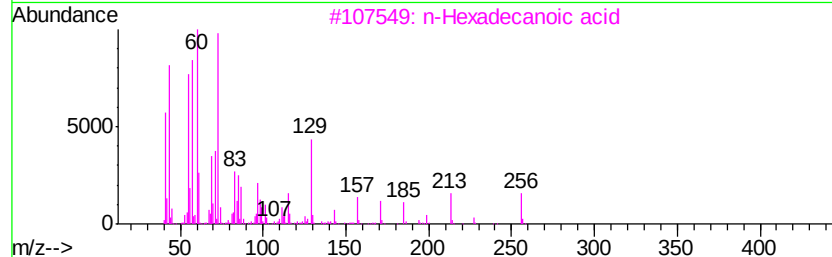
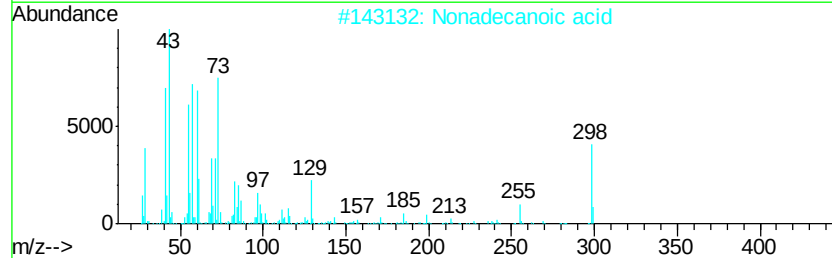
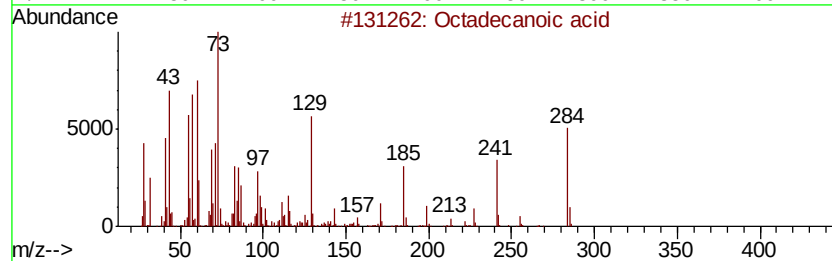
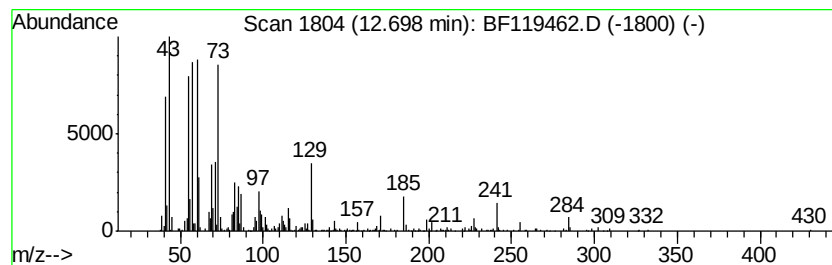
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	4.51 ng	510563	Phenanthrene-d10	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		Nonadecanoic acid	298	C19H38O2	000646-30-0	93
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	83



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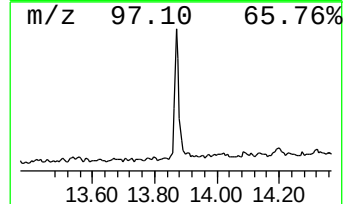
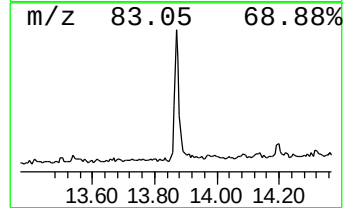
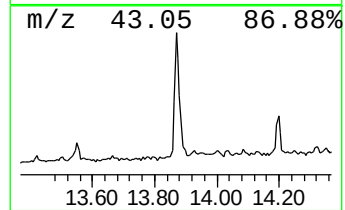
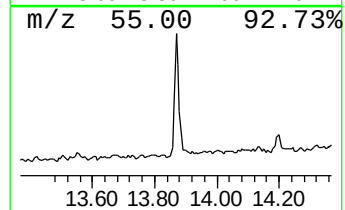
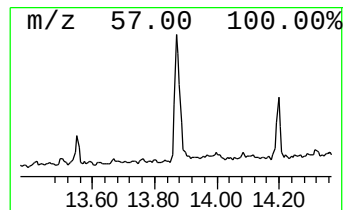
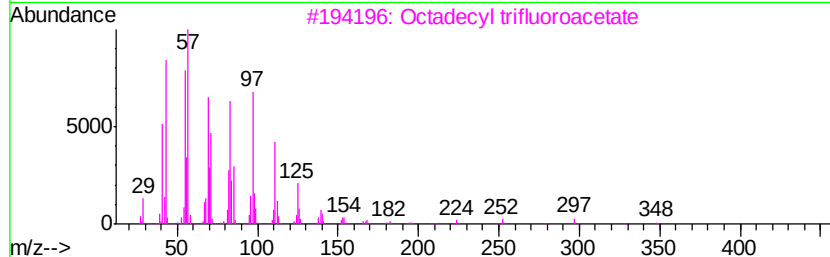
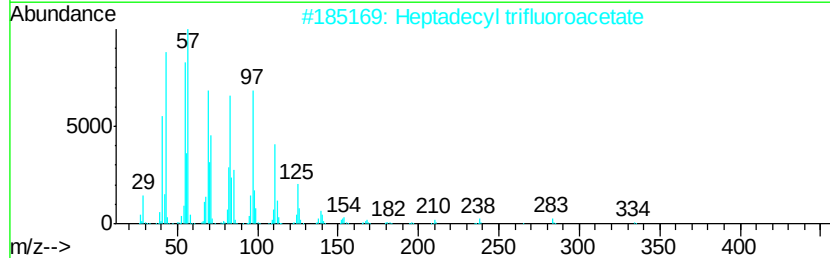
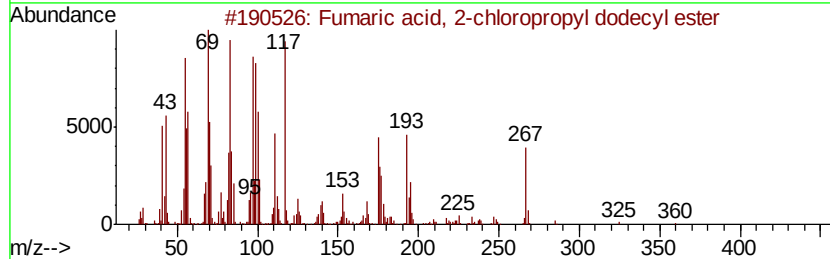
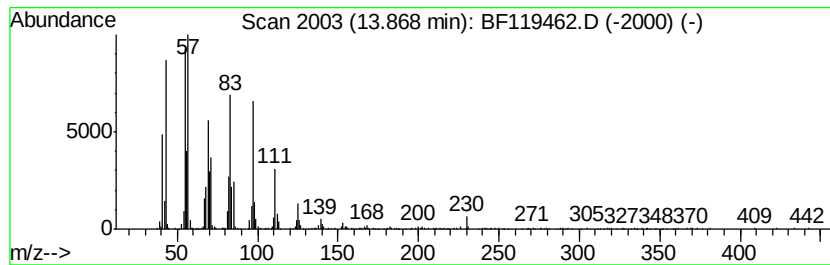
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Peak Number 6 Fumaric acid, 2-chloropropyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.87	7.72 ng	890287	Chrysene-d12	14.02		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Fumaric acid, 2-chloropropyl dod...	360	C19H33ClO4	1000348-57-0	96
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
4		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
