

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032720\
 Data File : BF119599.D
 Acq On : 28 Mar 2020 6:27
 Operator : CG/JU
 Sample : L2029-03
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-1C-(0-2)

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	2.216	18	22	28	rVB	114078	135902	1.77%	0.226%
2	5.039	495	502	510	rBV	874882	1119409	14.54%	1.864%
3	5.445	565	571	574	rBV	6751731	6422900	83.43%	10.697%
4	6.457	737	743	746	rBV	5943057	6256382	81.27%	10.420%
5	6.833	803	807	810	rBV	1879512	1632073	21.20%	2.718%
6	6.986	829	833	837	rBV	5157422	4754677	61.76%	7.919%
7	7.392	897	902	905	rBV	3919866	3669725	47.67%	6.112%
8	8.116	1020	1025	1028	rBV	2527616	2121750	27.56%	3.534%
9	9.198	1203	1209	1212	rBV	7787945	7452268	96.81%	12.411%
10	9.310	1220	1228	1232	rVB2	90858	104080	1.35%	0.173%
11	9.586	1271	1275	1279	rBV	548535	426485	5.54%	0.710%
12	9.874	1319	1324	1327	rBV	2951674	2528994	32.85%	4.212%
13	10.663	1453	1458	1461	rBV	4535991	3987177	51.79%	6.640%
14	11.363	1572	1577	1580	rBV	3170509	2715645	35.28%	4.523%
15	12.774	1814	1817	1820	rBV	470644	363671	4.72%	0.606%
16	12.851	1828	1830	1834	rVB	100450	81257	1.06%	0.135%
17	12.951	1842	1847	1851	rBV	7642639	7698145	100.00%	12.821%
18	13.186	1883	1887	1894	rBV	100764	95149	1.24%	0.158%
19	13.480	1934	1937	1941	rBV	328155	267134	3.47%	0.445%
20	13.527	1942	1945	1947	rBV	143351	115289	1.50%	0.192%
