

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010319\
 Data File : BF111830.D
 Acq On : 3 Jan 2019 19:27
 Operator : JU/SJ
 Sample : K1017-21
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-6

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-BF121918.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	2.205	15	20	29	rVB	169464	223760	3.17%	0.367%
2	3.446	227	231	247	rBV	82740	195306	2.77%	0.320%
3	5.128	507	517	524	rBV	310684	393844	5.59%	0.646%
4	5.540	582	587	590	rBV	5825500	5804006	82.33%	9.523%
5	6.545	752	758	763	rBV	5467974	6618862	93.89%	10.860%
6	6.681	776	781	784	rBV	6537183	6180255	87.67%	10.141%
7	6.898	815	818	822	rVB	1912330	1705235	24.19%	2.798%
8	7.063	841	846	849	rBV	5218031	4814910	68.30%	7.900%
9	7.463	908	914	917	rBV	4241883	4115608	58.38%	6.753%
10	8.187	1032	1037	1040	rBV	2442312	2243891	31.83%	3.682%
11	9.257	1214	1219	1222	rBV	7850323	7049370	100.00%	11.567%
12	9.645	1282	1285	1290	rBV	1139999	916329	13.00%	1.504%
13	9.939	1331	1335	1339	rBV	3033315	2526845	35.84%	4.146%
14	10.728	1465	1469	1473	rBV	4486704	4328484	61.40%	7.102%
15	10.851	1486	1490	1497	rVB	119388	152770	2.17%	0.251%
