

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
 Data File : BF111194.D
 Acq On : 7 Dec 2018 18:37
 Operator : JU/SJ
 Sample : J6214-05
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-9(13-15)

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-BF120518.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	3.228	191	194	207	rBV	247143	482169	3.83%	0.409%
2	5.022	489	499	507	rBV	674718	976708	7.76%	0.828%
3	5.422	562	567	571	rBV	11021134	12588045	100.00%	10.675%
4	6.439	733	740	744	rBV	10360061	12117832	96.26%	10.276%
5	6.575	758	763	766	rBV	10638389	11043120	87.73%	9.365%
6	6.804	798	802	806	rBV	3210345	2512282	19.96%	2.130%
7	6.869	810	813	819	rBV	133459	127997	1.02%	0.109%
8	6.963	825	829	832	rVB	9596704	8440910	67.05%	7.158%
9	7.363	892	897	900	rBV	7148582	7829244	62.20%	6.639%
10	8.086	1016	1020	1023	rBV	3972013	3279778	26.05%	2.781%
11	9.163	1198	1203	1206	rBV	12756030	12427772	98.73%	10.539%
12	9.557	1265	1270	1273	rBV	2735980	2300256	18.27%	1.951%
13	9.839	1312	1318	1322	rBV2	5209053	4404890	34.99%	3.735%
14	10.039	1349	1352	1355	rBV	146031	126750	1.01%	0.107%
15	10.627	1446	1452	1455	rBV	7386856	7088193	56.31%	6.011%
16	11.321	1566	1570	1573	rBV	4422596	3633171	28.86%	3.081%
17	11.863	1656	1662	1671	rBV	3974928	4178814	33.20%	3.544%
18	12.527	1772	1775	1779	rBV	179536	287905	2.29%	0.244%
19	12.645	1790	1795	1808	rBV	3195276	3240217	25.74%	2.748%
20	12.757	1812	1814	1817	rVB	179995	135616	1.08%	0.115%
21	12.910	1835	1840	1843	rBV	9366307	8628419	68.54%	7.317%
22	13.151	1878	1881	1885	rVB	260329	205285	1.63%	0.174%
23	13.492	1936	1939	1942	rBV	474829	381423	3.03%	0.323%
24	13.821	1991	1995	2002	rVB	1083348	1190437	9.46%	1.010%
25	13.957	2013	2018	2021	rBV	3235858	2922918	23.22%	2.479%
26	14.139	2046	2049	2053	rBV	846078	745541	5.92%	0.632%
27	14.451	2099	2102	2108	rVB	865061	752023	5.97%	0.638%
28	14.757	2151	2154	2160	rVB	765344	726528	5.77%	0.616%
29	14.833	2164	2167	2170	rBV	126713	129555	1.03%	0.110%
30	14.986	2191	2193	2201	rVB2	133078	248124	1.97%	0.210%
31	15.092	2207	2211	2215	rVB	616481	658983	5.23%	0.559%
32	15.404	2259	2264	2269	rBV	2103394	2574513	20.45%	2.183%
33	15.462	2270	2274	2279	rVB	474247	573876	4.56%	0.487%
34	15.886	2342	2346	2352	rBV2	391785	565029	4.49%	0.479%

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SB-9(13-15)