21	13.857	1997	2001	2021	rBV	394443	718127	9.33%	1.196%
22	14.004	2021	2026	2029	rBV	2309015	2186131	28.40%	3.641%
23	14.174	2051	2055	2059	rBV	358453	309370	4.02%	0.515%
24	14.480	2103	2107	2111	rBV	579596	501201	6.51%	0.835%
25	14.786	2155	2159	2164	rBV	570206	559760	7.27%	0.932%
26	14.862	2168	2172	2177	rVB	89402	80246	1.04%	0.134%
27	15.127	2212	2217	2226	rBV	516981	592729	7.70%	0.987%
28	15.462	2268	2274	2278	rBV2	1434726	1786589	23.21%	2.975%
29	15.509	2278	2282	2291	rVB	435905	596135	7.74%	0.993%
30	15.945	2350	2356	2362	rBV	302907	463294	6.02%	0.772%
31	16.456	2437	2443	2451	rBV	124593	214997	2.79%	0.358%
32	17.050	2538	2544	2553	rBV3	42592	86865	1.13%	0.145%

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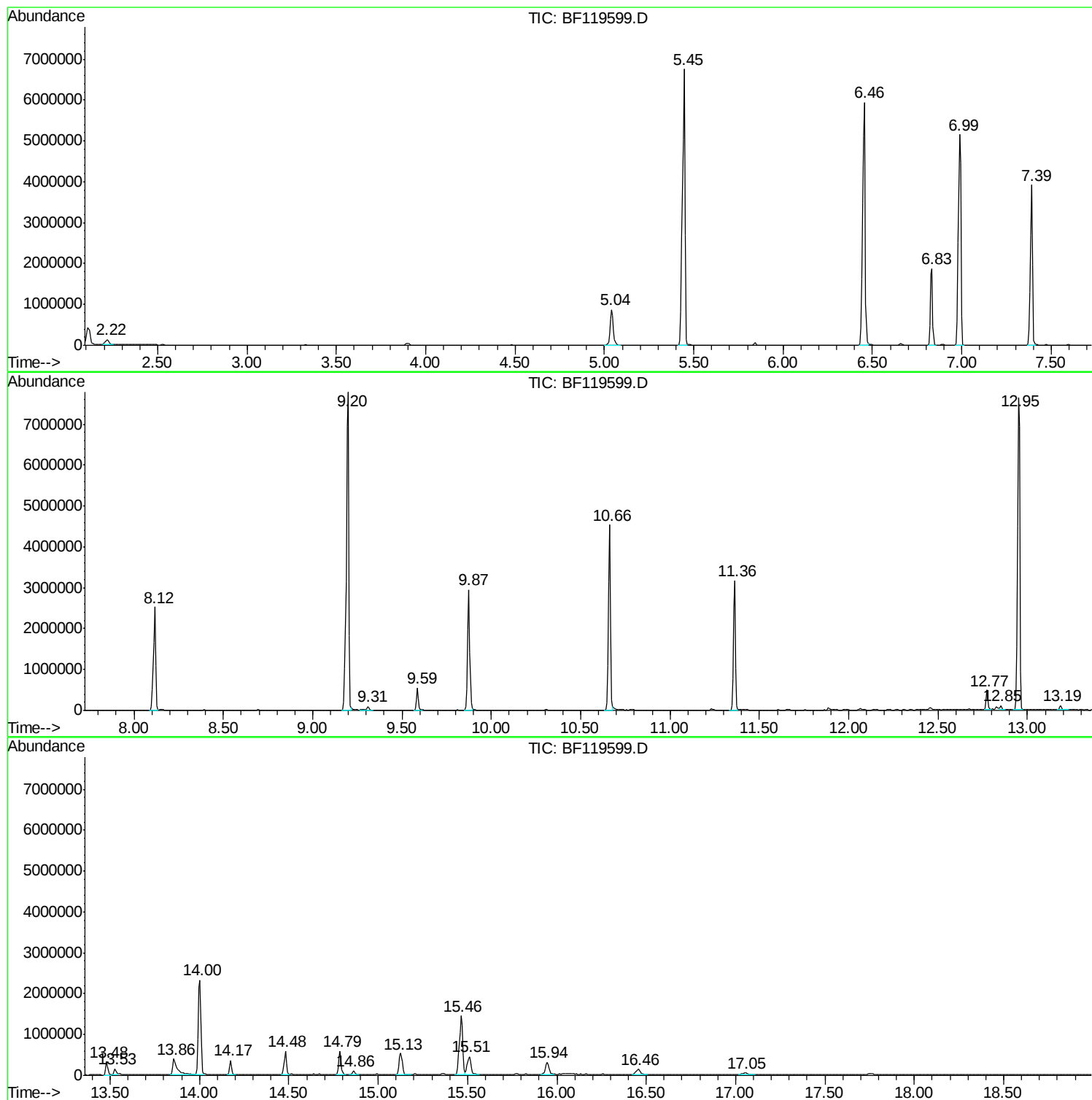
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF031820.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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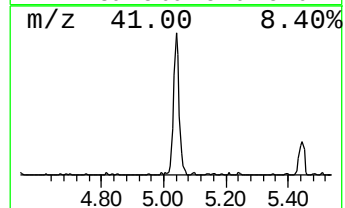
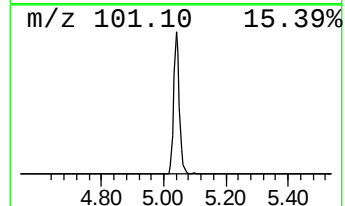
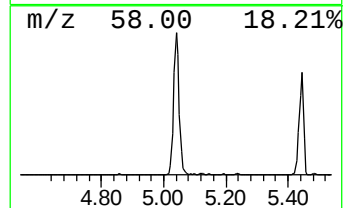
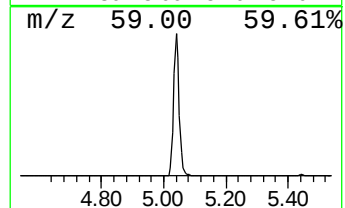
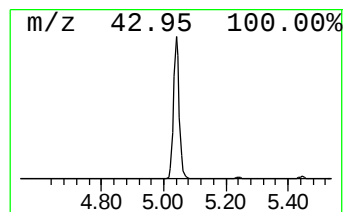
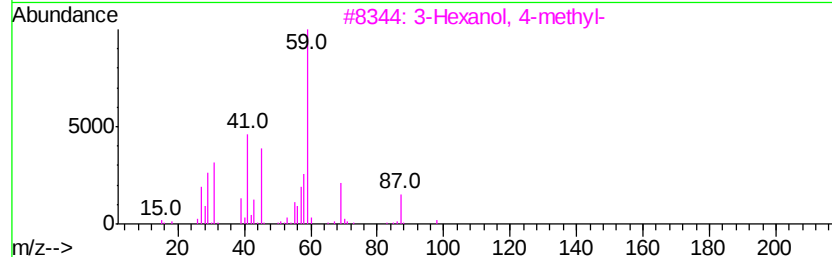
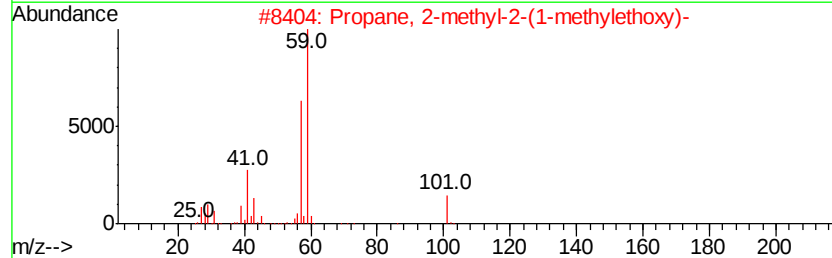
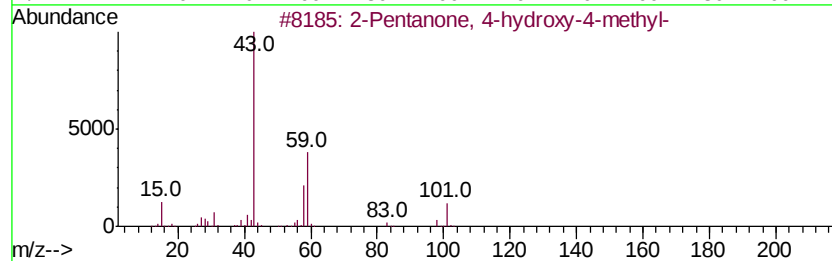
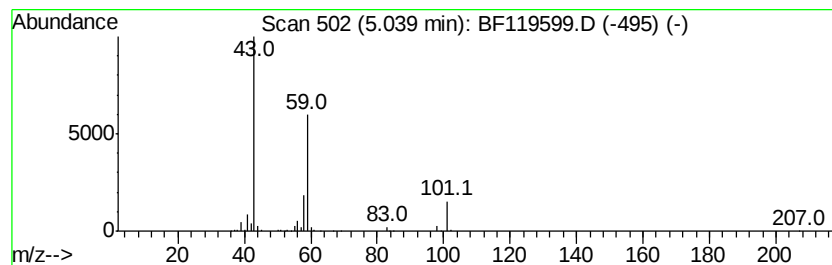
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	13.72 ng	1119410	1,4-Dichlorobenzene-d4	6.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	



