

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
 Data File : BF119662.D
 Acq On : 31 Mar 2020 19:55
 Operator : MA/SJ
 Sample : L2055-07
 Misc :
 ALS Vial : 16 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	2.204	16	20	28	rVB	119556	156172	2.73%	0.310%
2	5.039	497	502	508	rVB	145505	188926	3.30%	0.375%
3	5.445	566	571	574	rBV	5961240	5589238	97.76%	11.105%
4	6.457	738	743	746	rBV	5284743	5561767	97.28%	11.050%
5	6.828	803	806	810	rBV	2077056	1709623	29.90%	3.397%
6	6.986	829	833	836	rBV	5312293	4492660	78.58%	8.926%
7	7.392	894	902	905	rBV	3949018	3505117	61.31%	6.964%
8	8.116	1021	1025	1028	rBV	2702149	2112453	36.95%	4.197%
9	9.198	1204	1209	1212	rBV	6858338	5717140	100.00%	11.359%
10	9.592	1272	1276	1280	rVB	536978	462203	8.08%	0.918%
11	9.874	1321	1324	1328	rVB	2259502	2049673	35.85%	4.072%
12	10.669	1454	1459	1462	rBV	2948001	2702509	47.27%	5.370%
13	11.239	1549	1556	1558	rBV4	42622	74108	1.30%	0.147%
14	11.368	1574	1578	1580	rBV	2007688	1704165	29.81%	3.386%
15	11.392	1580	1582	1585	rVB	135318	110546	1.93%	0.220%
16	11.898	1665	1668	1679	rBV	733144	715244	12.51%	1.421%
17	12.580	1781	1784	1787	rBV	347246	310718	5.43%	0.617%
18	12.680	1798	1801	1809	rBV2	170351	225374	3.94%	0.448%
19	12.810	1820	1823	1826	rVB	287948	231890	4.06%	0.461%
20	12.957	1844	1848	1852	rBV	4233440	3824880	66.90%	7.600%
21	13.192	1885	1888	1893	rBV2	176950	221270	3.87%	0.440%
22	13.539	1944	1947	1950	rBV	107763	104723	1.83%	0.208%
23	13.651	1964	1966	1969	rVB2	85149	80394	1.41%	0.160%
24	13.868	2000	2003	2014	rVB	944258	1403778	24.55%	2.789%
25	14.015	2023	2028	2030	rBV	1532807	1598541	27.96%	3.176%
26	14.039	2030	2032	2034	rVB	152720	117232	2.05%	0.233%
27	14.121	2043	2046	2049	rBV2	149343	122175	2.14%	0.243%
28	14.186	2054	2057	2059	rBV	141423	129866	2.27%	0.258%
29	14.492	2106	2109	2110	rBV	508413	423697	7.41%	0.842%
30	14.515	2110	2113	2122	rVB2	668365	1187175	20.77%	2.359%
31	14.798	2159	2161	2164	rVB	146413	128928	2.26%	0.256%
32	14.945	2183	2186	2190	rVB	298569	316467	5.54%	0.629%
33	15.056	2202	2205	2213	rVB	181516	366512	6.41%	0.728%
34	15.139	2216	2219	2223	rBV	475186	528996	9.25%	1.051%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.186	2224	2227	2231	rBV	379194	654270	11.44%	1.300%
36	15.486	2274	2278	2281	rBV	901562	1078173	18.86%	2.142%
37	15.968	2356	2360	2365	rVB	300158	423934	7.42%	0.842%

