

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102618\
 Data File : BF110220.D
 Acq On : 26 Oct 2018 20:04
 Operator : JU/SJ
 Sample : J5515-10
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AOC3-01A

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-BF102318.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	2.340	36	43	49	rVB	243745	327668	8.26%	1.043%
2	5.228	530	534	542	rBV	120943	176412	4.45%	0.562%
3	5.598	592	597	600	rBV	3321281	3601528	90.79%	11.465%
4	6.598	760	767	780	rBV	3295045	3966827	100.00%	12.628%
5	6.740	786	791	794	rBV	3598103	3760748	94.80%	11.972%
6	6.969	826	830	833	rBV	987180	800925	20.19%	2.550%
7	7.128	852	857	860	rBV	3164636	2835543	71.48%	9.027%
8	7.534	920	926	929	rBV	2295630	2299220	57.96%	7.320%
9	8.251	1044	1048	1065	rVB	1148982	1023901	25.81%	3.260%
10	9.328	1225	1231	1234	rBV	4374836	3917211	98.75%	12.470%
11	9.716	1293	1297	1302	rBV	336381	292362	7.37%	0.931%
12	10.010	1343	1347	1354	rBV2	1089216	937771	23.64%	2.985%
13	10.804	1477	1482	1495	rBV	1905286	1802477	45.44%	5.738%
14	11.504	1597	1601	1609	rBV	881307	772309	19.47%	2.459%
15	13.092	1866	1871	1874	rBV	3078193	2956187	74.52%	9.411%
16	13.969	2016	2020	2028	rBV	188503	235667	5.94%	0.750%
17	14.151	2047	2051	2056	rBV	709379	653996	16.49%	2.082%