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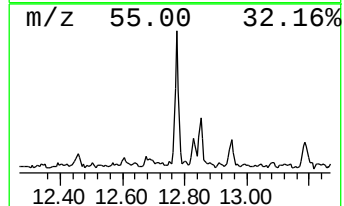
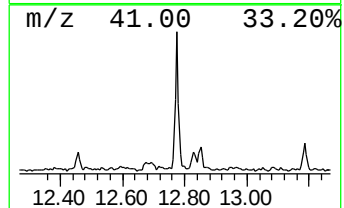
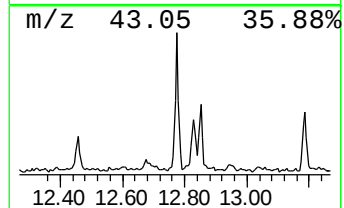
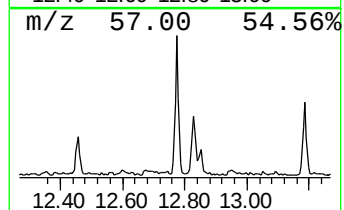
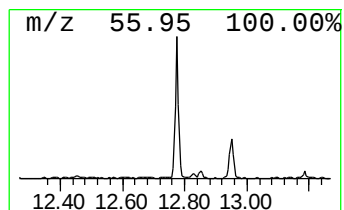
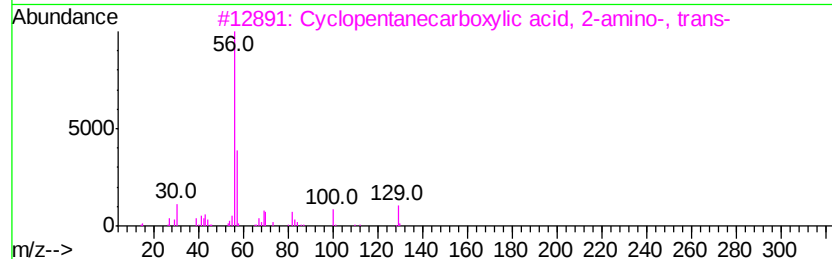
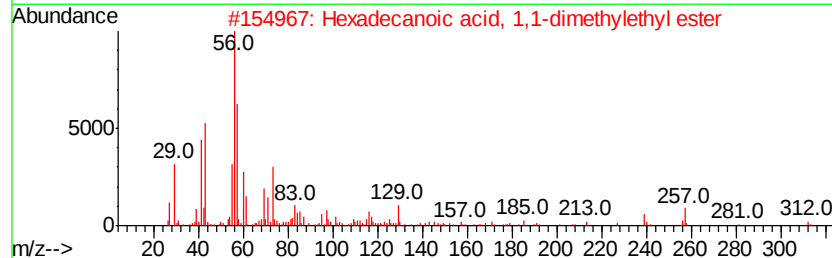
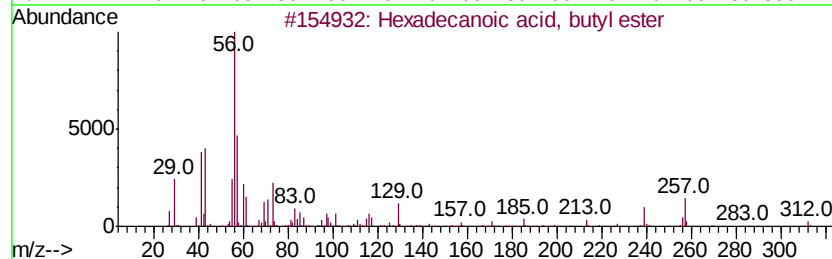
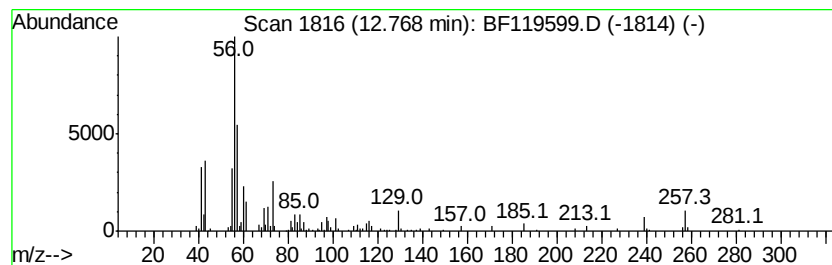
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	3.33 ng	363671	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
5		Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	40



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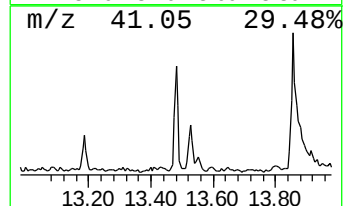
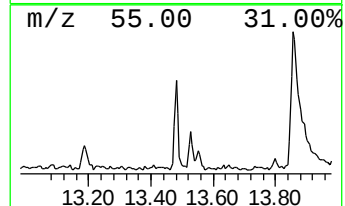
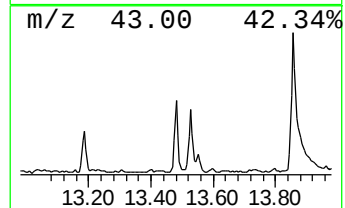
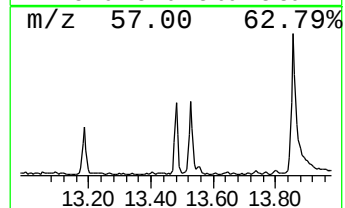
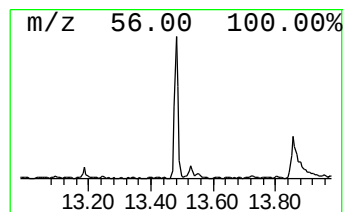
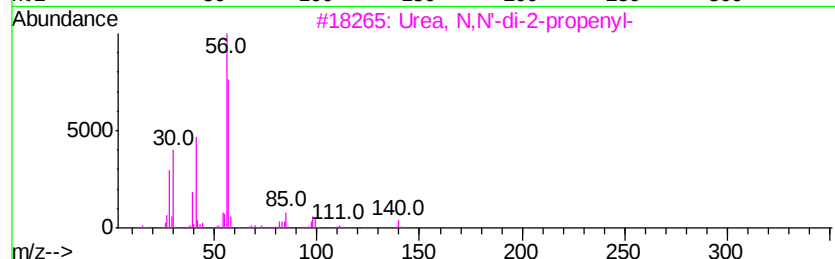
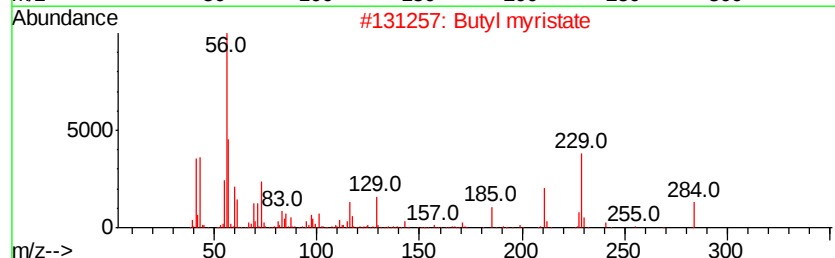
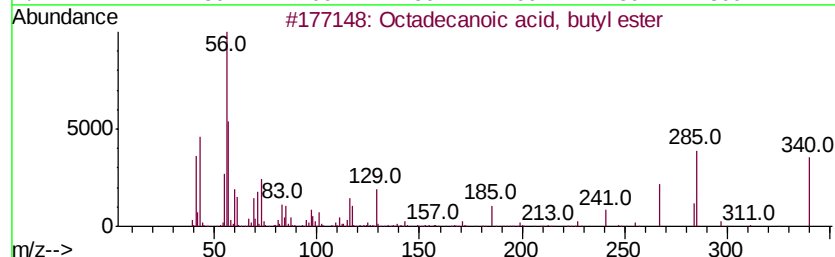
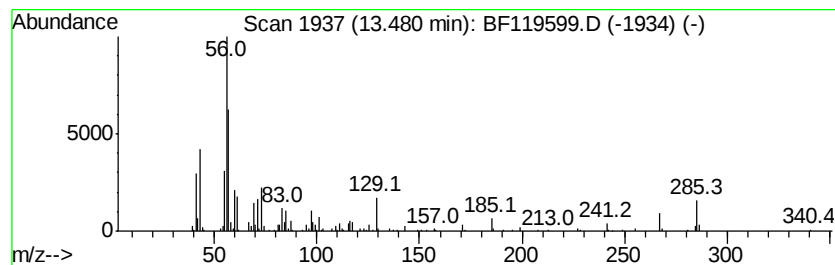
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	2.44 ng	267134	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		Butyl myristate	284	C18H36O2	000110-36-1	72
3		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38
4		Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	37
