

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040120\
 Data File : BF119700.D
 Acq On : 2 Apr 2020 6:40
 Operator : MA/SJ
 Sample : L2055-07
 Misc :
 ALS Vial : 50 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-9-(1-3)

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-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	2.169	10	14	22	rVB	88586	128776	2.66%	0.295%
2	5.022	493	499	506	rVB	124216	160869	3.33%	0.369%
3	5.422	562	567	570	rBV	4672238	4590250	94.96%	10.527%
4	6.439	735	740	743	rBV	4279588	4540676	93.94%	10.414%
5	6.810	800	803	807	rBV	1659164	1364094	28.22%	3.128%
6	6.969	826	830	833	rBV	4344539	3644255	75.39%	8.358%
7	7.375	892	899	902	rBV	3221543	2961942	61.28%	6.793%
8	8.098	1018	1022	1025	rBV	2203040	1725230	35.69%	3.957%
9	9.175	1200	1205	1208	rBV	5857201	4833739	100.00%	11.086%
10	9.569	1268	1272	1275	rBV	449622	385650	7.98%	0.884%
11	9.851	1315	1320	1324	rBV	2082078	1845999	38.19%	4.234%
12	10.639	1450	1454	1458	rBV	3188140	2868672	59.35%	6.579%
13	11.339	1568	1573	1576	rBV	2139150	1761486	36.44%	4.040%
14	11.363	1576	1577	1581	rVV	162141	95411	1.97%	0.219%
15	11.410	1581	1585	1588	rVB3	48516	69108	1.43%	0.158%
16	11.869	1660	1663	1669	rBV	835369	761322	15.75%	1.746%
17	12.551	1775	1779	1782	rBV	351187	307115	6.35%	0.704%
18	12.651	1793	1796	1804	rBV2	173044	225758	4.67%	0.518%
19	12.780	1814	1818	1821	rBV	282052	233937	4.84%	0.537%
20	12.927	1839	1843	1846	rBV	4283013	3601963	74.52%	8.261%
21	13.163	1877	1883	1888	rBV3	177891	276446	5.72%	0.634%
22	13.216	1888	1892	1895	rBV2	45285	72950	1.51%	0.167%
23	13.504	1939	1941	1944	rBV	90741	78458	1.62%	0.180%
24	13.833	1993	1997	2004	rBV	936344	1258745	26.04%	2.887%
25	13.980	2017	2022	2025	rBV	1383371	1381225	28.57%	3.168%
26	14.004	2025	2026	2029	rVB	135756	77034	1.59%	0.177%
27	14.151	2049	2051	2057	rBV2	97455	128603	2.66%	0.295%
28	14.468	2100	2105	2111	rBV2	659350	1270942	26.29%	2.915%
29	14.910	2177	2180	2185	rVB2	184055	195425	4.04%	0.448%
30	15.015	2195	2198	2206	rVB	180744	331890	6.87%	0.761%
31	15.098	2209	2212	2215	rBV	365524	432878	8.96%	0.993%
32	15.133	2215	2218	2223	rBV2	310486	456718	9.45%	1.047%
33	15.439	2266	2270	2273	rBV	961880	1113000	23.03%	2.553%
34	15.674	2308	2310	2314	rVB2	114896	145583	3.01%	0.334%

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Instrument :
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ClientSampleId :
SB-9-(1-3)