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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35	16.380	2426	2430	2437	rVB	233705	396867	3.15%	0.337%
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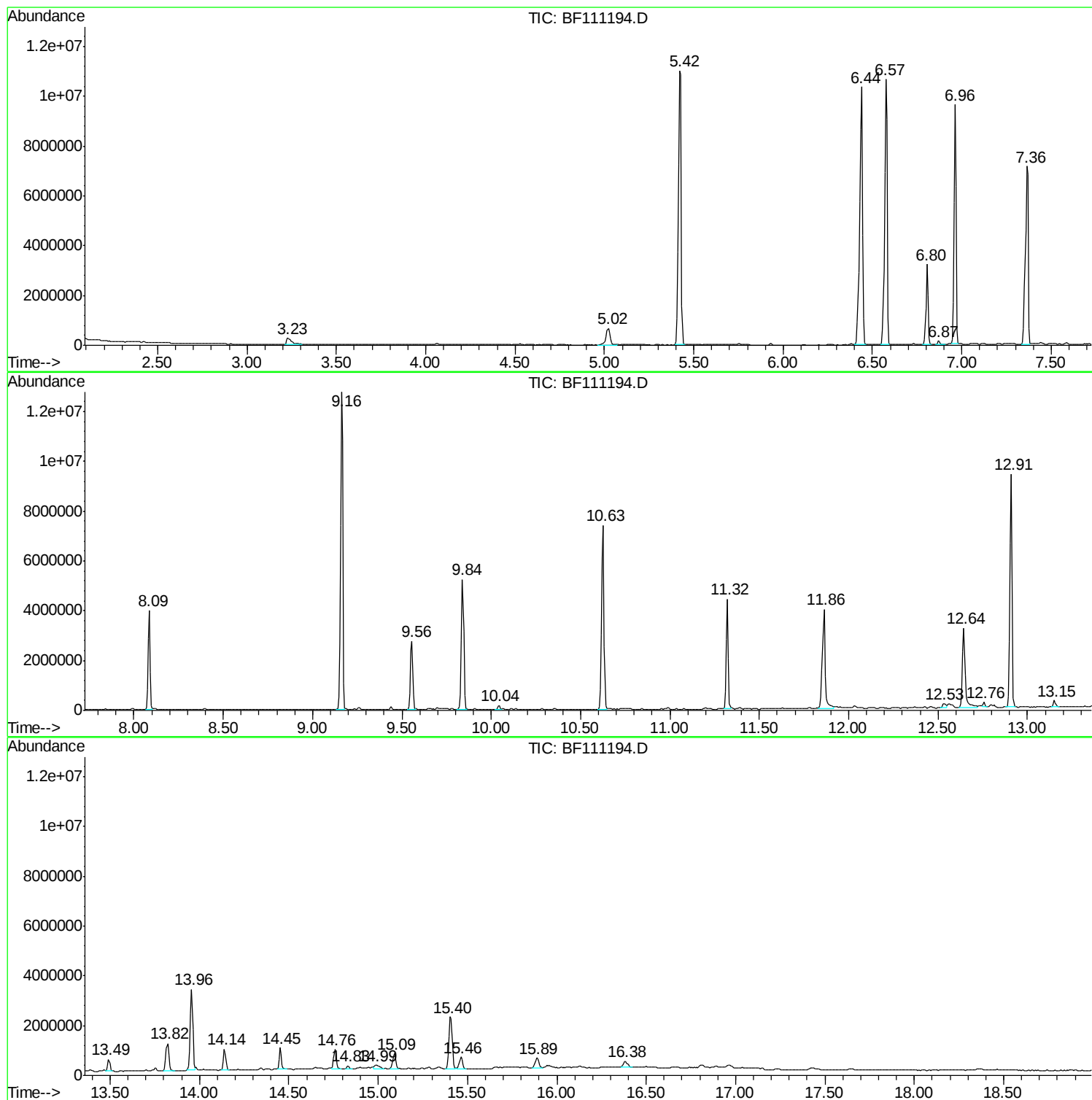
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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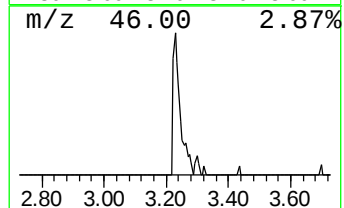
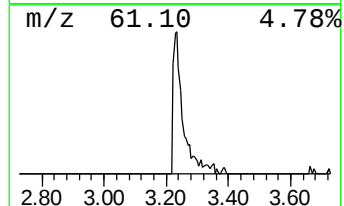
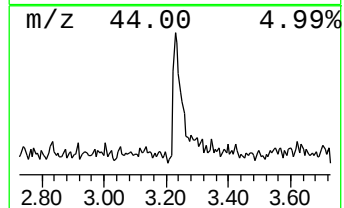
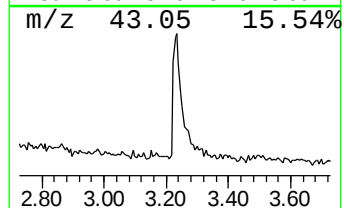
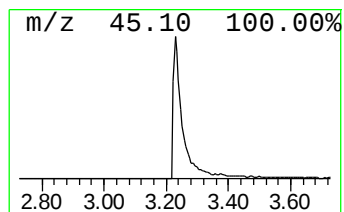
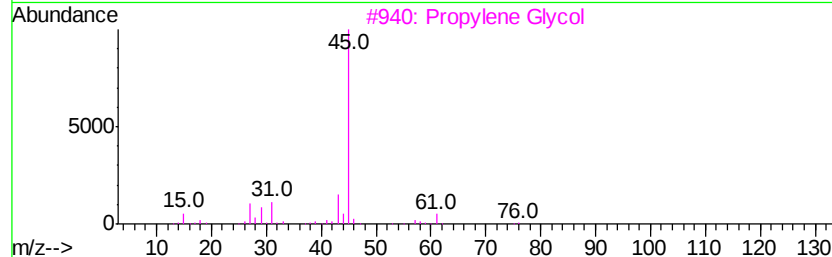
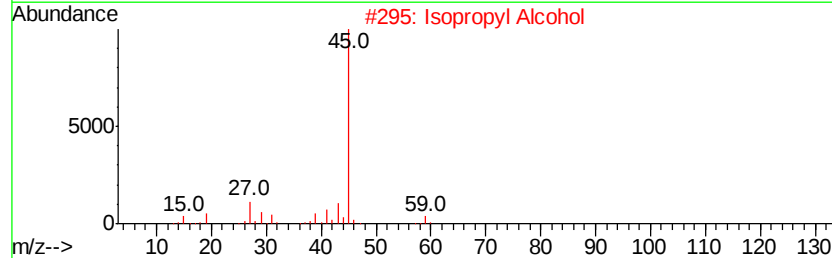
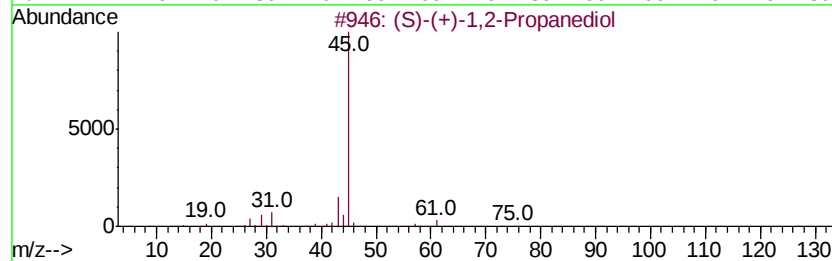
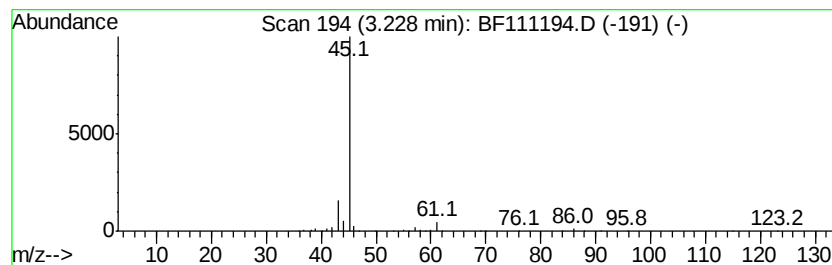
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	3.84 ng	482169	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3		Propylene Glycol	76	C3H8O2	000057-55-6	9
4		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9



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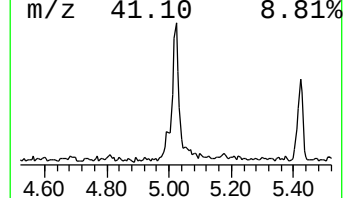
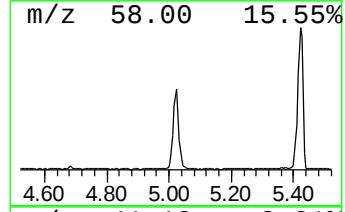
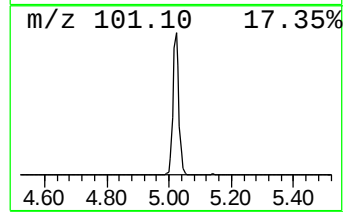
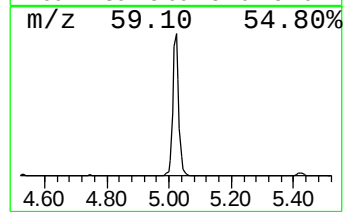
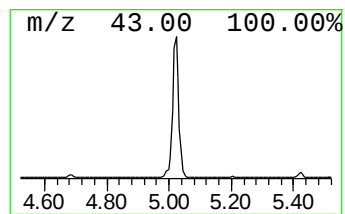
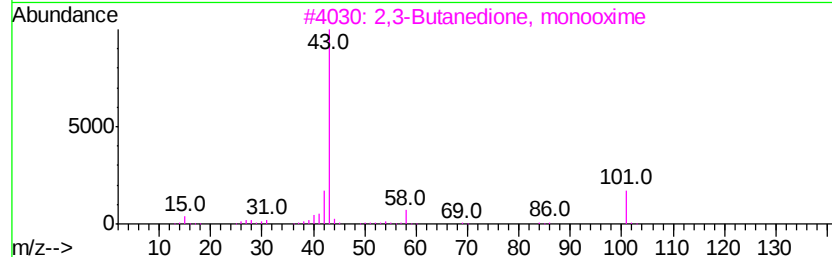
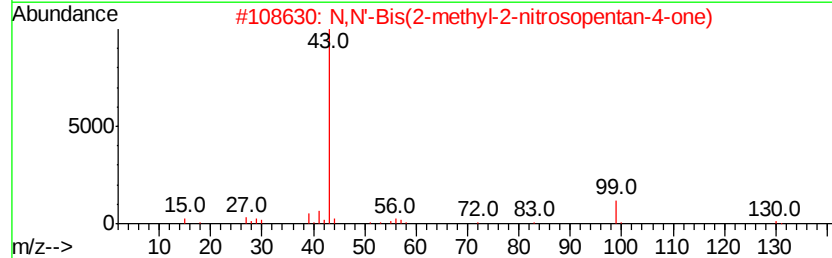
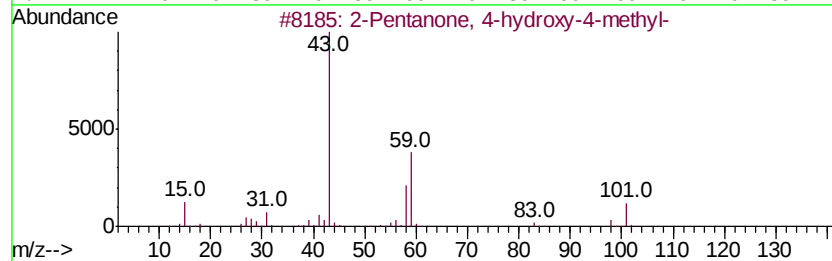
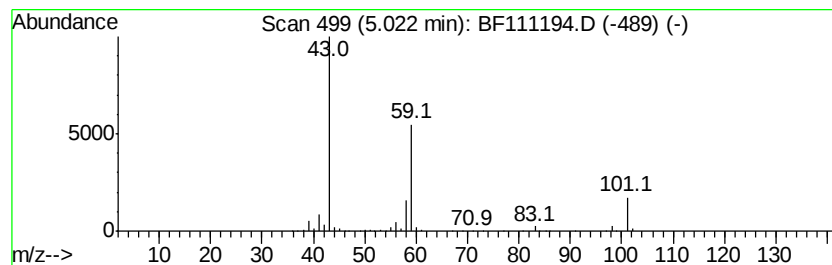
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	7.78 ng	976708	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