16	11.316	1566	1569	1575	rVB	83441	106771	1.51%	0.175%
17	11.422	1584	1587	1590	rBV	2232794	2178575	30.90%	3.575%
18	11.445	1590	1591	1594	rVB	332582	220347	3.13%	0.362%
19	11.945	1674	1676	1680	rVB2	141980	129408	1.84%	0.212%
20	12.039	1689	1692	1694	rBV	77622	79496	1.13%	0.130%
21	12.510	1769	1772	1775	rBV2	83122	77048	1.09%	0.126%
22	12.639	1790	1794	1798	rVB	427338	402352	5.71%	0.660%
23	12.863	1827	1832	1837	rBV	363620	466820	6.62%	0.766%
24	13.010	1852	1857	1860	rBV	5112578	4705825	66.76%	7.722%
25	13.904	2005	2009	2017	rVB2	324511	428289	6.08%	0.703%
26	14.063	2031	2036	2039	rBV	1848220	1815638	25.76%	2.979%
27	14.086	2039	2040	2046	rVB	198634	164187	2.33%	0.269%
28	14.221	2060	2063	2066	rBV	182554	158537	2.25%	0.260%
29	14.527	2112	2115	2120	rBV	226050	246545	3.50%	0.405%
30	14.839	2165	2168	2173	rVB	204359	193540	2.75%	0.318%
31	15.115	2211	2215	2218	rBV	139925	207795	2.95%	0.341%
32	15.186	2223	2227	2231	rBV	203894	233601	3.31%	0.383%
33	15.421	2264	2267	2273	rVB	80269	110502	1.57%	0.181%
34	15.480	2274	2277	2281	rVV	99034	136015	1.93%	0.223%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.551	2284	2289	2300	rVB	955152	1432564	20.32%	2.351%