18	14.286	2071	2074	2078	rBV	71346	70754	1.78%	0.225%
19	14.592	2124	2126	2134	rVB	84567	94921	2.39%	0.302%
20	14.916	2178	2181	2185	rVB	87186	86534	2.18%	0.275%
21	14.992	2192	2194	2199	rVB	59842	65339	1.65%	0.208%
22	15.268	2238	2241	2246	rVB	101502	115914	2.92%	0.369%
23	15.680	2306	2311	2316	rVB2	371761	514918	12.98%	1.639%
24	16.133	2385	2388	2392	rVB3	79413	102781	2.59%	0.327%

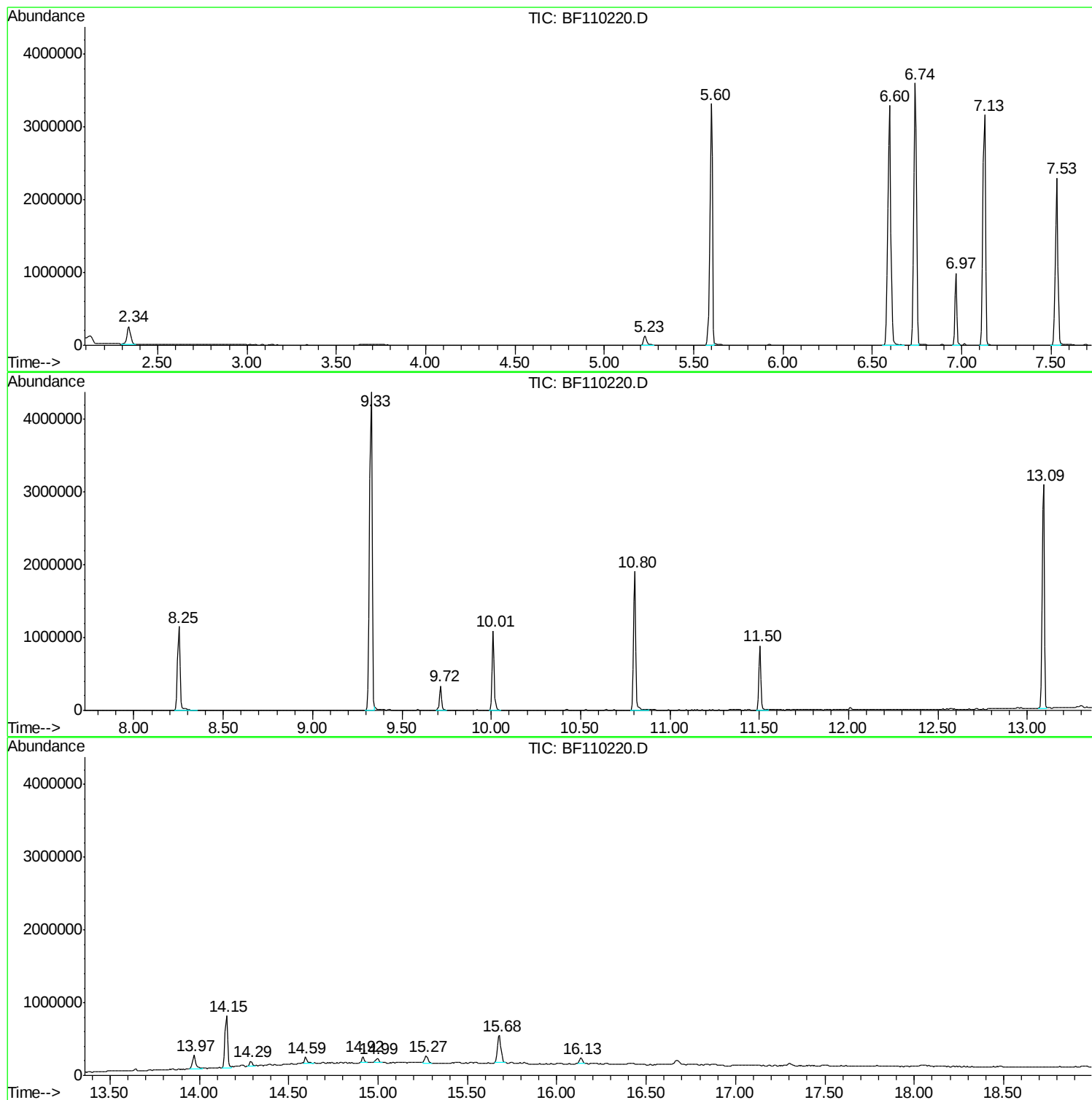
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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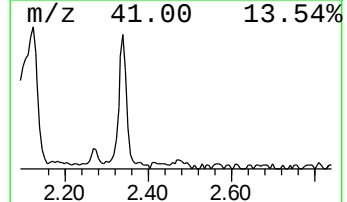
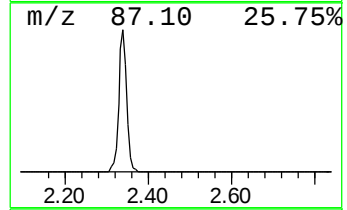
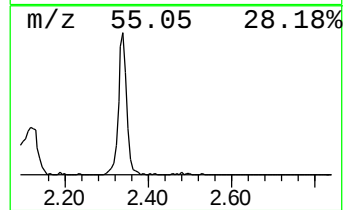
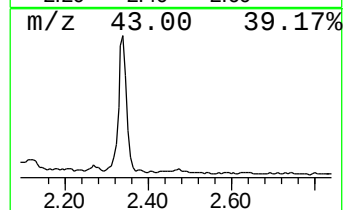
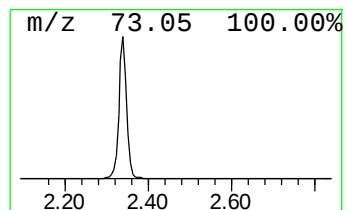
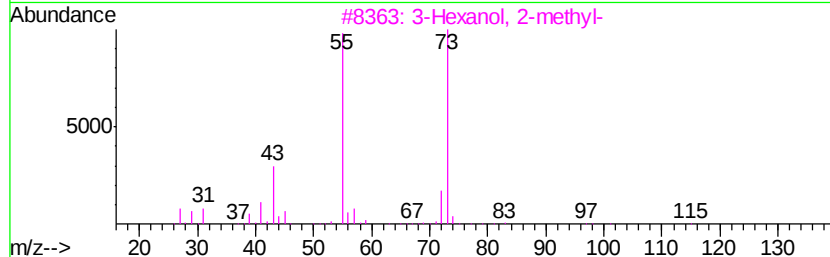
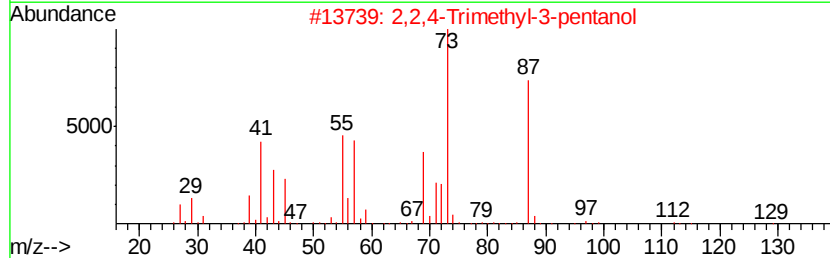
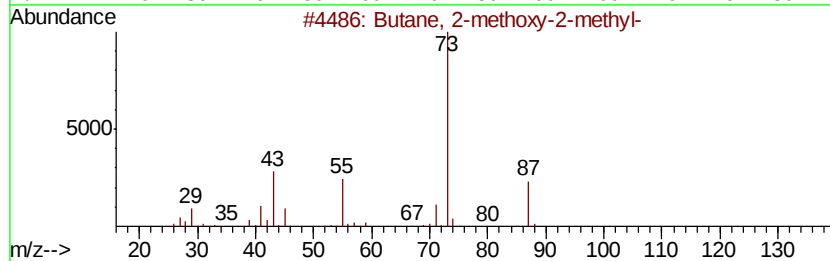
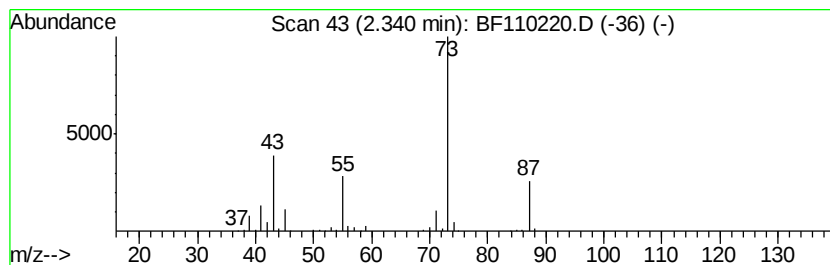
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.34	8.18 ng	327668	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	23
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22



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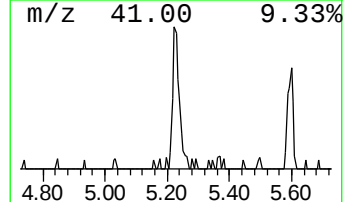
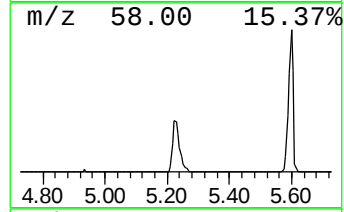
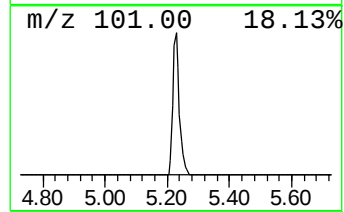
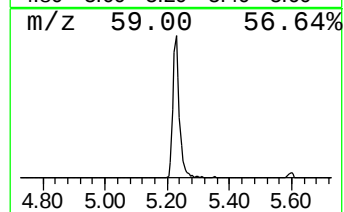