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

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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.915	2348	2351	2355	rVB	215258	276864	5.73%	0.635%
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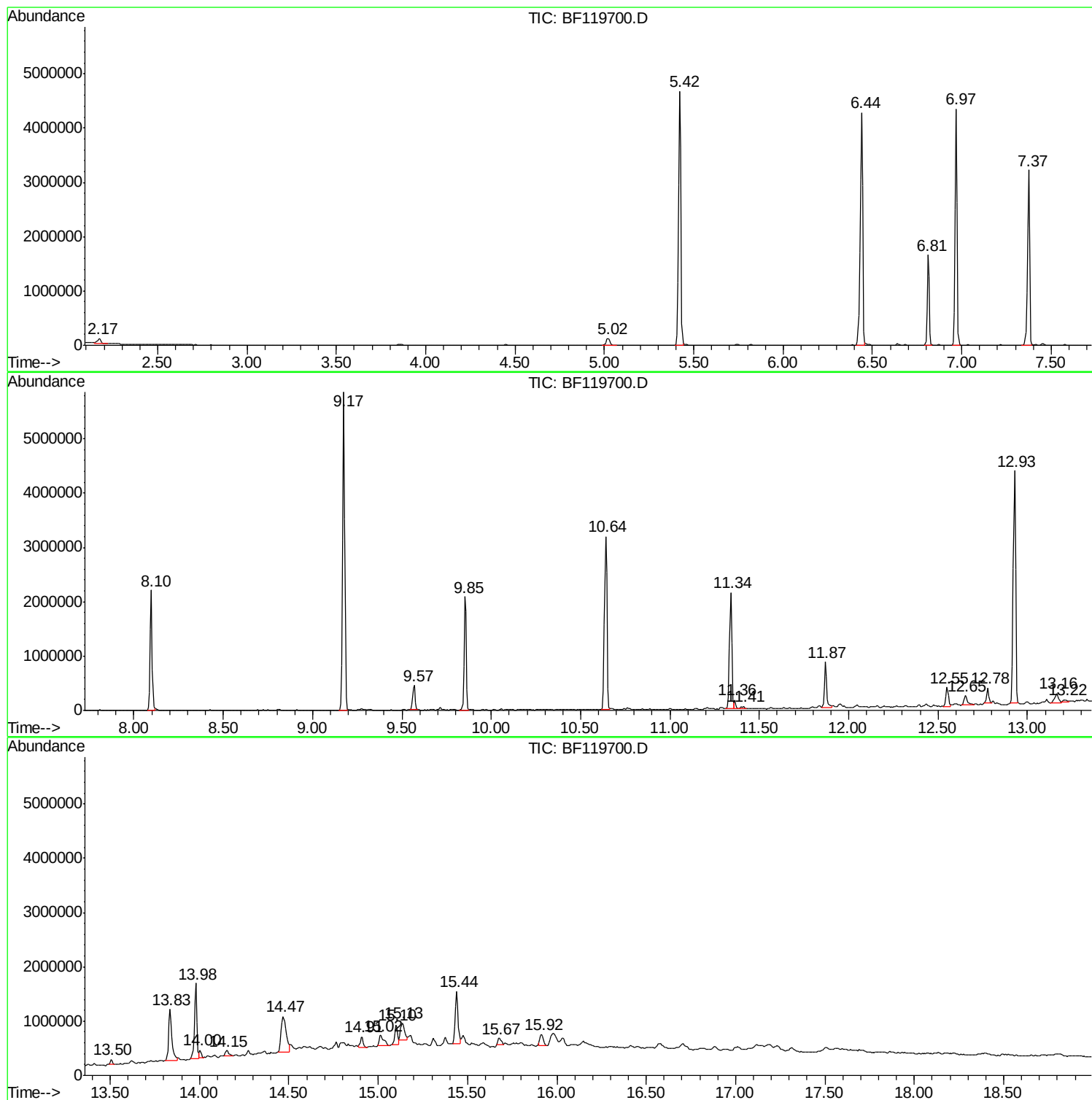
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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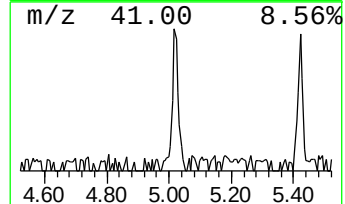
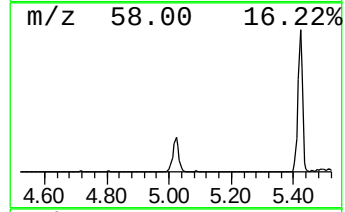
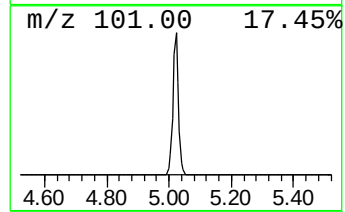
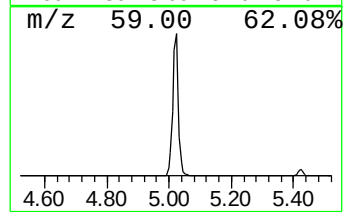
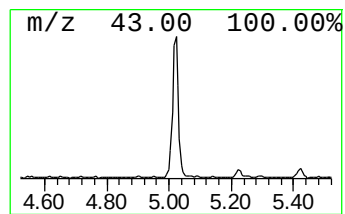
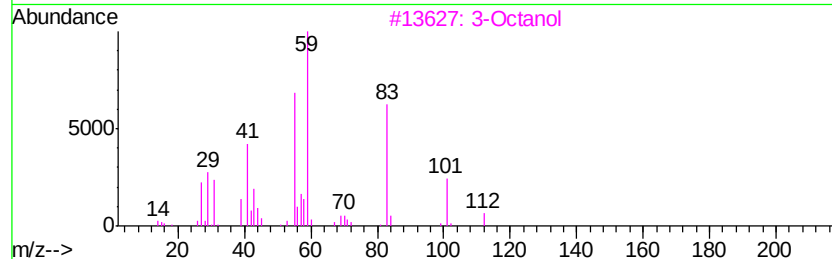
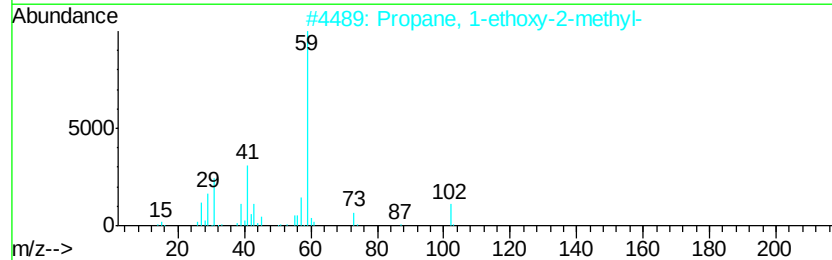
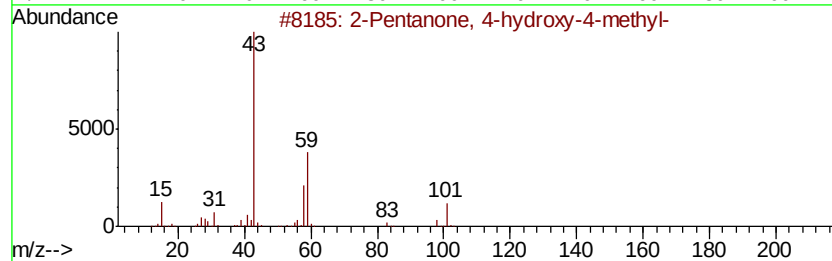
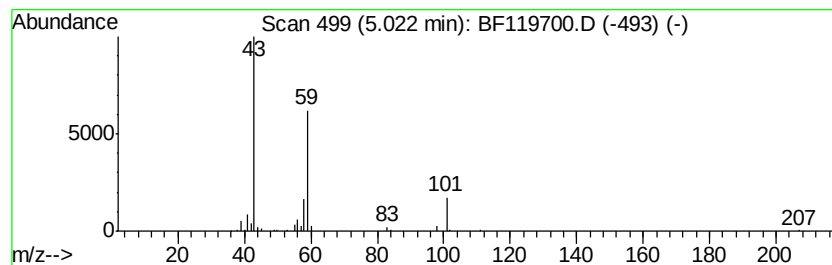
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	2.36 ng	160869	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	43