5		1-Docosene	308	C22H44	001599-67-3	94



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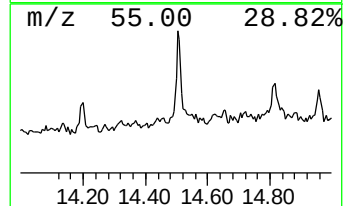
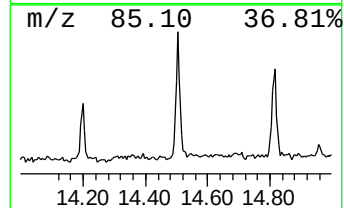
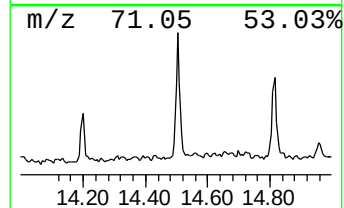
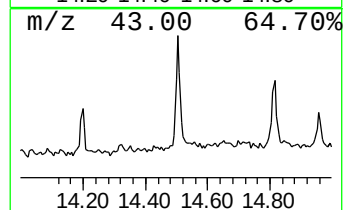
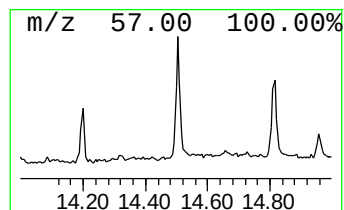
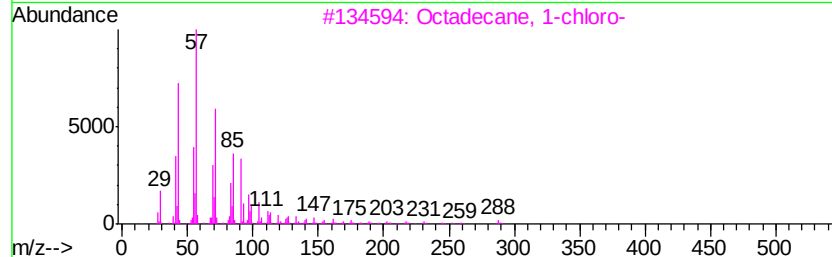
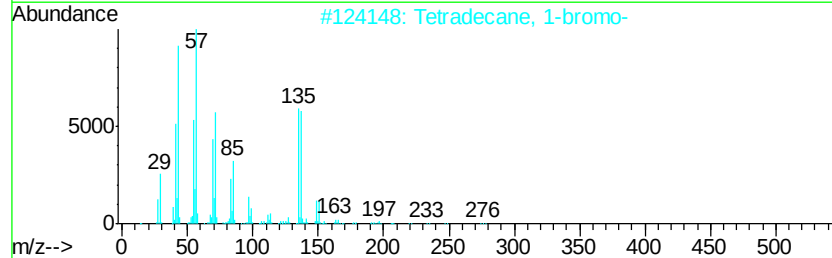
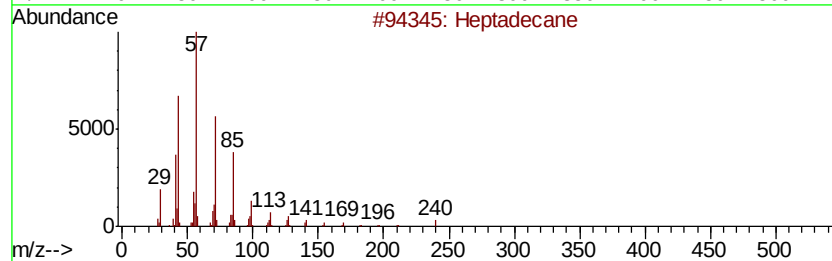
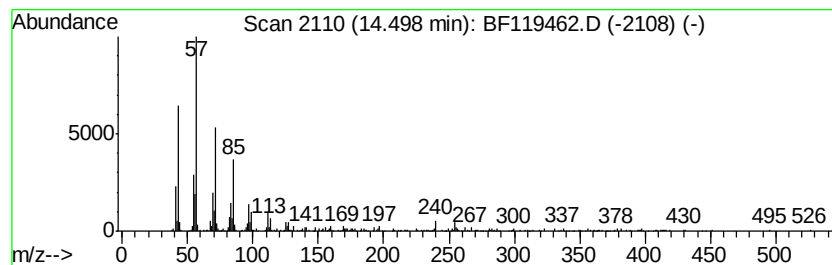
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.50	4.97 ng	572948	Chrysene-d12	14.02		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	95
2	Tetradecane, 1-bromo-		276	C14H29Br	000112-71-0	91
3	Octadecane, 1-chloro-		288	C18H37Cl	003386-33-2	91
4	Sulfurous acid, butyl heptadecyl...		376	C21H44O3S	1000309-18-4	91
5	Octacosane		394	C28H58	000630-02-4	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
Data File : BF119462.D
Acq On : 20 Mar 2020 2:44
Operator : CG/JU
Sample : L1965-01
Misc :
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Instrument :
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ClientSampleId :
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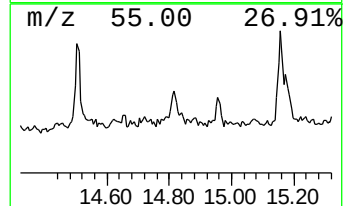
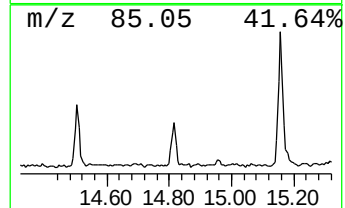
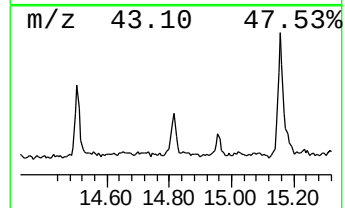