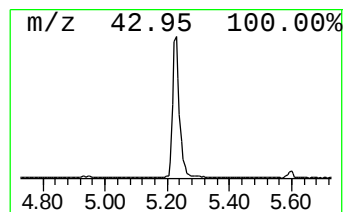
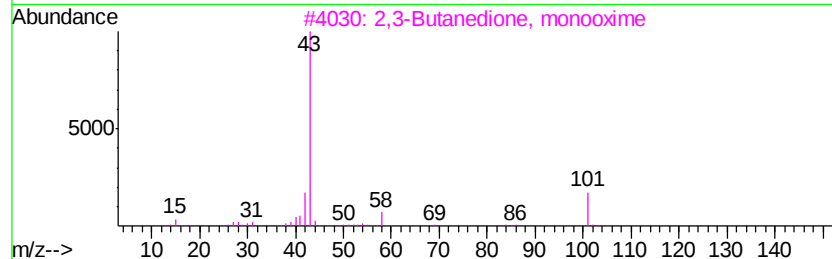
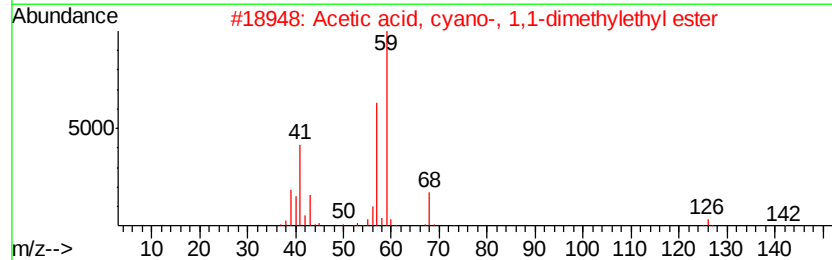
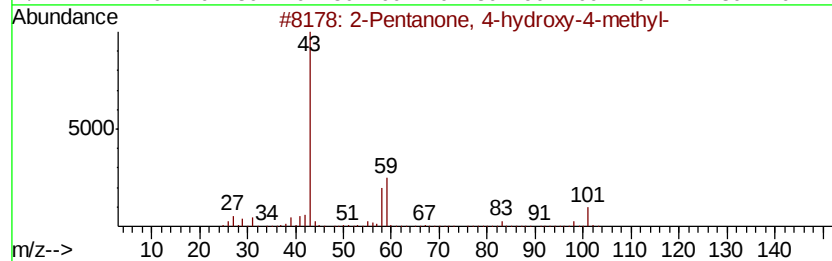
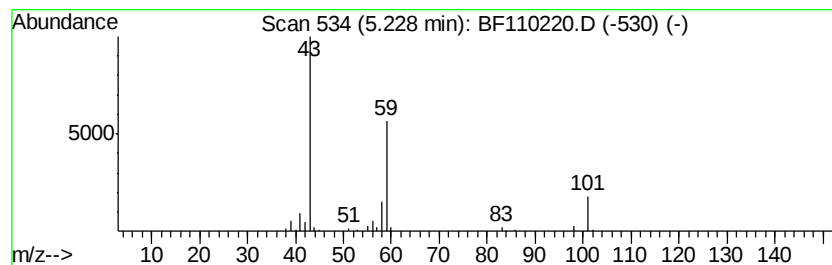
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	4.41 ng	176412	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9



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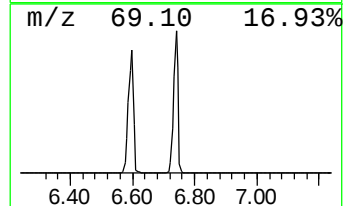
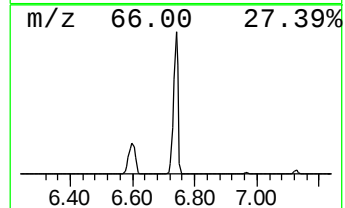
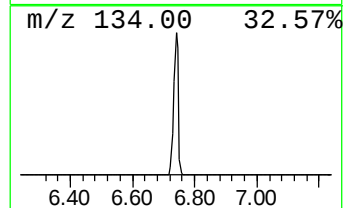
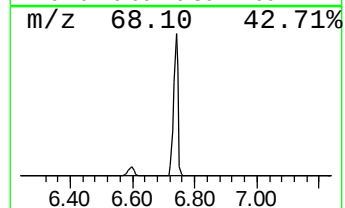
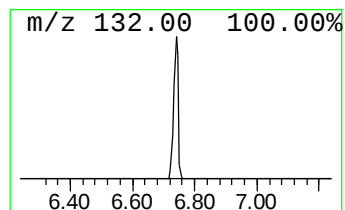
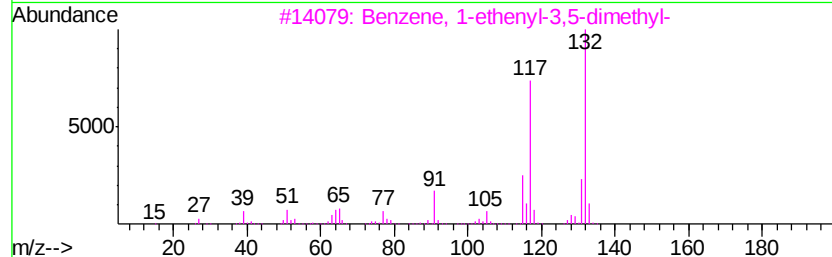
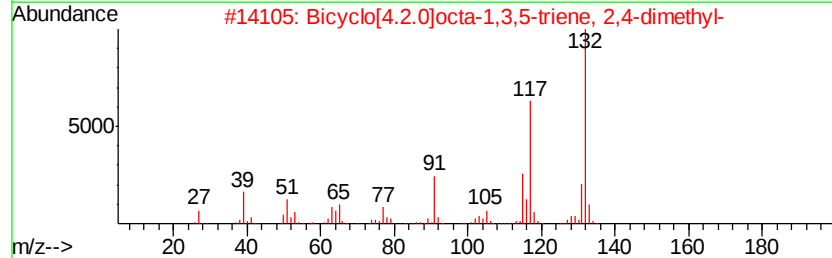
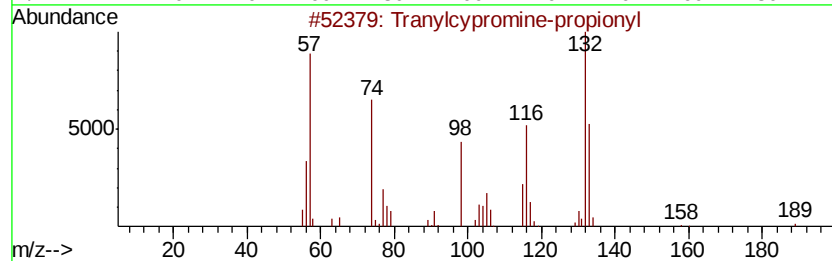
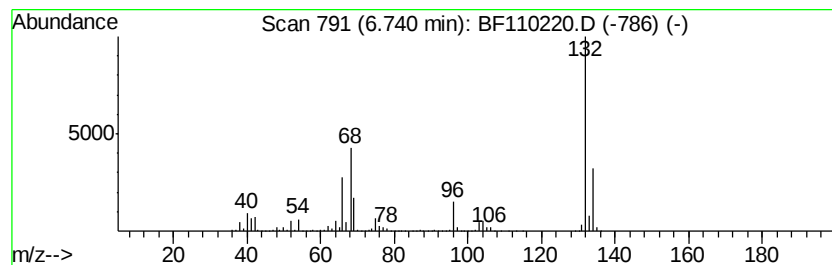
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Peak Number 3 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	93.91 ng	3760750	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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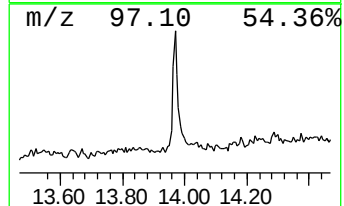
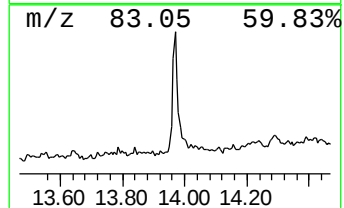
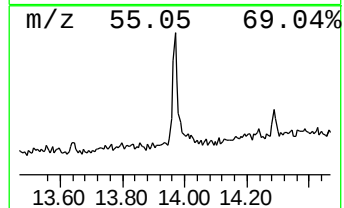
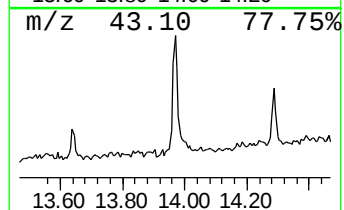
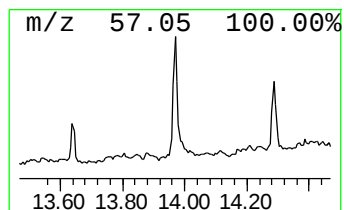
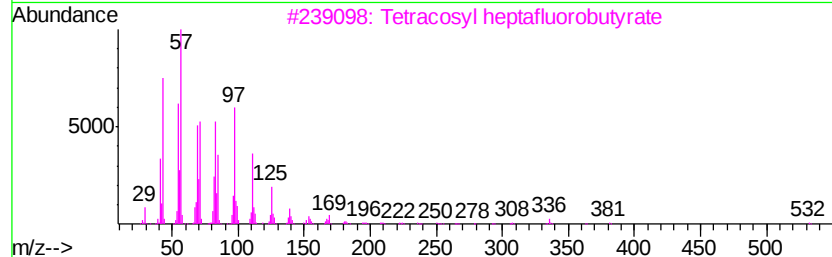
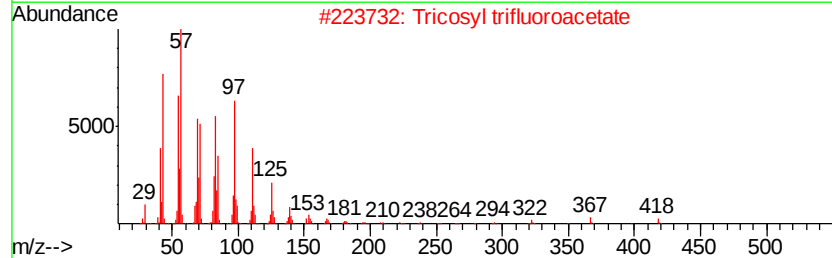
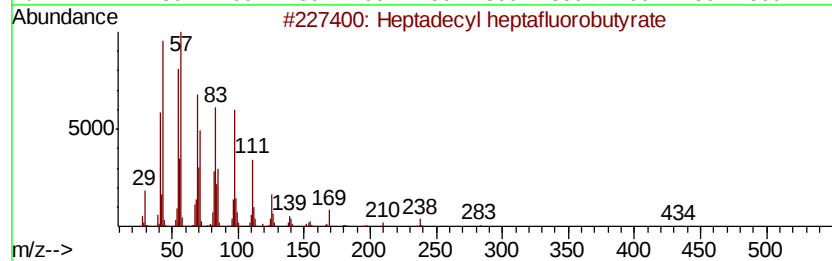