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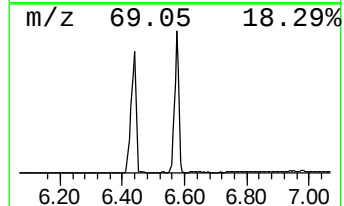
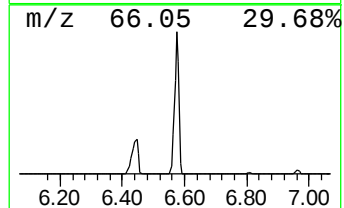
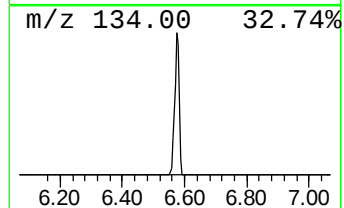
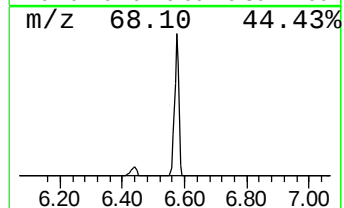
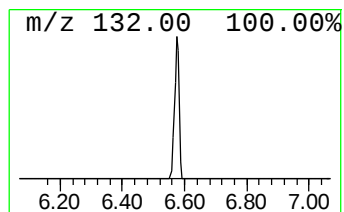
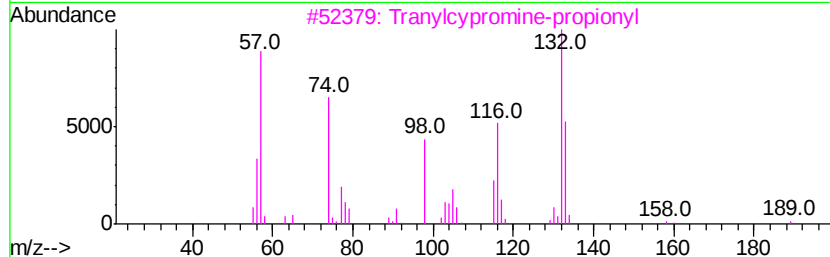
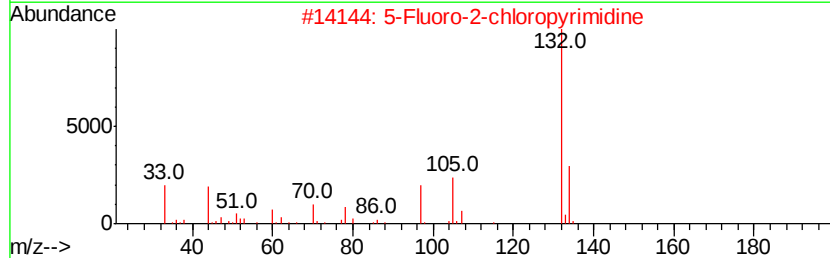
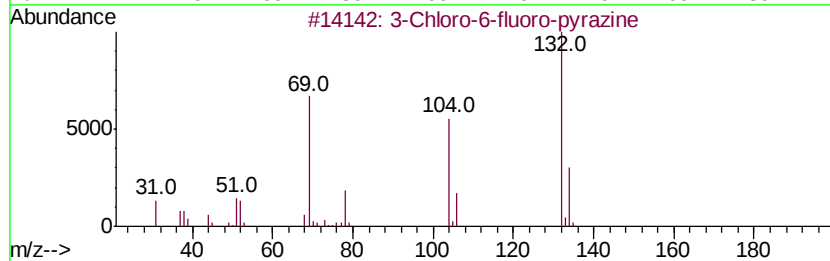
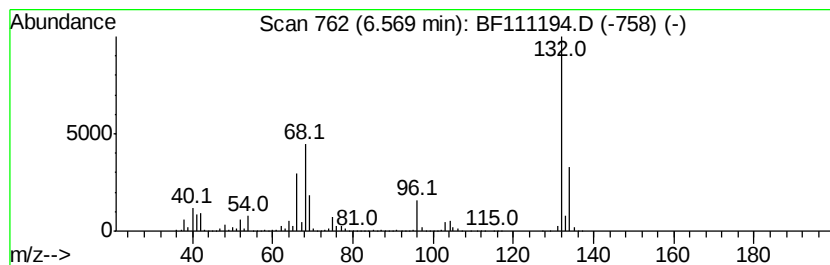
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	87.91 ng	11043100	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	12
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9