36	16.021	2365	2369	2374	rVB	128560	181108	2.57%	0.297%

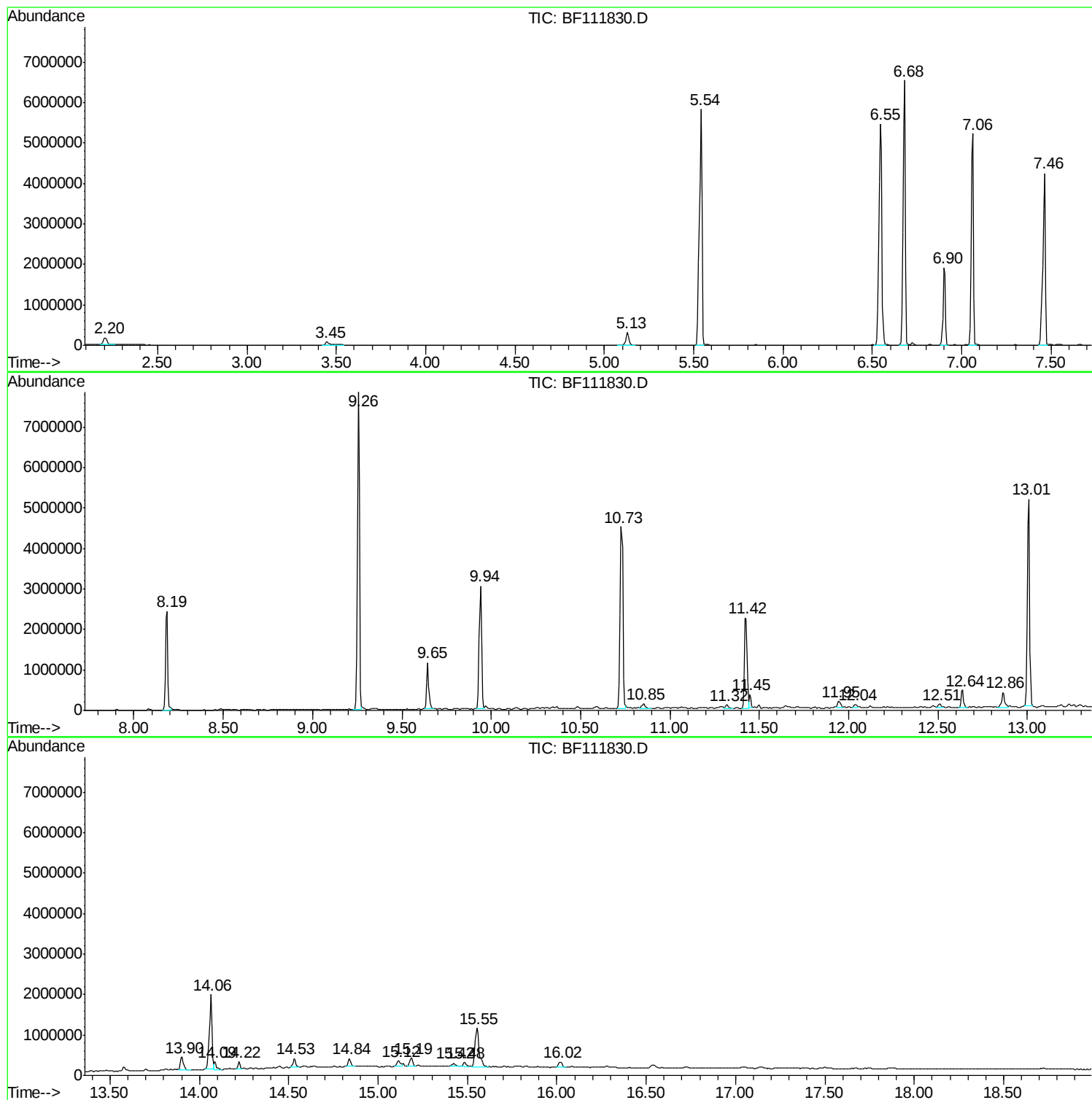
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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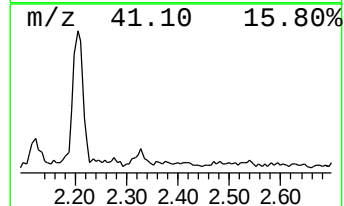
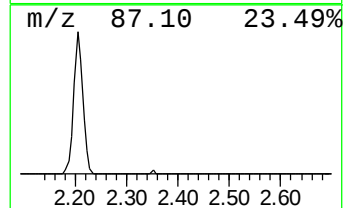
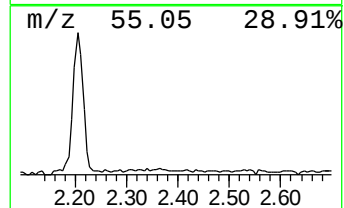
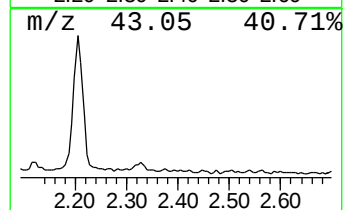
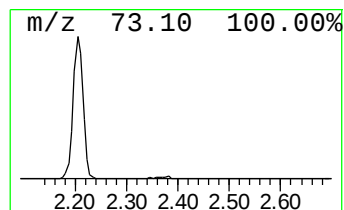
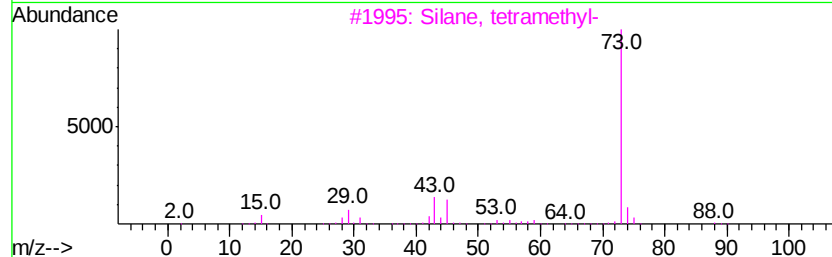
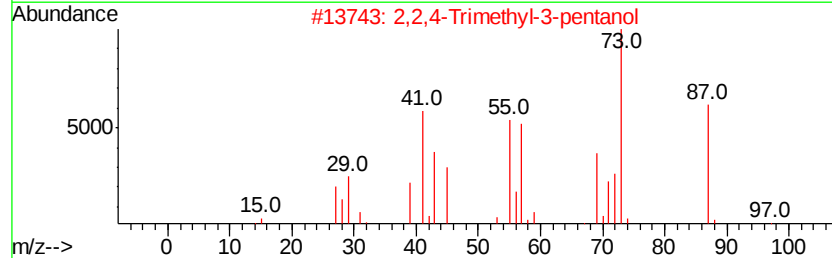
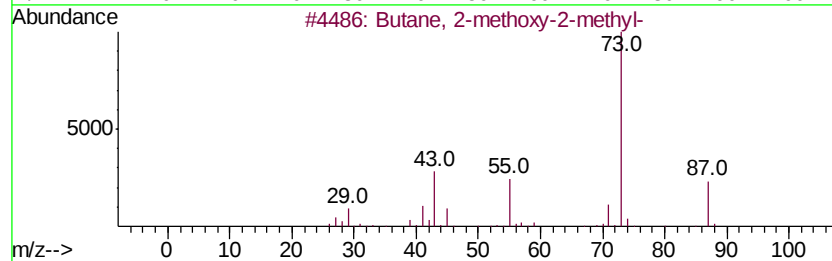
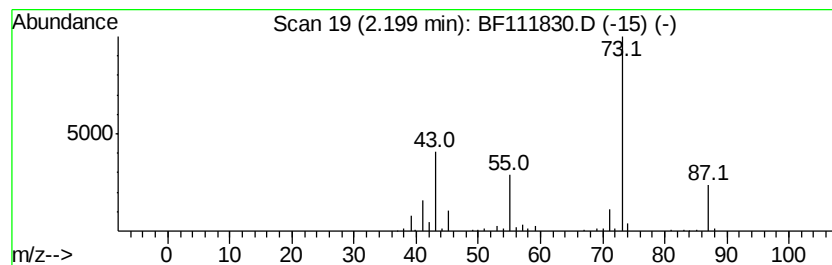
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	2.62 ng	223760	1,4-Dichlorobenzene-d4	6.90

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		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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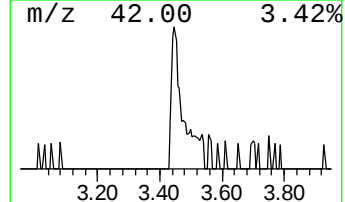
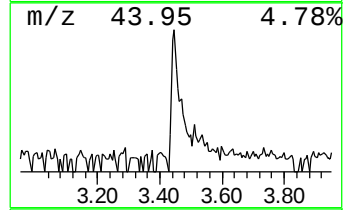
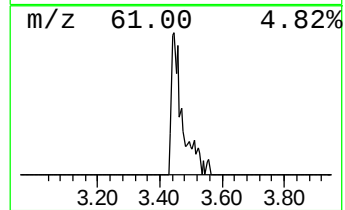
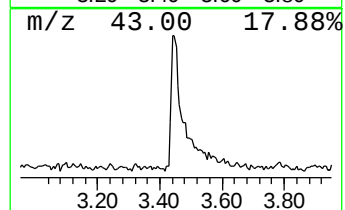
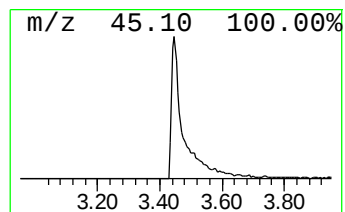
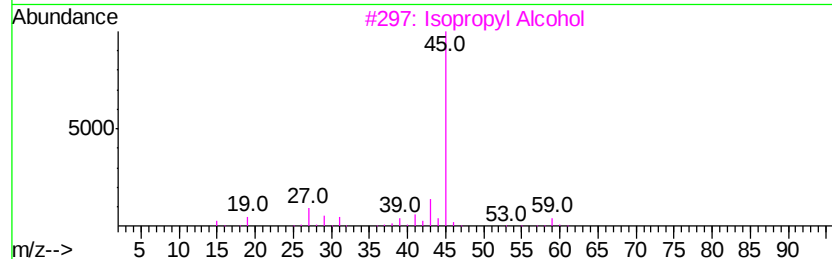
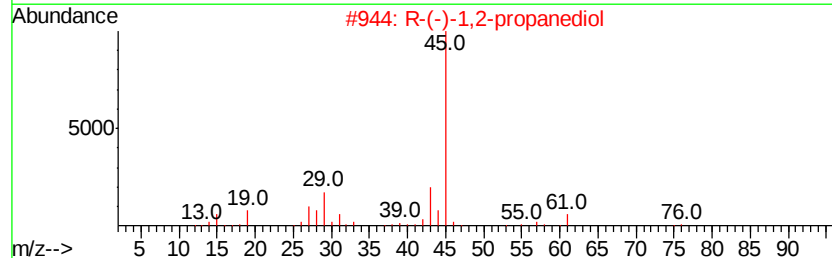