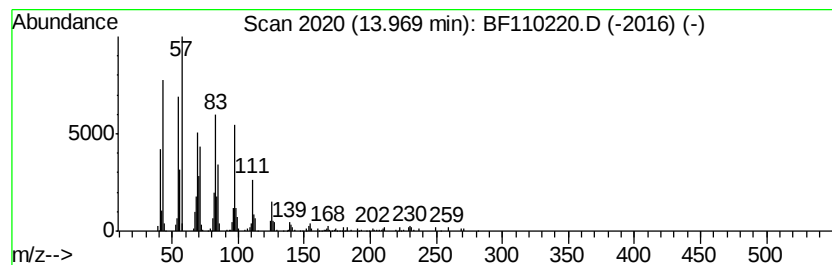
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Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	7.21 ng	235667	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	95
2		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
3		Tetracosyl heptafluorobutvrate	550	C28H49F7O2	1000351-83-7	91
4		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
5		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91



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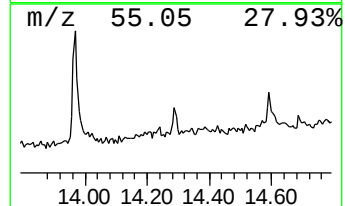
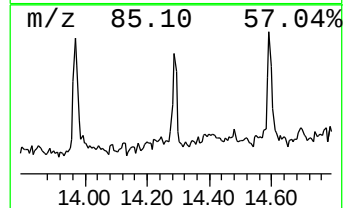
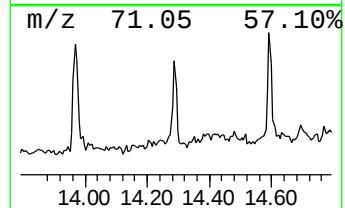
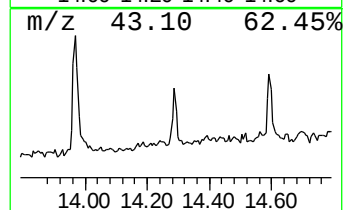
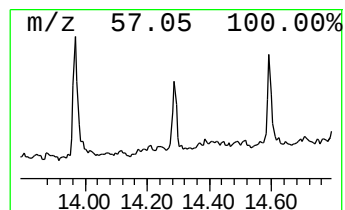
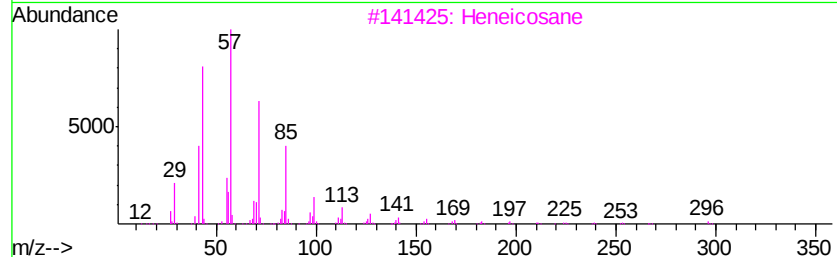
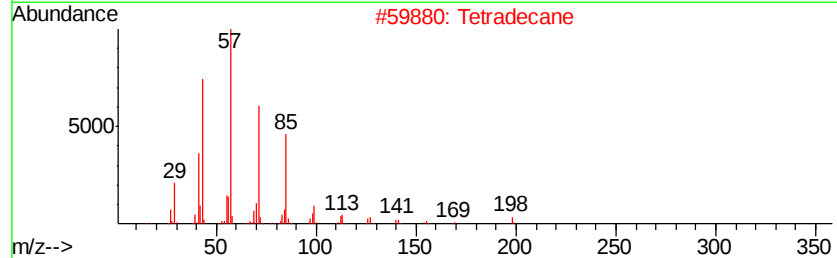
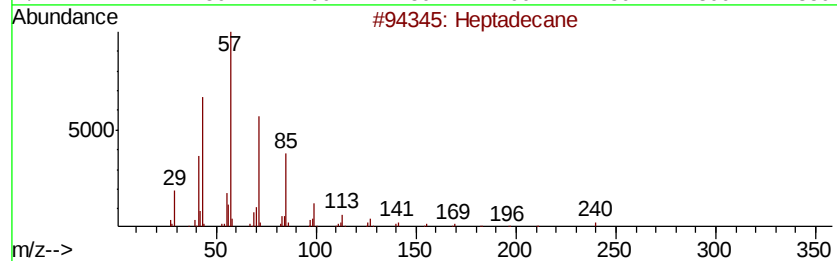
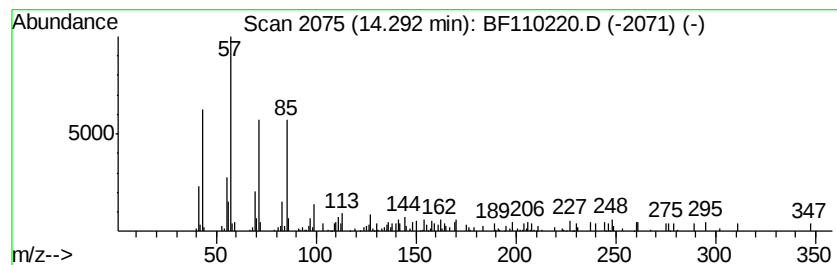
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	2.16 ng	70754	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	91
2		Tetradecane	198	C14H30	000629-59-4	81
3		Heneicosane	296	C21H44	000629-94-7	80
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
5		Dodecane	170	C12H26	000112-40-3	80



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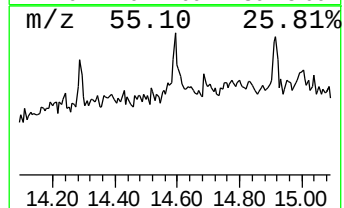
