

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011720\
 Data File : BF118580.D
 Acq On : 18 Jan 2020 1:33
 Operator : JU
 Sample : L1173-02
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 0053-DECANT-H2O-COMP-5

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-BF011720.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	2.163	7	13	20	rVB	5421234	7534623	53.54%	7.021%
2	5.098	503	512	519	rBV	545543	644011	4.58%	0.600%
3	5.498	575	580	584	rBV	5510859	5445359	38.69%	5.074%
4	6.504	746	751	759	rVB	4603025	4131514	29.36%	3.850%
5	6.657	772	777	780	rBV	9983428	9665483	68.68%	9.006%
6	6.886	812	816	820	rBV	2656047	2124161	15.09%	1.979%
7	6.945	823	826	830	rBV	213861	172712	1.23%	0.161%
8	7.045	839	843	846	rBV	9292299	8091656	57.50%	7.540%
9	7.445	905	911	914	rBV	6572083	6364685	45.22%	5.930%
10	8.169	1030	1034	1038	rBV	3312082	2694400	19.15%	2.511%
11	9.245	1212	1217	1221	rBV	12164296	12171056	86.48%	11.341%
12	9.633	1279	1283	1286	rBV	902690	688889	4.89%	0.642%
13	9.927	1328	1333	1336	rBV	3383638	3192243	22.68%	2.974%
14	10.339	1399	1403	1406	rBV	657293	519010	3.69%	0.484%
15	10.710	1461	1466	1469	rBV	8852043	8728240	62.02%	8.133%
16	11.410	1580	1585	1588	rBV	3678632	3396695	24.14%	3.165%
17	11.939	1670	1675	1684	rBV	1300279	1313035	9.33%	1.223%
18	12.721	1804	1808	1821	rBV	673767	700630	4.98%	0.653%
19	12.998	1850	1855	1858	rBV	13739674	14073647	100.00%	13.113%
20	13.886	2003	2006	2021	rBV	2888558	2989076	21.24%	2.785%
21	14.045	2028	2033	2036	rBV	3776075	3545576	25.19%	3.304%
22	14.215	2058	2062	2070	rVB	406708	384154	2.73%	0.358%
23	14.521	2110	2114	2120	rBV	738086	667535	4.74%	0.622%
24	14.804	2159	2162	2164	rBV	151625	174764	1.24%	0.163%
25	14.833	2164	2167	2177	rVB	764002	840107	5.97%	0.783%