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	32



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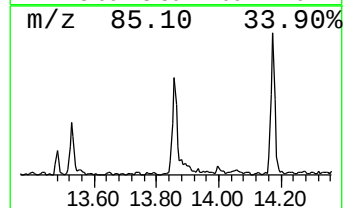
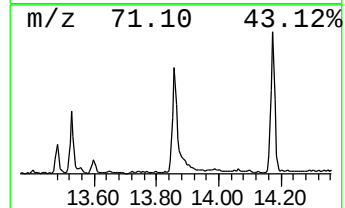
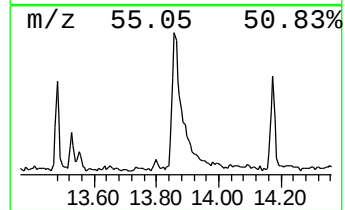
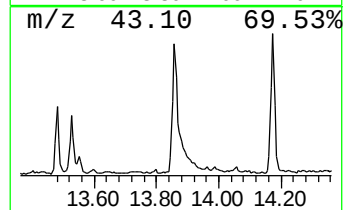
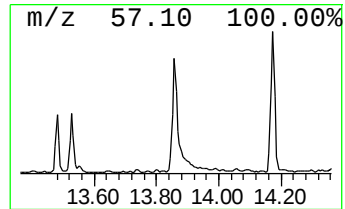
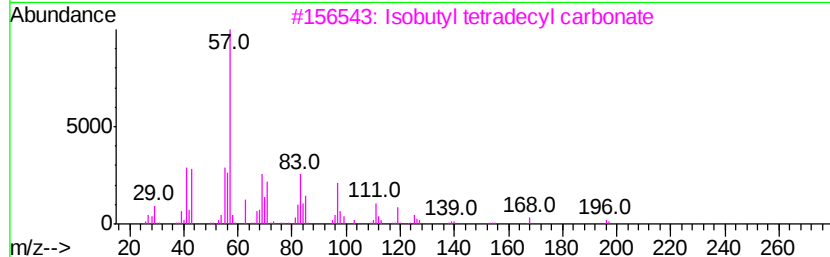
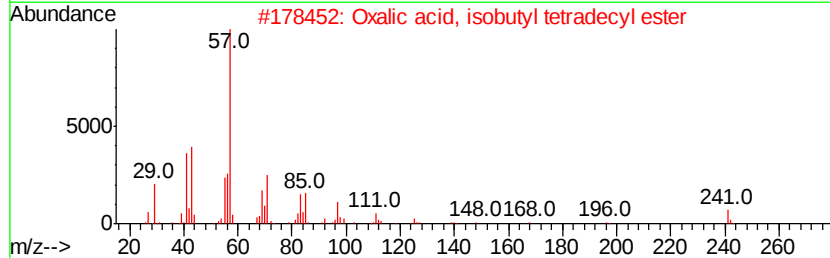
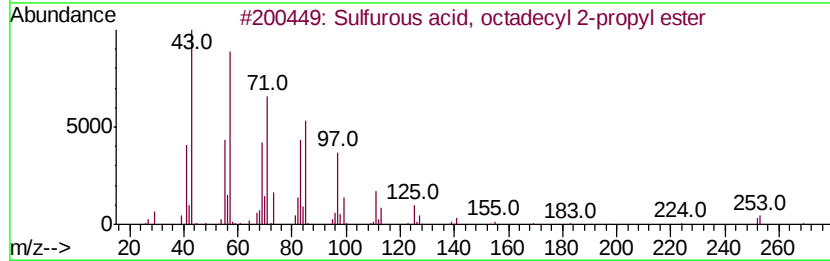
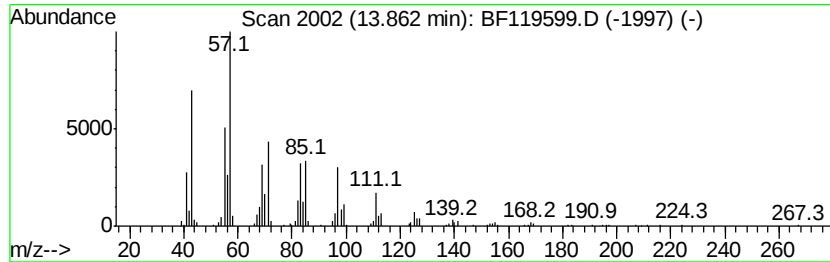
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Sulfurous acid, octadecyl 2... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	6.57 ng	718127	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	81
2		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	74
3		Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	68
4		Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	62
5		Tetradecane	198	C14H30	000629-59-4	53



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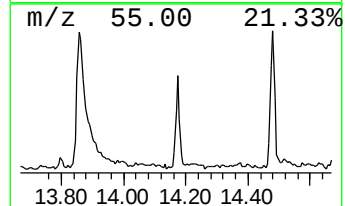
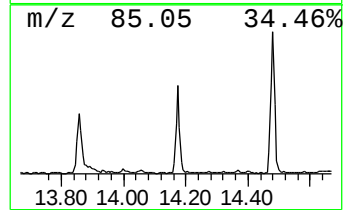
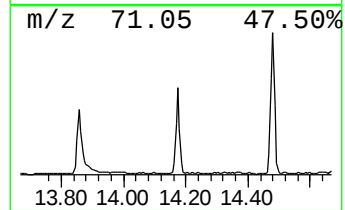
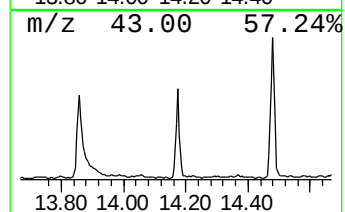
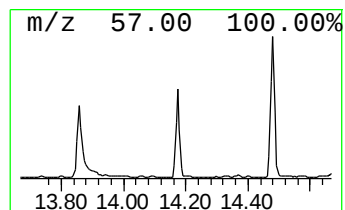
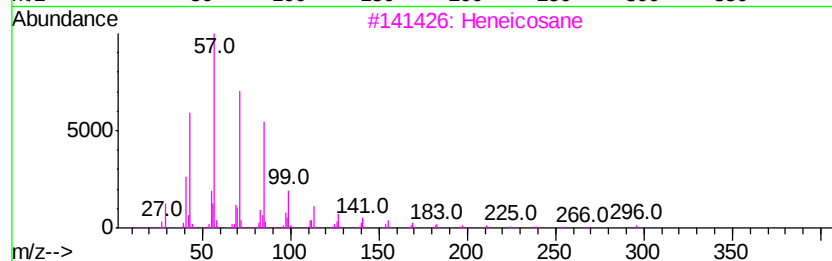
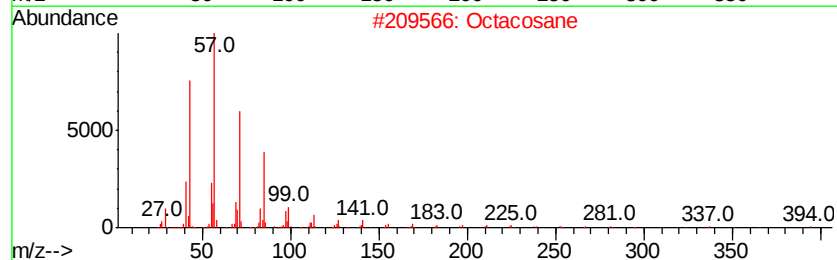
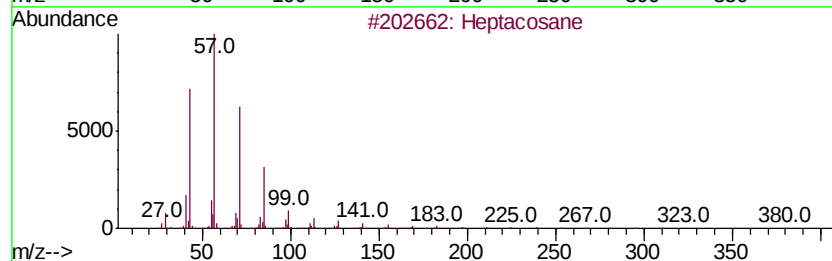
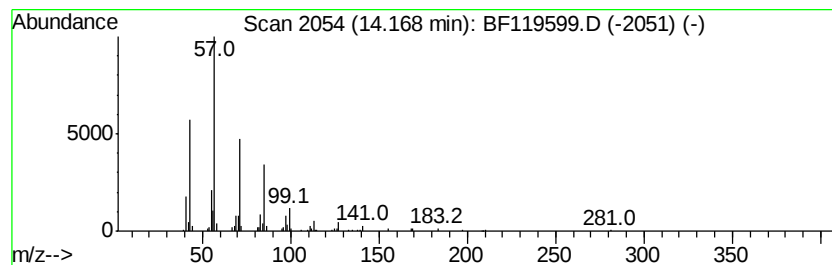