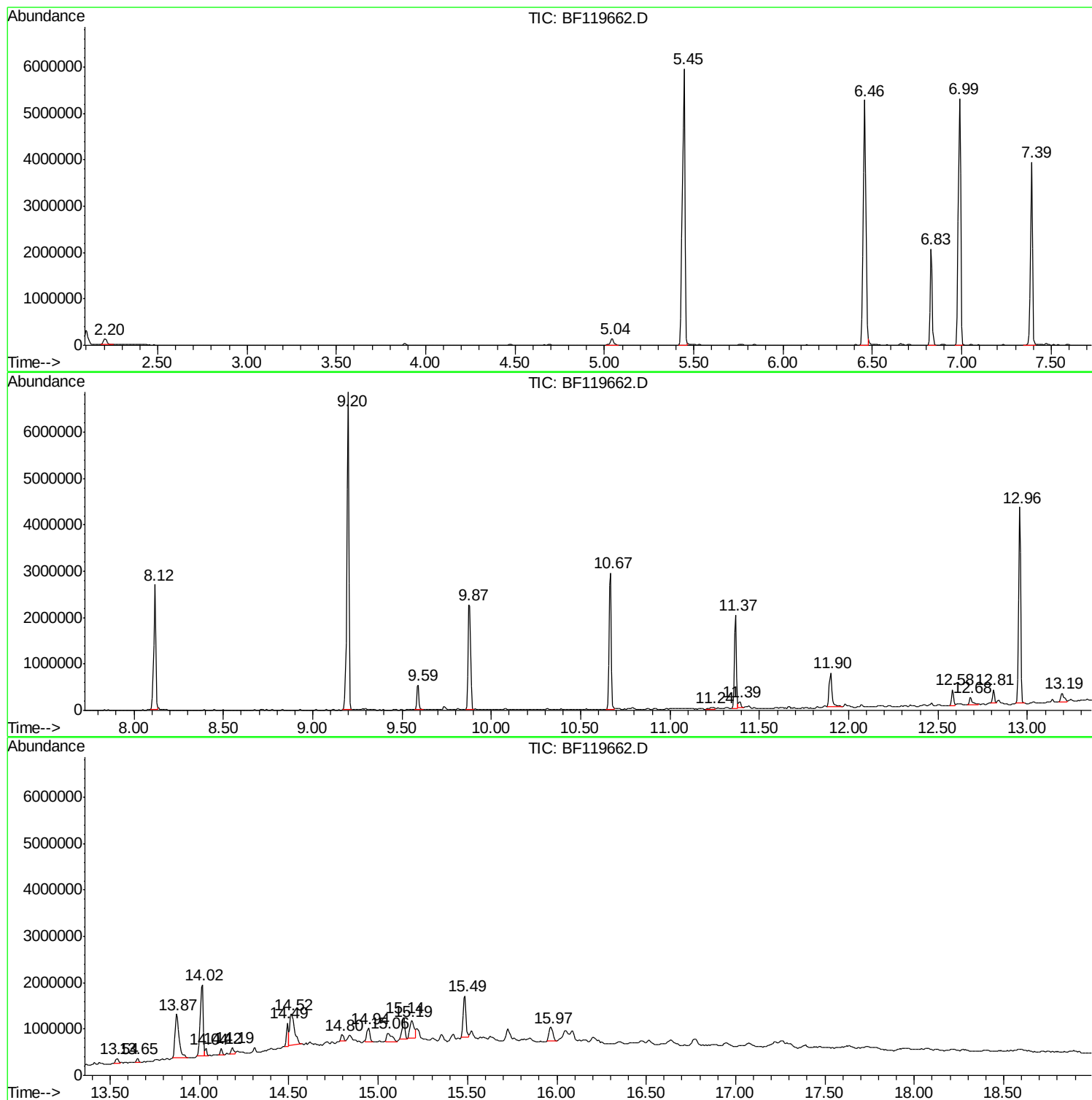
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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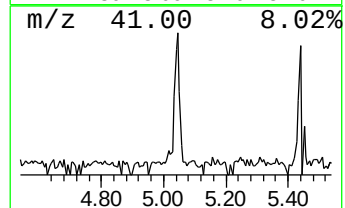
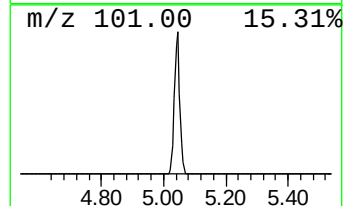
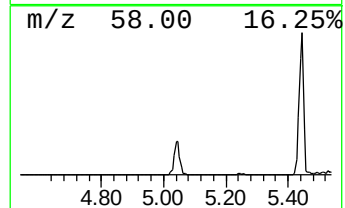
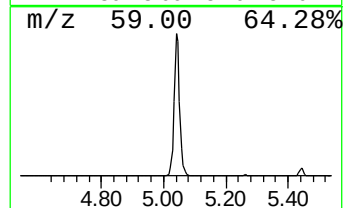
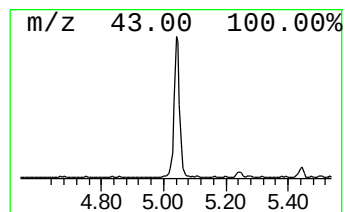
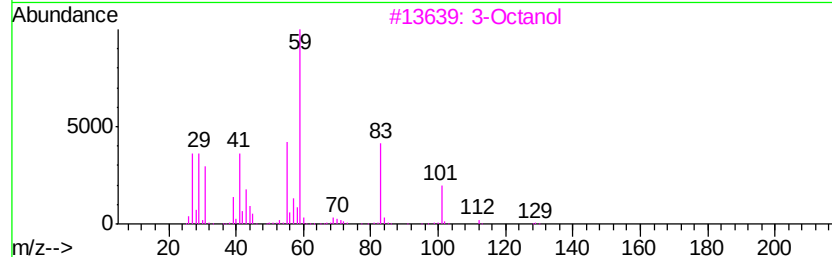
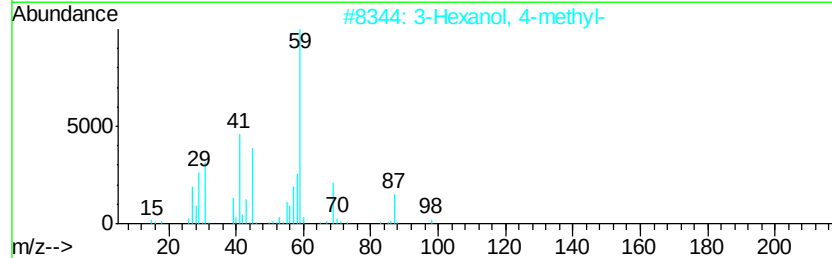
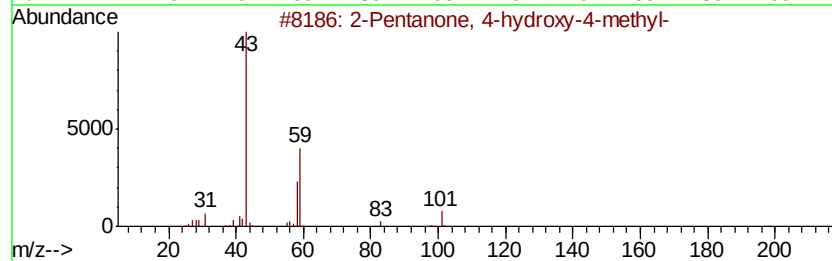
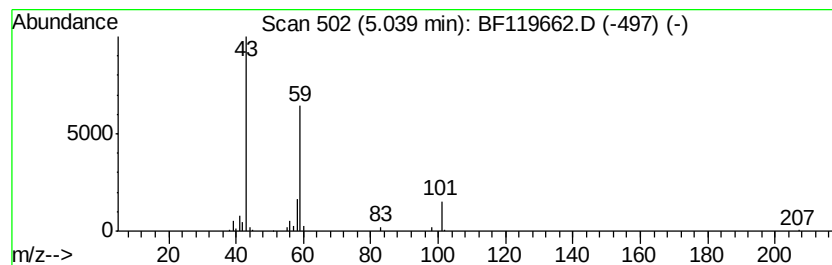
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	2.21 ng	188926	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		3-Octanol	130	C8H18O	000589-98-0	33
4		3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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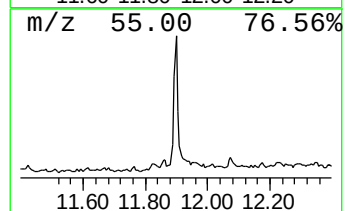
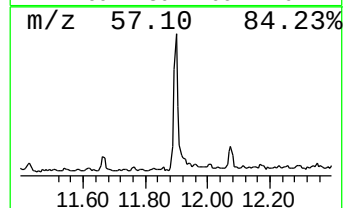
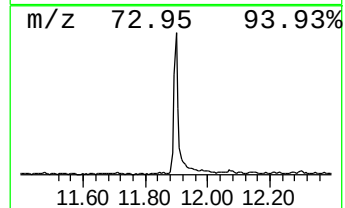
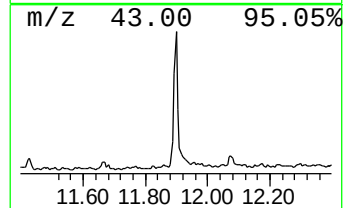
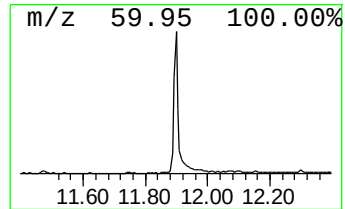
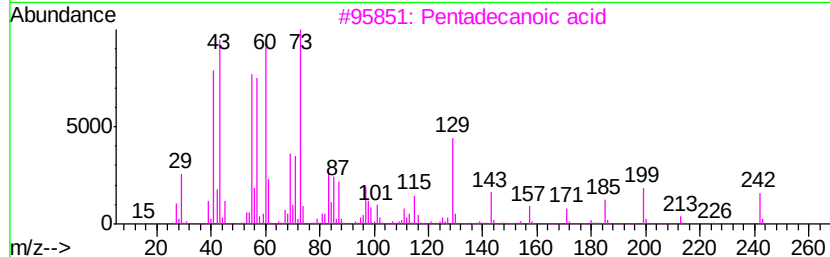
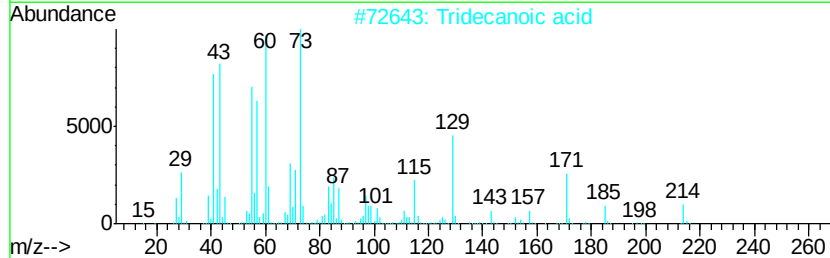
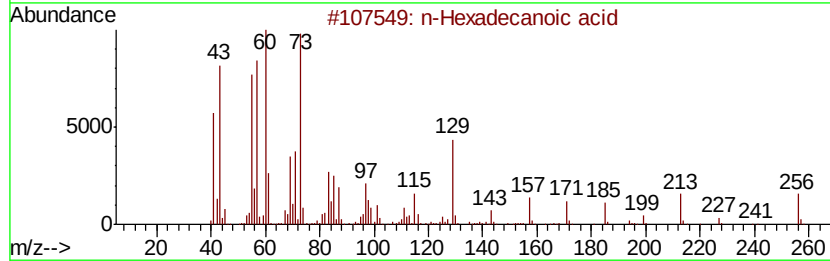
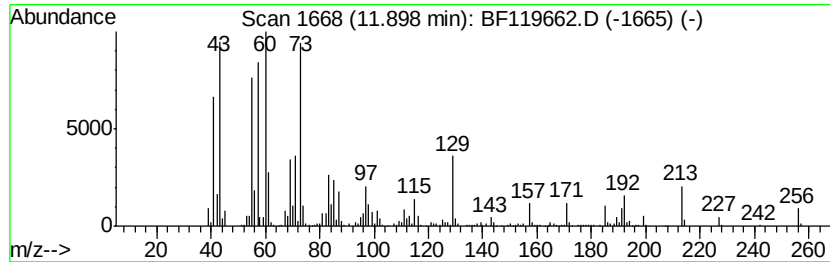
Instrument :
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SB-9-(1-3)