26	15.174	2221	2225	2236	rBV	800204	922548	6.56%	0.860%
27	15.515	2277	2283	2287	rBV	2762133	3371275	23.95%	3.141%
28	15.562	2287	2291	2304	rVB	678566	903103	6.42%	0.841%
29	16.009	2361	2367	2370	rBV	435008	705842	5.02%	0.658%
30	16.051	2370	2374	2383	rVB	351616	578787	4.11%	0.539%
31	16.521	2449	2454	2465	rVB	207918	389498	2.77%	0.363%
32	17.203	2566	2570	2580	rVB5	79325	197980	1.41%	0.184%

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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
0053-DECANT-H2O-COMP-5

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-BF011720.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

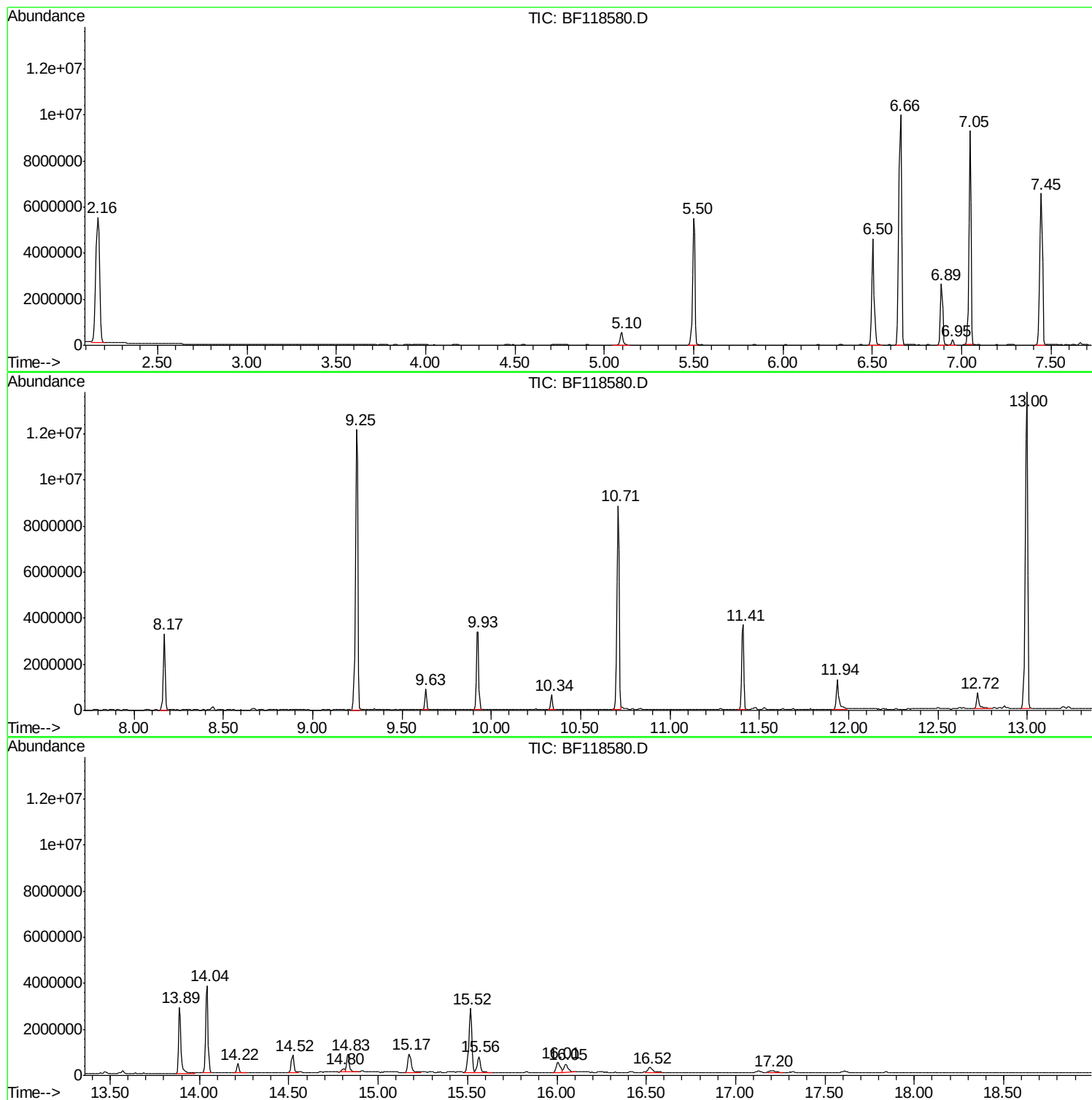
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF011720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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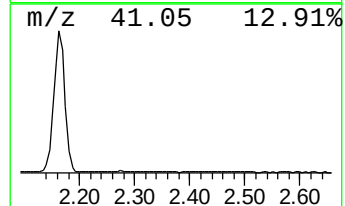
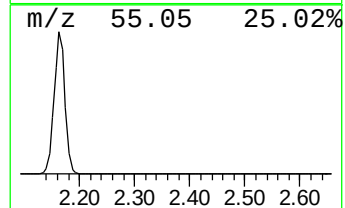
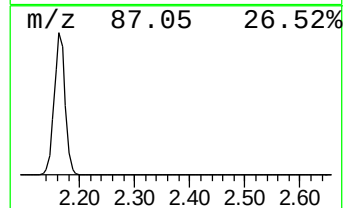
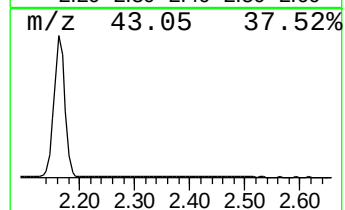
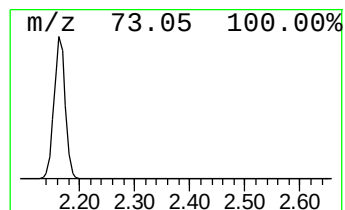
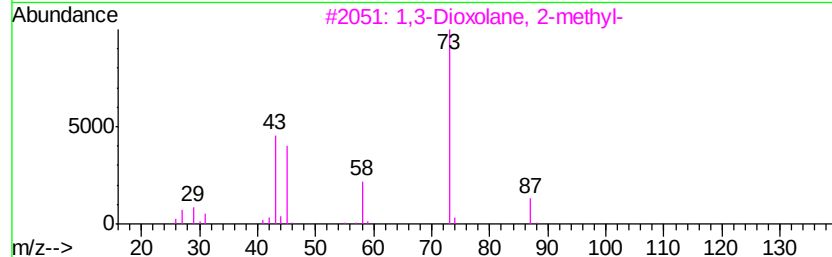
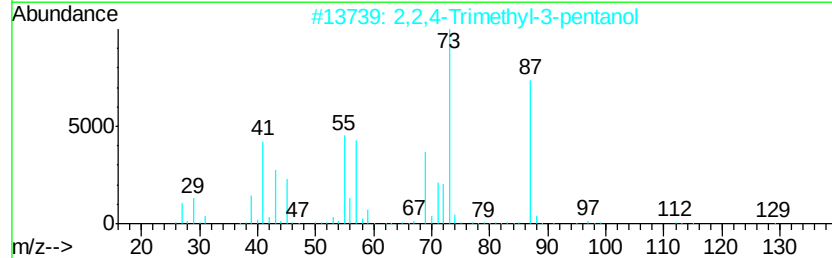
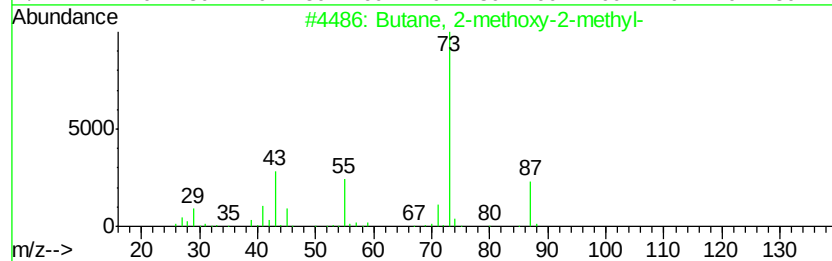
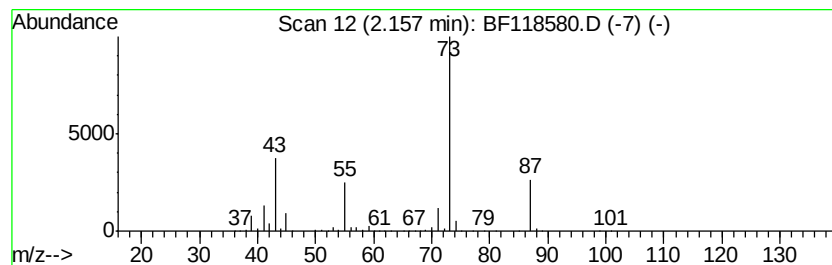
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	70.94 ng	7534620	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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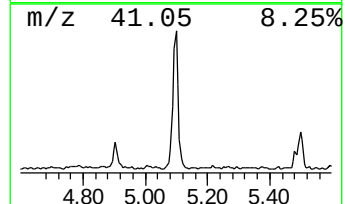
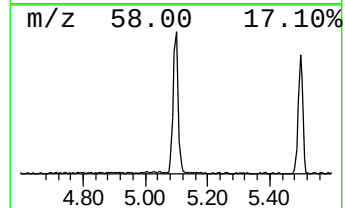
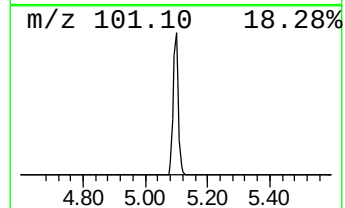
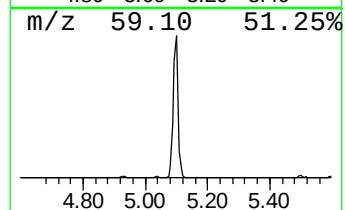
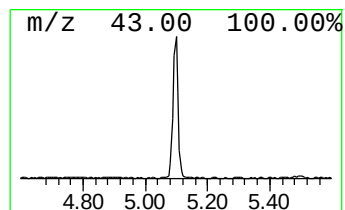
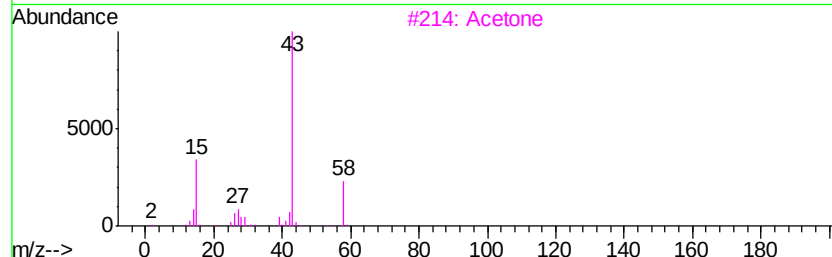
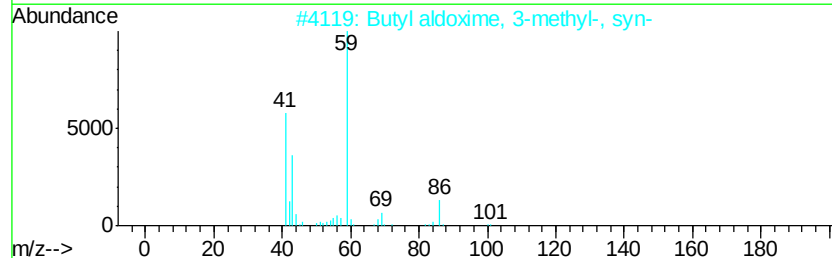
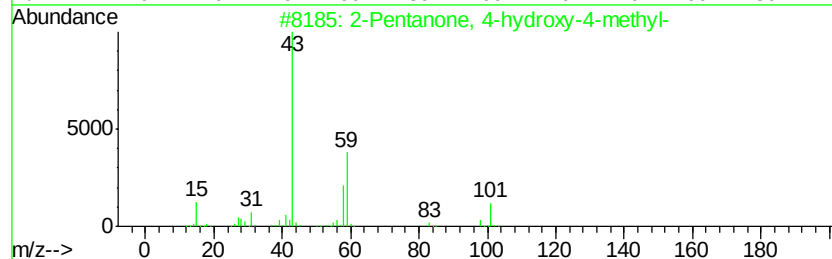
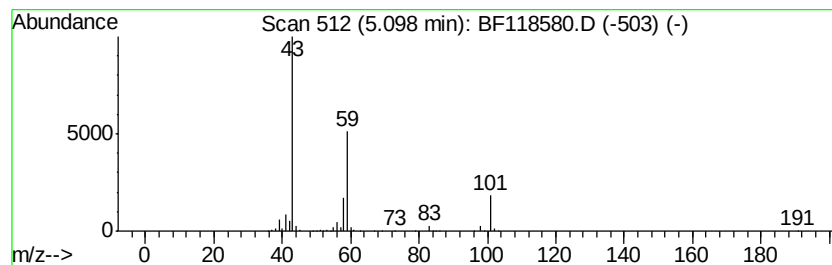