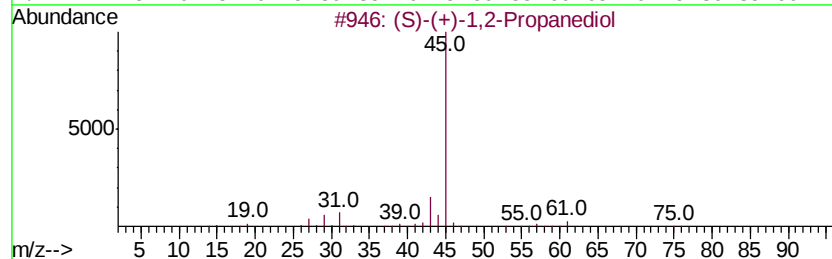
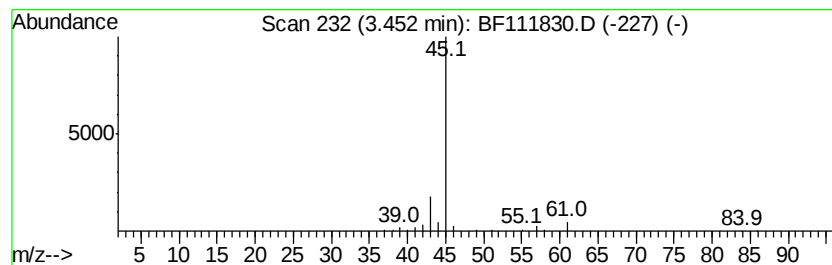
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.45	2.29 ng	195306	1,4-Dichlorobenzene-d4	6.90	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
5	Propylene Glycol	76	C3H8O2	000057-55-6	9



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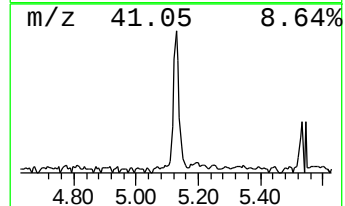
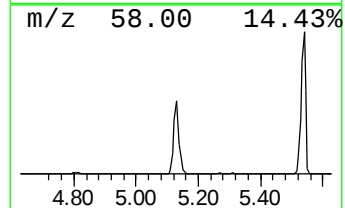
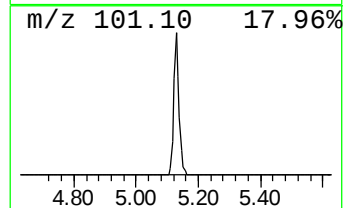
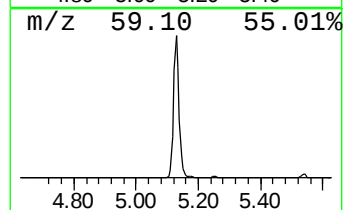
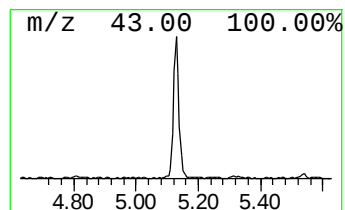
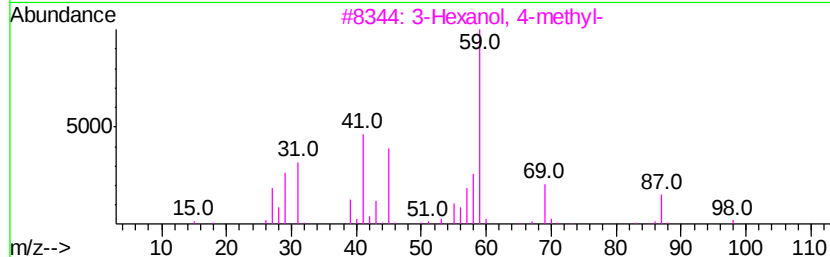
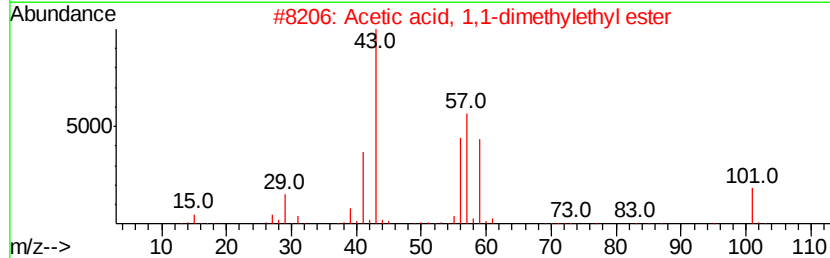
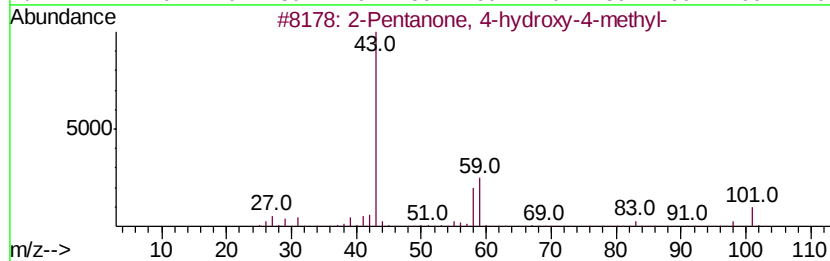
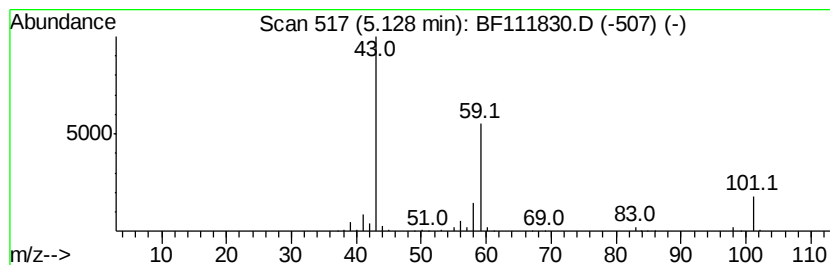
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	4.62 ng	393844	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5			3-Hexanol	102	C6H14O	000623-37-0	33



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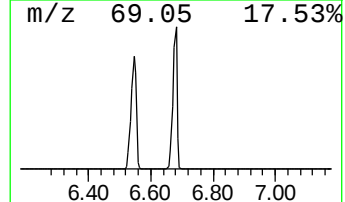
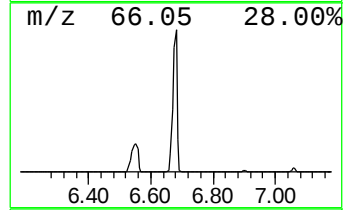
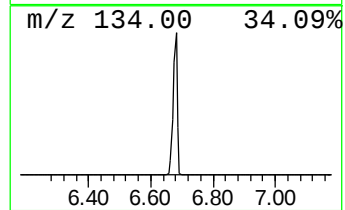
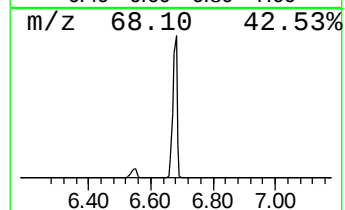
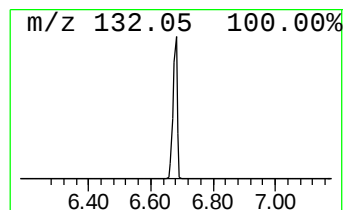
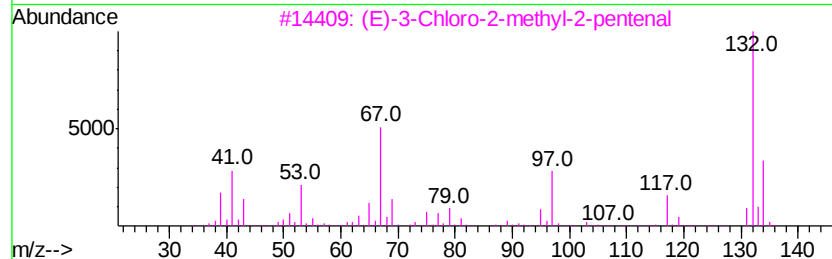