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 Peak Number 6 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	2.83 ng	309370	Chrysene-d12	14.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Octacosane		394	C28H58	000630-02-4	91
3	Heneicosane		296	C21H44	000629-94-7	90
4	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	87
5	Nonadecane, 9-methyl-		282	C20H42	013287-24-6	86



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ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1C-(0-2)

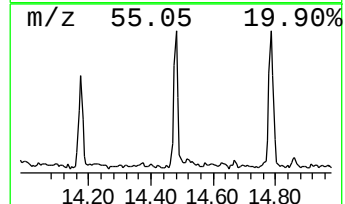
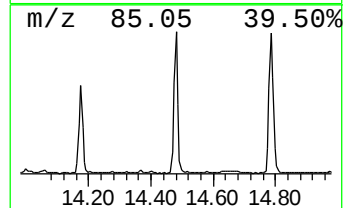
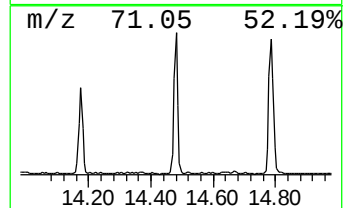
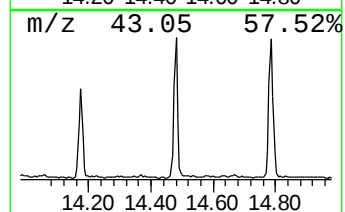
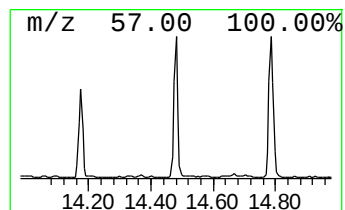
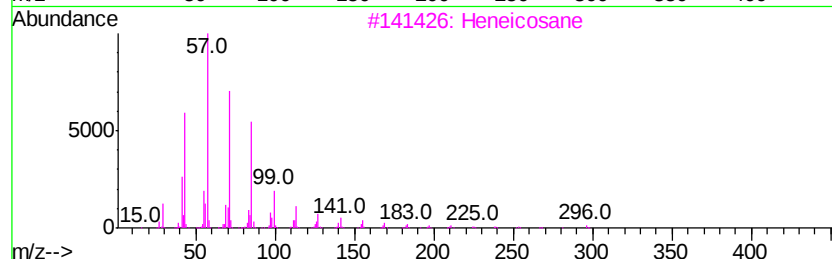
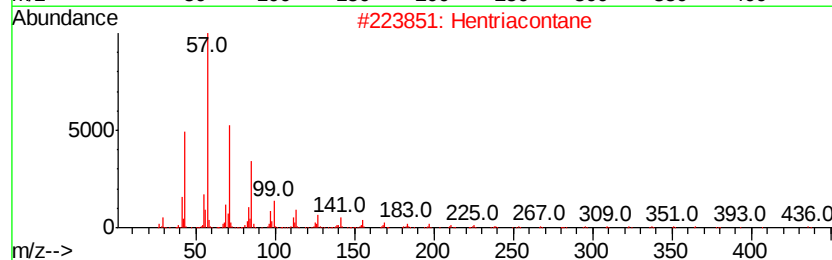
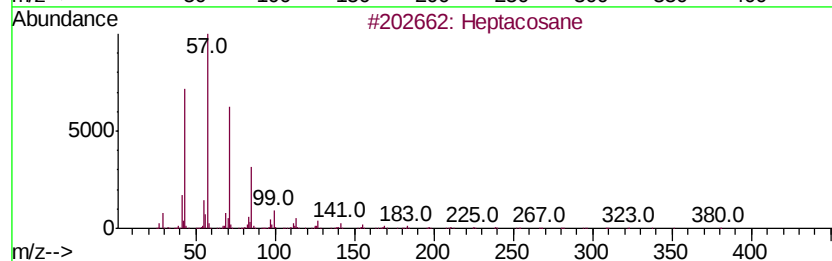
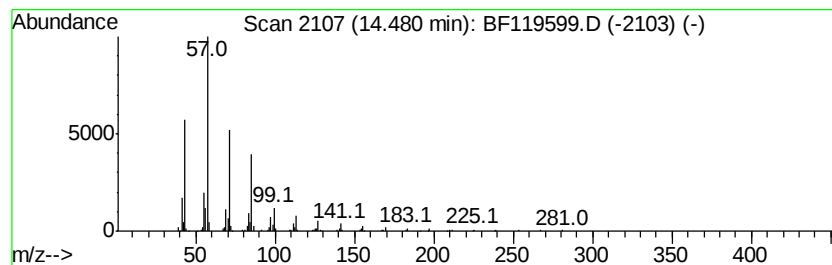
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.48	4.59 ng	501201	Chrysene-d12	14.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	91
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Octadecane	254	C18H38	000593-45-3	90
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032720\
Data File : BF119599.D
Acq On : 28 Mar 2020 6:27
Operator : CG/JU
Sample : L2029-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

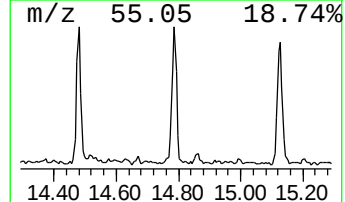
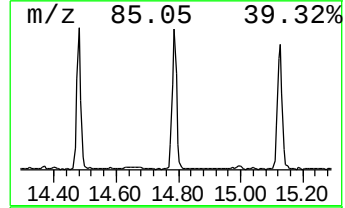
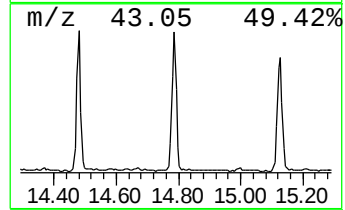
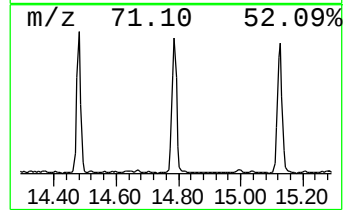