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.90	8.39 ng	715244	Phenanthrene-d10	11.37	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55



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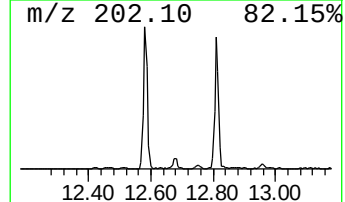
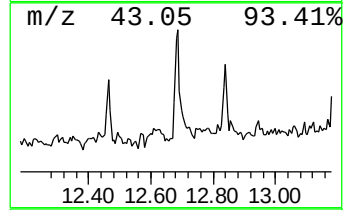
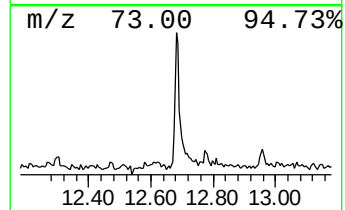
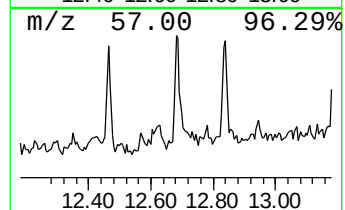
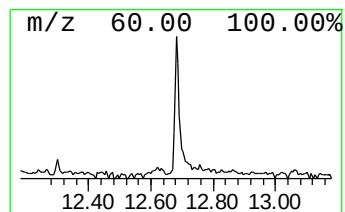
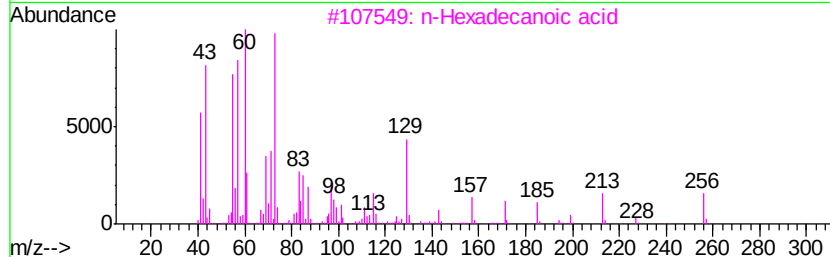
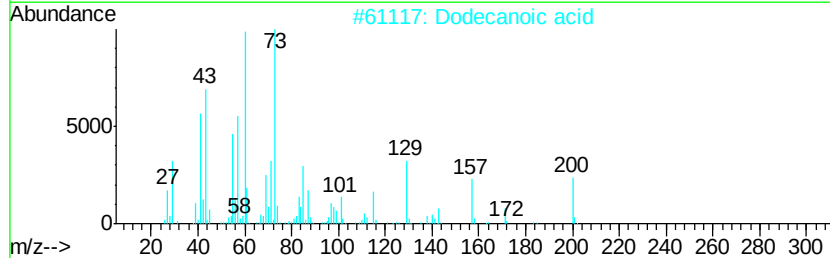
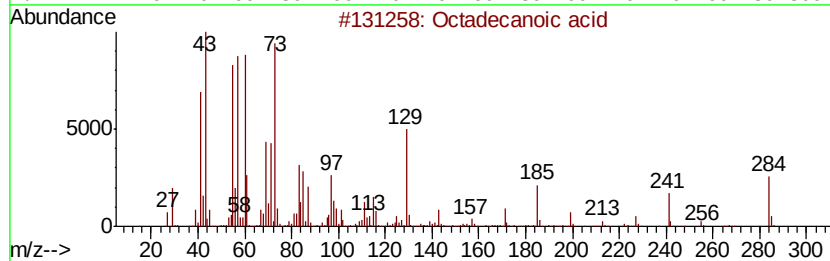
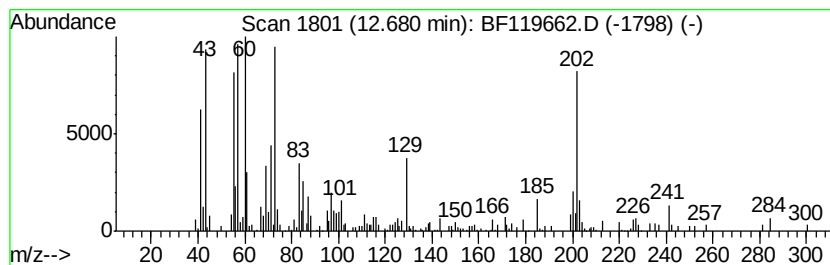
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	2.64 ng	225374	Phenanthrene-d10	11.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	95
2		Dodecanoic acid	200	C12H24O2	000143-07-7	78
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5		Fluoranthene	202	C16H10	000206-44-0	25



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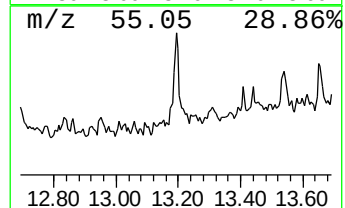
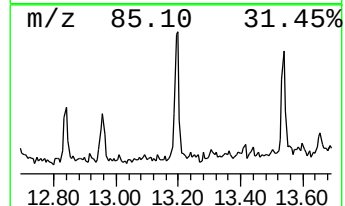
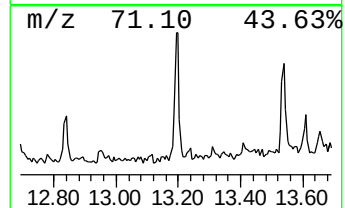
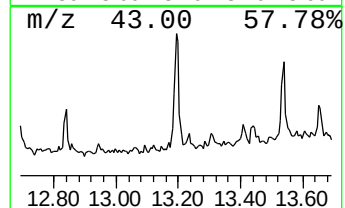
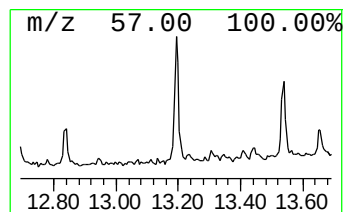
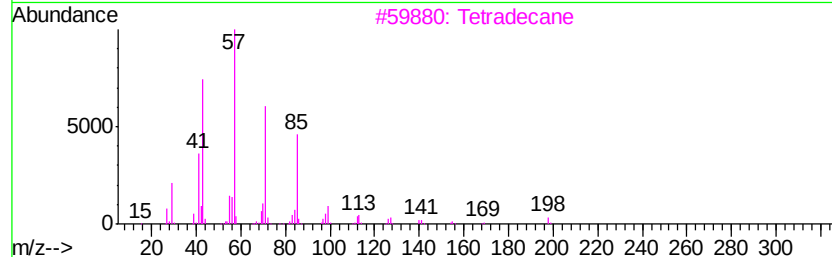
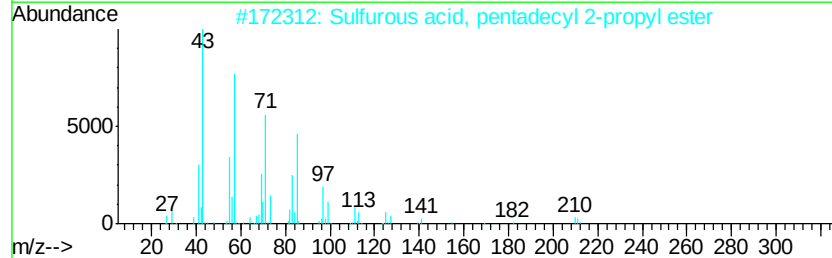
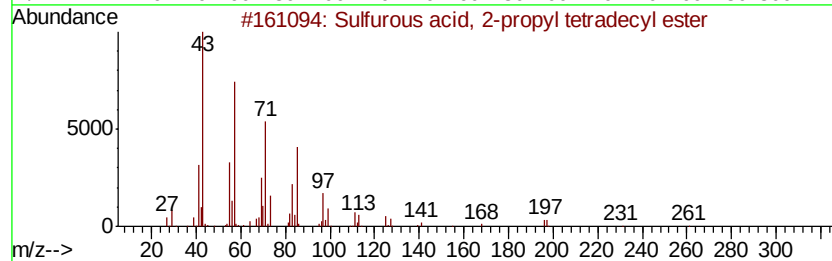
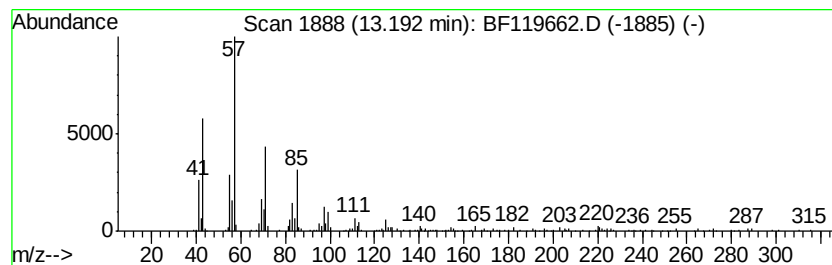
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Sulfurous acid, 2-propyl te... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	2.77 ng	221270	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	74
2		Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	74
3		Tetradecane	198	C14H30	000629-59-4	74
4		Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	72
5		Tritetracontane	605	C43H88	007098-21-7	72