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	6.06 ng	644011	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
3			Acetone	58	C3H6O	000067-64-1	12
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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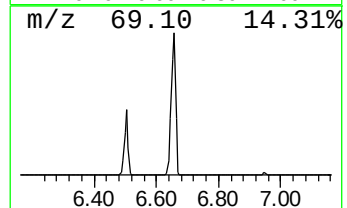
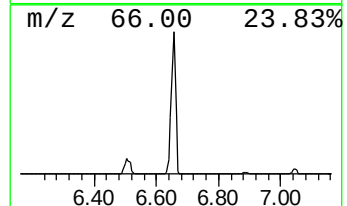
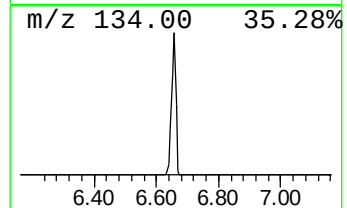
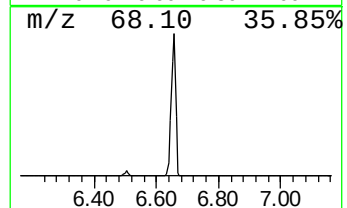
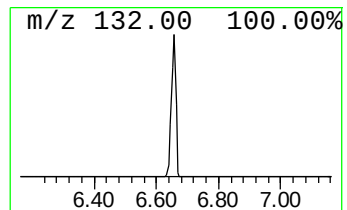
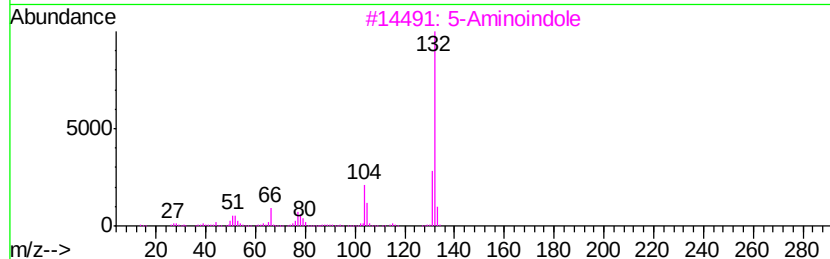
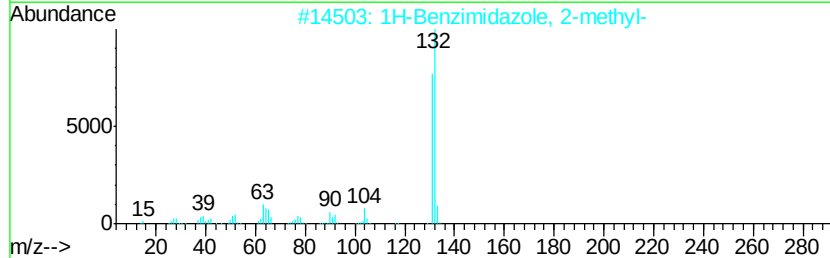
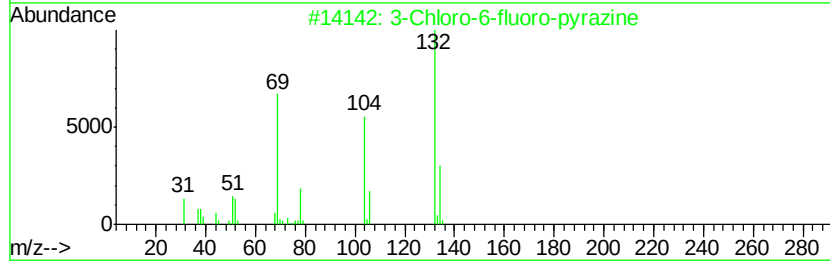
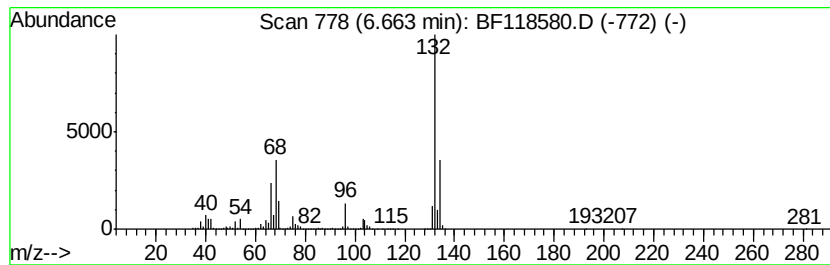
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	91.01 ng	9665480	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		5-Aminoindole	132	C8H8N2	005192-03-0	22
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12



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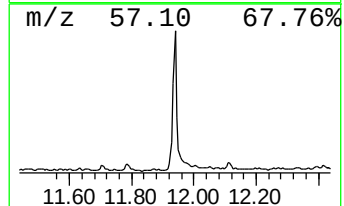
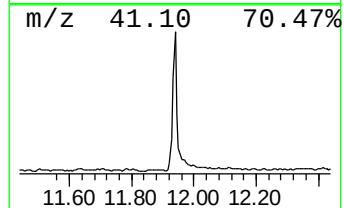
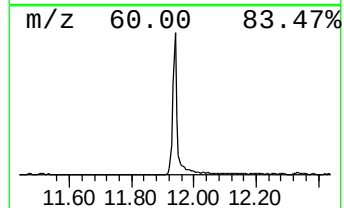
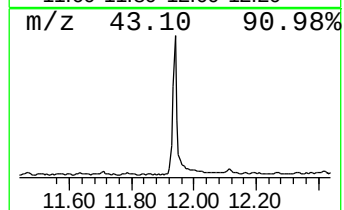
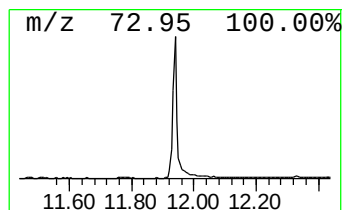
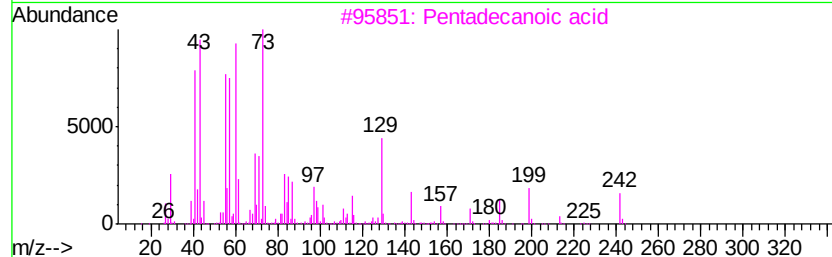
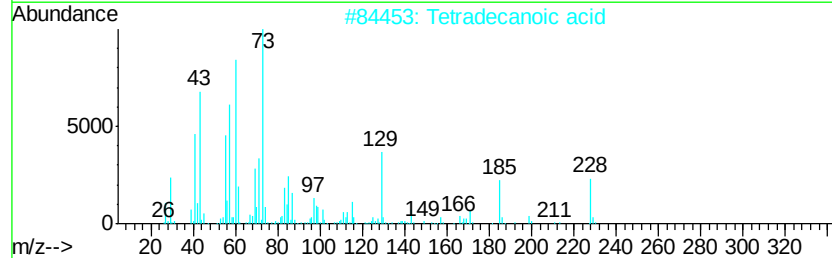
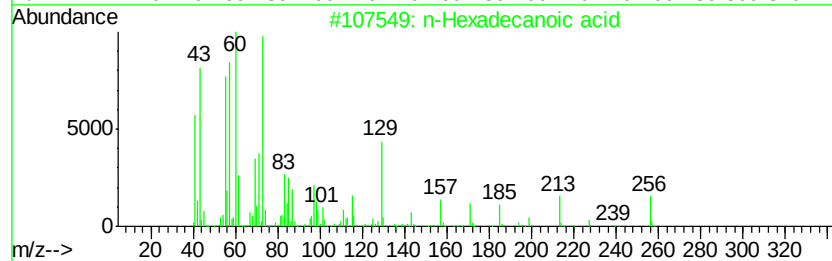
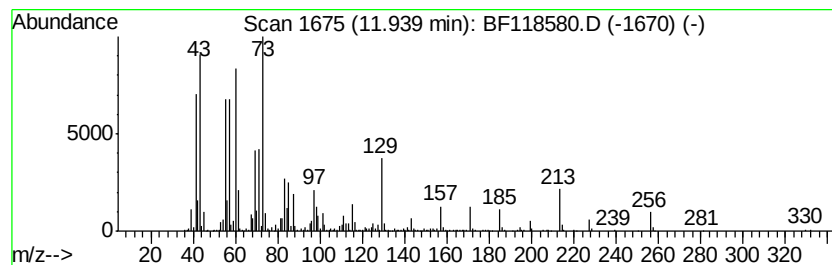
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	7.73 ng	1313040	Phenanthrene-d10	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Octadecanoic acid	284	C18H36O2	000057-11-4	76
5		Tridecanoic acid	214	C13H26O2	000638-53-9	72



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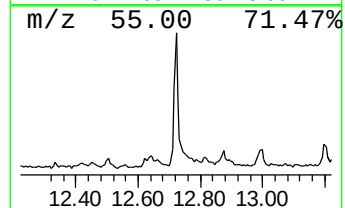
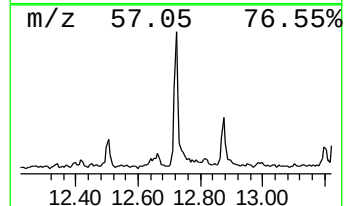
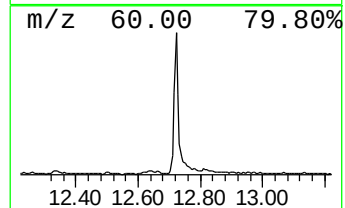
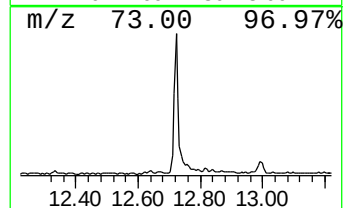
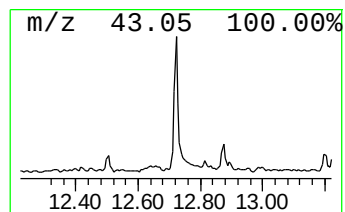