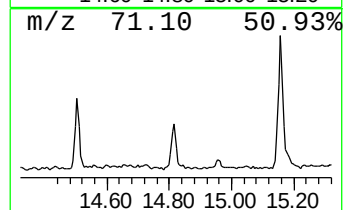
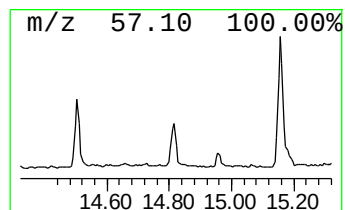
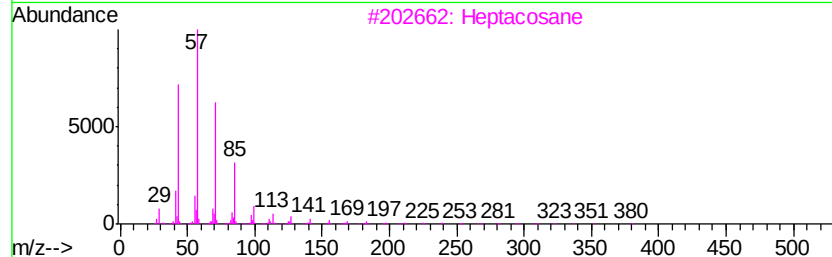
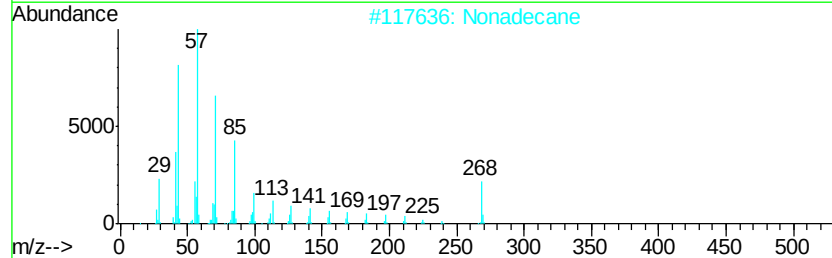
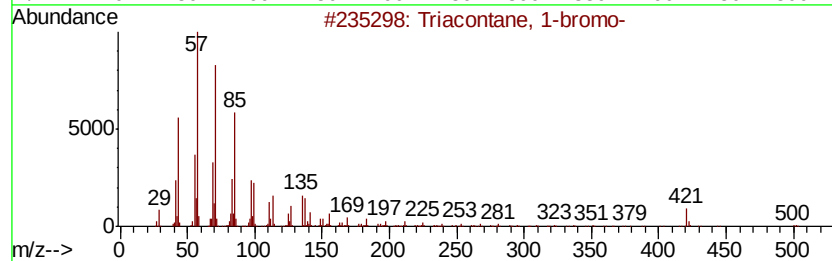
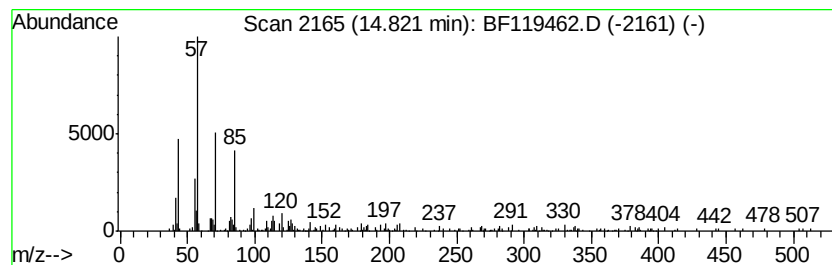
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triacontane, 1-bromo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	4.23 ng	345451	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane, 1-bromo-	500	C30H61Br	004209-22-7	86
2		Nonadecane	268	C19H40	000629-92-5	83
3		Heptacosane	380	C27H56	000593-49-7	83
4		Tridecane, 2-methyl-	198	C14H30	001560-96-9	80
5		Hexacosane	366	C26H54	000630-01-3	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
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Acq On : 20 Mar 2020 2:44
Operator : CG/JU
Sample : L1965-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

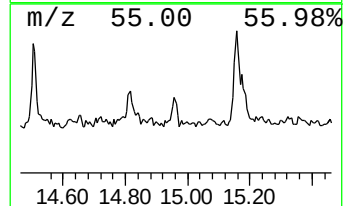
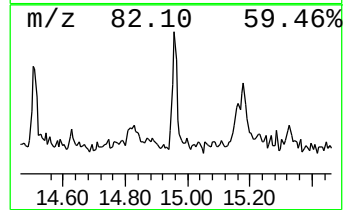
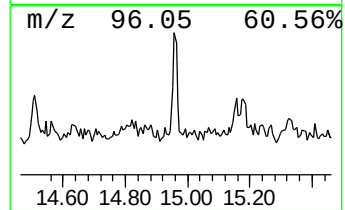
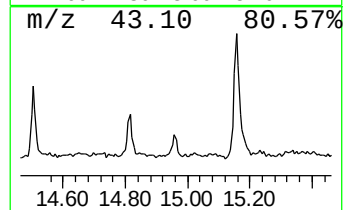
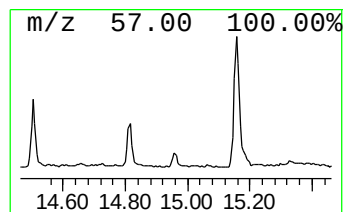
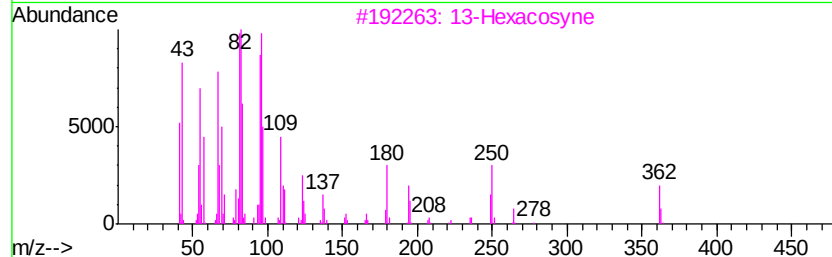
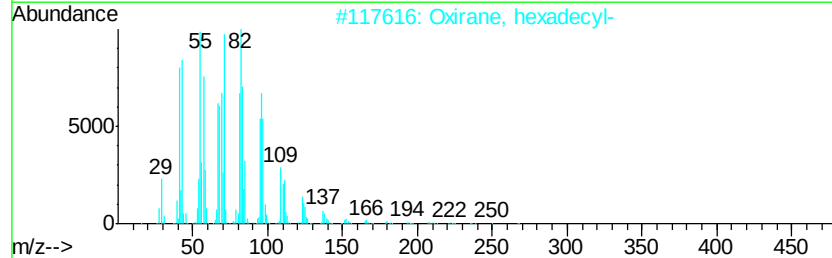
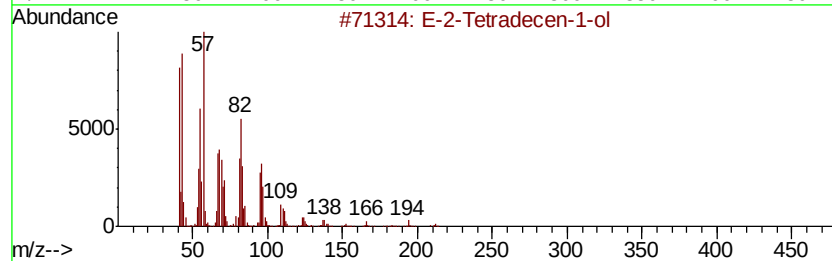
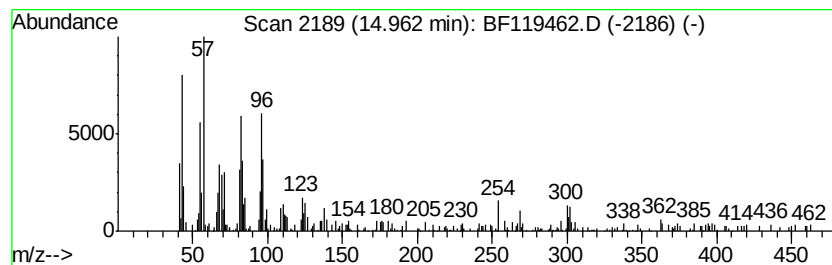