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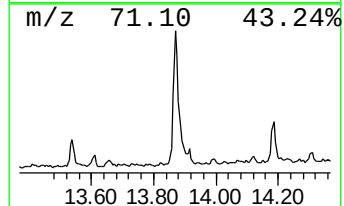
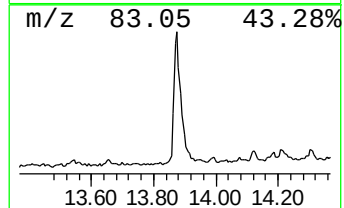
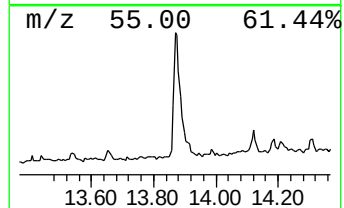
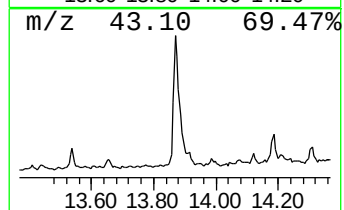
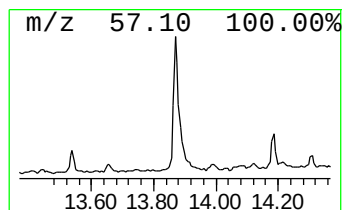
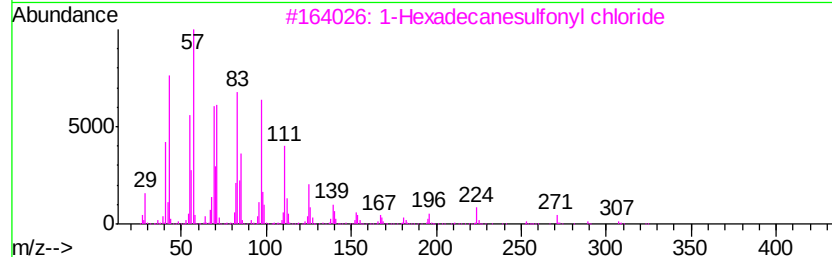
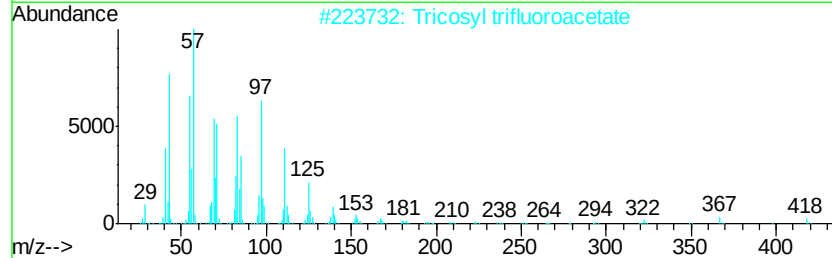
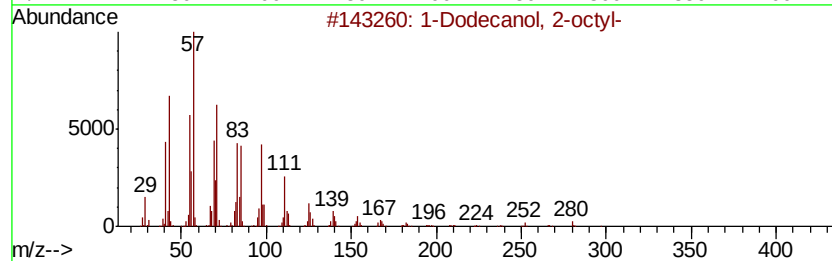
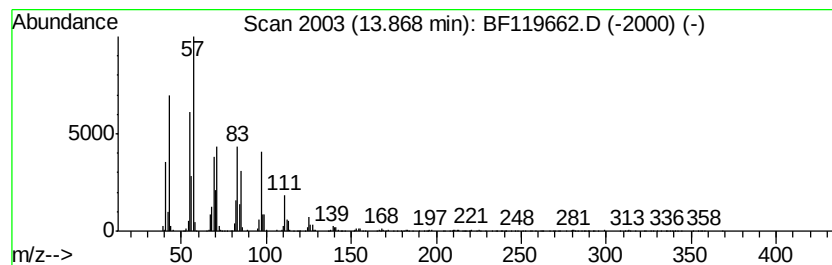
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 Peak Number 6 1-Dodecanol, 2-octyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	17.56 ng	1403780	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
2		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
3		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
4		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
5		Triacontyl heptafluorobutyrate	634	C34H61F7O2	1000351-83-2	90



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Sample : L2055-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

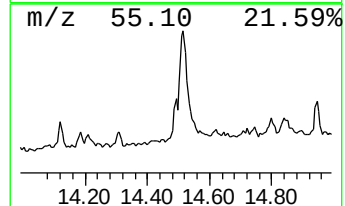
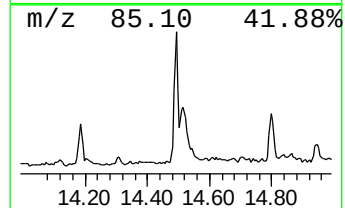
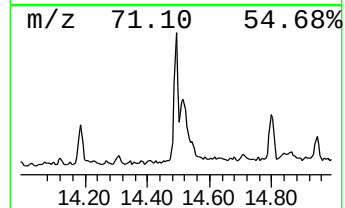
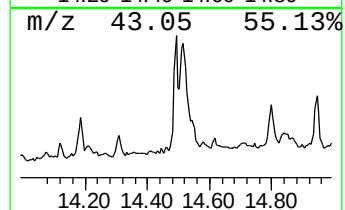
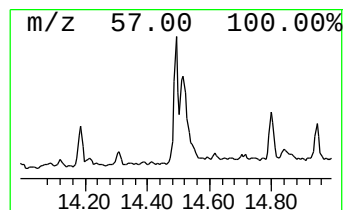
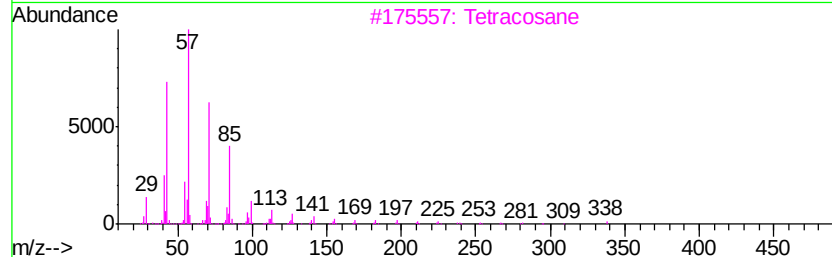
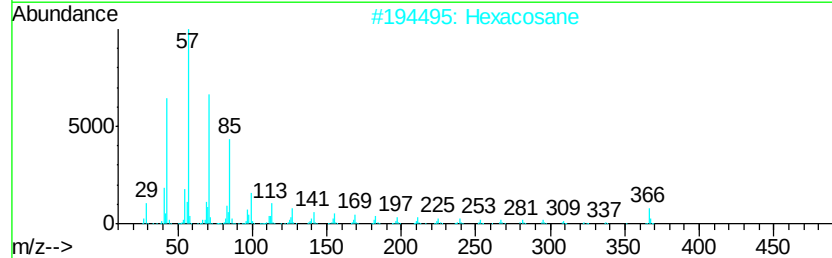
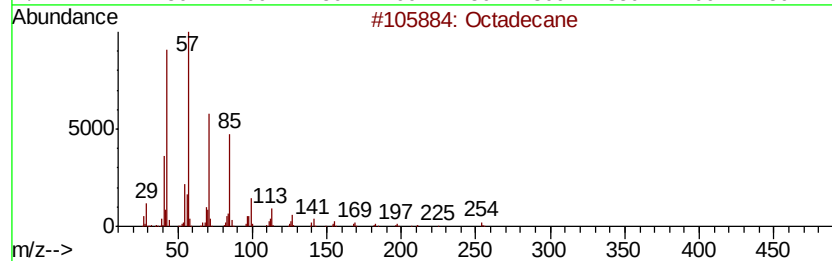
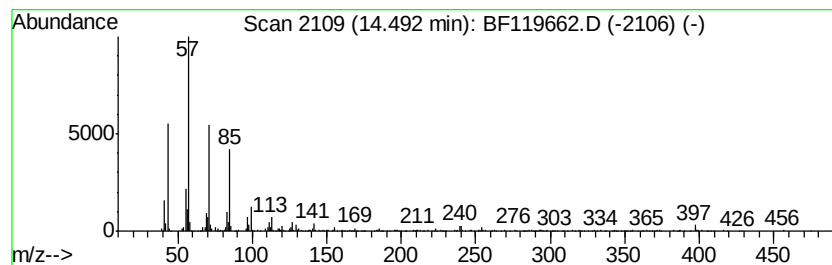
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BNA_F
ClientSampleId :
SB-9-(1-3)