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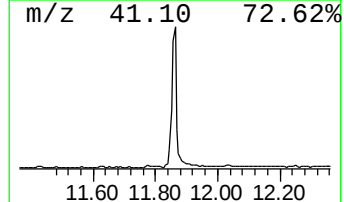
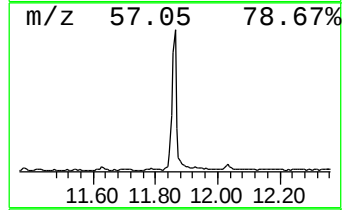
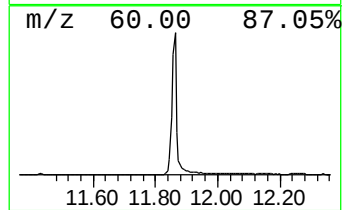
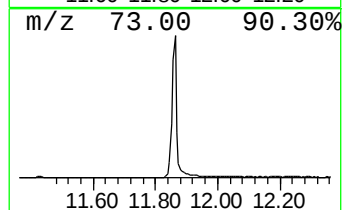
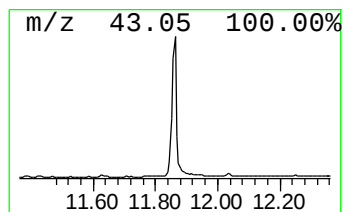
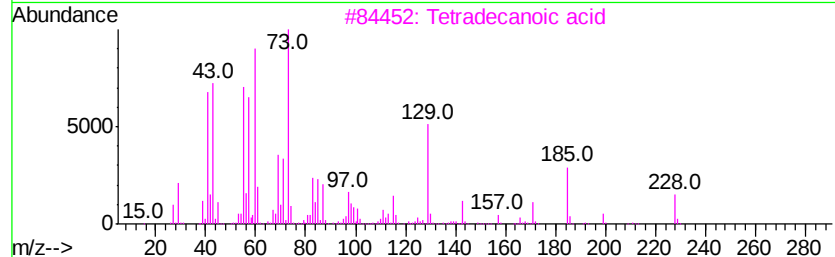
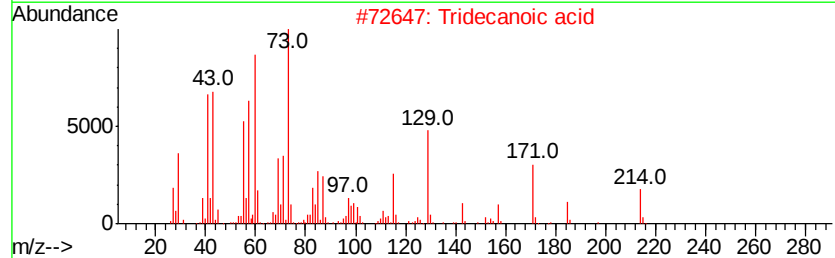
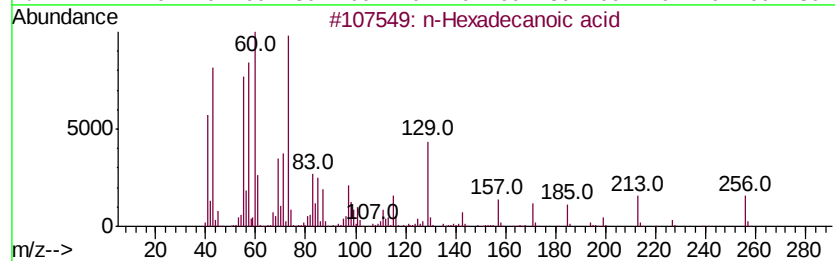
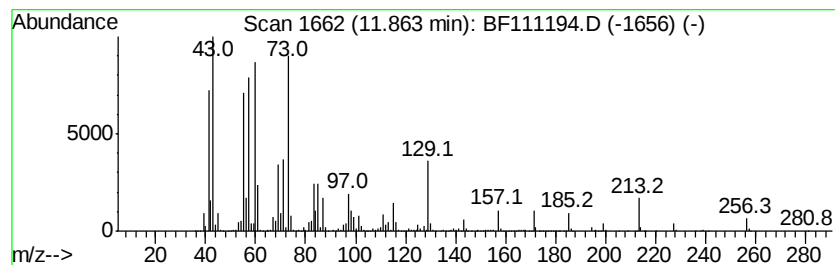
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	23.00 ng	4178810	Phenanthrene-d10	11.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5		n-Decanoic acid	172	C10H20O2	000334-48-5	60



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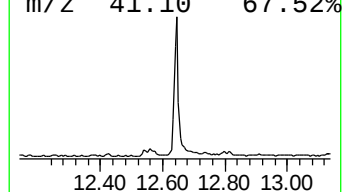
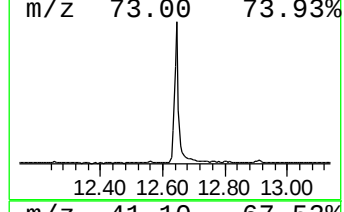
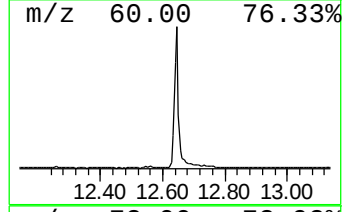
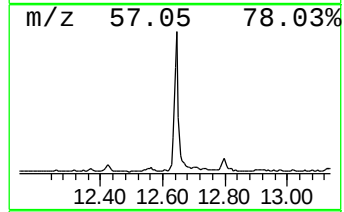
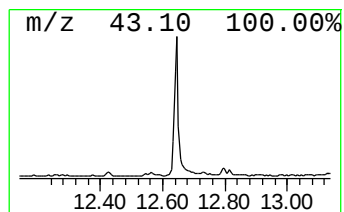
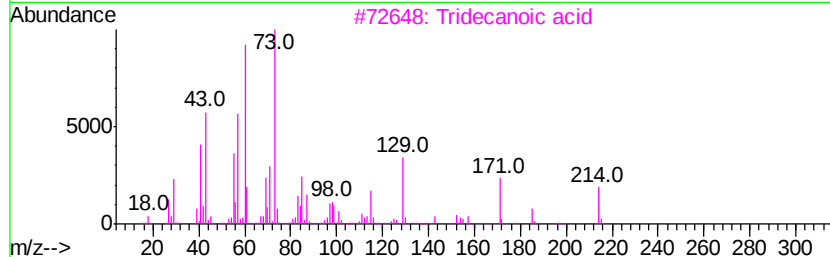
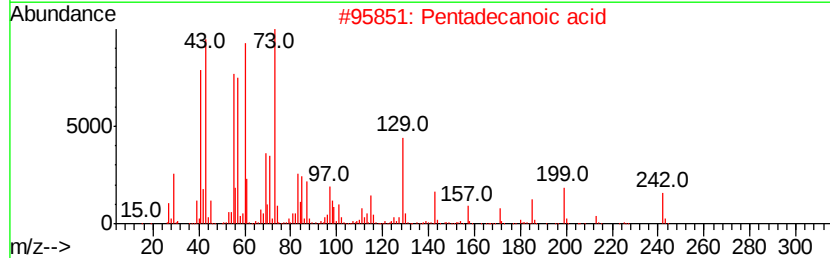
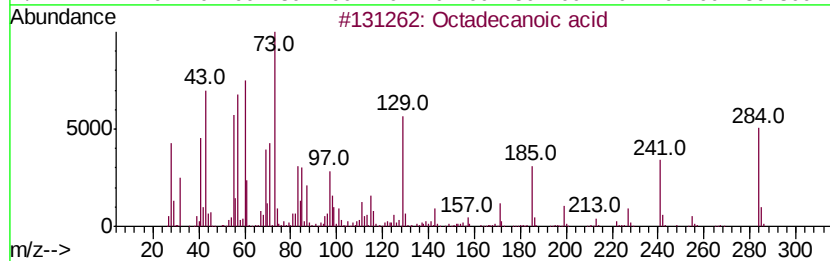
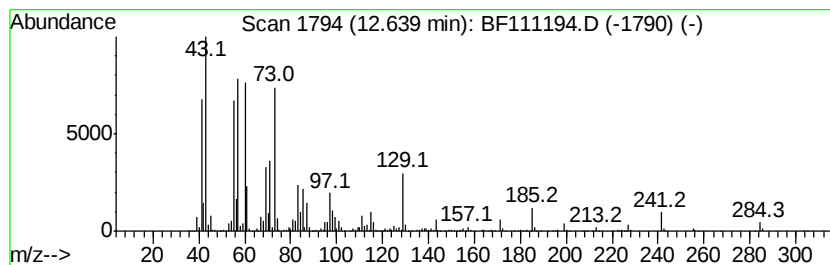
Instrument :
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Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.		
12.64	22.17 ng	3240220	Chrysene-d12		13.96		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
Data File : BF111194.D
Acq On : 7 Dec 2018 18:37
Operator : JU/SJ
Sample : J6214-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