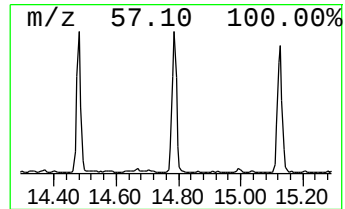
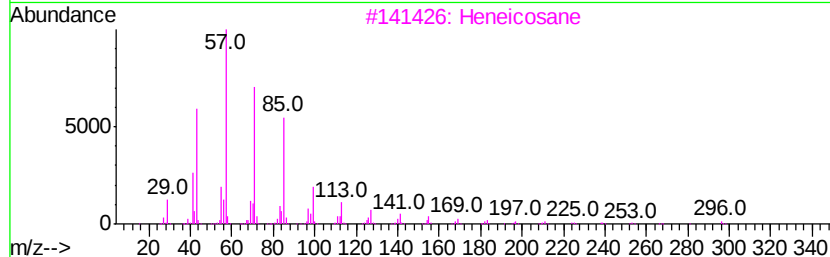
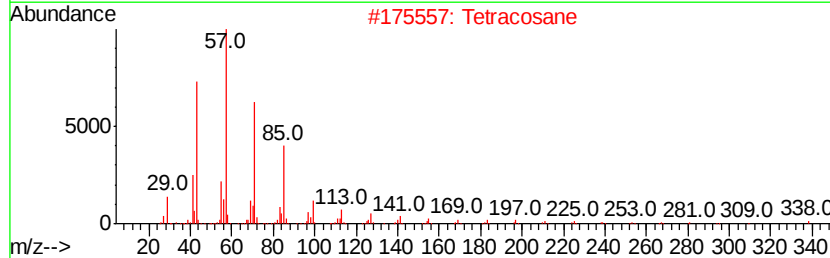
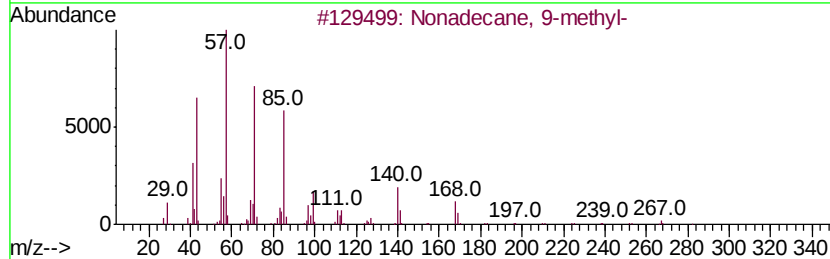
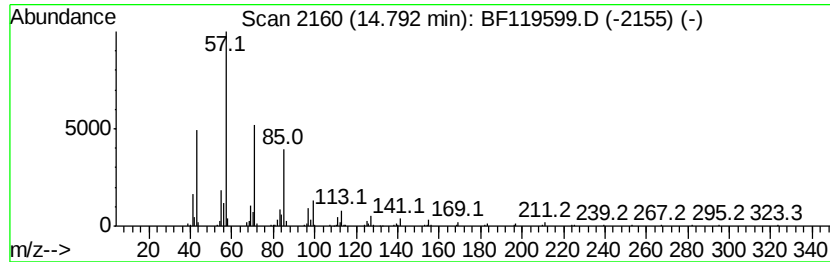
Instrument :
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ClientSampleId :
SB-1C-(0-2)

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 8 Nonadecane, 9-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.79	6.27 ng	559760	Perylene-d12	15.46	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2	Tetracosane	338	C24H50	000646-31-1	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Hentriacontane	437	C31H64	000630-04-6	90
5	Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032720\
Data File : BF119599.D
Acq On : 28 Mar 2020 6:27
Operator : CG/JU
Sample : L2029-03
Misc :
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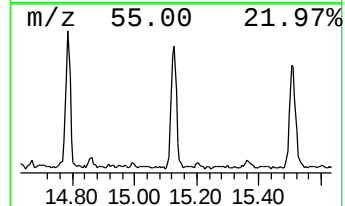
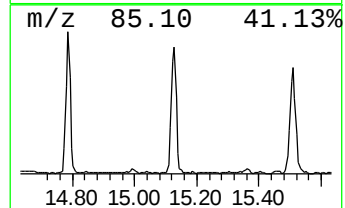
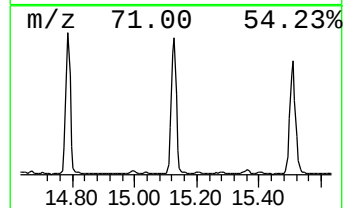
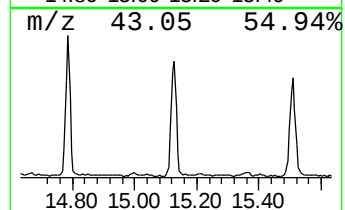
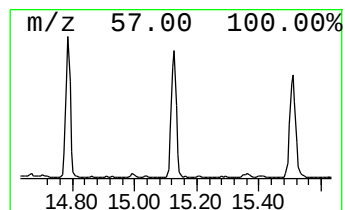
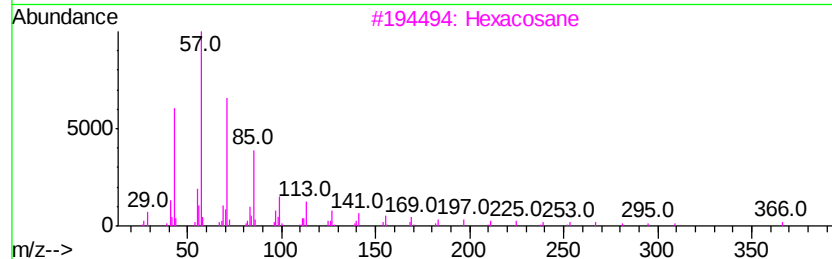
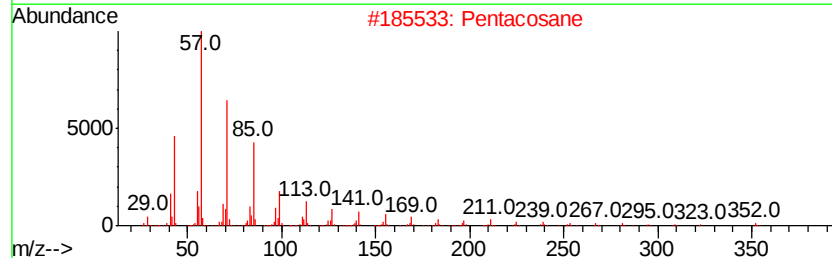
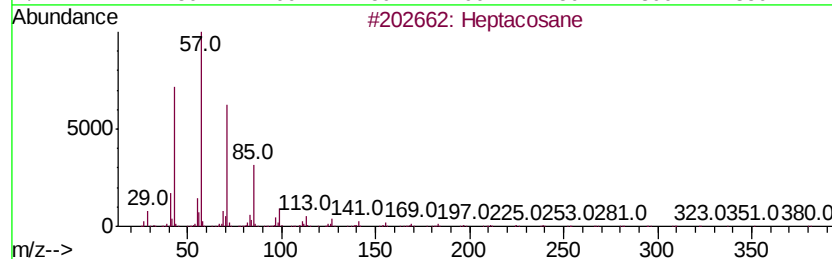
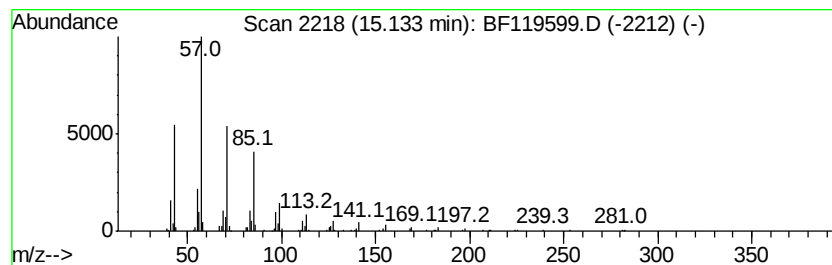
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	6.64 ng	592729	Perylene-d12	15.46
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane	380 C27H56	000593-49-7	91