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 E-2-Tetradecen-1-ol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.33 ng	190024	Perylene-d12	15.50
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	E-2-Tetradecen-1-ol	212 C14H28O	1000130-83-7	86
2	Oxirane, hexadecyl-	268 C18H36O	007390-81-0	86
3	13-Hexacosyne	362 C26H50	034291-68-4	78
4	E-5-Octadecen-1-ol acetate	310 C20H38O2	1000130-94-6	58
5	1,19-Eicosadiene	278 C20H38	014811-95-1	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
 Data File : BF119462.D
 Acq On : 20 Mar 2020 2:44
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 Sample : L1965-01
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Instrument :
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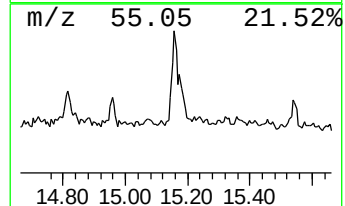
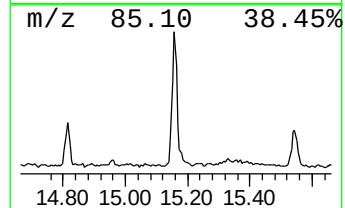
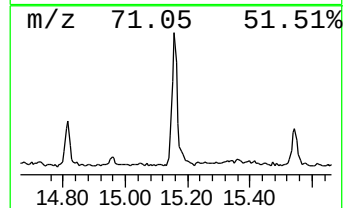
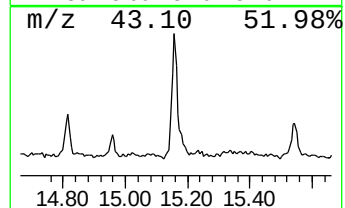
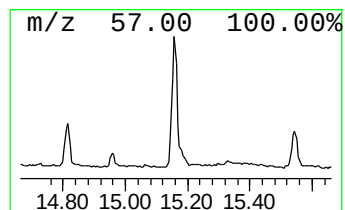
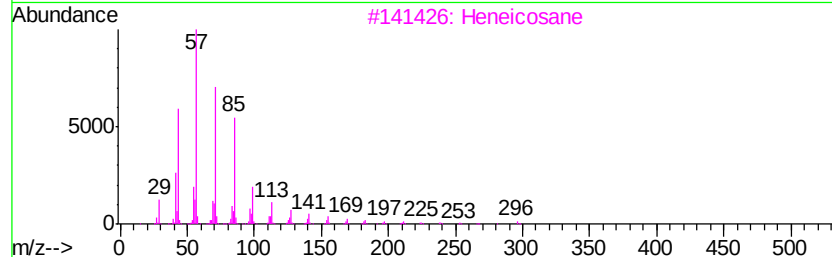
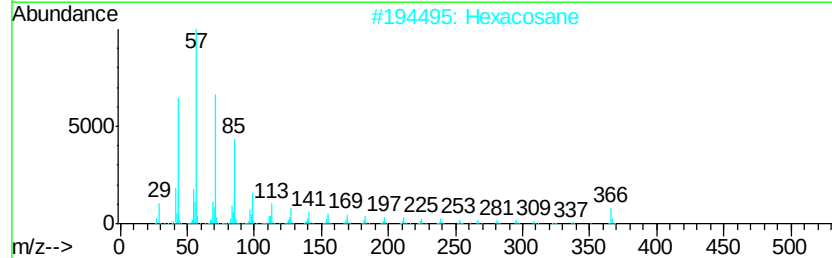
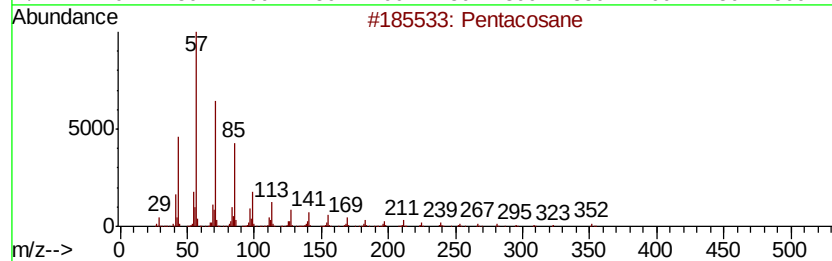
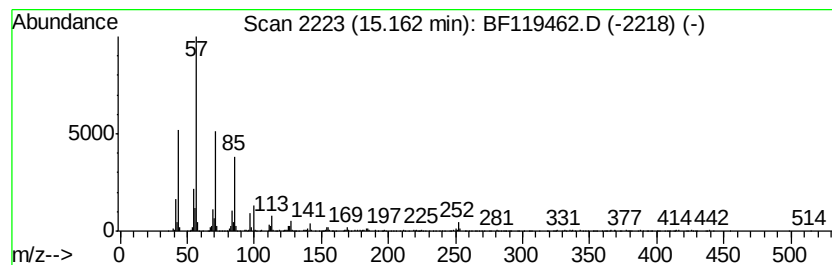
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 10 Pentacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	13.73 ng	1120830	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	93