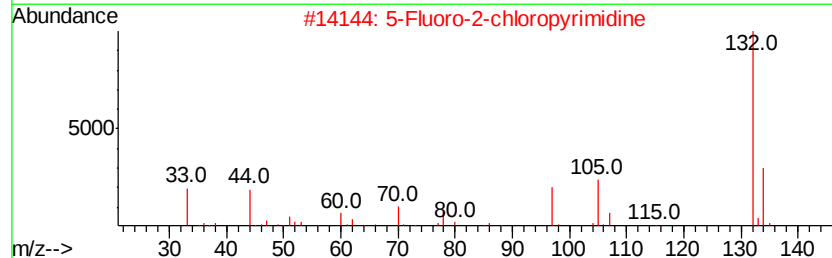
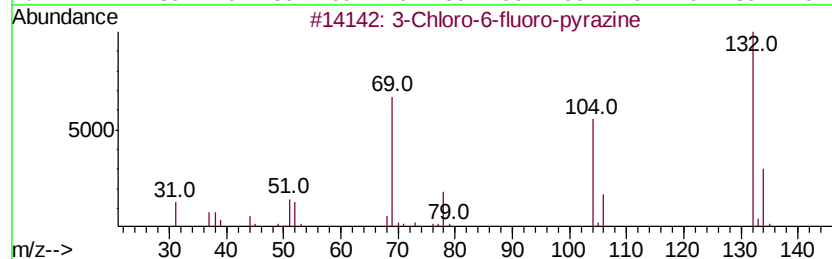
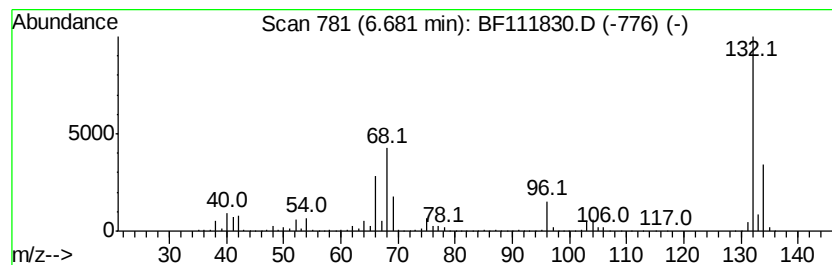
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	72.49 ng	6180260	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16	
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16	
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12	
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9	



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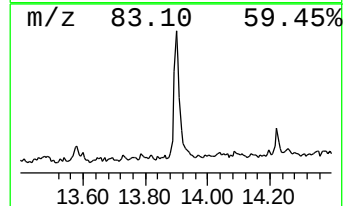
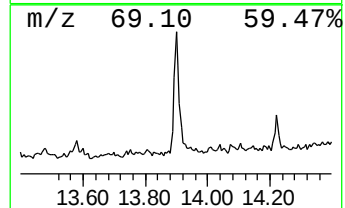
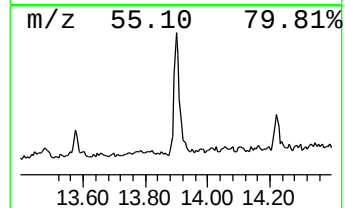
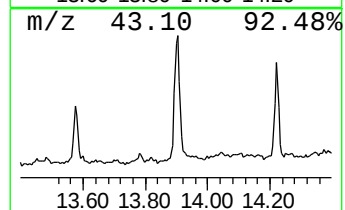
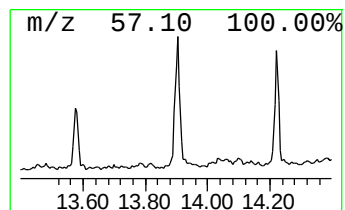
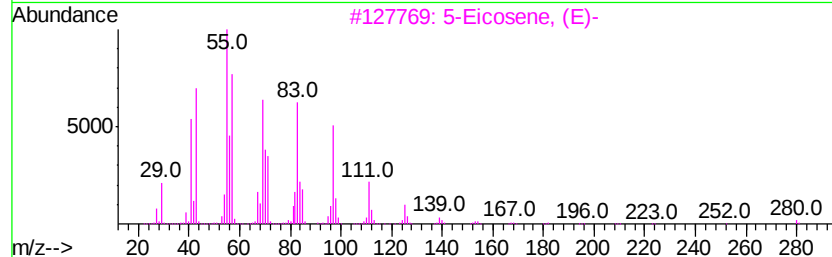
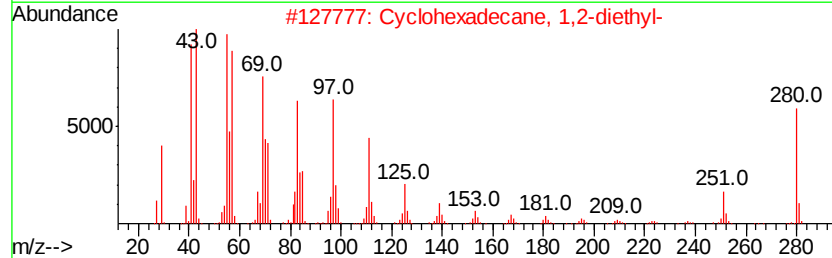
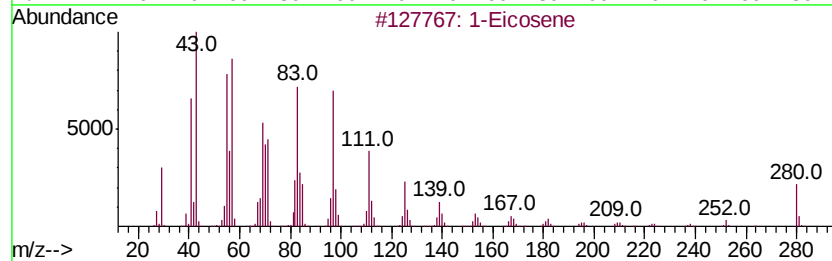
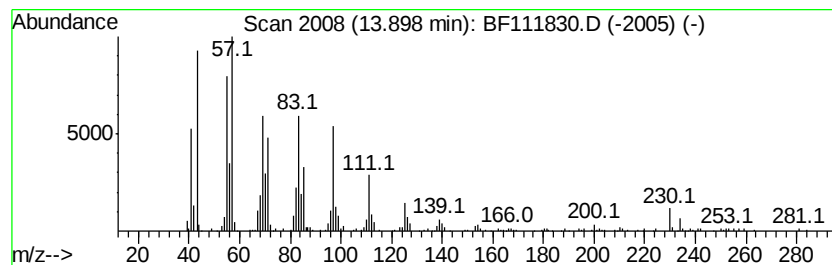
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Eicosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	4.72 ng	428289	Chrysene-d12	14.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Eicosene		280 C20H40	003452-07-1 95
2	Cyclohexadecane, 1,2-diethyl-		280 C20H40	1000155-85-3 95