2	Pentacosane	352 C25H52	000629-99-2	91
3	Hexacosane	366 C26H54	000630-01-3	91
4	Octadecane	254 C18H38	000593-45-3	90
5	2-methyloctacosane	408 C29H60	1000376-72-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032720\
Data File : BF119599.D
Acq On : 28 Mar 2020 6:27
Operator : CG/JU
Sample : L2029-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1C-(0-2)

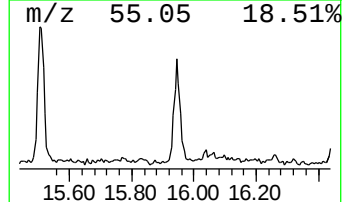
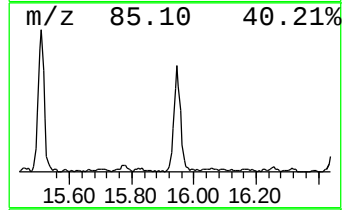
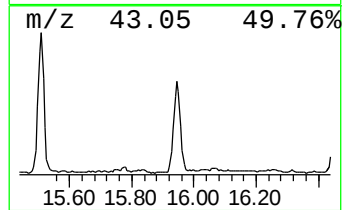
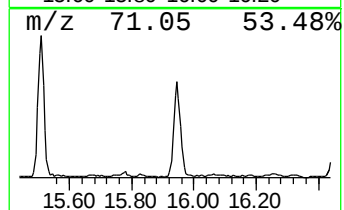
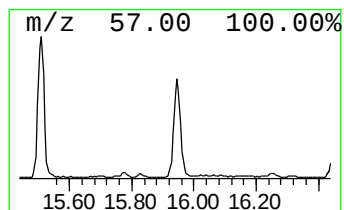
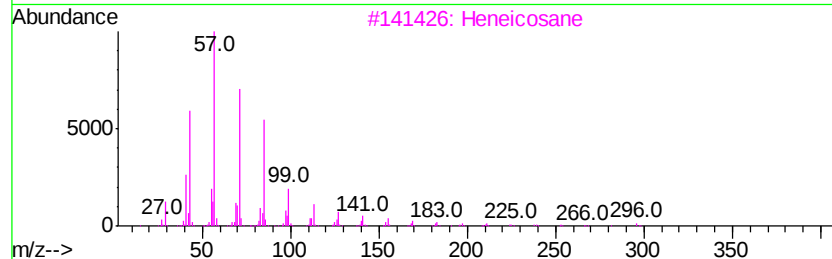
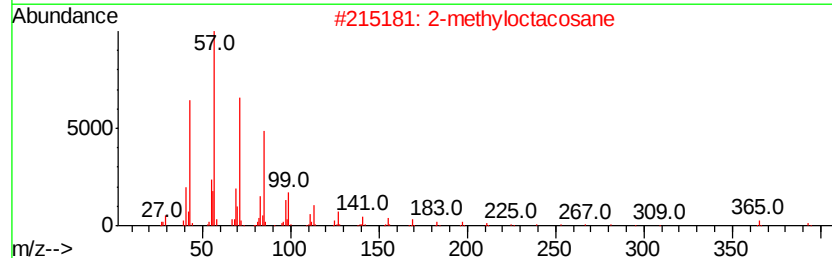
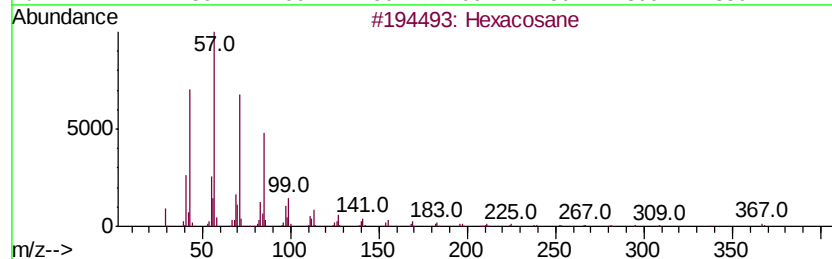
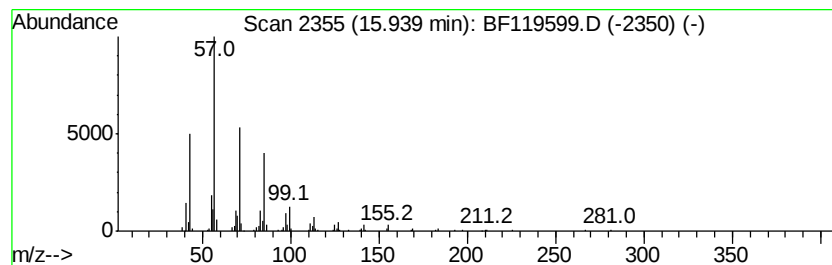
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	5.19 ng	463294	Perylene-d12	15.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5		Docosane	310	C22H46	000629-97-0	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032720\
Data File : BF119599.D
Acq On : 28 Mar 2020 6:27
Operator : CG/JU
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Misc :
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ClientSampleId :
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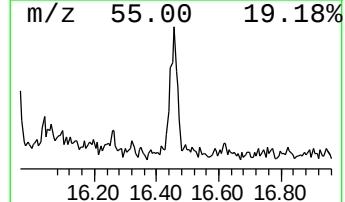
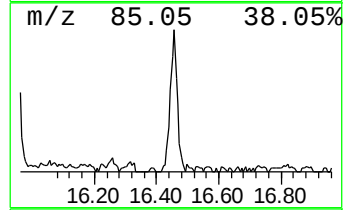
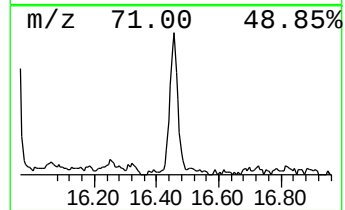
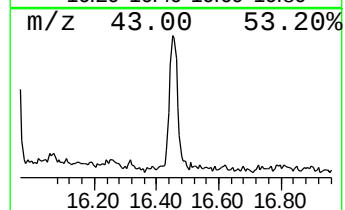