3			3-Octanol	130	C8H18O	000589-98-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32



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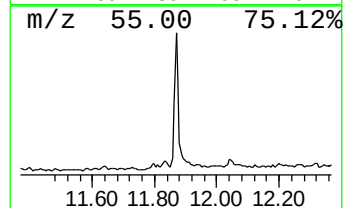
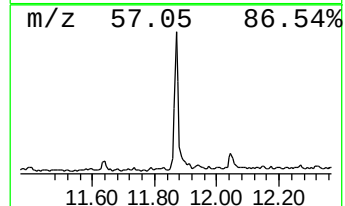
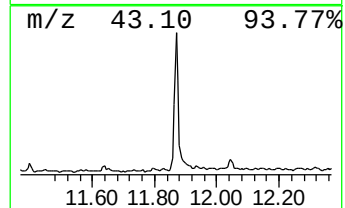
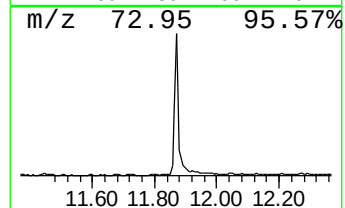
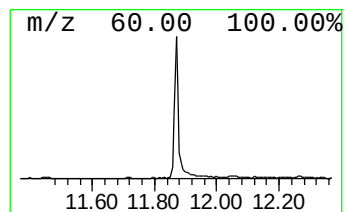
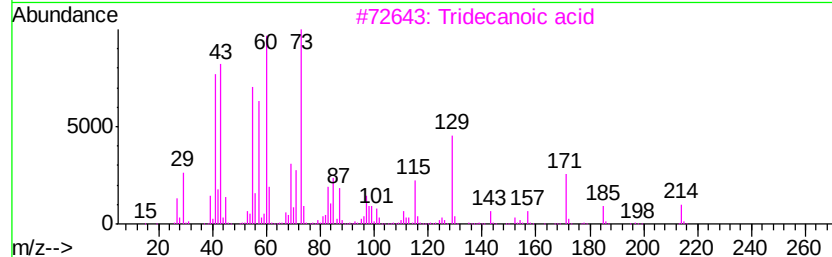
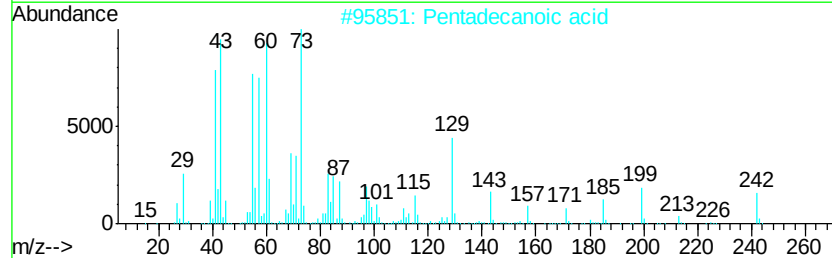
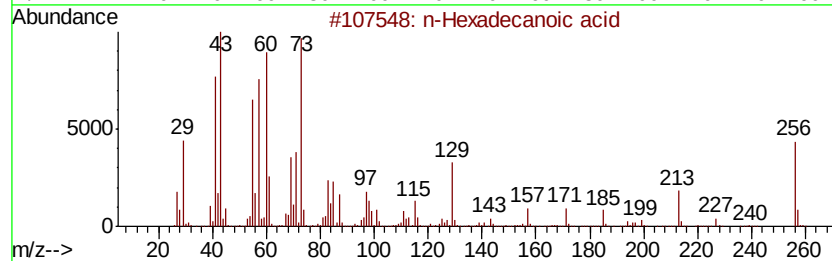
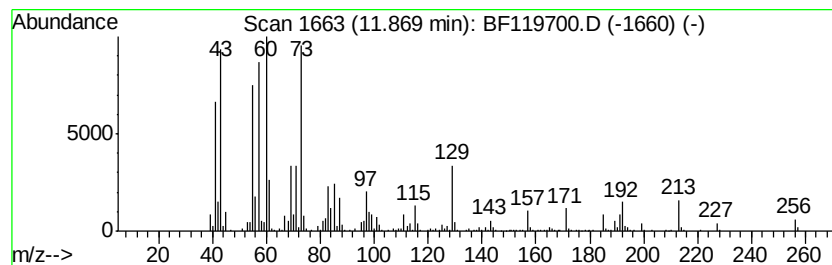
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF031820.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	8.64 ng	761322	Phenanthrene-d10	11.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Tridecanoic acid	214	C13H26O2	000638-53-9	70
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		n-Decanoic acid	172	C10H20O2	000334-48-5	47