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

Peak Number 7 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	5.30 ng	423697	Chrysene-d12	14.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecane	254 C18H38	000593-45-3	91
2	Hexacosane	366 C26H54	000630-01-3	87
3	Tetracosane	338 C24H50	000646-31-1	83
4	Heneicosane	296 C21H44	000629-94-7	81
5	3,5-Dimethyldodecane	198 C14H30	107770-99-0	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119662.D
Acq On : 31 Mar 2020 19:55
Operator : MA/SJ
Sample : L2055-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

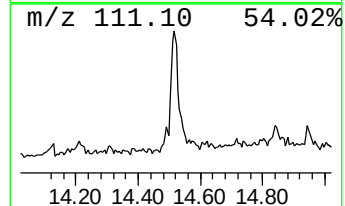
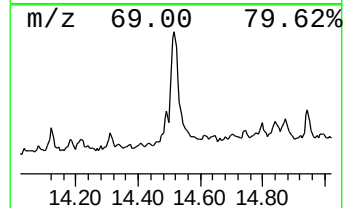
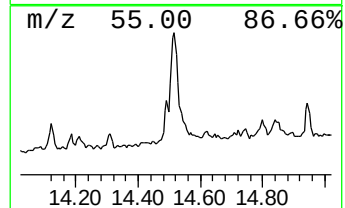
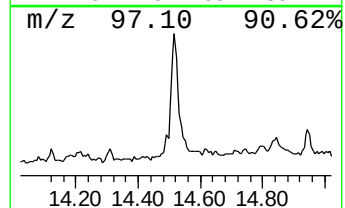
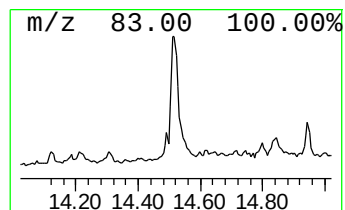
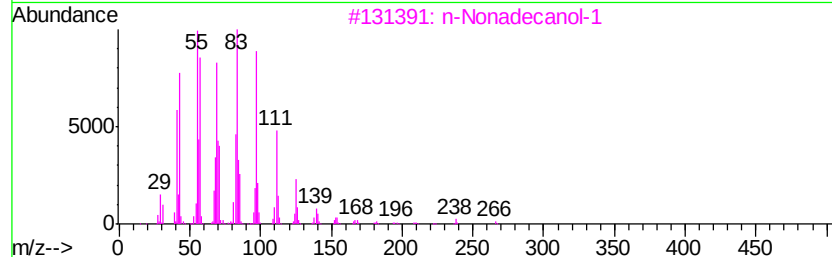
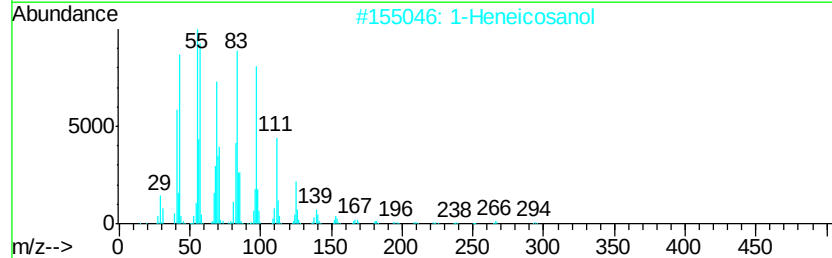
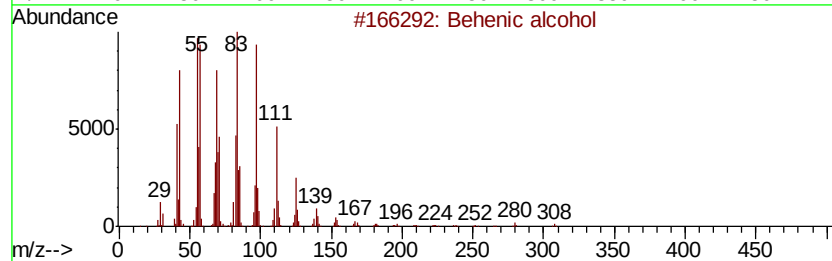
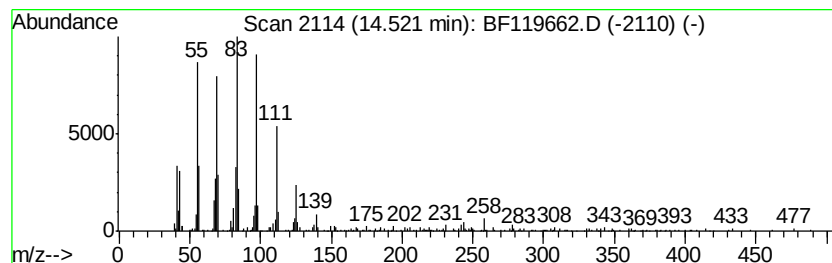
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	14.85 ng	1187180	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Behenic alcohol	326	C22H46O	000661-19-8	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	91
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	83
4		1-Octadecanol	270	C18H38O	000112-92-5	62
5		1-Docosene	308	C22H44	001599-67-3	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119662.D
Acq On : 31 Mar 2020 19:55
Operator : MA/SJ
Sample : L2055-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