3	5-Eicosene, (E)-		280 C20H40	074685-30-6 90
4	1-Decanol, 2-octyl-		270 C18H38O	045235-48-1 87
5	Sulfurous acid, octadecyl 2-prop...		376 C21H44O3S	1000309-12-7 76



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010319\
 Data File : BF111830.D
 Acq On : 3 Jan 2019 19:27
 Operator : JU/SJ
 Sample : K1017-21
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-6

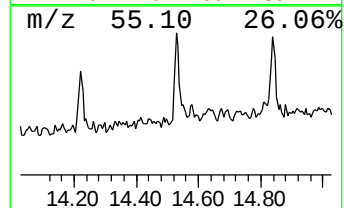
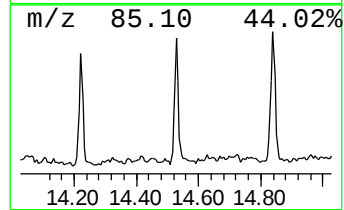
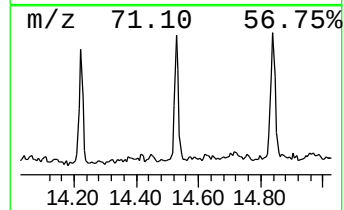
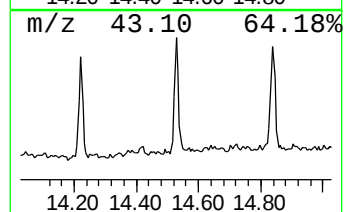
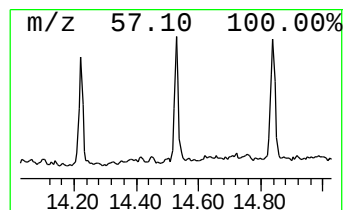
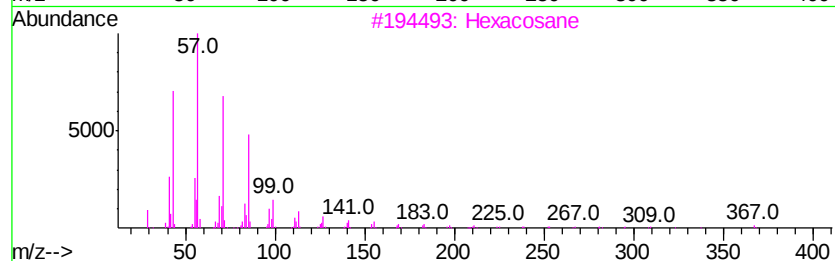
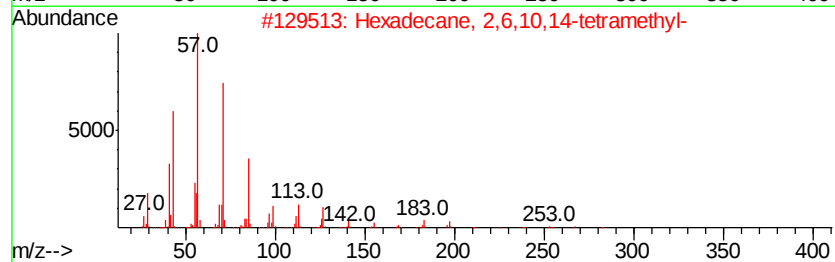
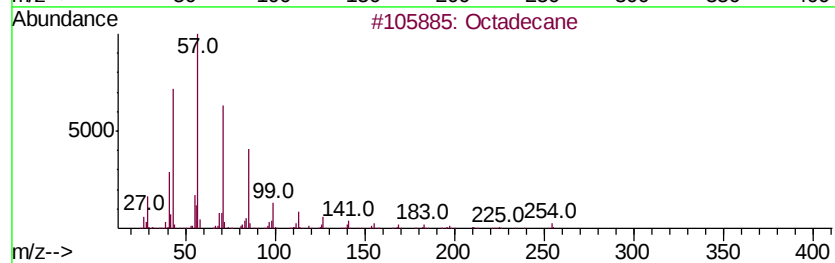
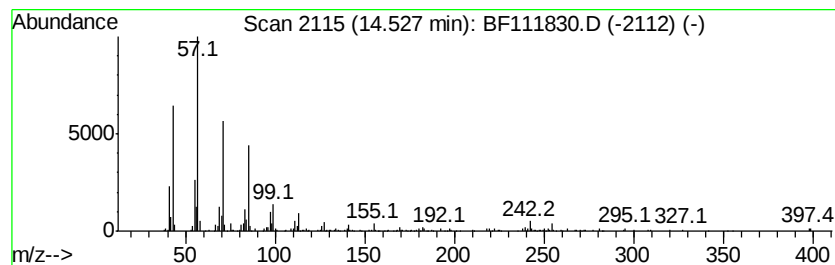
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	2.72 ng	246545	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	93
2		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	89
3		Hexacosane	366	C26H54	000630-01-3	87
4		Octacosane	394	C28H58	000630-02-4	87
5		Eicosane, 10-methyl-	296	C21H44	054833-23-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010319\
Data File : BF111830.D