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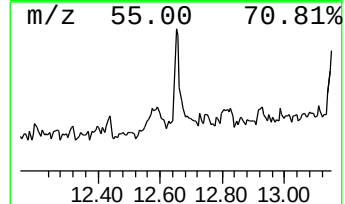
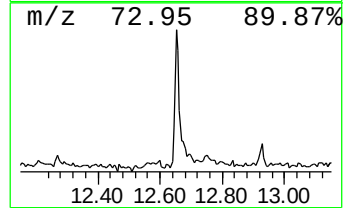
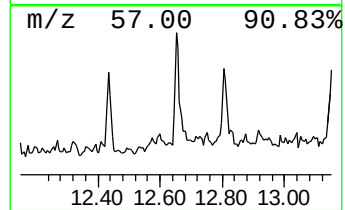
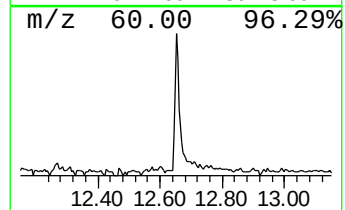
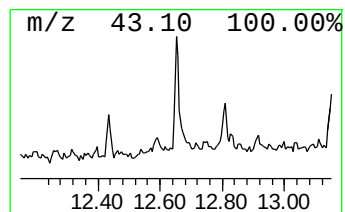
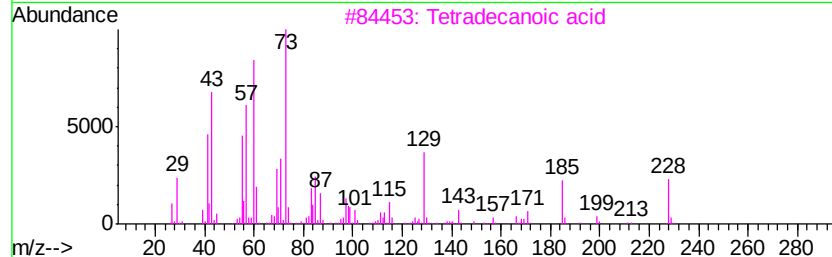
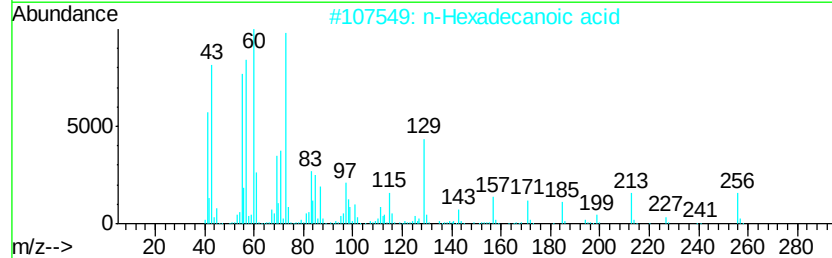
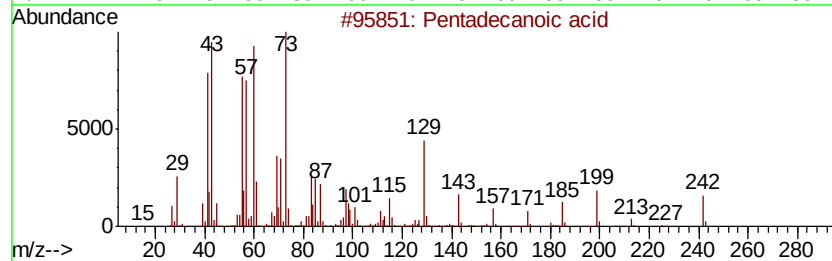
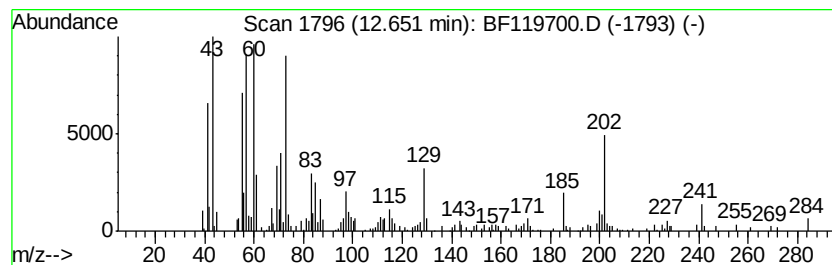
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.65	2.56 ng	225758	Phenanthrene-d10		11.34
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60