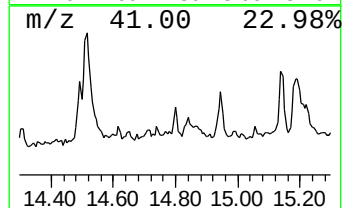
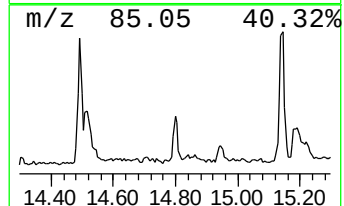
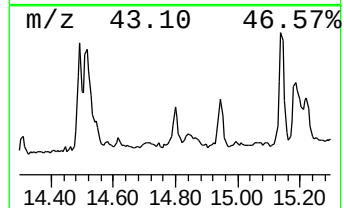
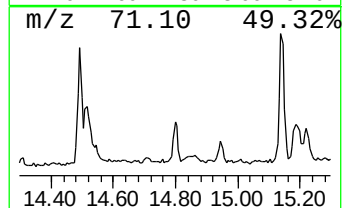
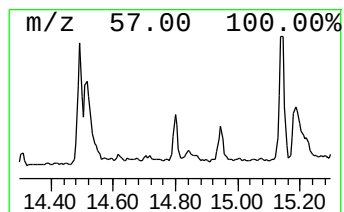
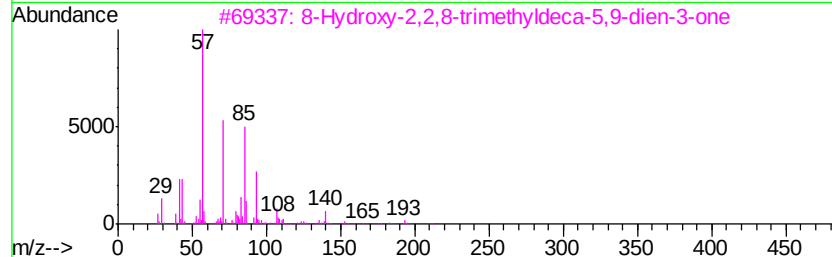
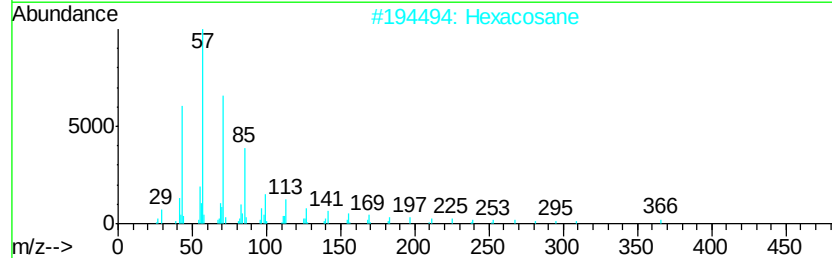
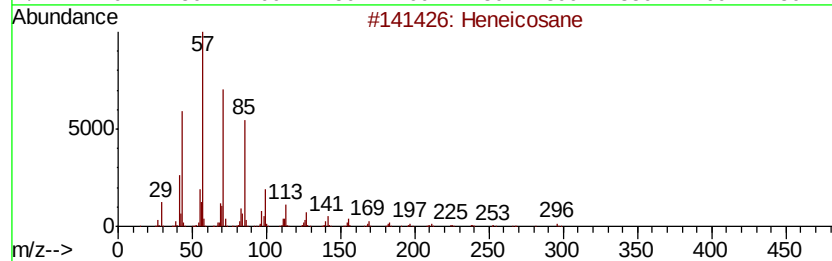
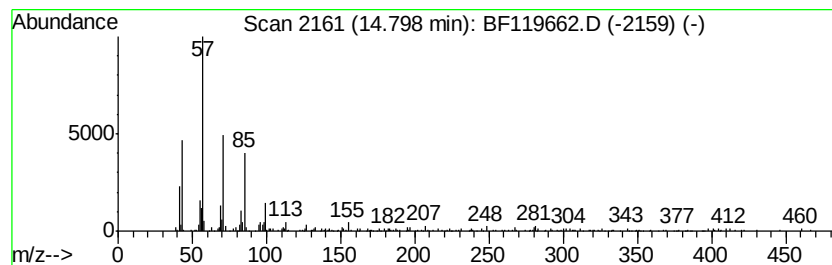
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	2.39 ng	128928	Perylene-d12	15.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	81
2	Hexacosane		366	C26H54	000630-01-3	72
3	8-Hydroxy-2,2,8-trimethyldeca-5,...		210	C13H22O2	083040-92-0	64
4	Nonadecane		268	C19H40	000629-92-5	64
5	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119662.D
Acq On : 31 Mar 2020 19:55
Operator : MA/SJ
Sample : L2055-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