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ClientSampleId :
SB-9(13-15)

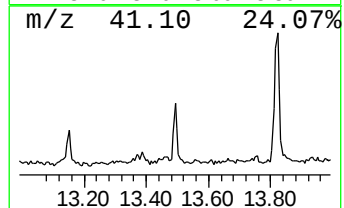
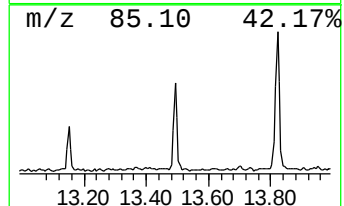
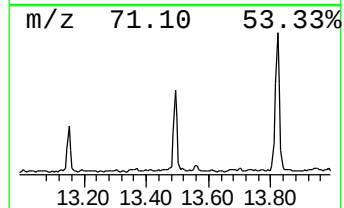
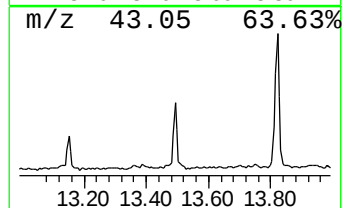
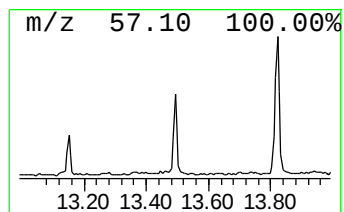
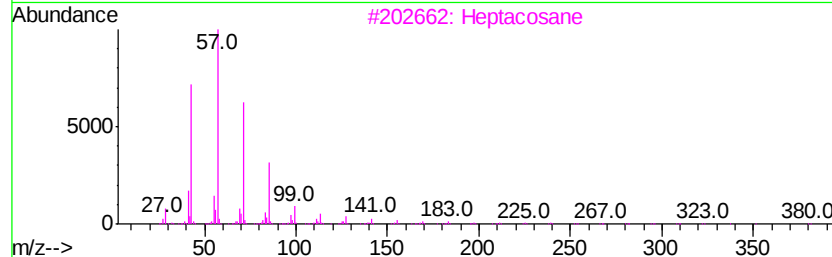
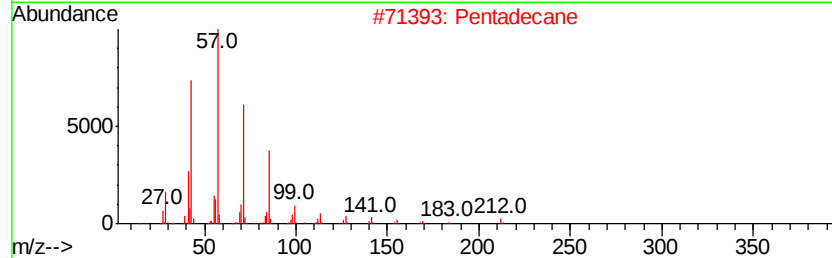
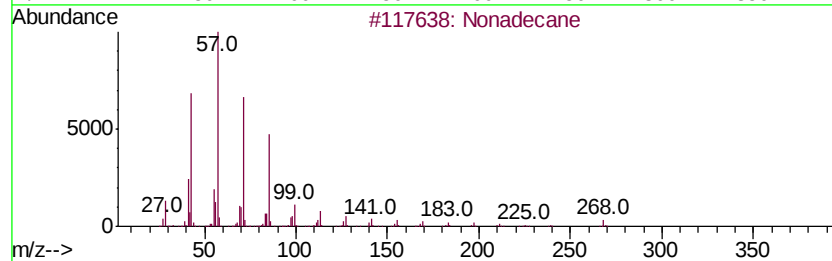
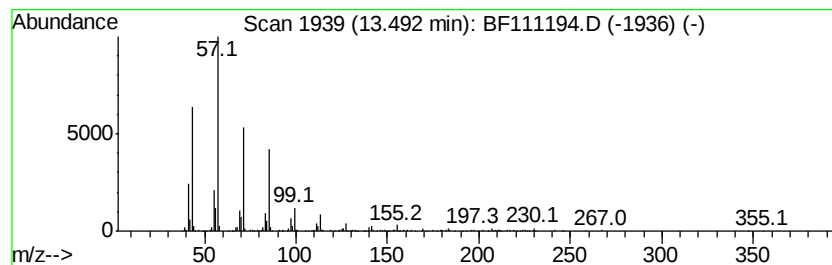
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	2.61 ng	381423	Chrysene-d12	13.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	90
2	Pentadecane		212	C15H32	000629-62-9	86
3	Heptacosane		380	C27H56	000593-49-7	81
4	Dodecane, 4-methyl-		184	C13H28	006117-97-1	81
5	Octadecane		254	C18H38	000593-45-3	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
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ClientSampleId :
SB-9(13-15)

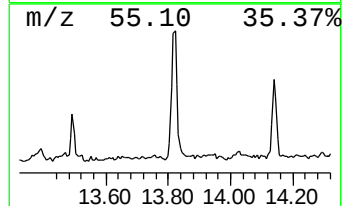
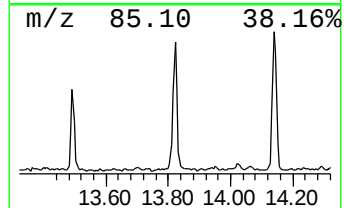
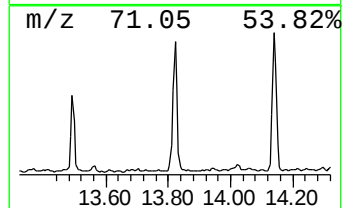
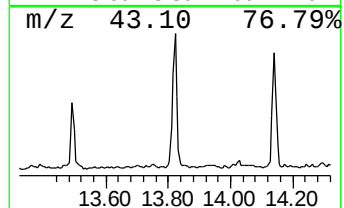
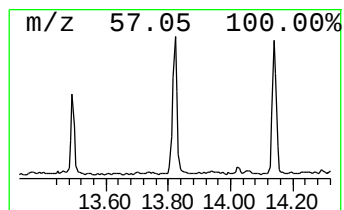
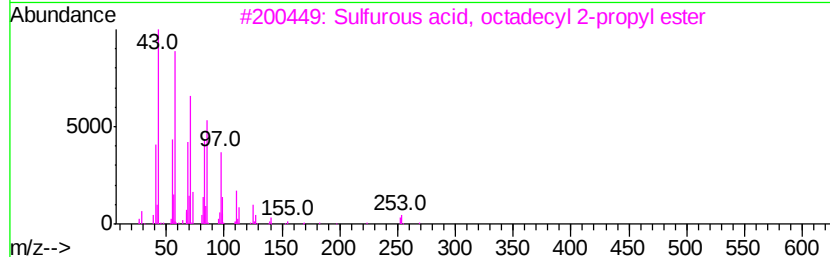
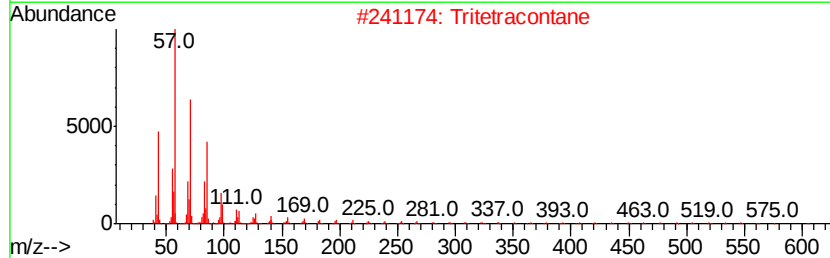
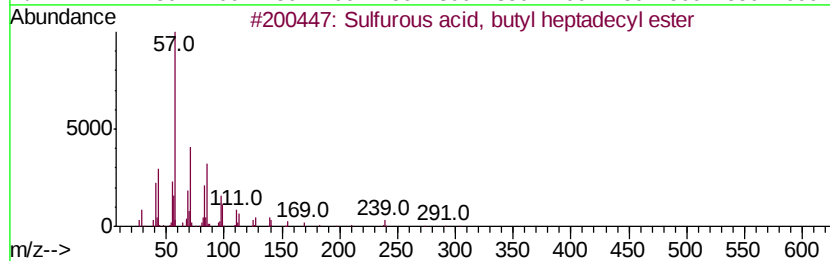
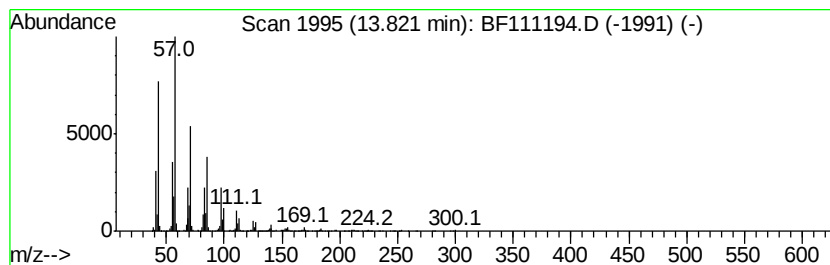
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Sulfurous acid, butyl hepta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	8.15 ng	1190440	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	91
2		Tritetracontane	605	C43H88	007098-21-7	91
3		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	74
4		Heneicosane	296	C21H44	000629-94-7	68
5		Eicosane	282	C20H42	000112-95-8	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
Data File : BF111194.D
Acq On : 7 Dec 2018 18:37
Operator : JU/SJ
Sample : J6214-05
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ClientSampleId :
SB-9(13-15)