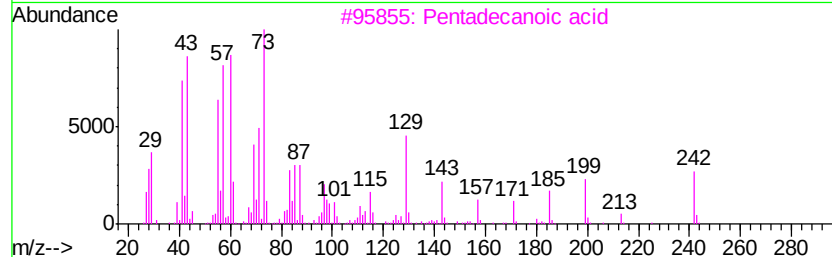
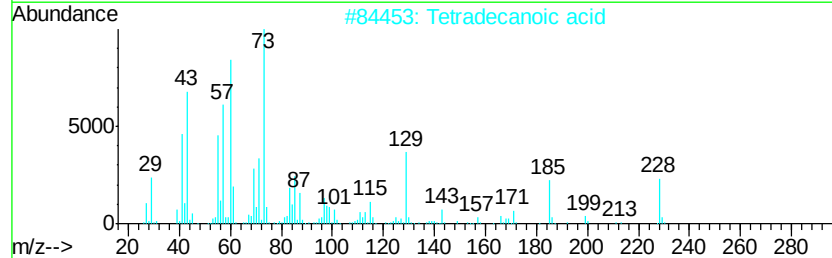
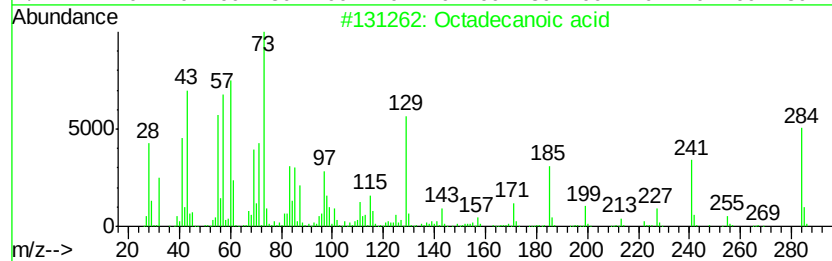
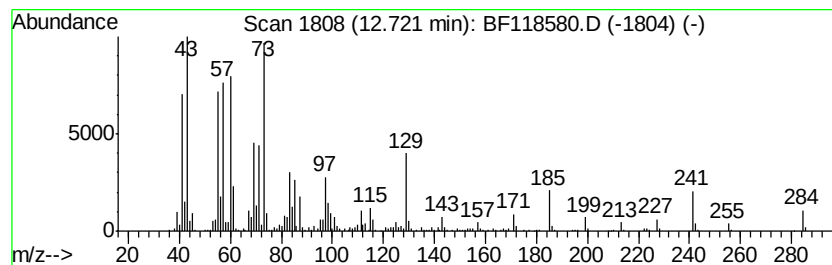
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	4.13 ng	700630	Phenanthrene-d10	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		n-Decanoic acid	172	C10H20O2	000334-48-5	64
5		n-PROPYL NONYL ETHER	186	C12H26O	1000130-69-3	25



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ALS Vial : 21 Sample Multiplier: 1

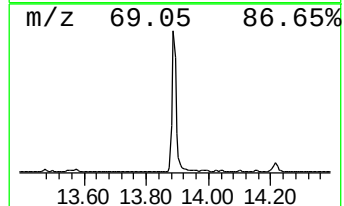
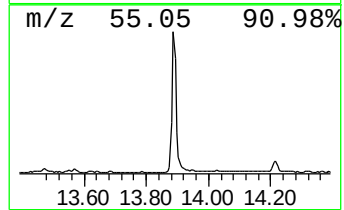
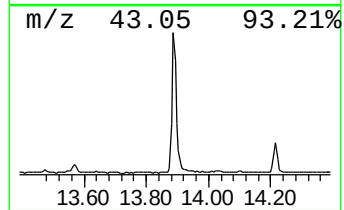
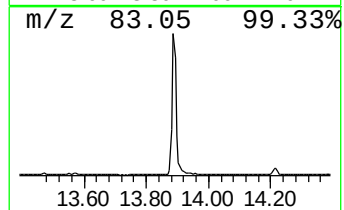
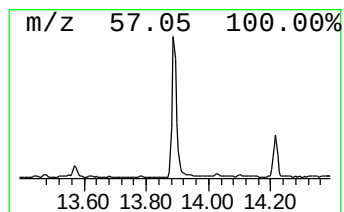
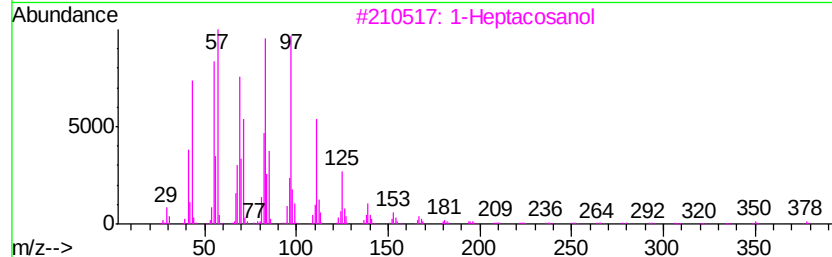
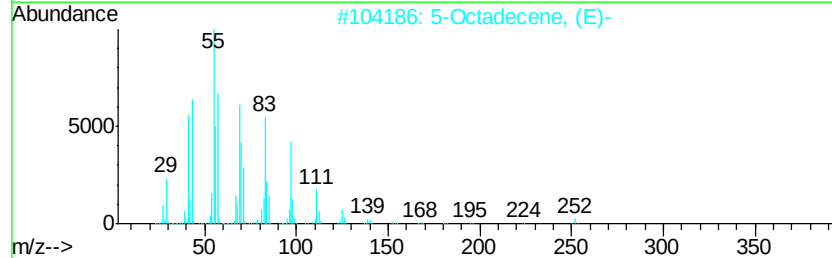
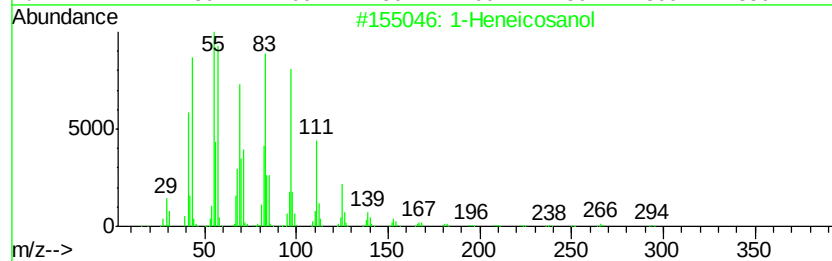
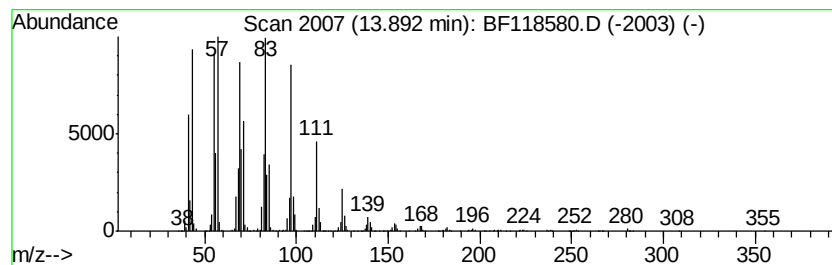
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ClientSampleId :
0053-DECANT-H2O-COMP-5

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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 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	16.86 ng	2989080	Chrysene-d12	14.04
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosanol	312 C21H44O	015594-90-8	95
2	5-Octadecene, (E)-	252 C18H36	007206-21-5	94
3	1-Heptacosanol	396 C27H56O	002004-39-9	94
4	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	94
5	Cyclohexadecane	224 C16H32	000295-65-8	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011720\
Data File : BF118580.D
Acq On : 18 Jan 2020 1:33
Operator : JU
Sample : L1173-02
Misc :
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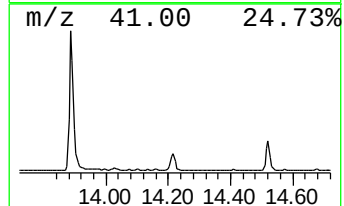
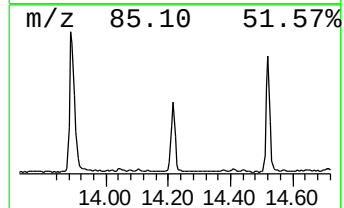
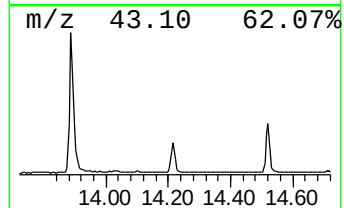