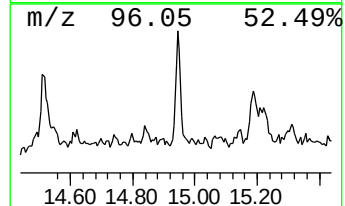
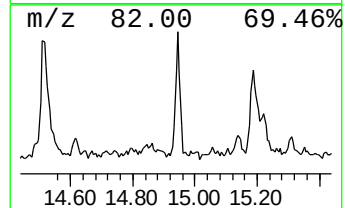
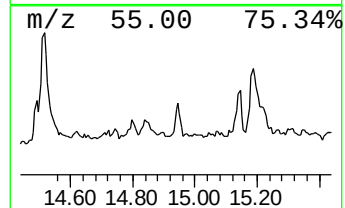
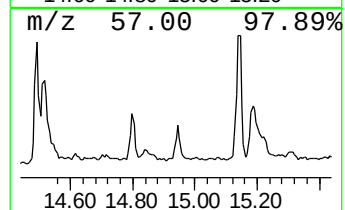
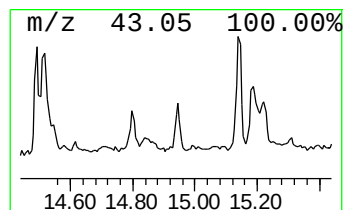
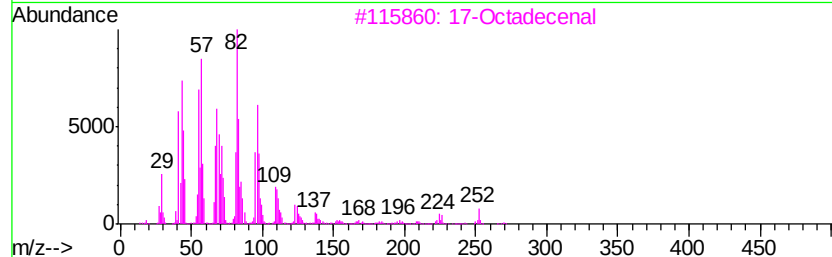
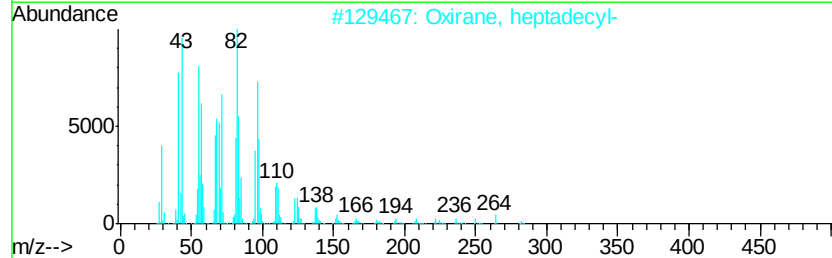
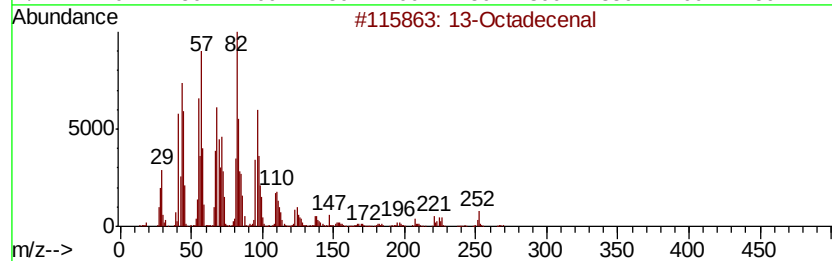
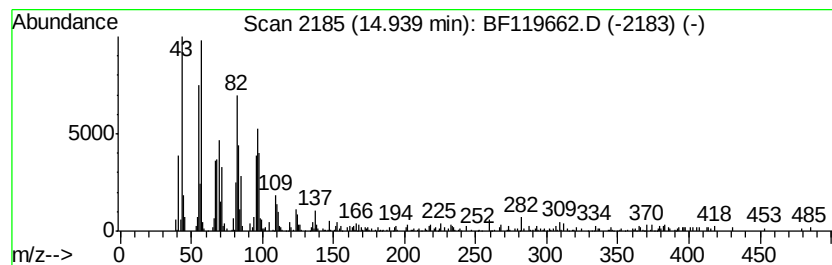
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 13-Octadecenal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.94	5.87 ng	316467	Perylene-d12	15.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Octadecenal	266	C18H34O	056554-90-6	94
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	93
3	17-Octadecenal	266	C18H34O	056554-86-0	93
4	16-Octadecenal	266	C18H34O	056554-87-1	93
5	Octadecanal	268	C18H36O	000638-66-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119662.D
Acq On : 31 Mar 2020 19:55
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ClientSampleId :
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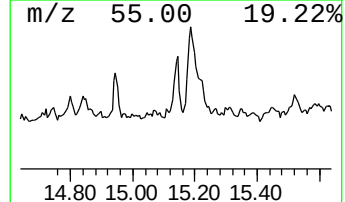
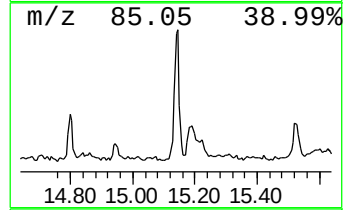
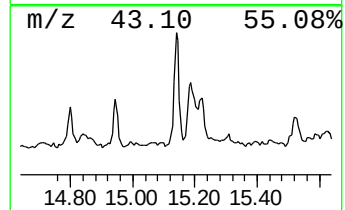
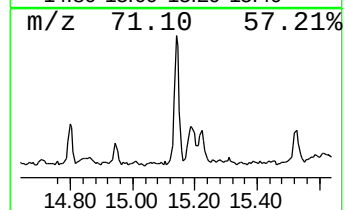
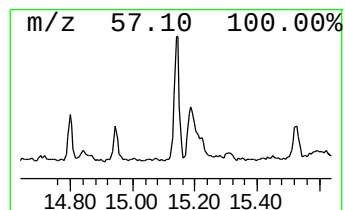
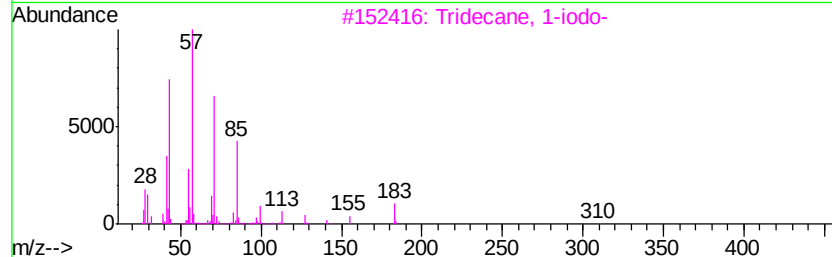
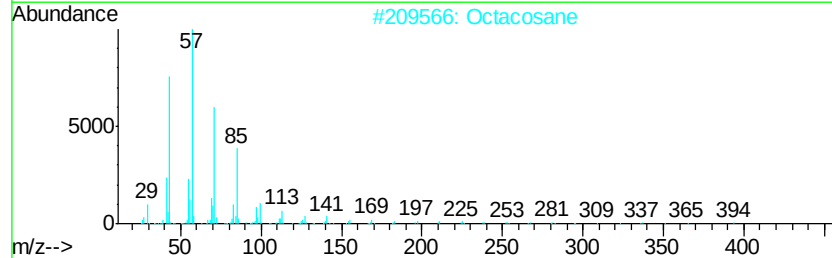
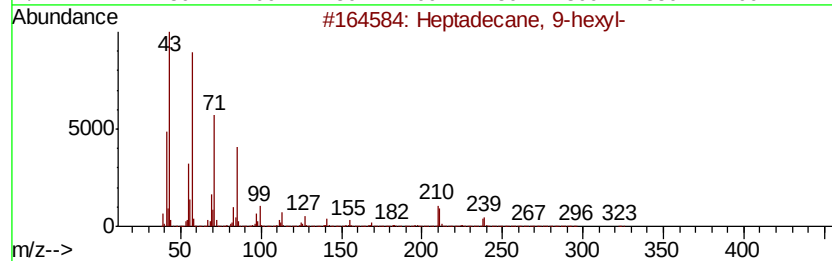
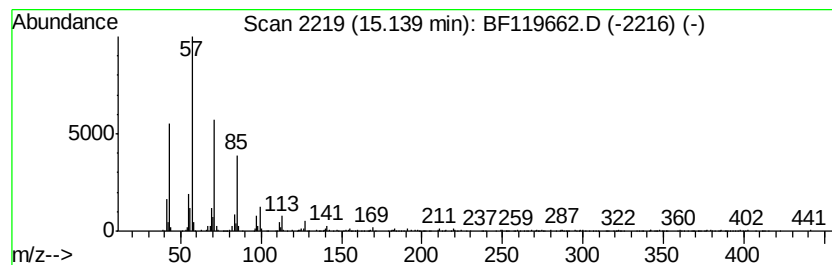
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane, 9-hexyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	9.81 ng	528996	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	90
2		Octacosane	394	C28H58	000630-02-4	87
3		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83
4		Tricosane	324	C23H48	000638-67-5	83
5		3,5-Dimethyldodecane	198	C14H30	107770-99-0	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119662.D
Acq On : 31 Mar 2020 19:55
Operator : MA/SJ
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Misc :
ALS Vial : 16 Sample Multiplier: 1

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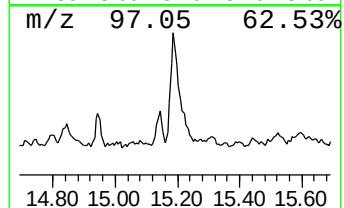
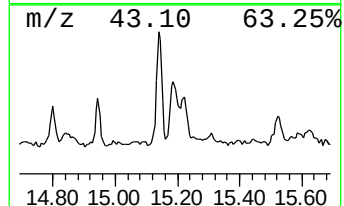
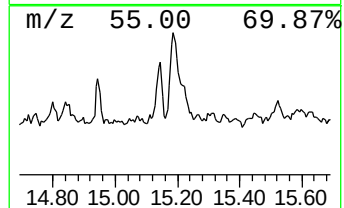
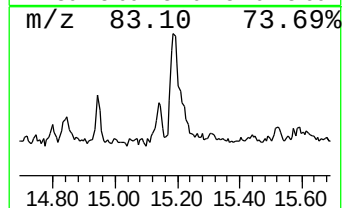
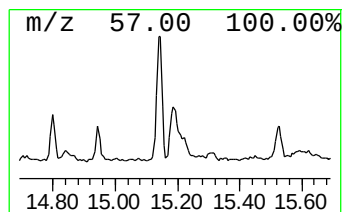
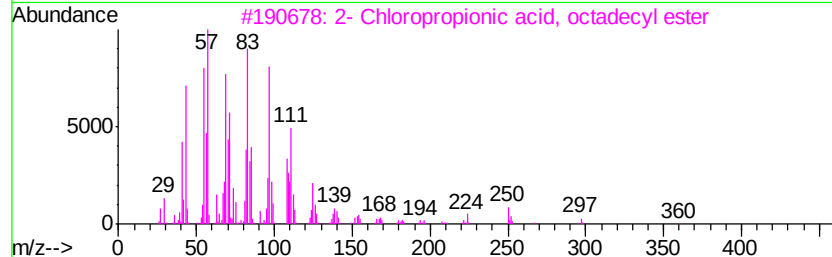
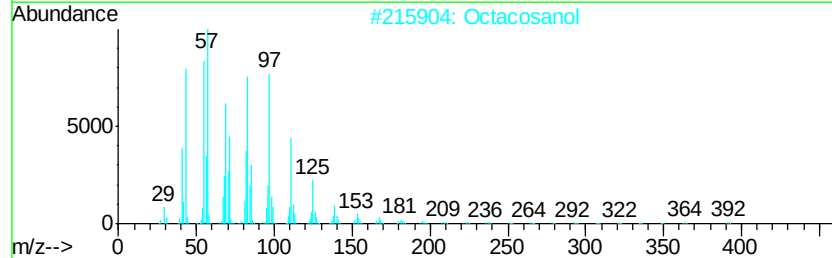
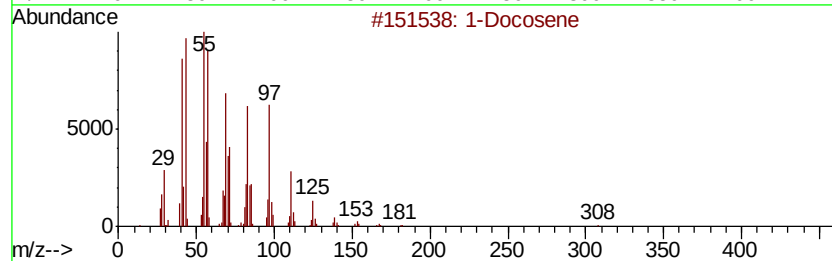
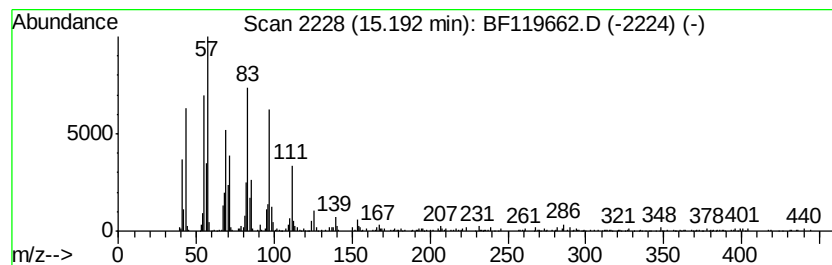
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	12.14 ng	654270	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	95
2		Octacosanol	410	C28H58O	000557-61-9	94
3		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	93
4		9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119662.D
Acq On : 31 Mar 2020 19:55
Operator : MA/SJ
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Misc :
ALS Vial : 16 Sample Multiplier: 1