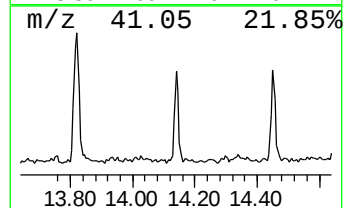
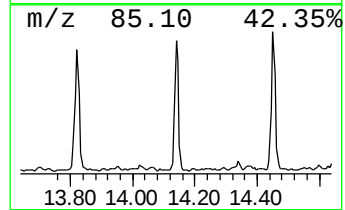
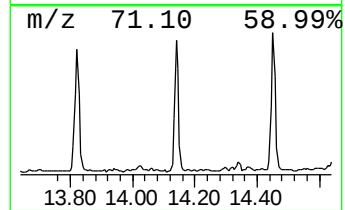
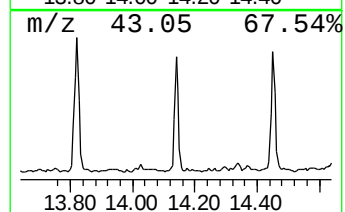
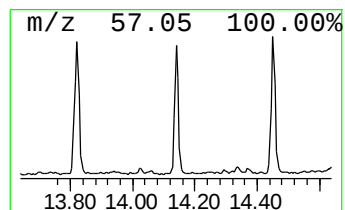
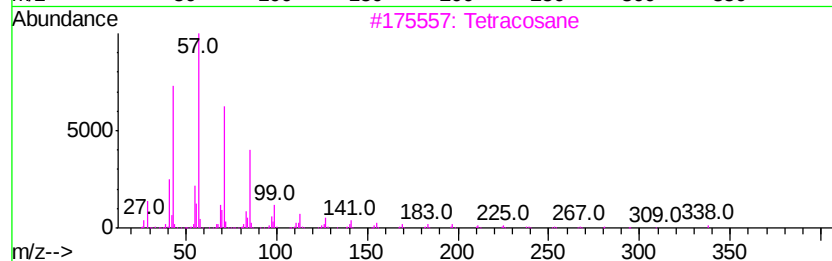
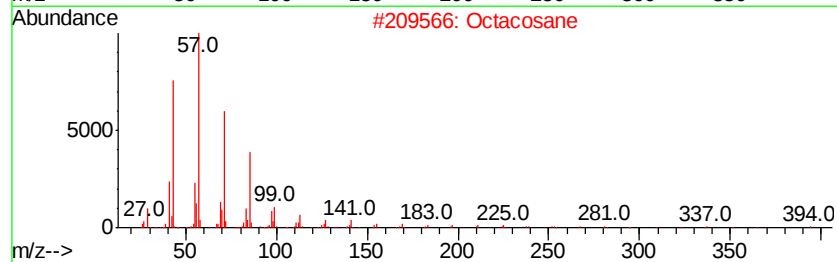
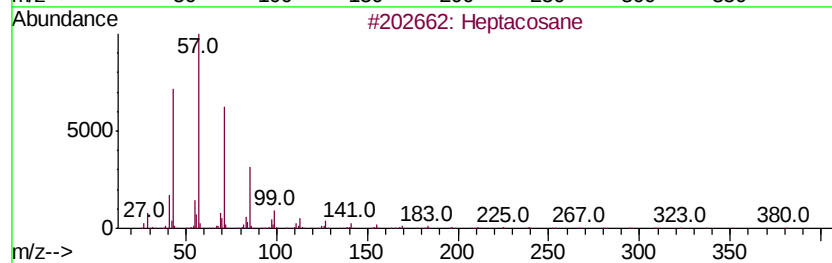
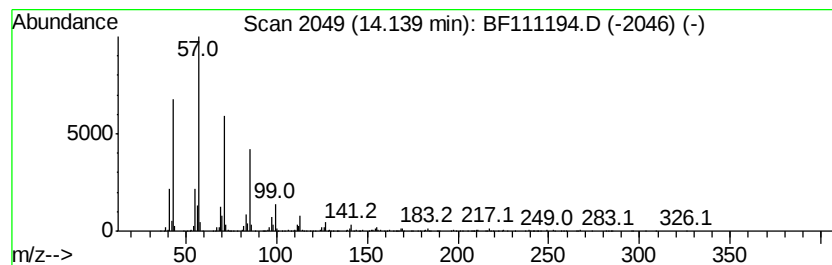
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	5.10 ng	745541	Chrysene-d12	13.96

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	Tetracosane		338	C24H50	000646-31-1	91
4	Heneicosane		296	C21H44	000629-94-7	90
5	Hexacosane		366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
Data File : BF111194.D
Acq On : 7 Dec 2018 18:37
Operator : JU/SJ
Sample : J6214-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

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SB-9(13-15)