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Sample : K1017-21
Misc :
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ClientSampleId :
TP-6

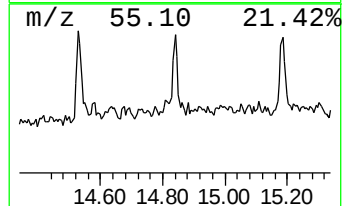
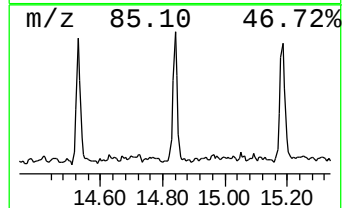
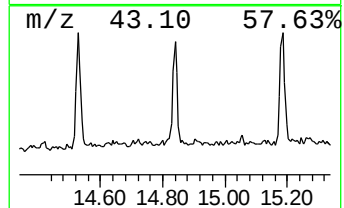
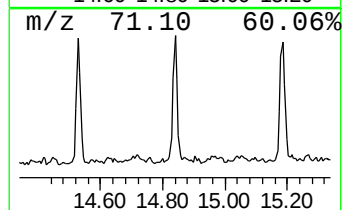
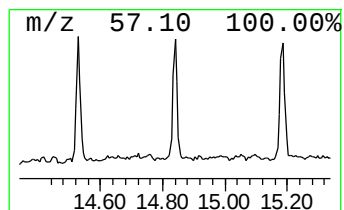
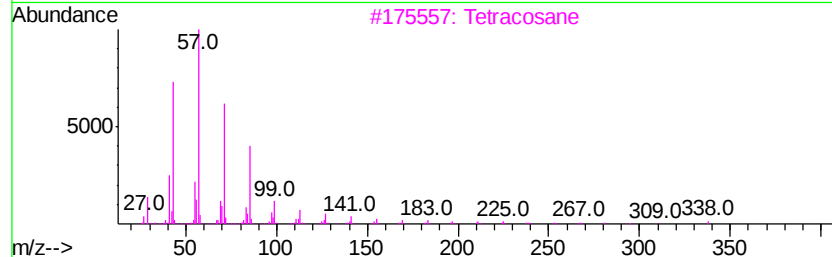
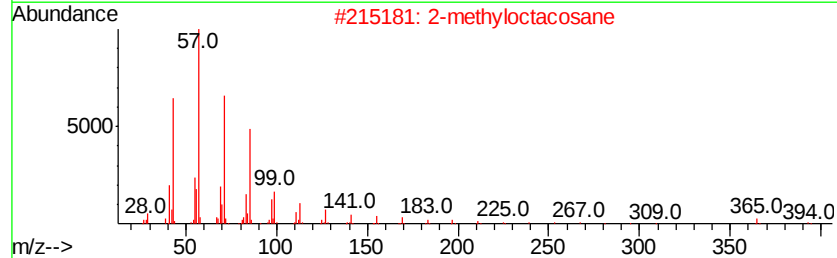
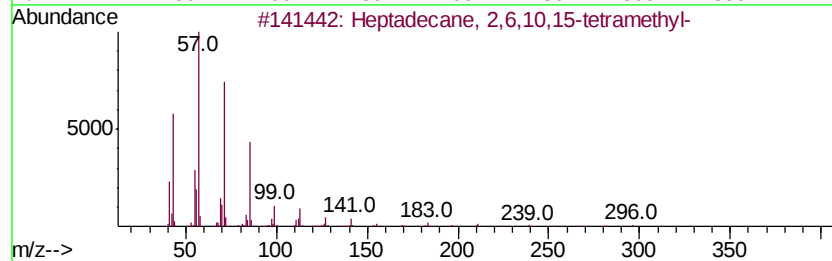
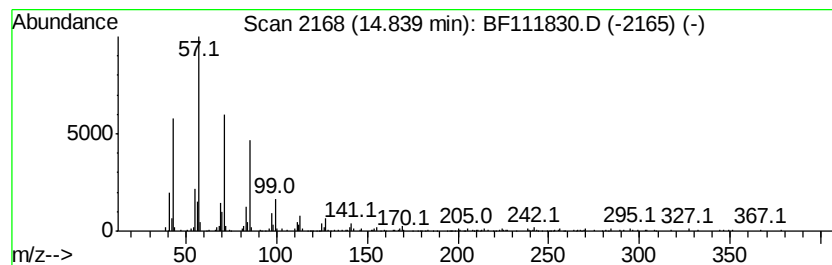
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane, 2,6,10,15-tetr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	2.70 ng	193540	Perylene-d12	15.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
2		2-methyloctacosane	408	C29H60	1000376-72-8	87
3		Tetracosane	338	C24H50	000646-31-1	86
4		Heneicosane	296	C21H44	000629-94-7	86
5		Octadecane, 2-methyl-	268	C19H40	001560-88-9	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010319\
Data File : BF111830.D
Acq On : 3 Jan 2019 19:27
Operator : JU/SJ
Sample : K1017-21
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

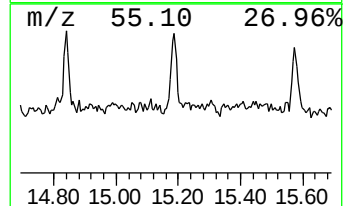