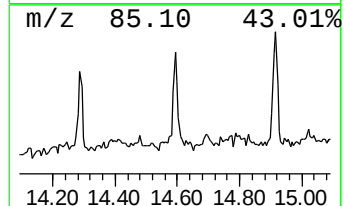
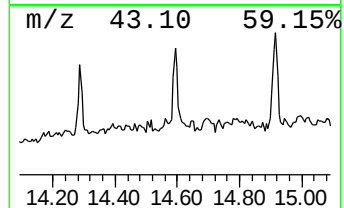
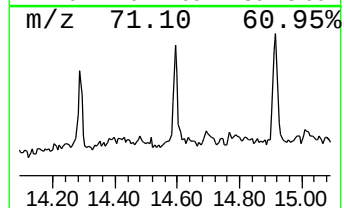
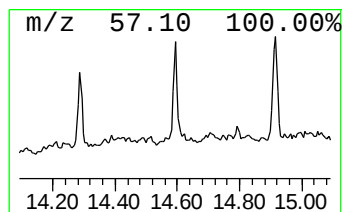
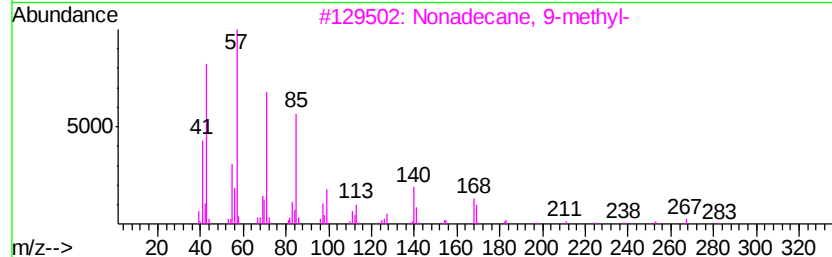
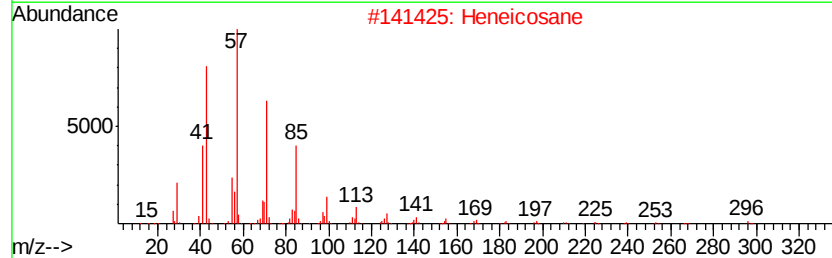
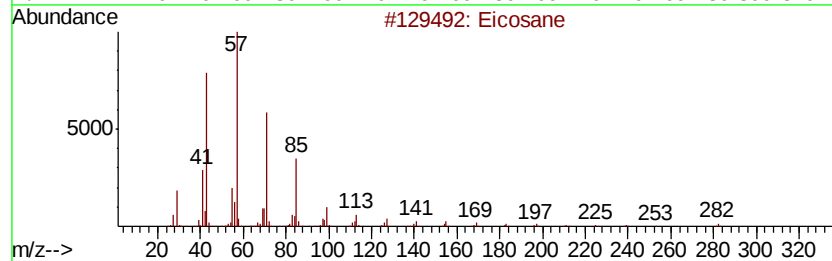
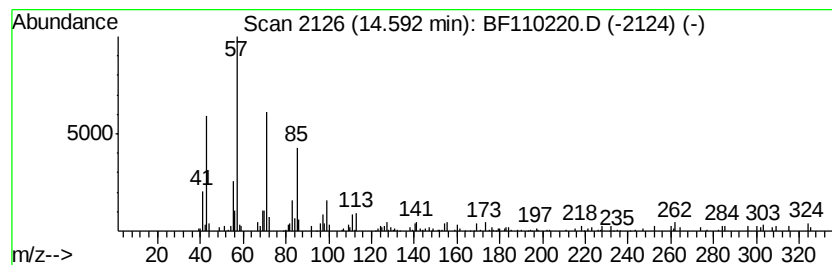
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ClientSampleId :
AOC3-01A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.90 ng	94921	Chrysene-d12	14.15
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	95
2	Heneicosane	296 C21H44	000629-94-7	93
3	Nonadecane, 9-methyl-	282 C20H42	013287-24-6	93
4	Tridecane, 6-propyl-	226 C16H34	055045-10-8	91
5	Tricosane	324 C23H48	000638-67-5	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102618\
Data File : BF110220.D
Acq On : 26 Oct 2018 20:04
Operator : JU/SJ
Sample : J5515-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AOC3-01A

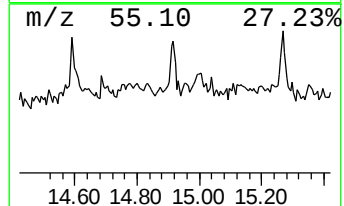
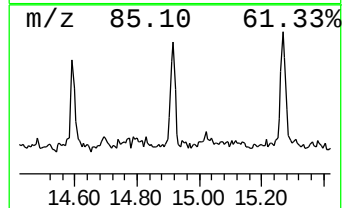
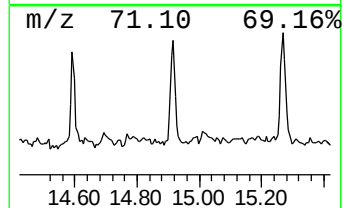
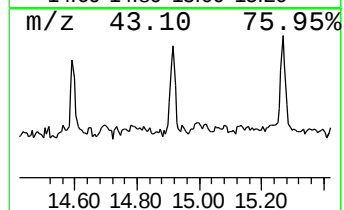
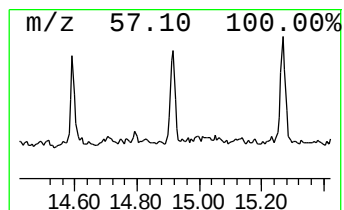
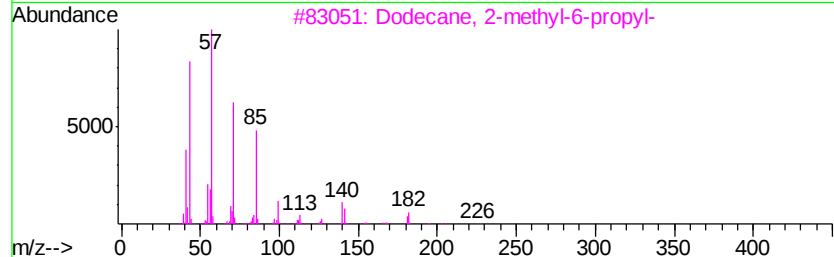
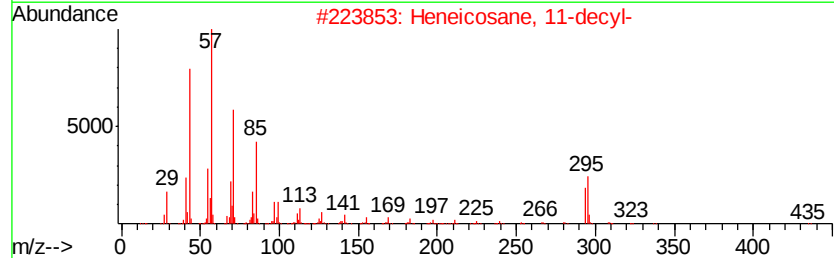
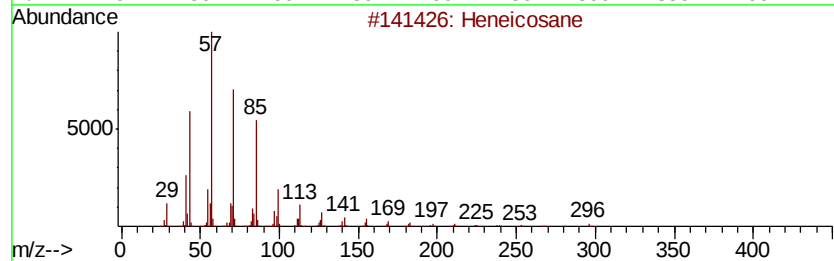
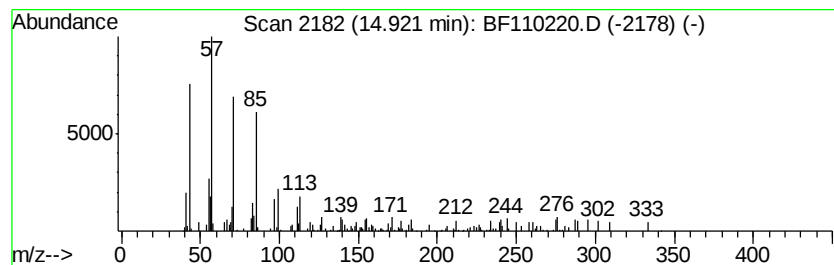