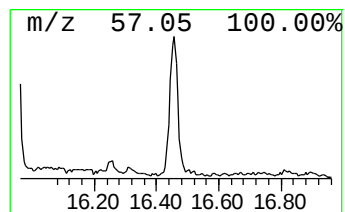
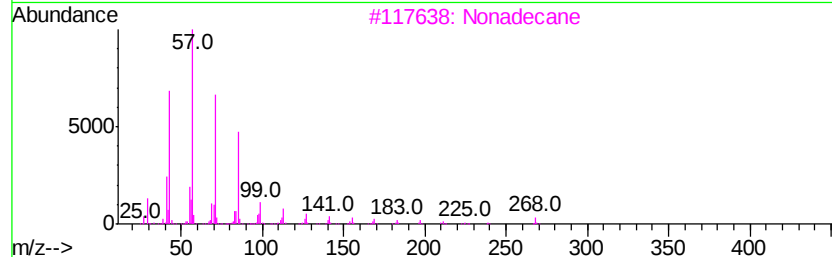
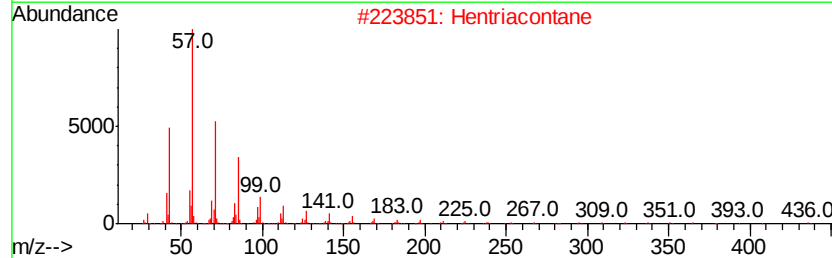
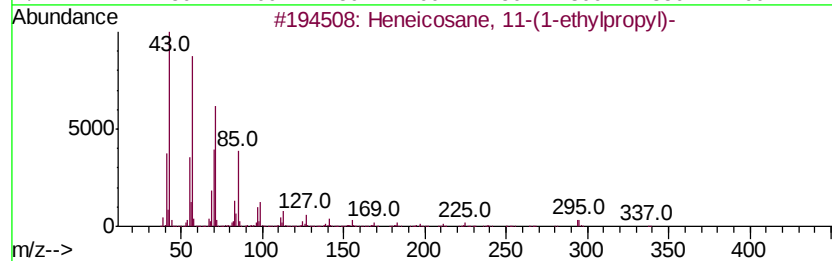
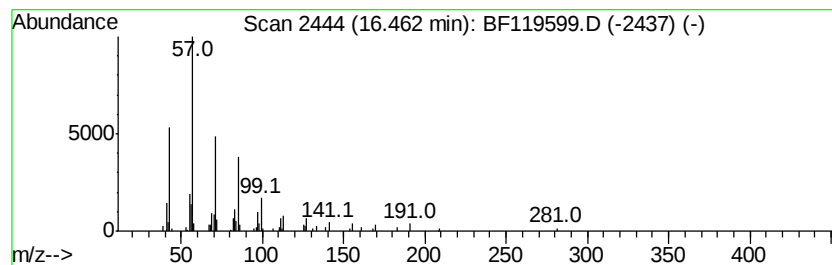
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane, 11-(1-ethylpro... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	2.41 ng	214997	Perylene-d12	15.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
2		Hentriacontane	437	C31H64	000630-04-6	86
3		Nonadecane	268	C19H40	000629-92-5	83
4		Octacosane	394	C28H58	000630-02-4	74
5		Heptacosane	380	C27H56	000593-49-7	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032720\
Data File : BF119599.D
Acq On : 28 Mar 2020 6:27
Operator : CG/JU
Sample : L2029-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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
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Hexadecanoic acid...	12.77	3.3	ng	363671	5	14.00	2186130	20.0
Octadecanoic acid...	13.48	2.4	ng	267134	5	14.00	2186130	20.0
Sulfurous acid, o...	13.86	6.6	ng	718127	5	14.00	2186130	20.0
Heptacosane	14.17	2.8	ng	309370	5	14.00	2186130	20.0
Hentriacontane	14.48	4.6	ng	501201	5	14.00	2186130	20.0
Nonadecane, 9-met...	14.79	6.3	ng	559760	6	15.46	1786590	20.0
Pentacosane	15.13	6.6	ng	592729	6	15.46	1786590	20.0
Hexacosane	15.94	5.2	ng	463294	6	15.46	1786590	20.0
Heneicosane, 11-(...	16.46	2.4	ng	214997	6	15.46	1786590	20.0