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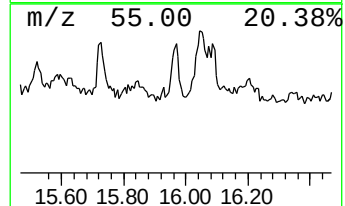
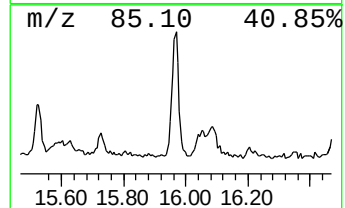
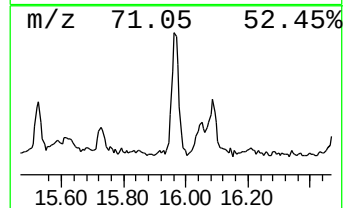
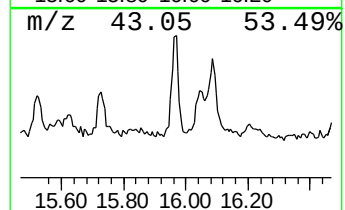
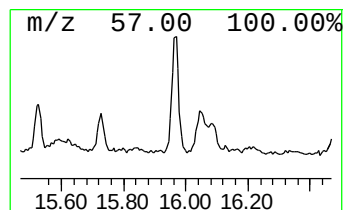
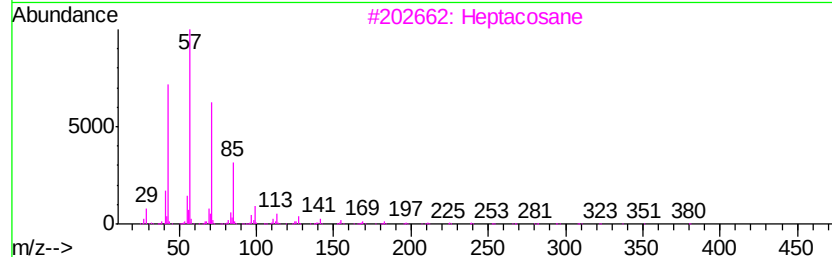
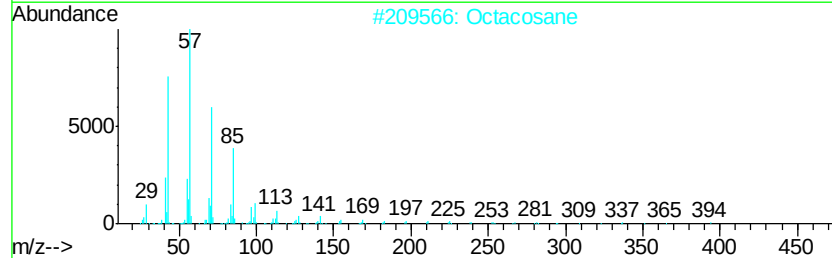
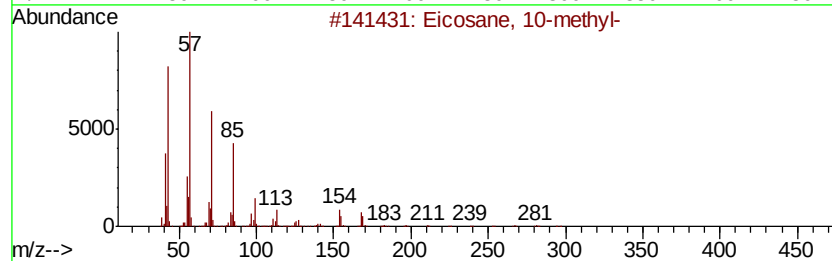
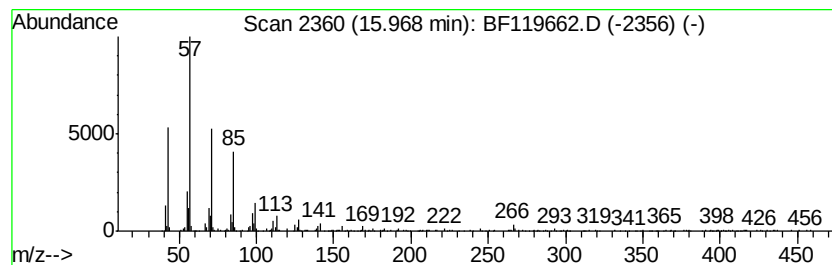
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Eicosane, 10-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	7.86 ng	423934	Perylene-d12	15.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 10-methyl-	296	C21H44	054833-23-7	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Heptacosane	380	C27H56	000593-49-7	90
4			Hexadecane, 3-methyl-	240	C17H36	006418-43-5	87
5			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF033120\
 Data File : BF119662.D
 Acq On : 31 Mar 2020 19:55
 Operator : MA/SJ
 Sample : L2055-07
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

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

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
2-Pentanone, 4-hy...	5.04	2.2	ng	188926	1	6.83	1709620	20.0
n-Hexadecanoic acid	11.90	8.4	ng	715244	4	11.37	1704170	20.0
Octadecanoic acid	12.68	2.6	ng	225374	4	11.37	1704170	20.0
Sulfurous acid, 2...	13.19	2.8	ng	221270	5	14.02	1598540	20.0
1-Dodecanol, 2-oc...	13.87	17.6	ng	1403780	5	14.02	1598540	20.0
Octadecane	14.49	5.3	ng	423697	5	14.02	1598540	20.0
Behenic alcohol	14.52	14.9	ng	1187180	5	14.02	1598540	20.0
Heneicosane	14.80	2.4	ng	128928	6	15.49	1078170	20.0
13-Octadecenal	14.94	5.9	ng	316467	6	15.49	1078170	20.0
Heptadecane, 9-he...	15.14	9.8	ng	528996	6	15.49	1078170	20.0
1-Docosene	15.19	12.1	ng	654270	6	15.49	1078170	20.0
Eicosane, 10-methyl-	15.97	7.9	ng	423934	6	15.49	1078170	20.0