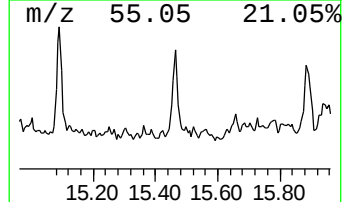
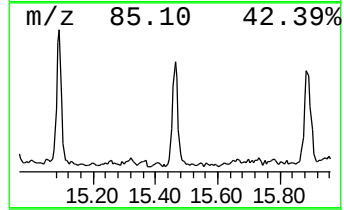
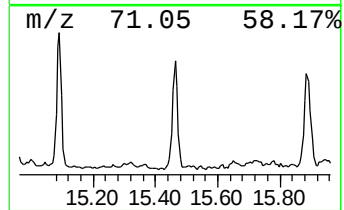
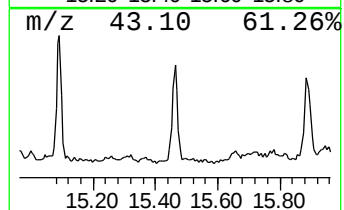
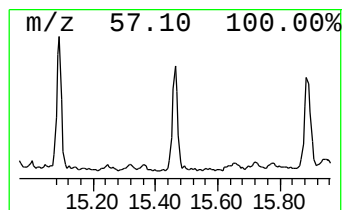
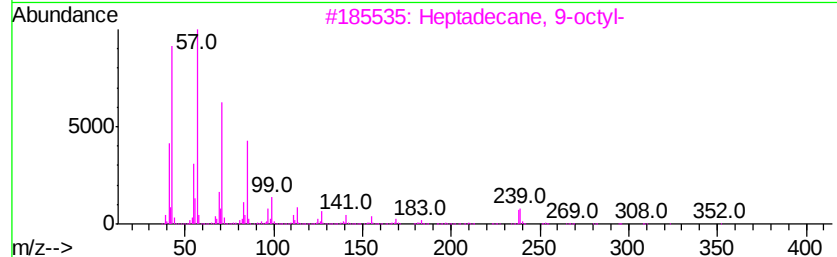
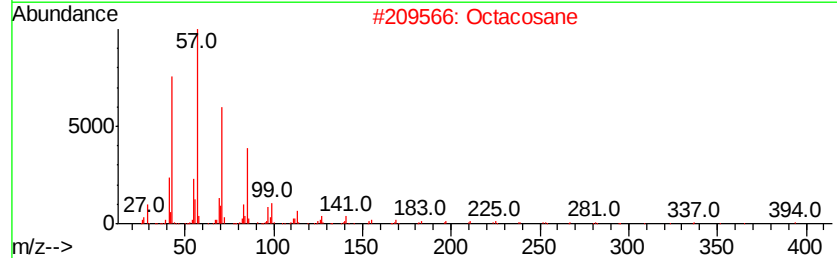
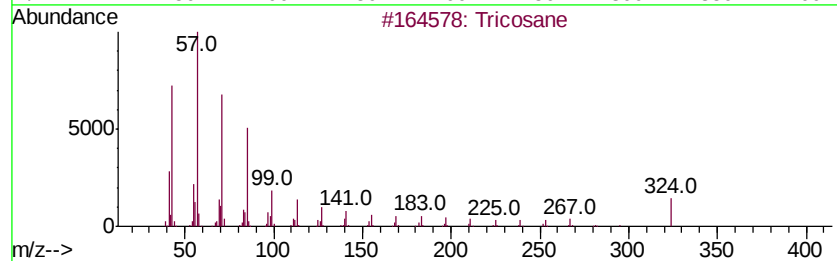
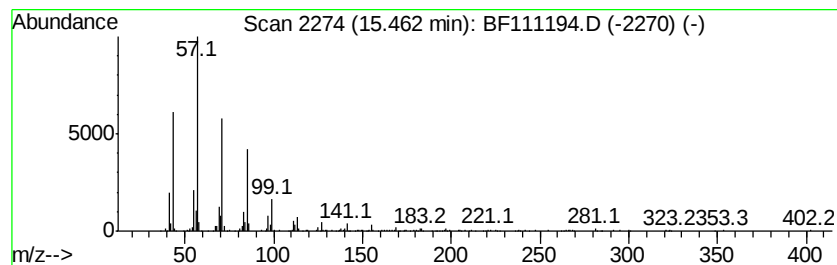
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Tricosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.46	4.46 ng	573876	Perylene-d12	15.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosane	324	C23H48	000638-67-5	95
2			Octacosane	394	C28H58	000630-02-4	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4			Nonadecane	268	C19H40	000629-92-5	91
5			Pentacosane	352	C25H52	000629-99-2	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
Data File : BF111194.D
Acq On : 7 Dec 2018 18:37
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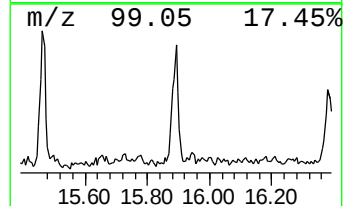
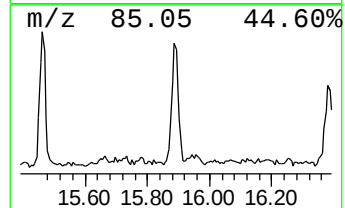
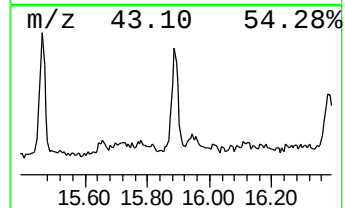
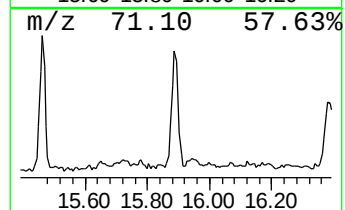
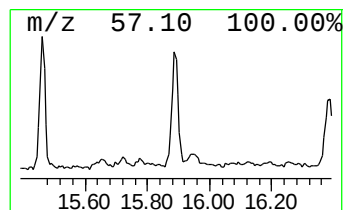
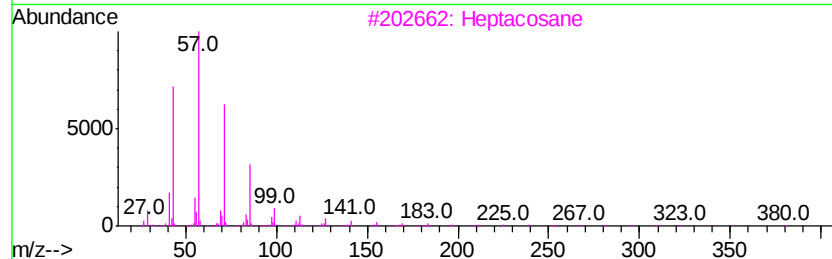
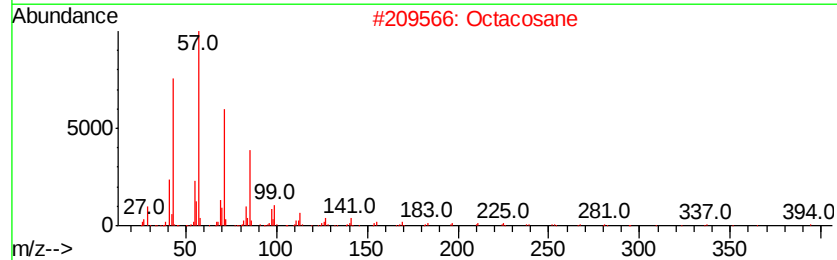
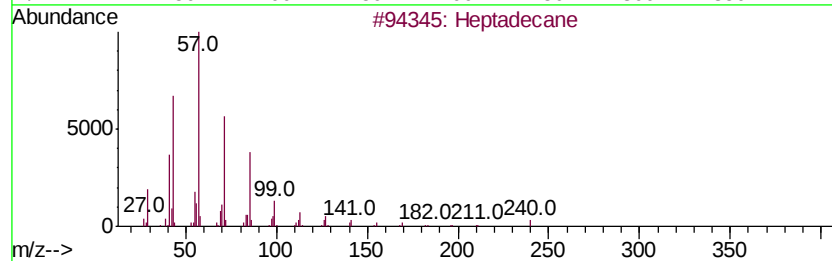
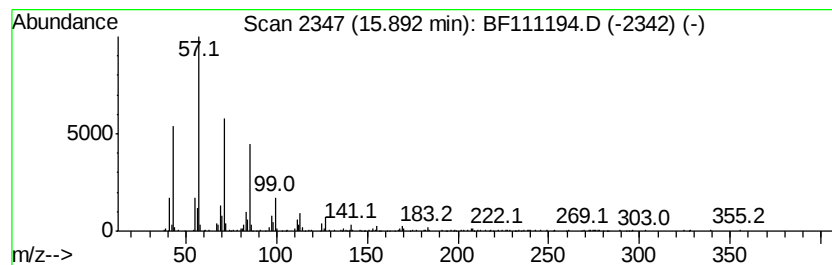
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	4.39 ng	565029	Perylene-d12	15.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	94
2			Octacosane	394	C28H58	000630-02-4	91
3			Heptacosane	380	C27H56	000593-49-7	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Tetracosane	338	C24H50	000646-31-1	91