2		Hexacosane	366	C26H54	000630-01-3	93
3		Heneicosane	296	C21H44	000629-94-7	87
4		Octadecane	254	C18H38	000593-45-3	87
5		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
Data File : BF119462.D
Acq On : 20 Mar 2020 2:44
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Sample : L1965-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

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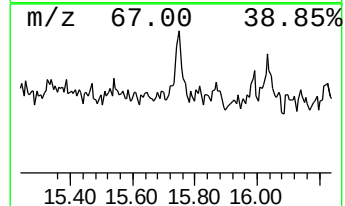
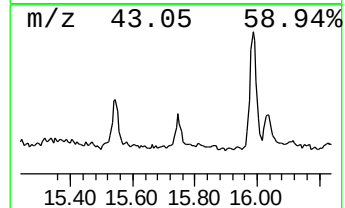
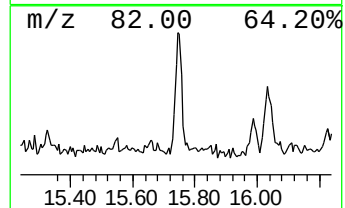
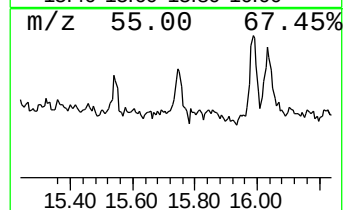
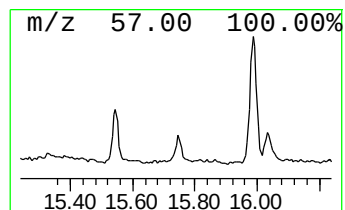
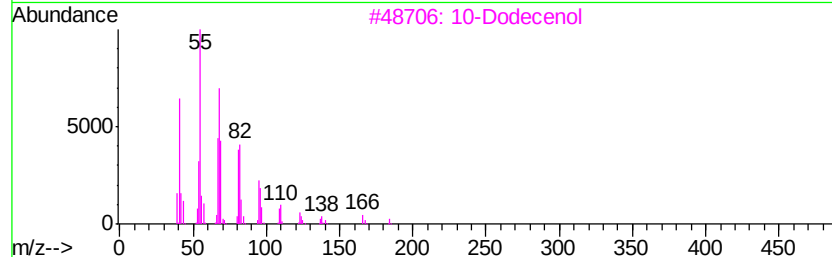
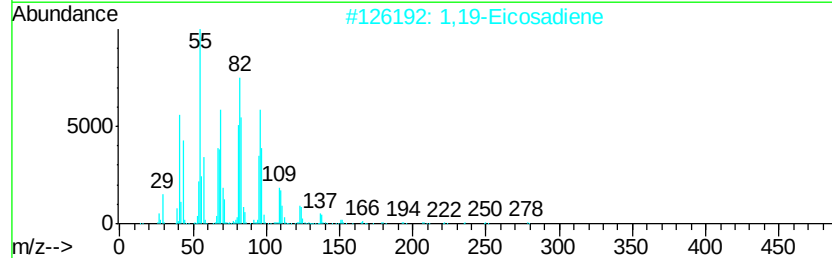
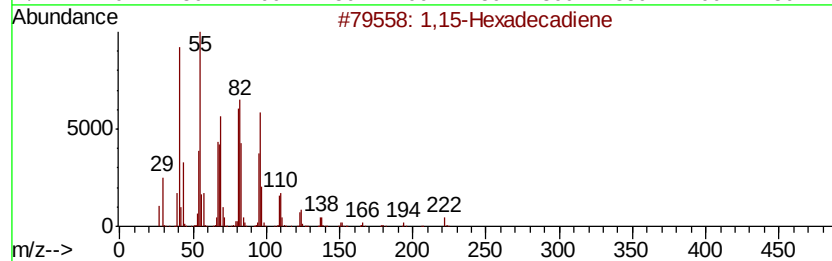
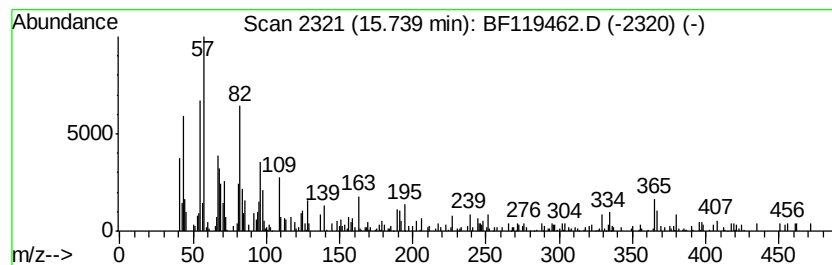
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1,15-Hexadecadiene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	3.07 ng	250751	Perylene-d12	15.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,15-Hexadecadiene	222	C16H30	021964-51-2	78
2			1,19-Eicosadiene	278	C20H38	014811-95-1	72
3			10-Dodecenol	184	C12H24O	035237-63-9	64
4			Cyclododecanol	184	C12H24O	001724-39-6	59
5			Z-14-Octadecen-1-ol acetate	310	C20H38O2	1000131-07-6	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