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	3.36 ng	86534	Perylene-d12	15.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	87
2	Heneicosane, 11-decyl-		437	C31H64	055320-06-4	86
3	Dodecane, 2-methyl-6-propyl-		226	C16H34	055045-08-4	83
4	Octacosane		394	C28H58	000630-02-4	76
5	Hexatriacontane		507	C36H74	000630-06-8	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102618\
Data File : BF110220.D
Acq On : 26 Oct 2018 20:04
Operator : JU/SJ
Sample : J5515-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

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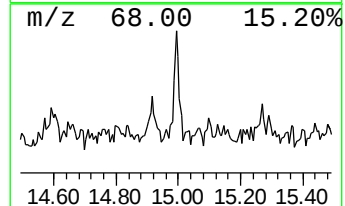
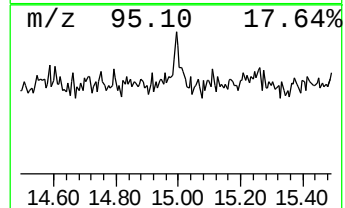
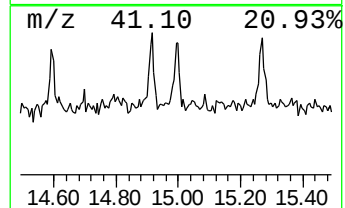
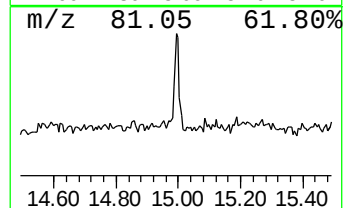
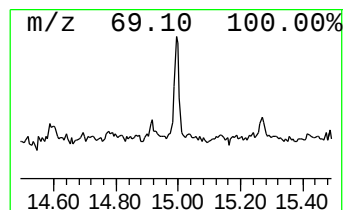
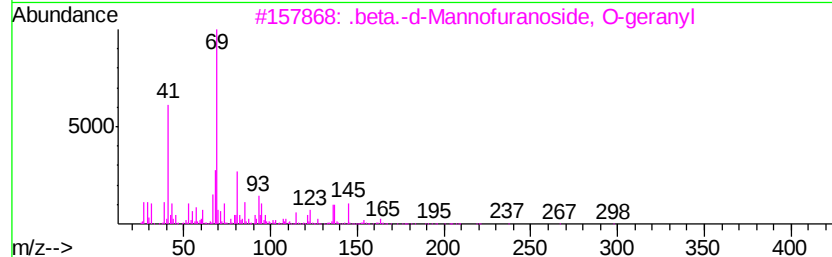
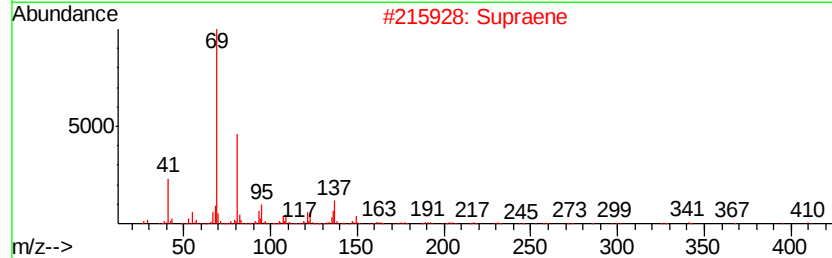
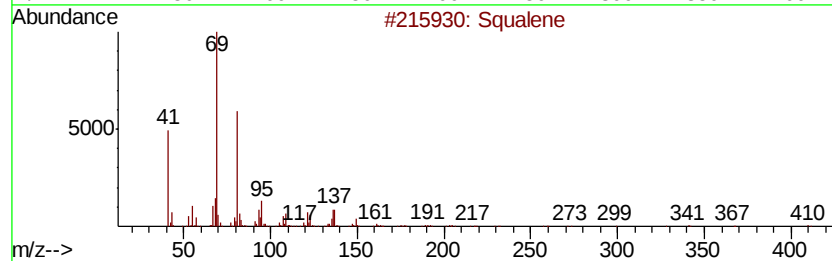
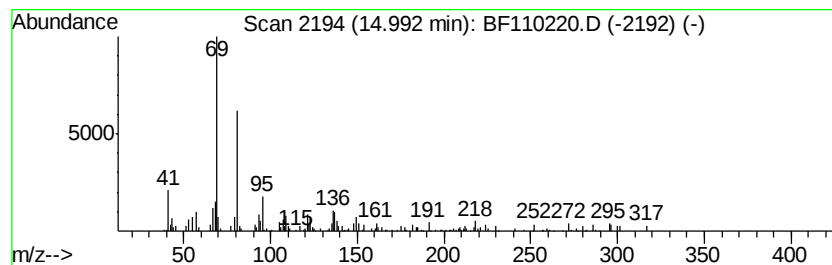
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	2.54 ng	65339	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	74
2		Supraene	410	C30H50	007683-64-9	64
3		.beta.-d-Mannofuranoside, O-geranyl	316	C16H28O6	1000154-77-2	64
4		6,10,14-Hexadecatrien-1-ol, 3,7,...	292	C20H36O	036237-66-8	64
5		1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102618\