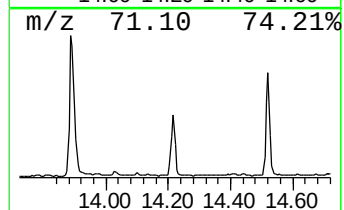
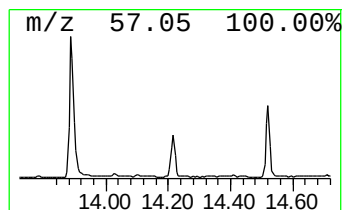
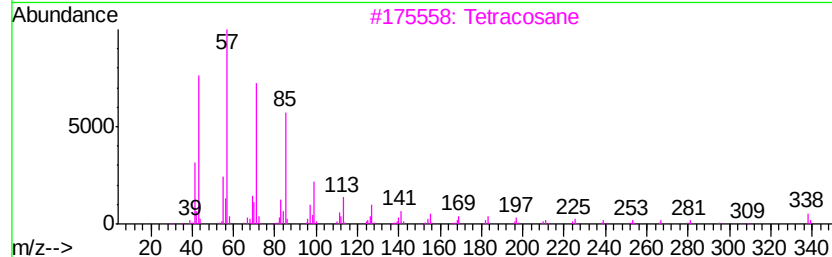
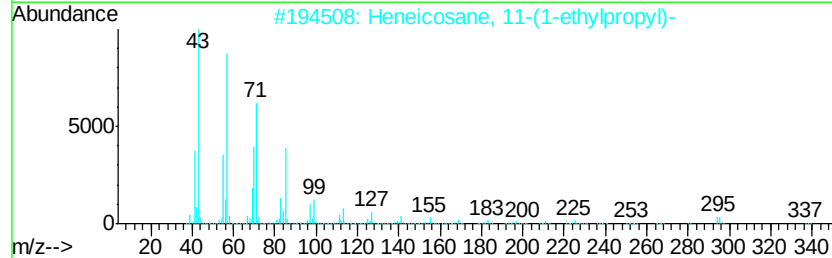
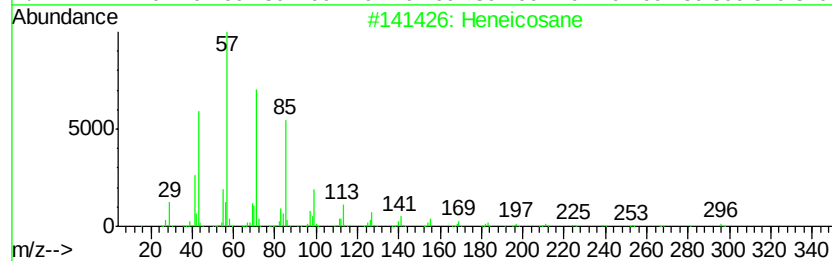
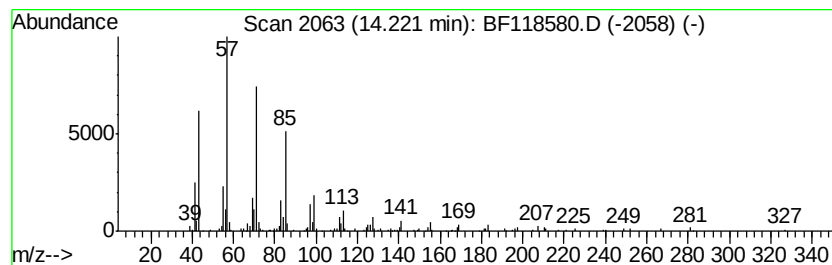
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF011720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.22	2.17 ng	384154	Chrysene-d12	14.04
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	91
2	Heneicosane, 11-(1-ethylpropyl)-	366 C26H54	055282-11-6	91
3	Tetracosane	338 C24H50	000646-31-1	91
4	Eicosane, 7-hexyl-	366 C26H54	055333-99-8	91
5	Pentadecane	212 C15H32	000629-62-9	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011720\
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Sample : L1173-02
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ALS Vial : 21 Sample Multiplier: 1

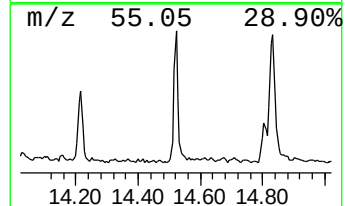
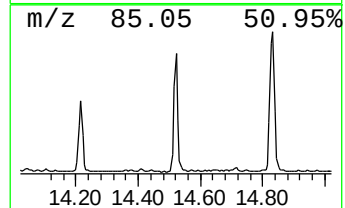
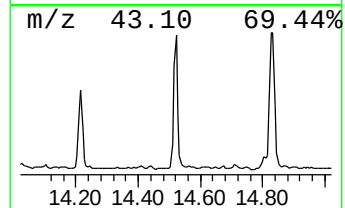
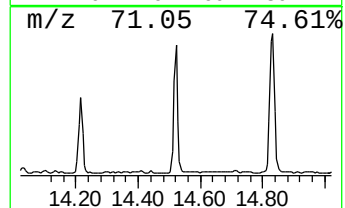
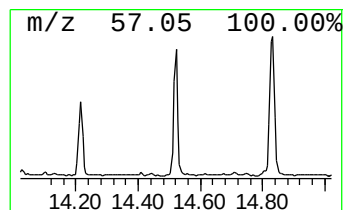
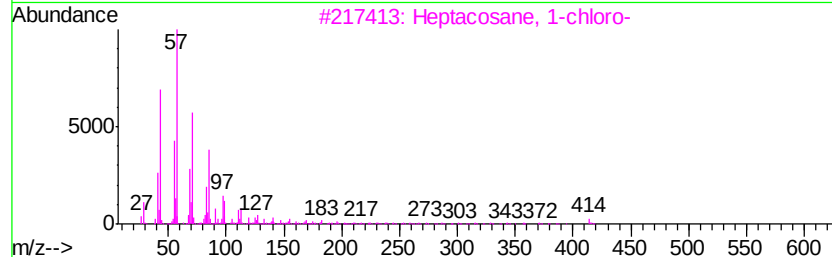
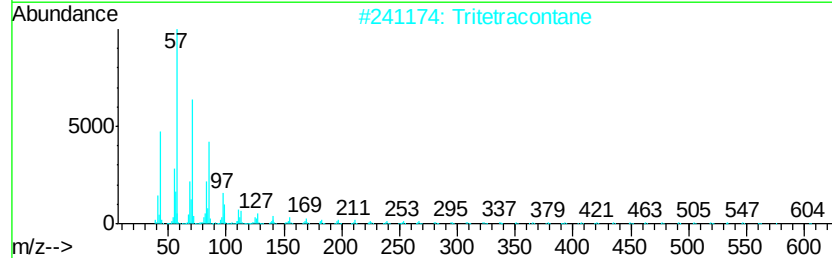
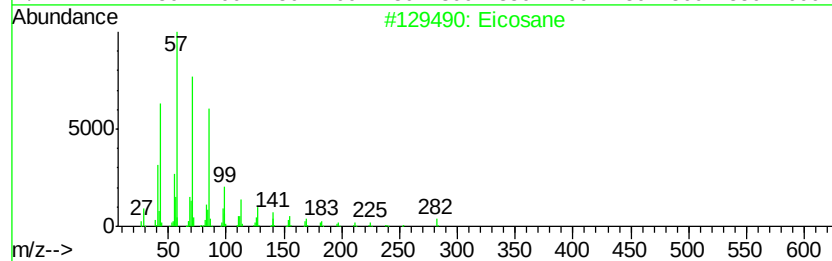
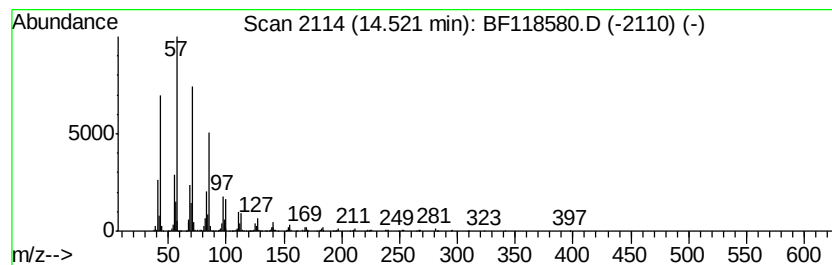
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF011720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	3.77 ng	667535	Chrysene-d12	14.04
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	95
2	Tritetracontane	605 C43H88	007098-21-7	91
3	Heptacosane, 1-chloro-	414 C27H55Cl	062016-79-9	91
4	Sulfurous acid, dodecyl 2-propyl...	292 C15H32O3S	1000309-12-3	91
5	Hexacosane	366 C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011720\
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Acq On : 18 Jan 2020 1:33