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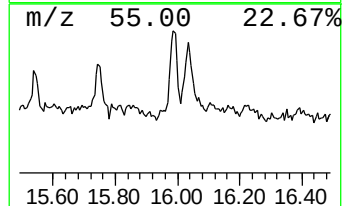
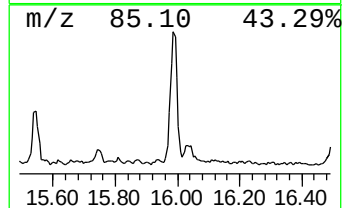
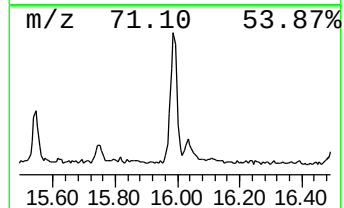
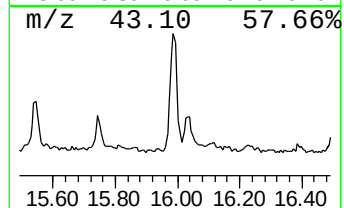
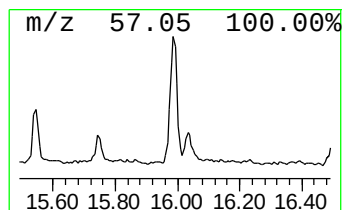
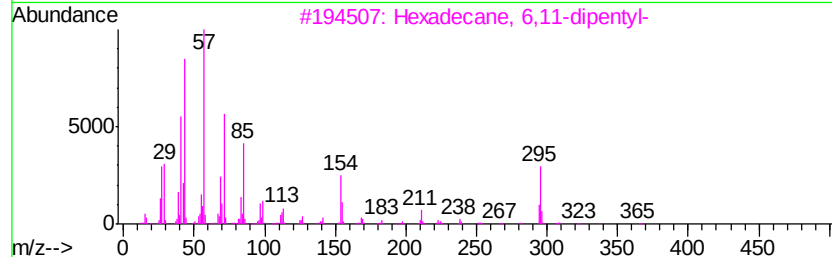
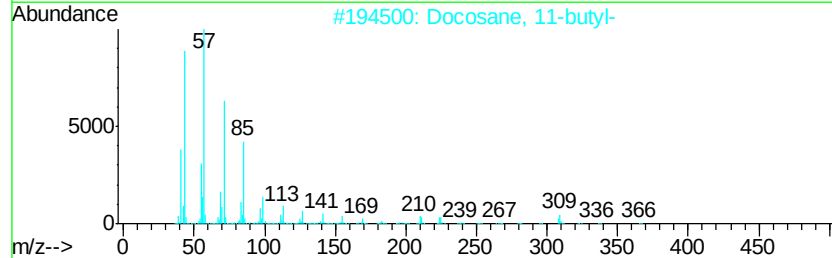
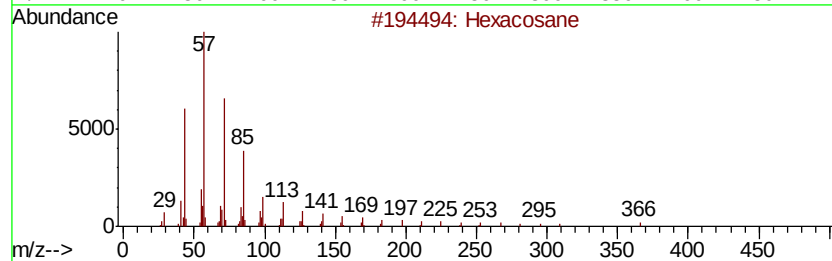
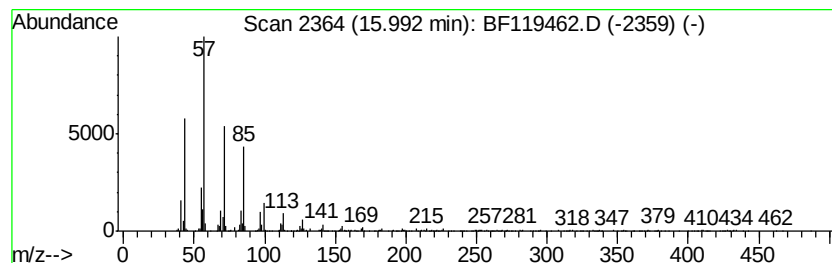
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	9.86 ng	805489	Perylene-d12	15.50
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexacosane	366 C26H54	000630-01-3	93
2	Docosane, 11-butyl-	366 C26H54	013475-76-8	87
3	Hexadecane, 6,11-dipentyl-	366 C26H54	015874-03-0	87
4	Heptacosane	380 C27H56	000593-49-7	87
5	2-methyloctacosane	408 C29H60	1000376-72-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
Data File : BF119462.D
Acq On : 20 Mar 2020 2:44
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Sample : L1965-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

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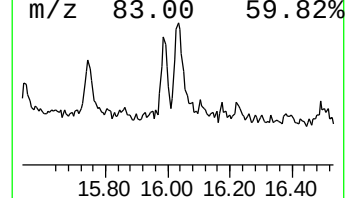
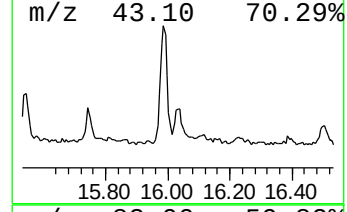
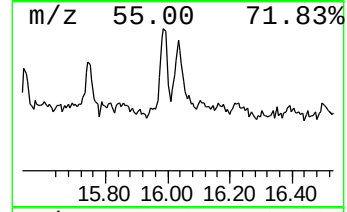
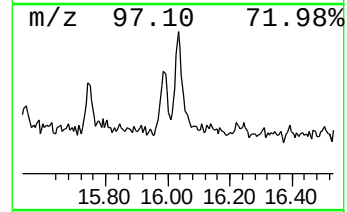