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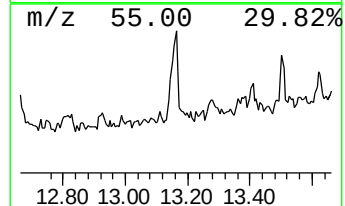
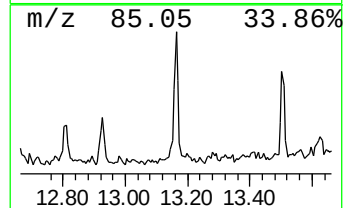
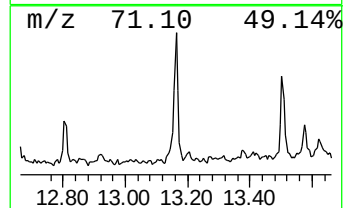
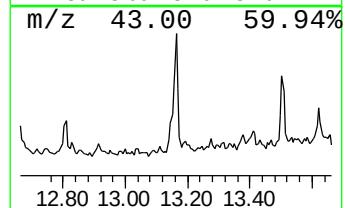
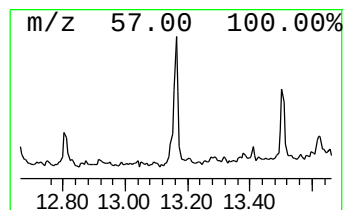
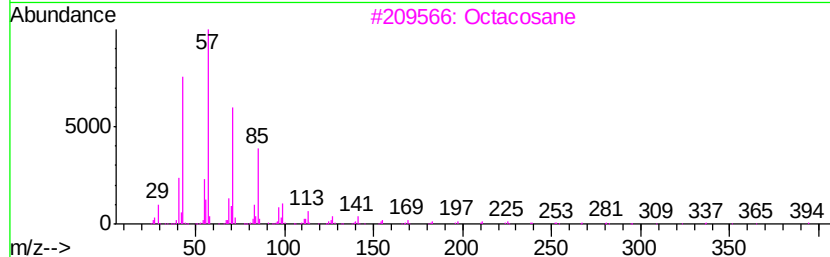
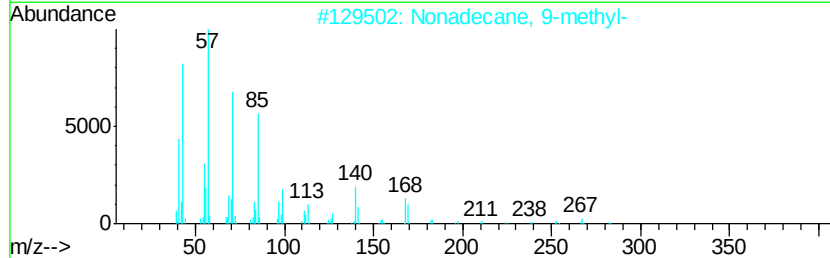
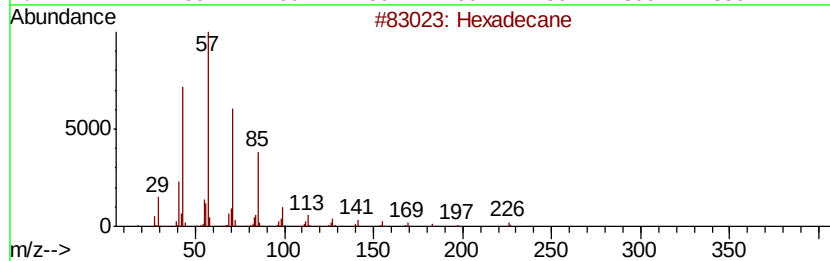
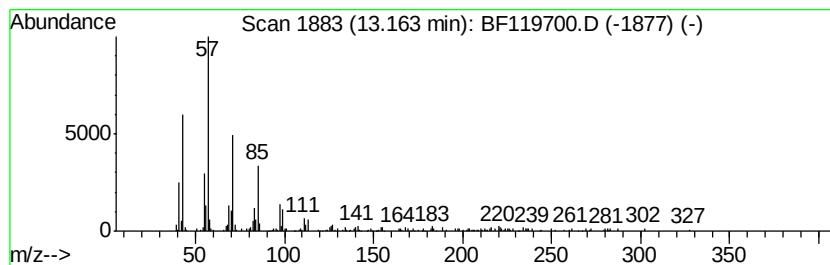
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.16	4.00 ng	276446	Chrysene-d12	13.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	95
2	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	91
3	Octacosane	394	C28H58	000630-02-4	87
4	Hentriacontane	437	C31H64	000630-04-6	87
5	Tetracosane	338	C24H50	000646-31-1	83



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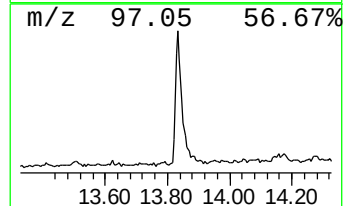
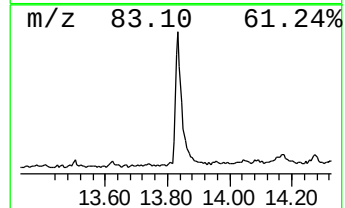
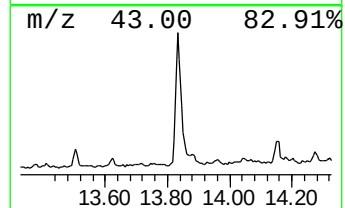
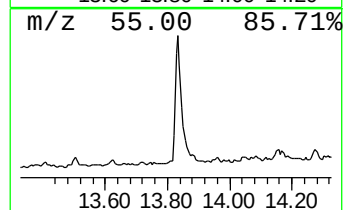
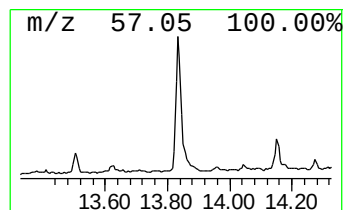
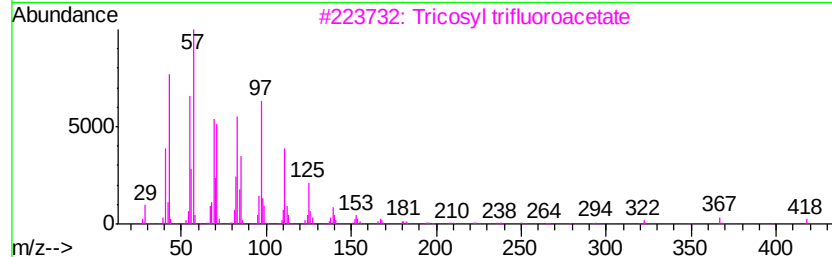
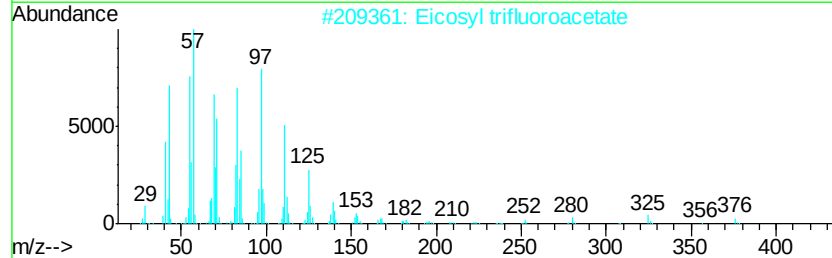
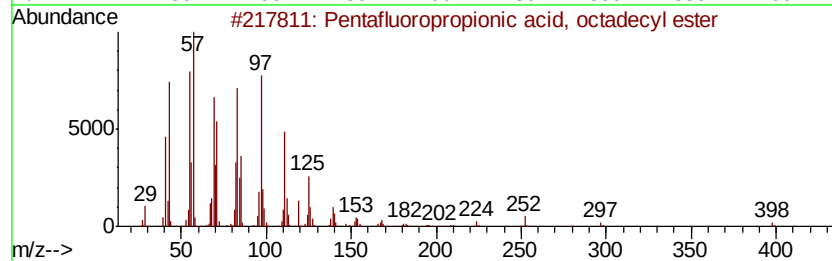
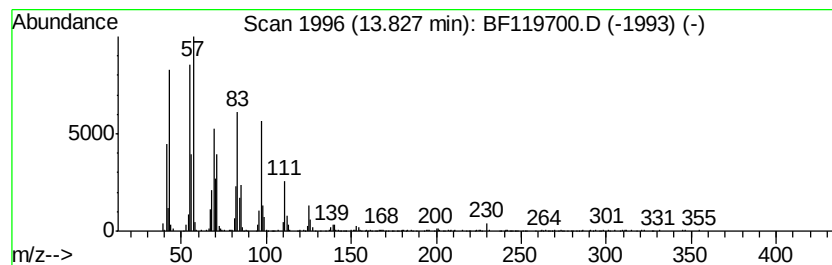
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	18.23 ng	1258750	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
2		Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
3		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
4		17-Pentatriacontene	491	C35H70	006971-40-0	91
5		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