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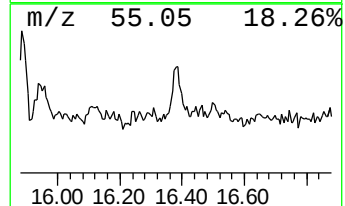
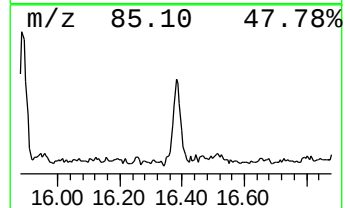
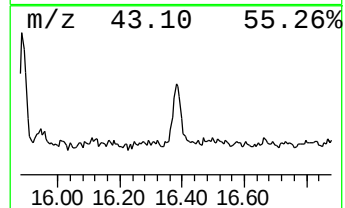
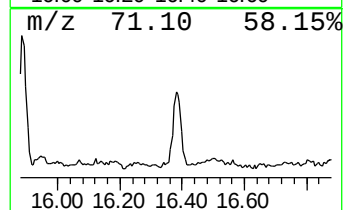
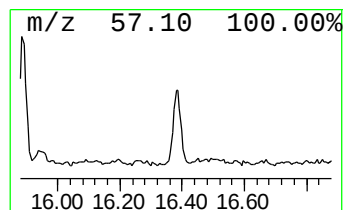
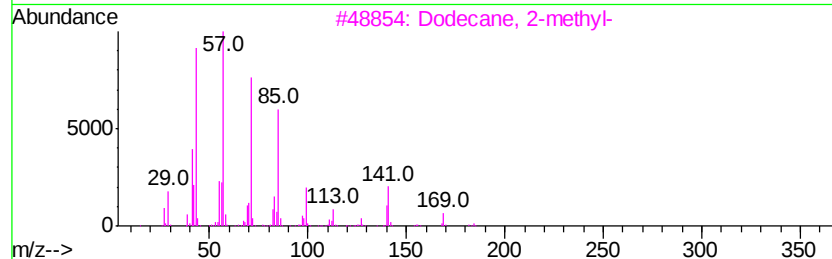
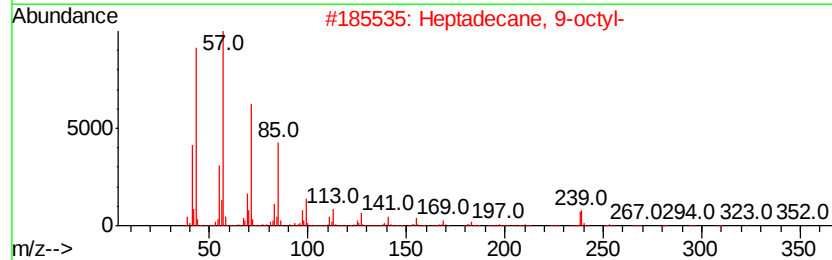
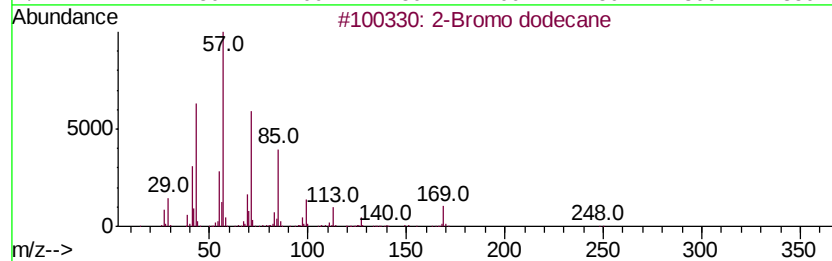
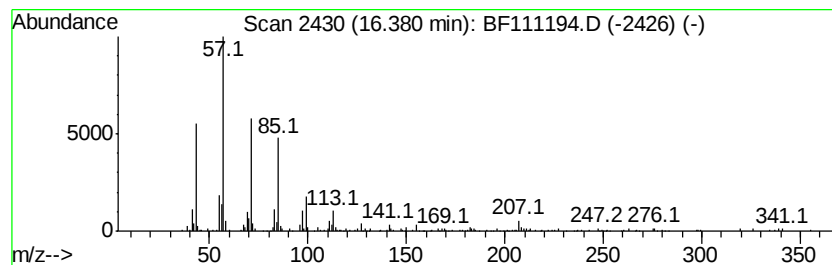
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 2-Bromo dodecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.38	3.08 ng	396867	Perylene-d12	15.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Bromo dodecane	248	C12H25Br	013187-99-0	90
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
3			Dodecane, 2-methyl-	184	C13H28	001560-97-0	81
4			Undecane, 5-methyl-	170	C12H26	001632-70-8	72
5			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120718\
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ALS Vial : 18 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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.02	7.8	ng	976708	1	6.80	2512280	20.0
unknown6.57	6.57	87.9	ng	11043100	1	6.80	2512280	20.0
n-Hexadecanoic acid	11.86	23.0	ng	4178810	4	11.32	3633170	20.0
Octadecanoic acid	12.64	22.2	ng	3240220	5	13.96	2922920	20.0
Nonadecane	13.49	2.6	ng	381423	5	13.96	2922920	20.0
Sulfurous acid, b...	13.82	8.2	ng	1190440	5	13.96	2922920	20.0
Heptacosane	14.14	5.1	ng	745541	5	13.96	2922920	20.0
Tricosane	15.46	4.5	ng	573876	6	15.40	2574510	20.0
Heptadecane	15.89	4.4	ng	565029	6	15.40	2574510	20.0
2-Bromo dodecane	16.38	3.1	ng	396867	6	15.40	2574510	20.0