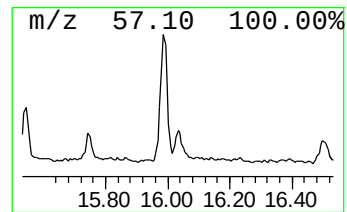
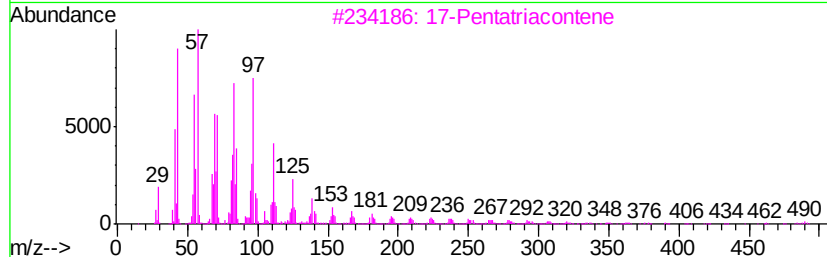
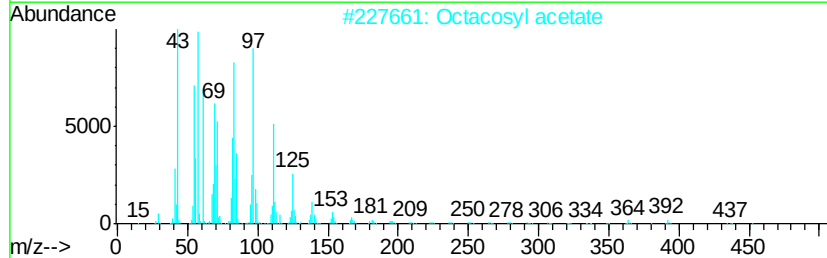
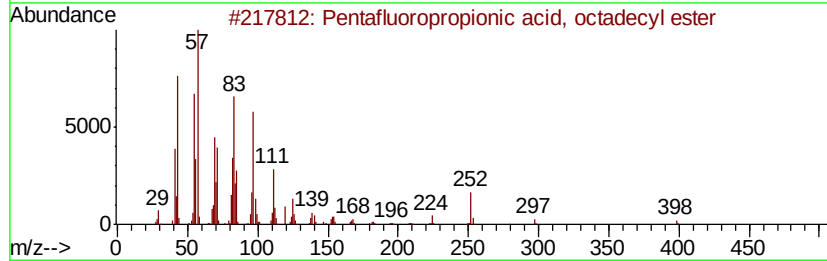
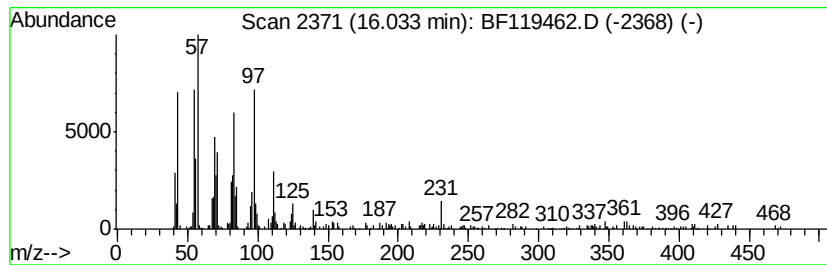
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	6.10 ng	498001	Perylene-d12	15.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
2			Octacosyl acetate	452	C30H60O2	018206-97-8	91
3			17-Pentatriacontene	491	C35H70	006971-40-0	91
4			Cyclotriacontane	420	C30H60	000297-35-8	90
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
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Instrument :
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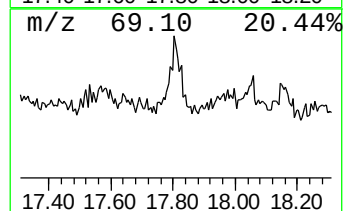
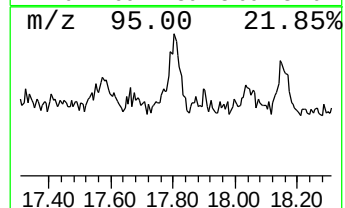
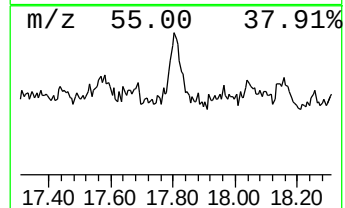
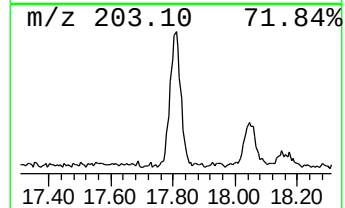
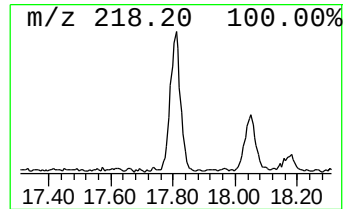
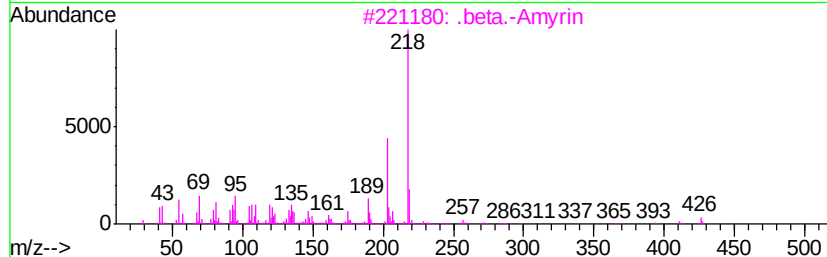
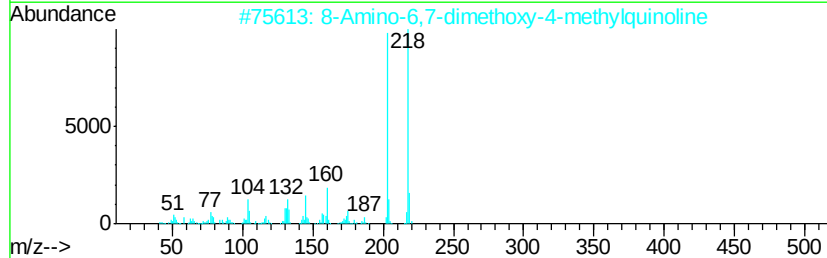
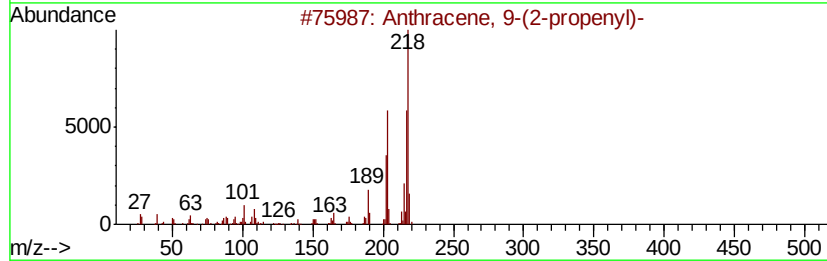
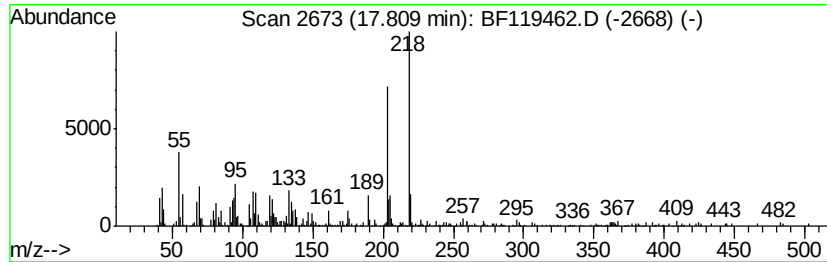
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Anthracene, 9-(2-propenyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.81	9.06 ng	739912	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	68
2		8-Amino-6,7-dimethoxy-4-methylqu...	218	C12H14N2O2	1000213-07-2	64