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ClientSampleId :
SB-9-(1-3)

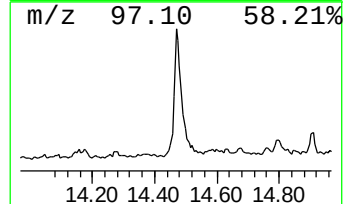
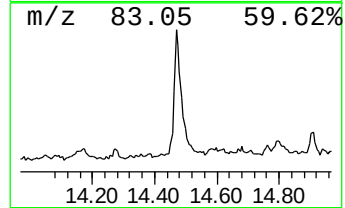
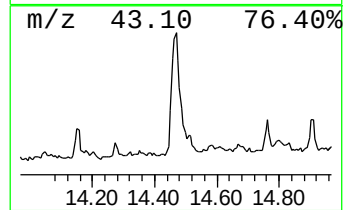
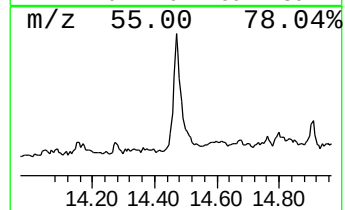
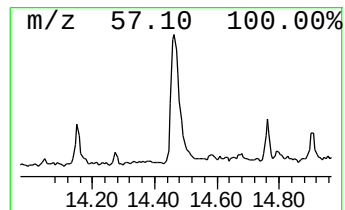
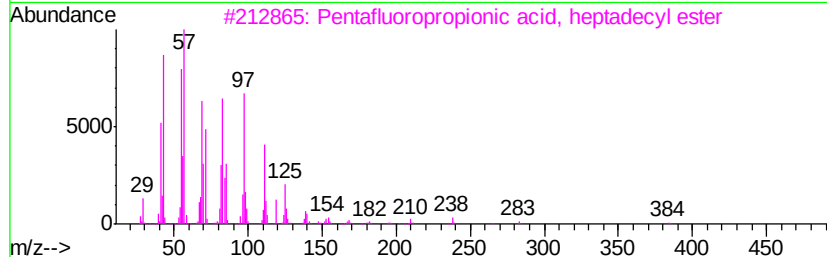
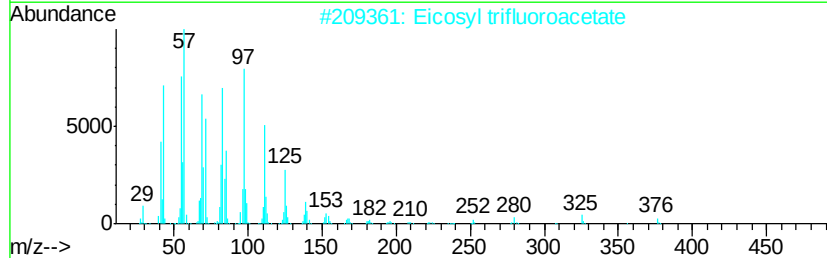
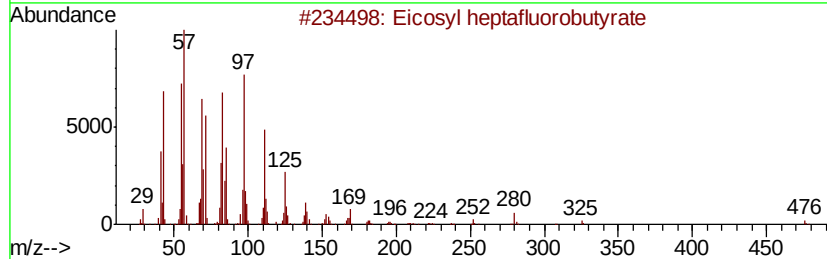
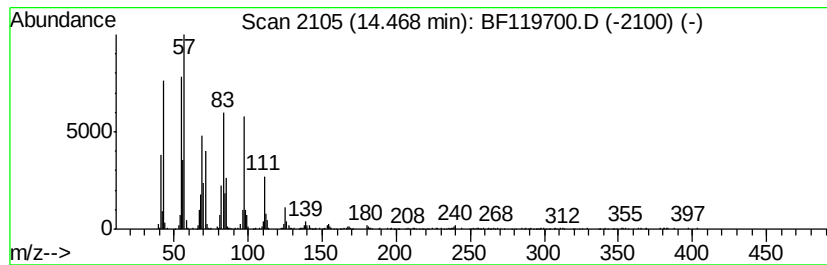
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	18.40 ng	1270940	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
2		Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4		Heneicosyl trifluoroacetate	408	C23H43F3O2	1000351-76-5	91
5		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040120\
Data File : BF119700.D
Acq On : 2 Apr 2020 6:40
Operator : MA/SJ
Sample : L2055-07
Misc :
ALS Vial : 50 Sample Multiplier: 1

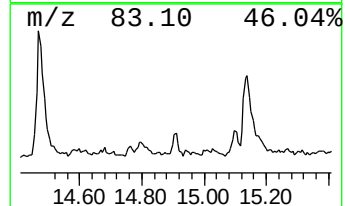
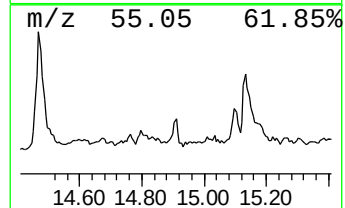
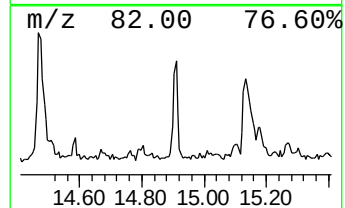
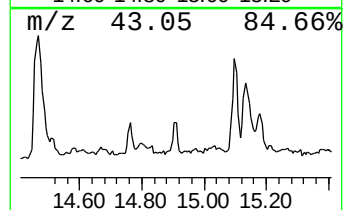
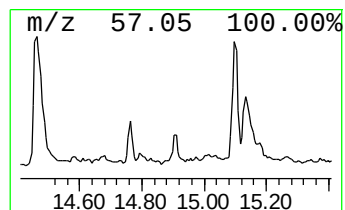
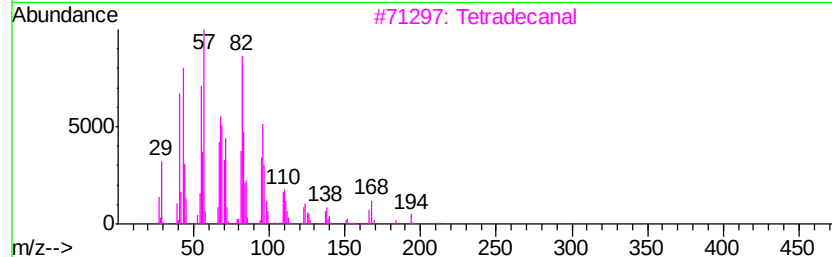
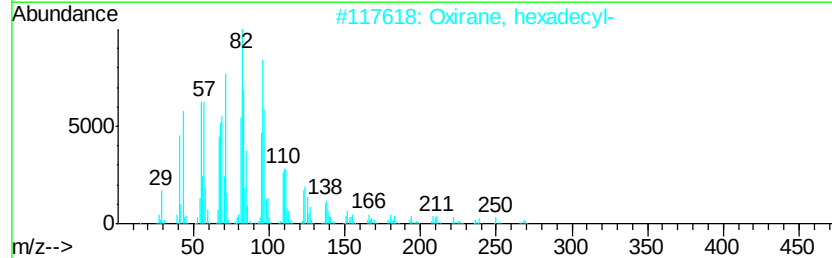
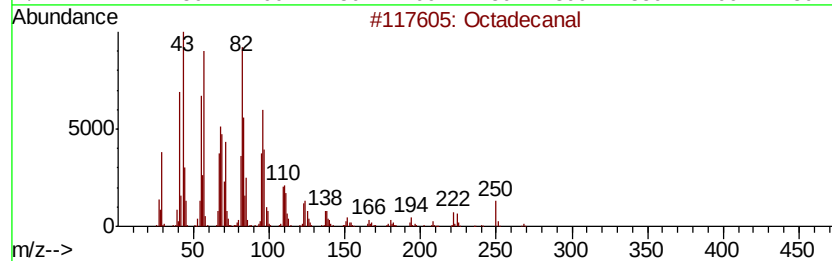
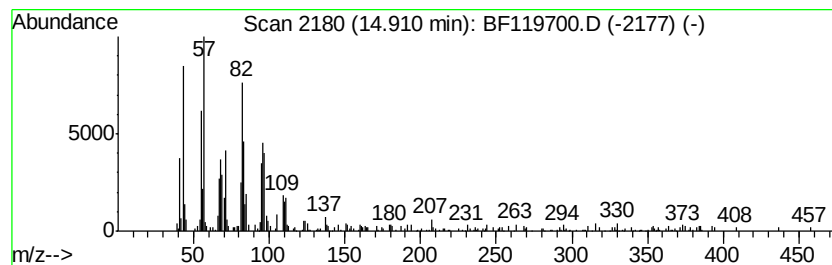
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.91	3.51 ng	195425	Perylene-d12		15.44
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
3	Tetradecanal	212	C14H28O	000124-25-4	87
4	Hexadecanal	240	C16H32O	000629-80-1	87
5	11-Tetradecyn-1-ol acetate	252	C16H28O2	033925-72-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040120\
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Sample : L2055-07
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-9-(1-3)