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Misc :
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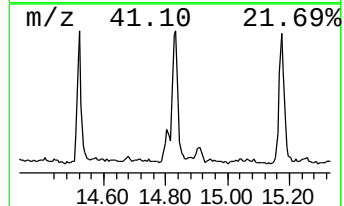
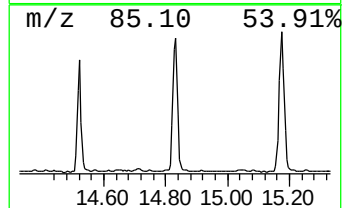
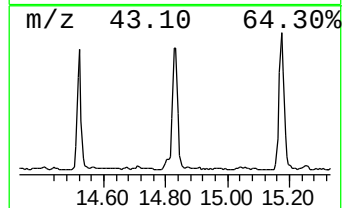
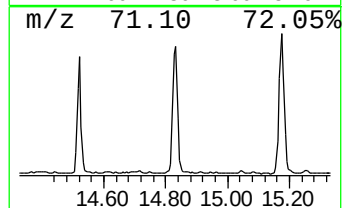
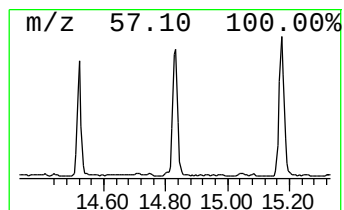
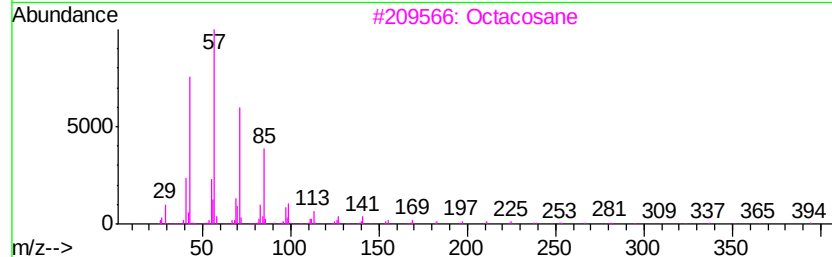
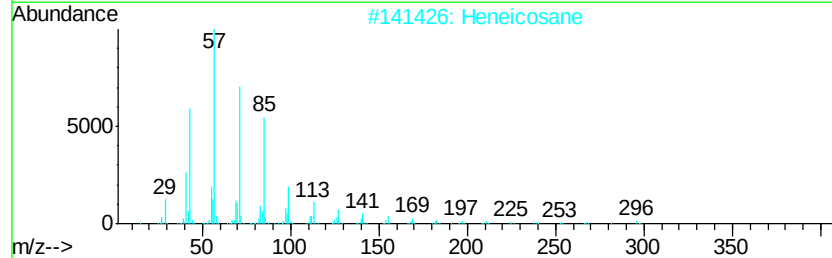
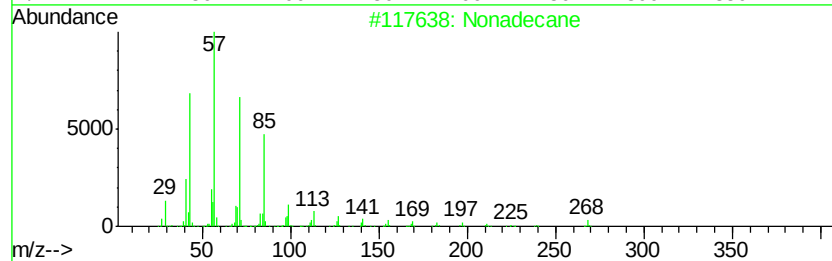
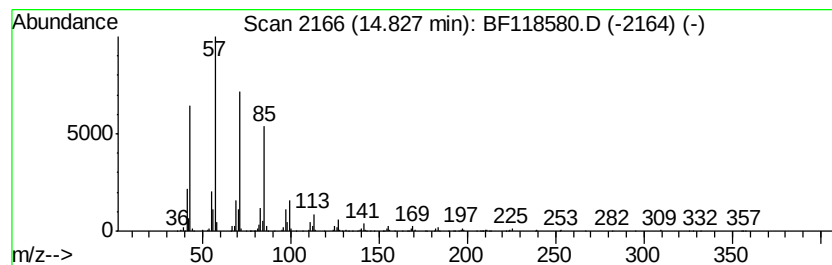
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	4.98 ng	840107	Perylene-d12	15.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonadecane	268 C19H40	000629-92-5	93
2	Heneicosane	296 C21H44	000629-94-7	91
3	Octacosane	394 C28H58	000630-02-4	91
4	Hexacosane	366 C26H54	000630-01-3	91
5	Heneicosane, 11-(1-ethylpropyl)-	366 C26H54	055282-11-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011720\
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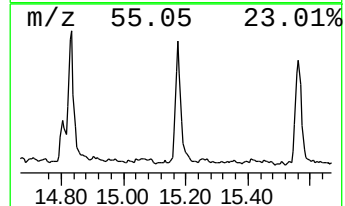
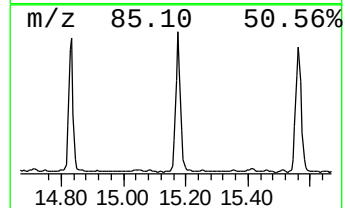
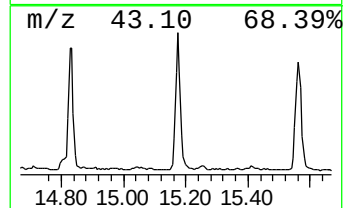
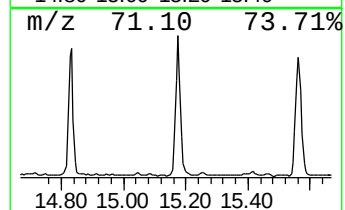
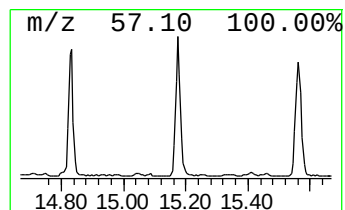
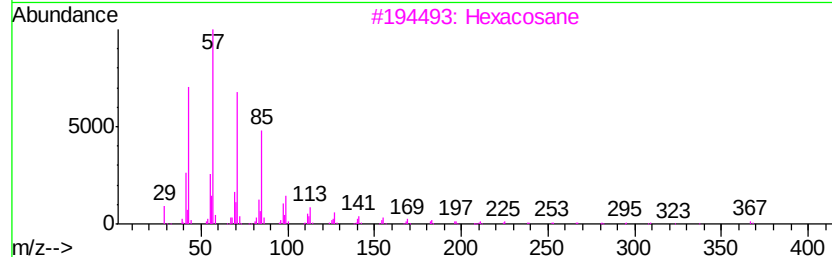
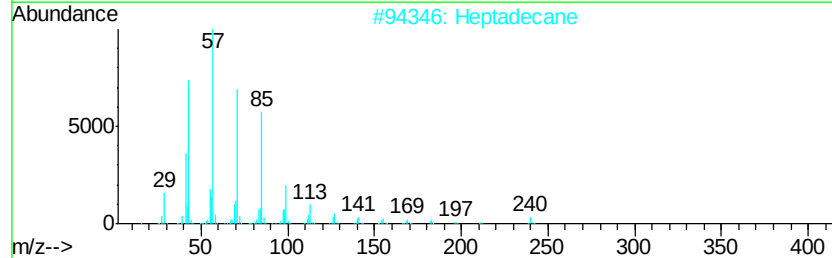
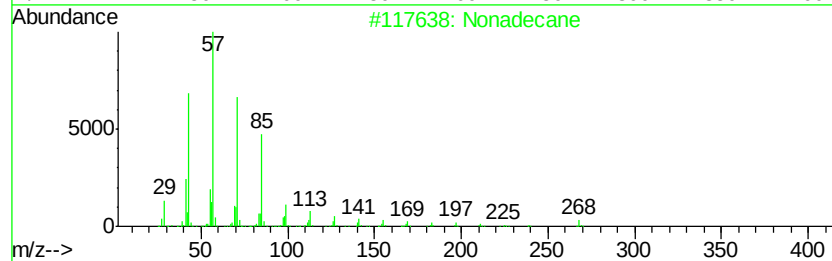
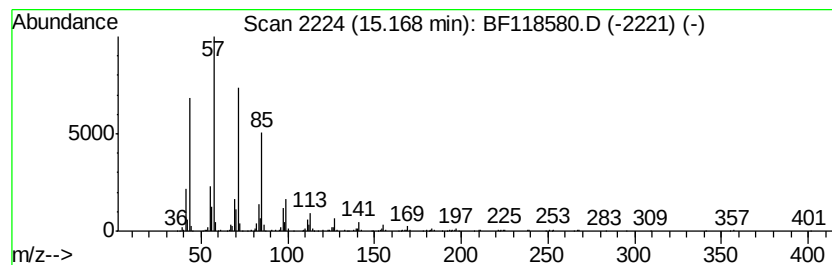
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	5.47 ng	922548	Perylene-d12	15.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonadecane	268 C19H40	000629-92-5	94
2	Heptadecane	240 C17H36	000629-78-7	94
3	Hexacosane	366 C26H54	000630-01-3	91
4	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	91
5	Heneicosane	296 C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011720\
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Acq On : 18 Jan 2020 1:33