Data File : BF110220.D
Acq On : 26 Oct 2018 20:04
Operator : JU/SJ
Sample : J5515-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

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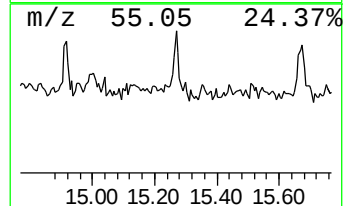
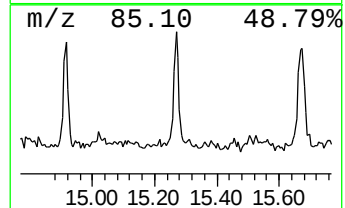
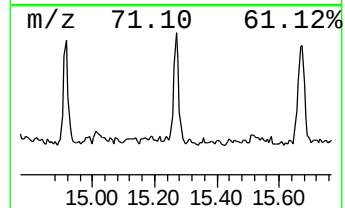
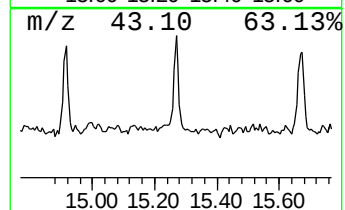
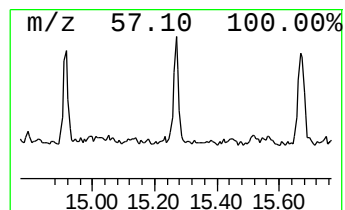
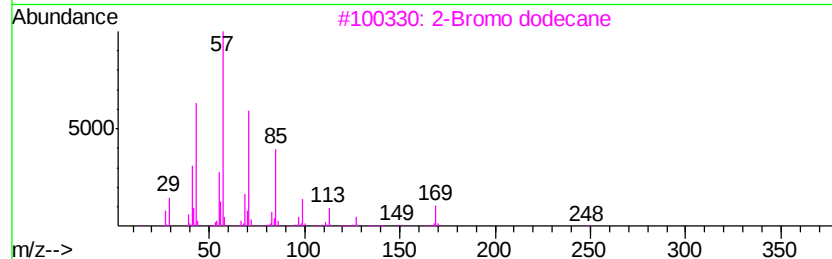
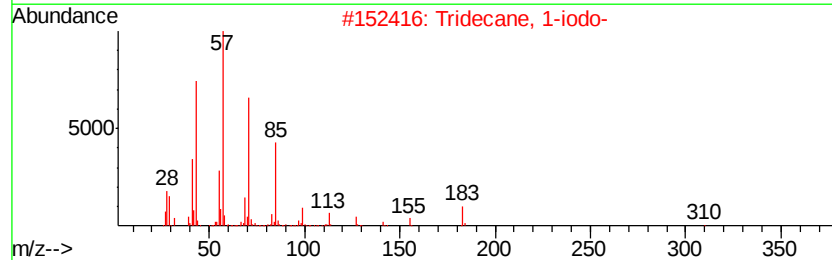
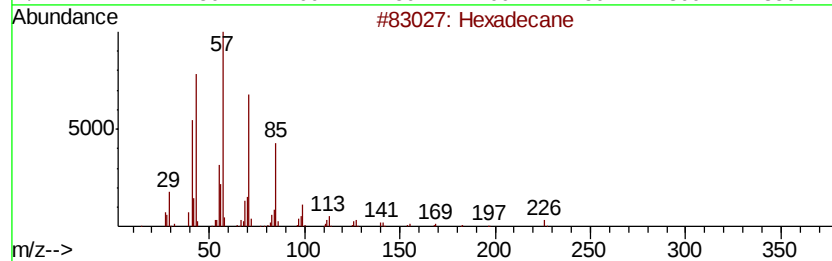
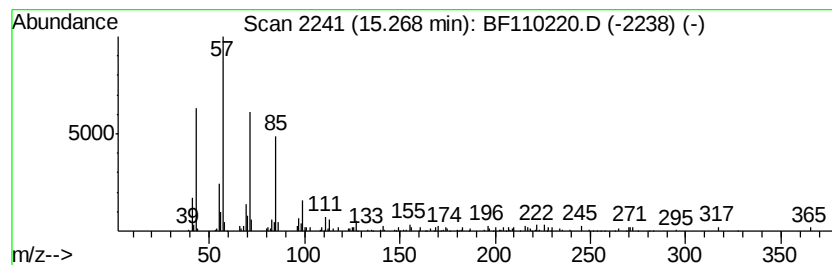
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	4.50 ng	115914	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	86
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83
3		2-Bromo dodecane	248	C12H25Br	013187-99-0	72
4		Eicosane	282	C20H42	000112-95-8	62
5		Heptacosane	380	C27H56	000593-49-7	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102618\
Data File : BF110220.D
Acq On : 26 Oct 2018 20:04
Operator : JU/SJ
Sample : J5515-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

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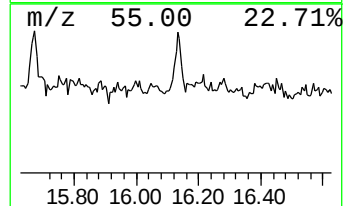
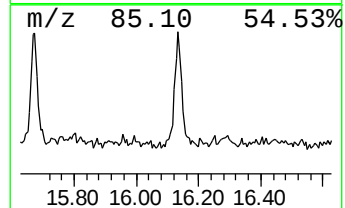
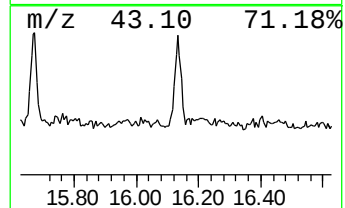
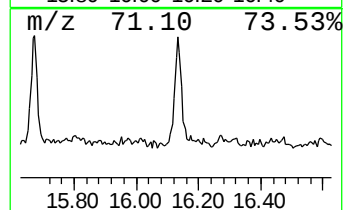