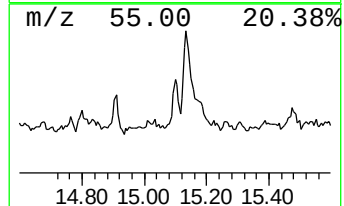
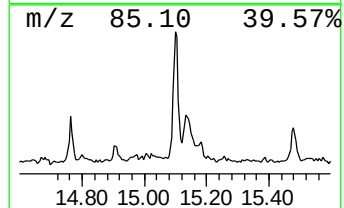
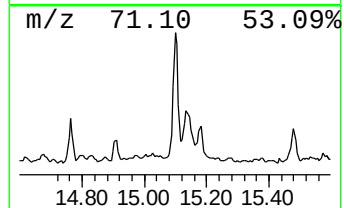
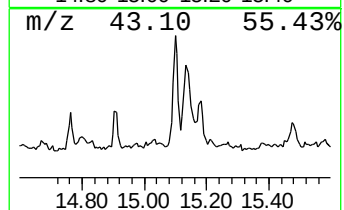
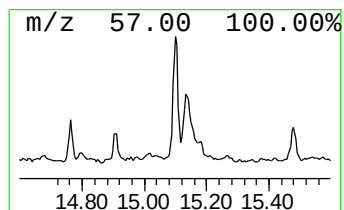
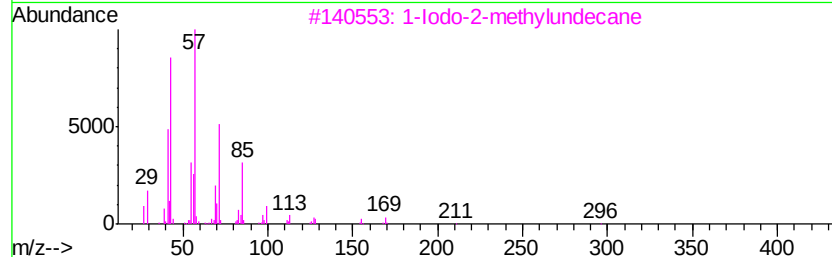
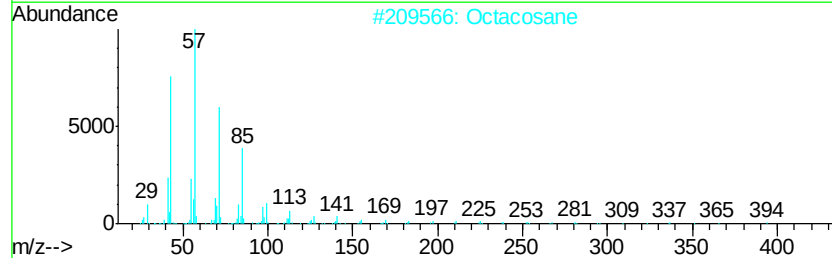
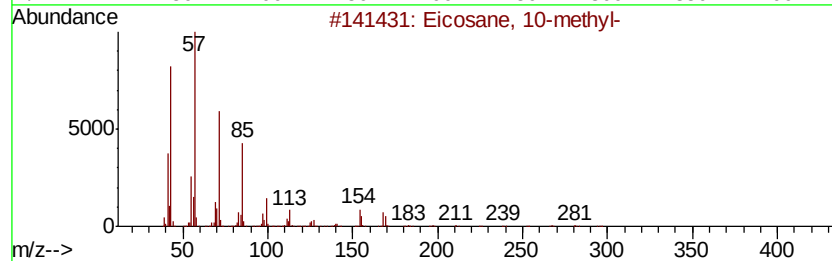
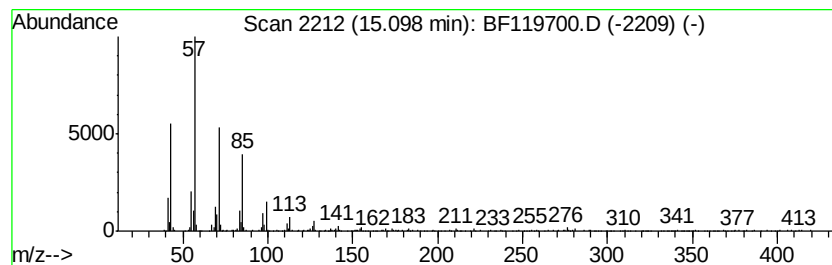
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane, 10-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	7.78 ng	432878	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
2		Octacosane	394	C28H58	000630-02-4	93
3		1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	90
4		Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	90
5		Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040120\
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Acq On : 2 Apr 2020 6:40
Operator : MA/SJ
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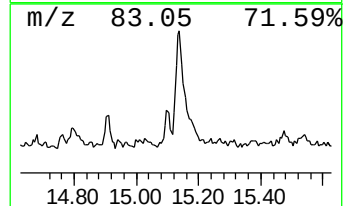
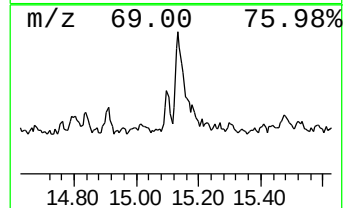
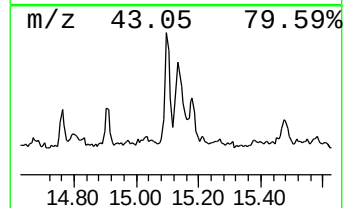
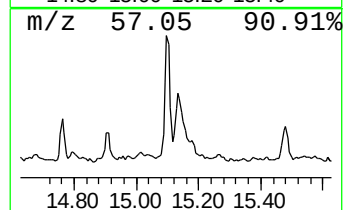
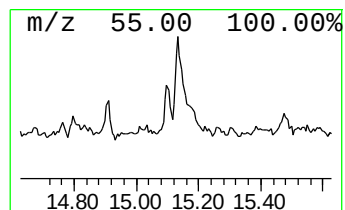
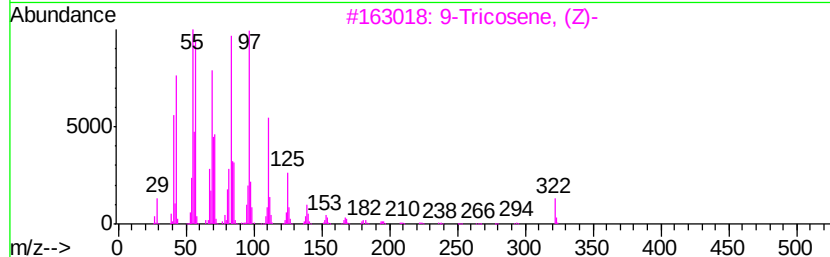
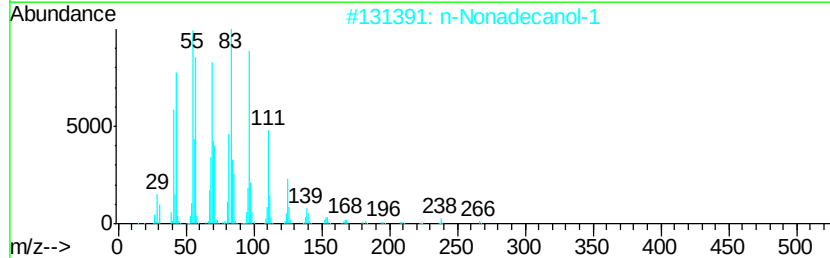
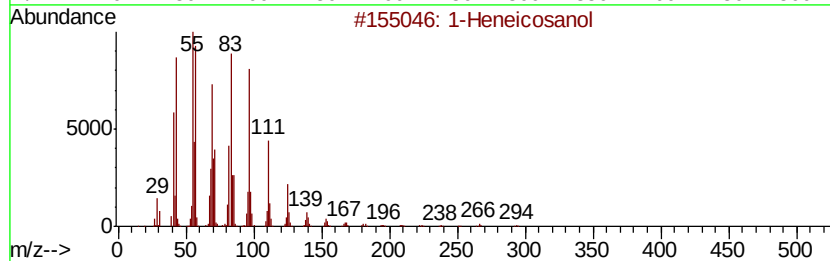
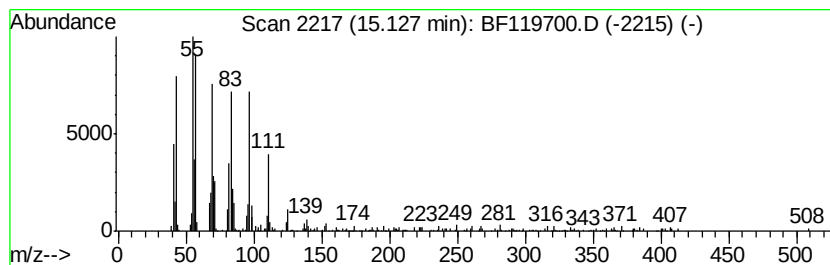
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	8.21 ng	456718	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	94
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3		9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
4		1-Octadecanol	270	C18H38O	000112-92-5	74
5		1-Hexadecene, 16-bromo-	302	C16H31Br	118625-56-2	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040120\
Data File : BF119700.D
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Sample : L2055-07
Misc :
ALS Vial : 50 Sample Multiplier: 1