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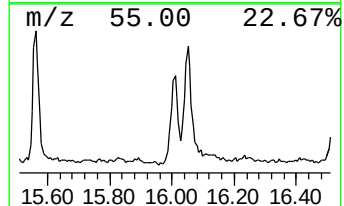
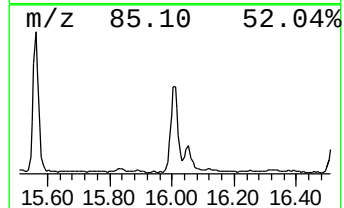
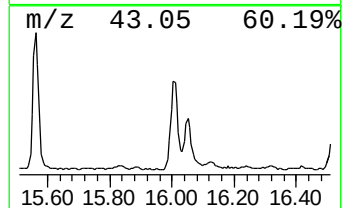
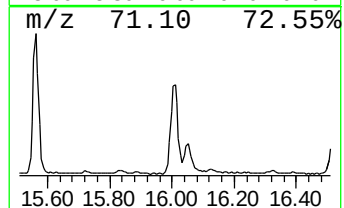
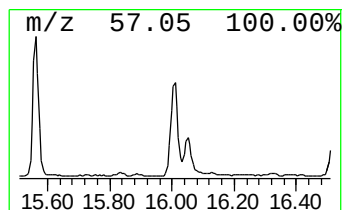
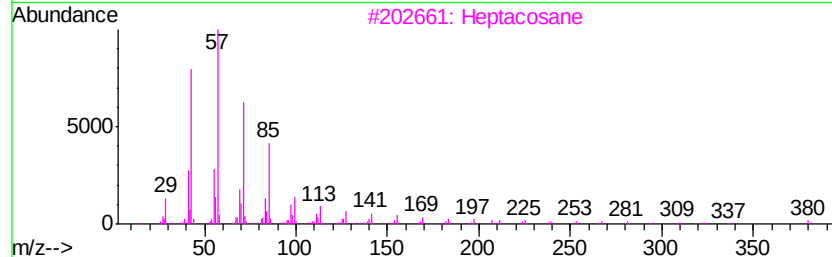
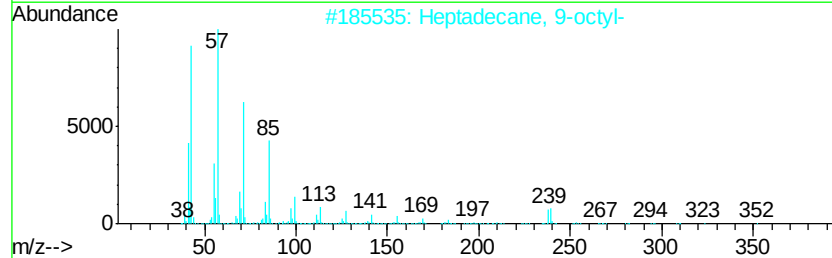
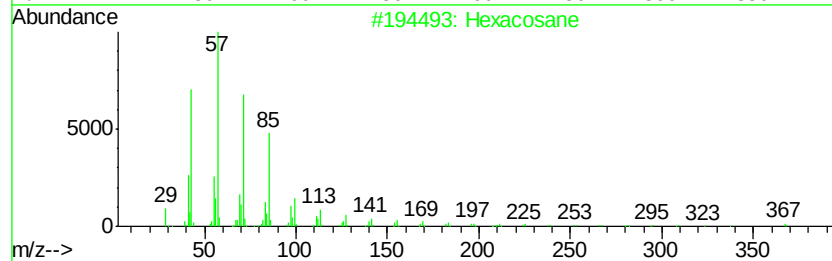
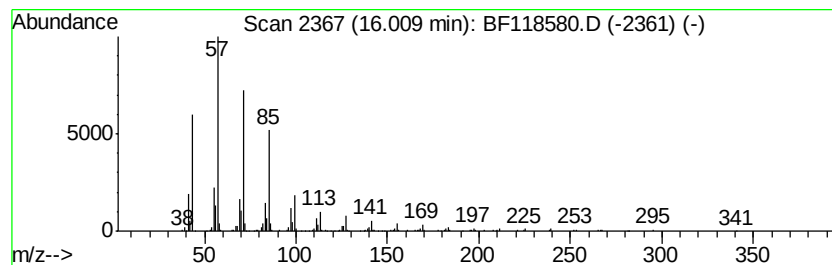
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	4.19 ng	705842	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	94
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Tetratetracontane	619	C44H90	007098-22-8	91
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011720\
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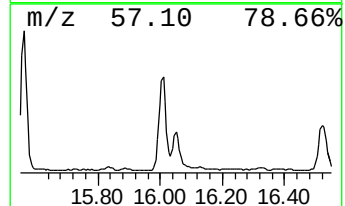
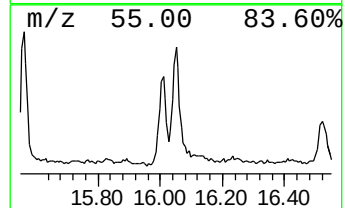
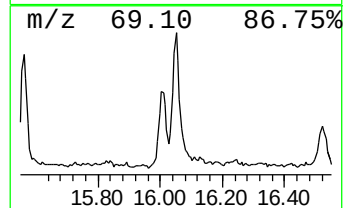
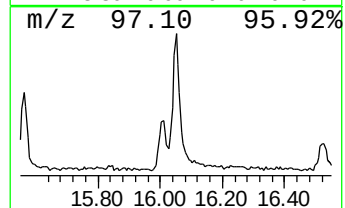
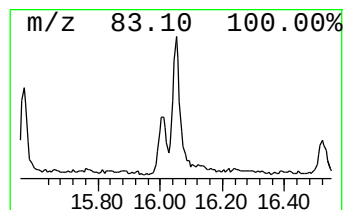
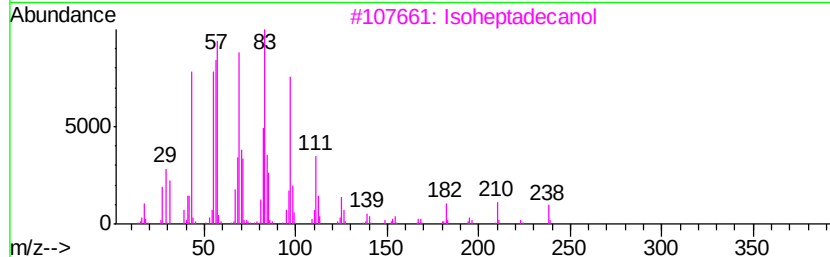
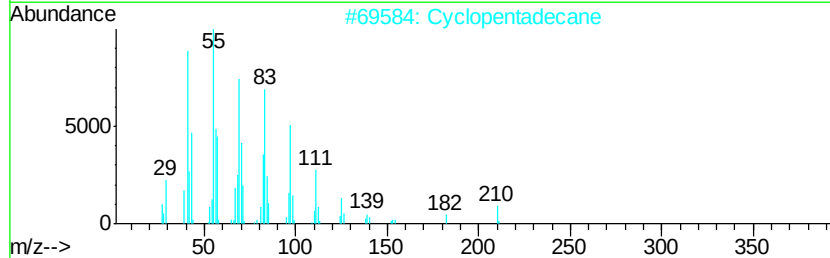
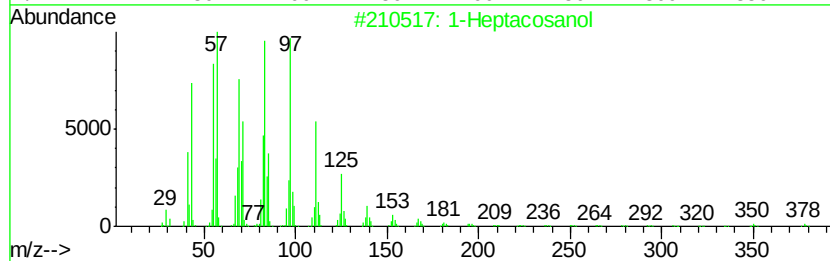
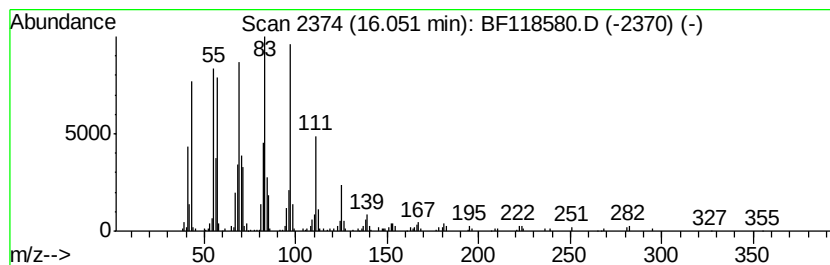
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-Heptacosanol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.05	3.43 ng	578787	Perylene-d12	15.52	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	Cyclopentadecane	210	C15H30	000295-48-7	74
3	Isoheptadecanol	256	C17H36O	057289-07-3	72
4	Fumaric acid, 3,5-difluorophenyl...	424	C24H34F2O4	1000339-37-9	64
5	1-Hexadecanol	242	C16H34O	036653-82-4	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011720\
Data File : BF118580.D
Acq On : 18 Jan 2020 1:33
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Sample : L1173-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0053-DECANT-H2O-COMP-5