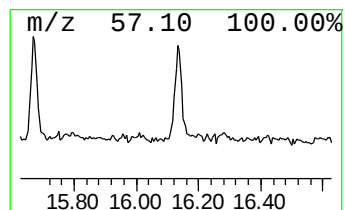
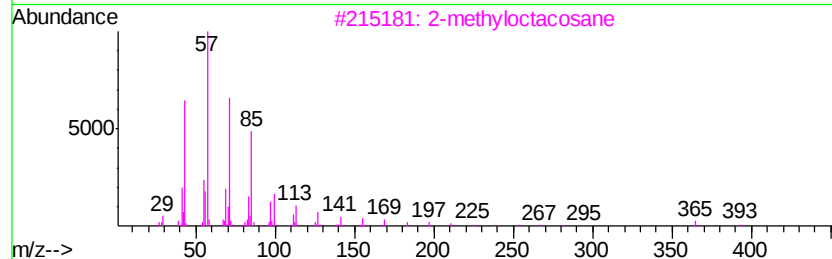
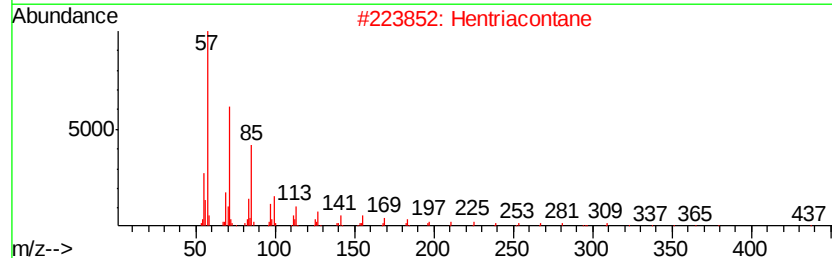
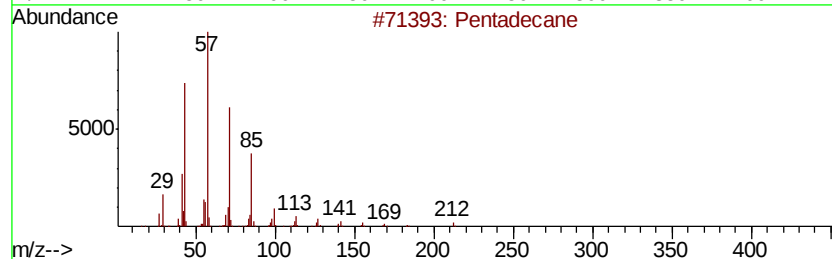
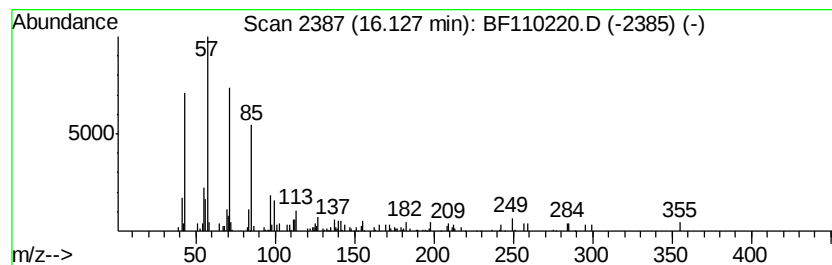
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	3.99 ng	102781	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	95
2		Hentriacontane	437	C31H64	000630-04-6	87
3		2-methyloctacosane	408	C29H60	1000376-72-8	87
4		Hexacosane	366	C26H54	000630-01-3	87
5		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102618\
Data File : BF110220.D
Acq On : 26 Oct 2018 20:04
Operator : JU/SJ
Sample : J5515-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AOC3-01A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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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2-Pentanone, 4-hy...	5.23	4.4	ng	176412	1	6.97	800925	20.0
unknown6.74	6.74	93.9	ng	3760750	1	6.97	800925	20.0
Heptadecyl heptaf...	13.97	7.2	ng	235667	5	14.15	653996	20.0
Heptadecane	14.29	2.2	ng	70754	5	14.15	653996	20.0
Eicosane	14.59	2.9	ng	94921	5	14.15	653996	20.0
Heneicosane	14.92	3.4	ng	86534	6	15.68	514918	20.0
Squalene	14.99	2.5	ng	65339	6	15.68	514918	20.0
Hexadecane	15.27	4.5	ng	115914	6	15.68	514918	20.0
Pentadecane	16.13	4.0	ng	102781	6	15.68	514918	20.0