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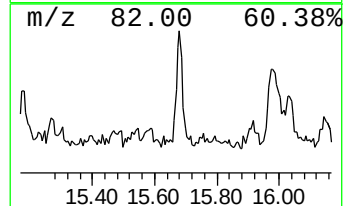
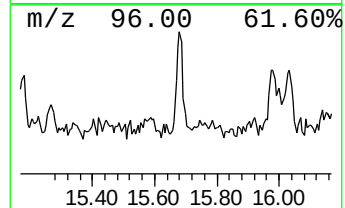
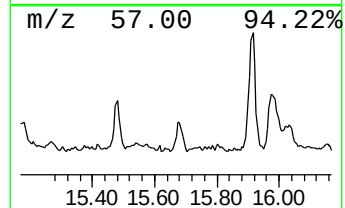
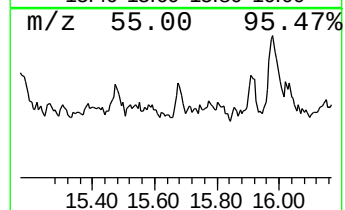
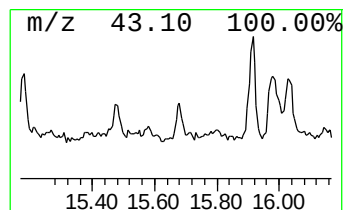
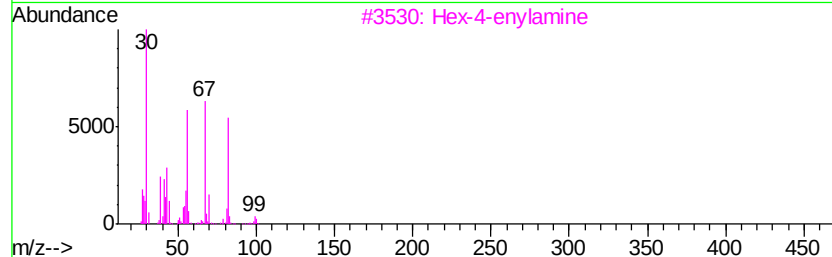
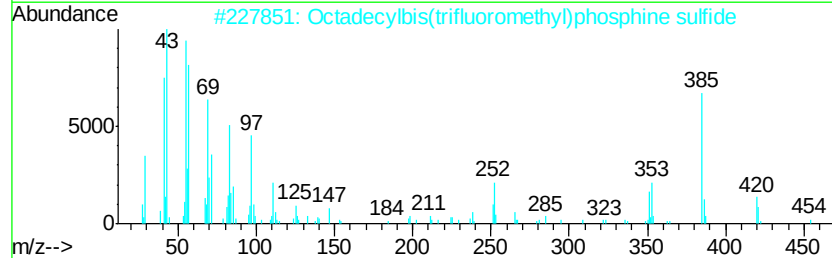
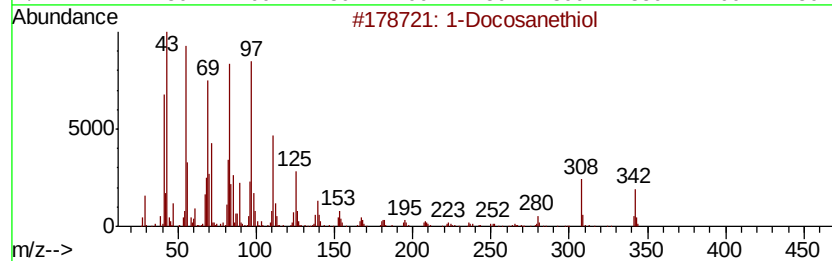
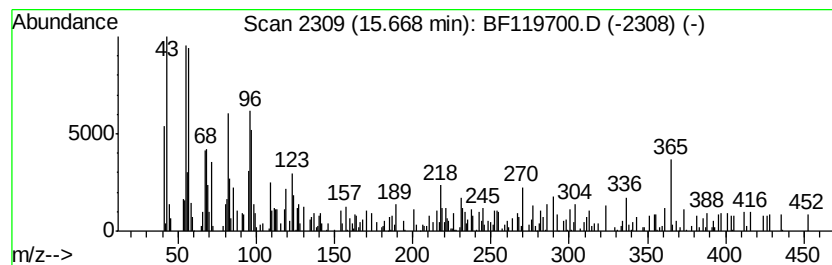
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown15.67 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	2.62 ng	145583	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosanethiol	342	C22H46S	007773-83-3	38
2		Octadecylbis(trifluoromethyl)pho...	454	C20H37F6PS	146920-13-0	10
3		Hex-4-enylamine	99	C6H13N	055108-01-5	10
4		Stigmasta-5,22-diene, 3-methoxy-...	426	C30H50O	010453-25-5	9
5		1,5-Dichloro-2,3-dinitrobenzene	236	C6H2Cl2N2O4	028689-08-9	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040120\
Data File : BF119700.D
Acq On : 2 Apr 2020 6:40
Operator : MA/SJ
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Misc :
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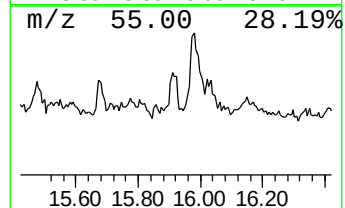
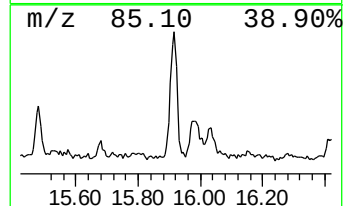
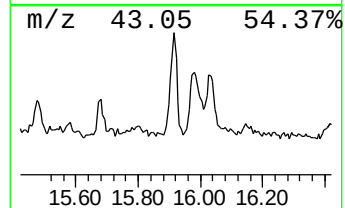
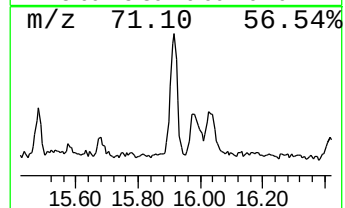
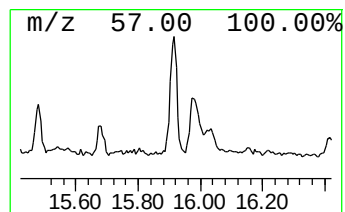
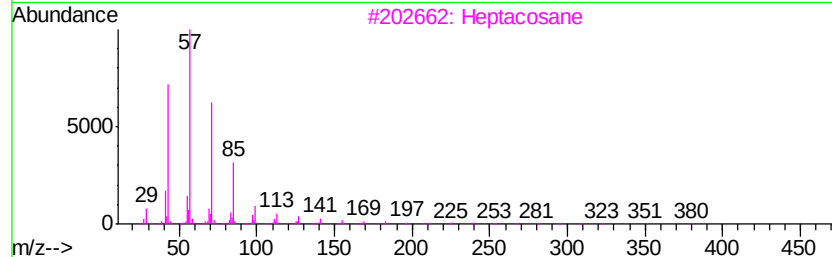
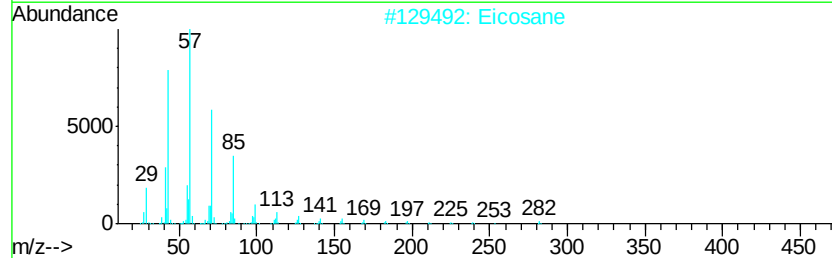
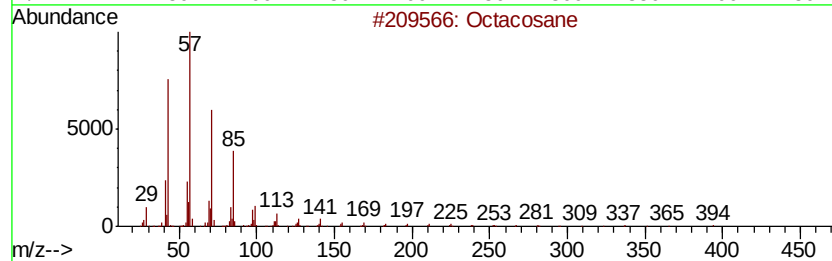
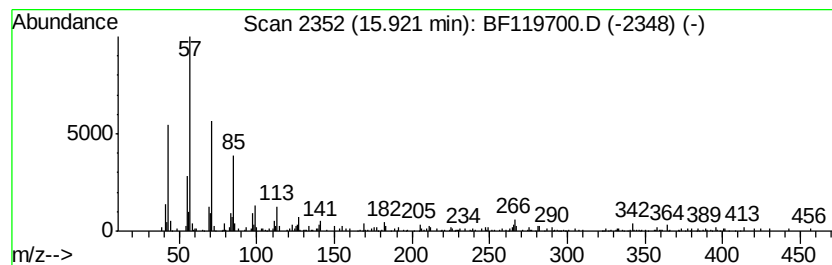
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	4.98 ng	276864	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	96
2		Eicosane	282	C20H42	000112-95-8	92
3		Heptacosane	380	C27H56	000593-49-7	90
4		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
5		Hentriacontane	437	C31H64	000630-04-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040120\
 Data File : BF119700.D
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 Sample : L2055-07
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 ALS Vial : 50 Sample Multiplier: 1

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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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n-Hexadecanoic acid	11.87	8.6	ng	761322	4	11.34	1761490	20.0
Pentadecanoic acid	12.65	2.6	ng	225758	4	11.34	1761490	20.0
Hexadecane	13.16	4.0	ng	276446	5	13.98	1381230	20.0
Pentafluoropropio...	13.83	18.2	ng	1258750	5	13.98	1381230	20.0
Eicosyl heptaflu...	14.47	18.4	ng	1270940	5	13.98	1381230	20.0
Octadecanal	14.91	3.5	ng	195425	6	15.44	1113000	20.0
Eicosane, 10-methyl-	15.10	7.8	ng	432878	6	15.44	1113000	20.0
1-Heneicosanol	15.13	8.2	ng	456718	6	15.44	1113000	20.0
unknown15.67	15.67	2.6	ng	145583	6	15.44	1113000	20.0
Octacosane	15.92	5.0	ng	276864	6	15.44	1113000	20.0