3		.beta.-Amyrin	426	C30H50O	000559-70-6	64
4		3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	64
5		Olean-12-ene	410	C30H50	000471-68-1	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031920\
 Data File : BF119462.D
 Acq On : 20 Mar 2020 2:44
 Operator : CG/JU
 Sample : L1965-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 80564952

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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
Butane, 2-methoxy...	2.14	4.0	ng	435861	1	6.85	2154200	20.0
cis-9-Hexadecenoic...	11.84	3.8	ng	426653	4	11.38	2262240	20.0
n-Hexadecanoic acid	11.91	8.0	ng	909468	4	11.38	2262240	20.0
Octadecanoic acid	12.70	4.5	ng	510563	4	11.38	2262240	20.0
Fumaric acid, 2-c...	13.87	7.7	ng	890287	5	14.02	2306510	20.0
Heptadecane	14.50	5.0	ng	572948	5	14.02	2306510	20.0
Triacotane, 1-br...	14.82	4.2	ng	345451	6	15.50	1633130	20.0
E-2-Tetradecen-1-ol	14.96	2.3	ng	190024	6	15.50	1633130	20.0
Pentacosane	15.16	13.7	ng	1120830	6	15.50	1633130	20.0
1,15-Hexadecadiene	15.74	3.1	ng	250751	6	15.50	1633130	20.0
Hexacosane	15.99	9.9	ng	805489	6	15.50	1633130	20.0
Pentafluoropropio...	16.03	6.1	ng	498001	6	15.50	1633130	20.0
Anthracene, 9-(2-...	17.81	9.1	ng	739912	6	15.50	1633130	20.0