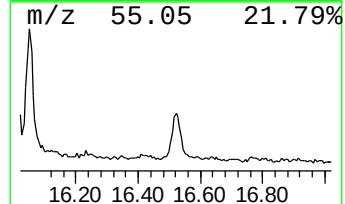
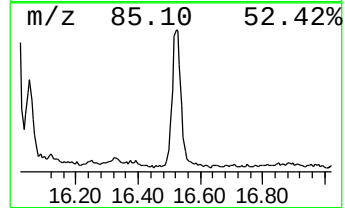
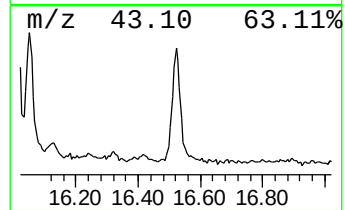
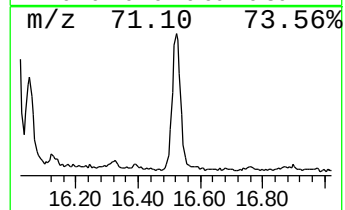
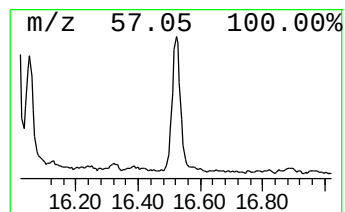
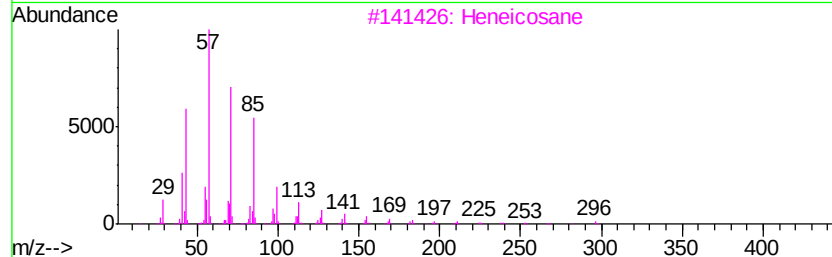
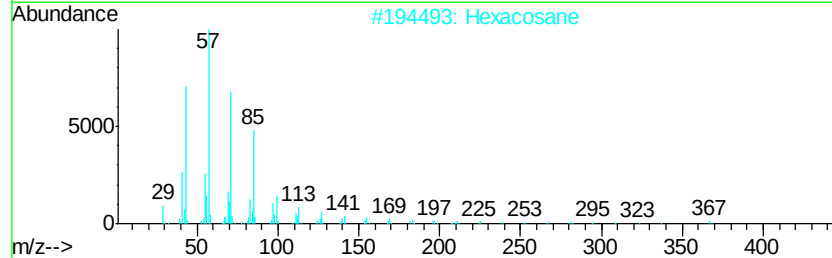
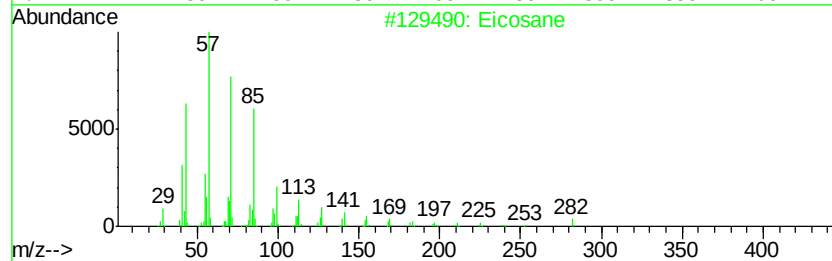
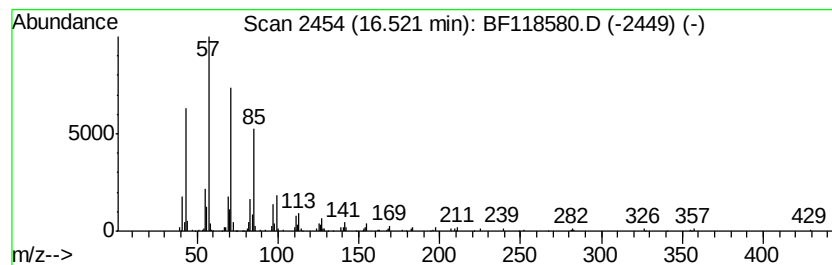
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Tetratetracontane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.52	2.31 ng	389498	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	95
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Tetratetracontane	619	C44H90	007098-22-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011720\
 Data File : BF118580.D
 Acq On : 18 Jan 2020 1:33
 Operator : JU
 Sample : L1173-02
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 0053-DECANT-H2O-COMP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011720.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...	2.16	70.9	ng	7534620	1	6.89	2124160	20.0
2-Pentanone, 4-hy...	5.10	6.1	ng	644011	1	6.89	2124160	20.0
unknown6.66	6.66	91.0	ng	9665480	1	6.89	2124160	20.0
n-Hexadecanoic acid	11.94	7.7	ng	1313040	4	11.41	3396700	20.0
Octadecanoic acid	12.72	4.1	ng	700630	4	11.41	3396700	20.0
1-Heneicosanol	13.89	16.9	ng	2989080	5	14.04	3545580	20.0
Heneicosane	14.22	2.2	ng	384154	5	14.04	3545580	20.0
Eicosane	14.52	3.8	ng	667535	5	14.04	3545580	20.0
Nonadecane	14.83	5.0	ng	840107	6	15.52	3371280	20.0
Heptadecane	15.17	5.5	ng	922548	6	15.52	3371280	20.0
Hexacosane	16.01	4.2	ng	705842	6	15.52	3371280	20.0
1-Heptacosanol	16.05	3.4	ng	578787	6	15.52	3371280	20.0
Tetratetracontane	16.52	2.3	ng	389498	6	15.52	3371280	20.0