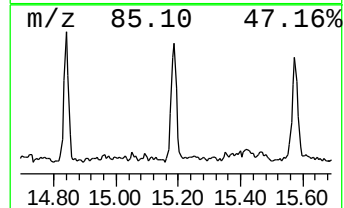
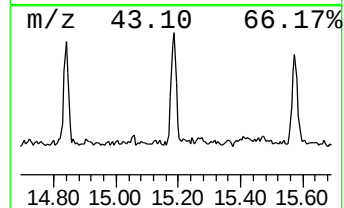
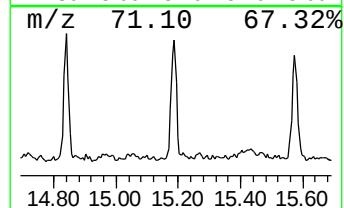
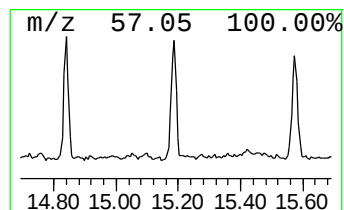
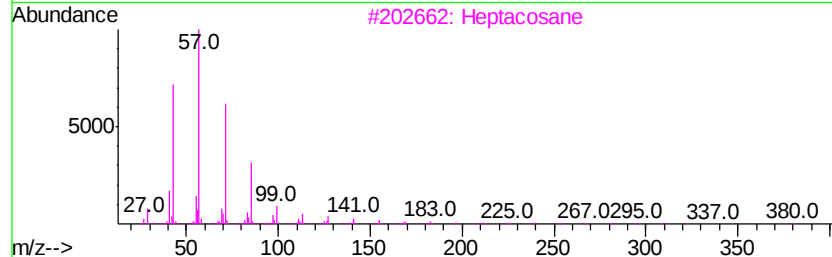
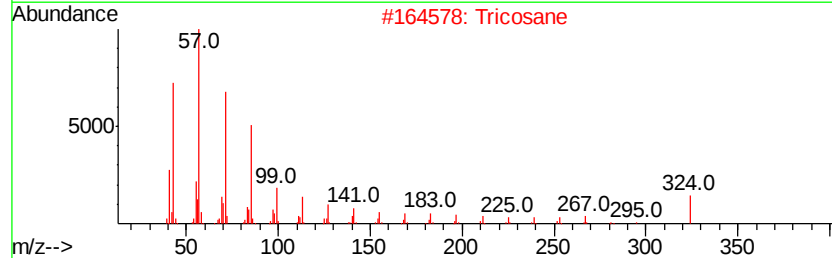
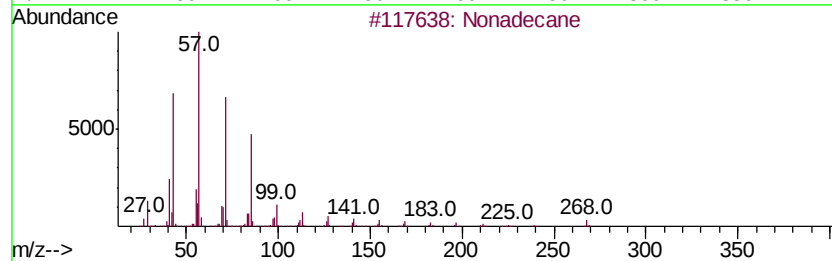
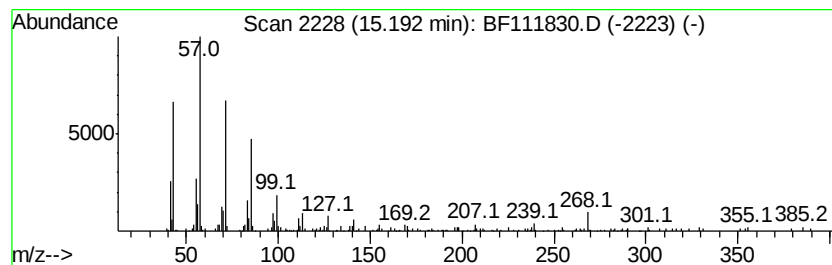
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	3.26 ng	233601	Perylene-d12	15.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	98
2	Tricosane		324	C23H48	000638-67-5	91
3	Heptacosane		380	C27H56	000593-49-7	90
4	Octacosane		394	C28H58	000630-02-4	90
5	2-methyloctacosane		408	C29H60	1000376-72-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010319\
 Data File : BF111830.D
 Acq On : 3 Jan 2019 19:27
 Operator : JU/SJ
 Sample : K1017-21
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

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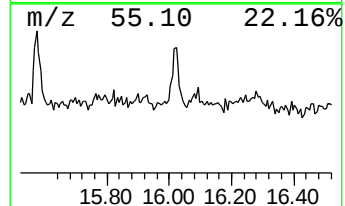
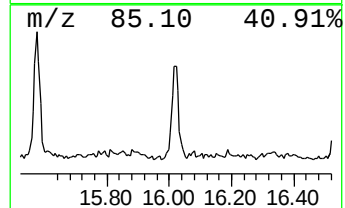
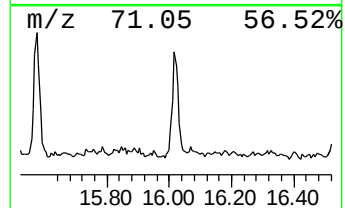
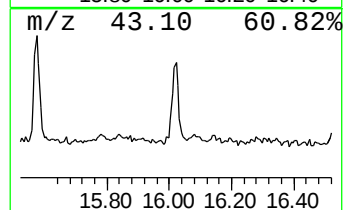
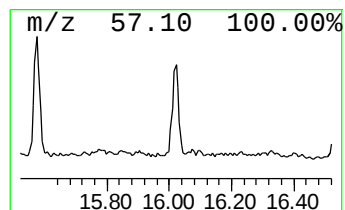
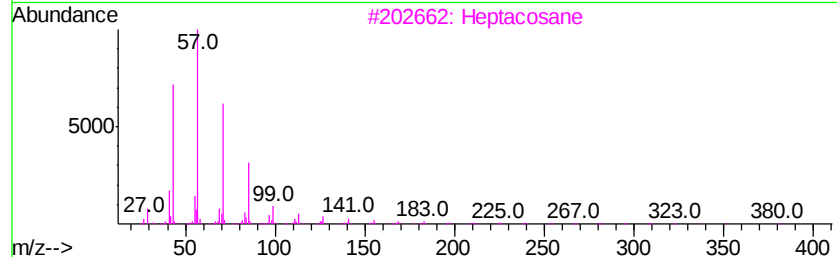
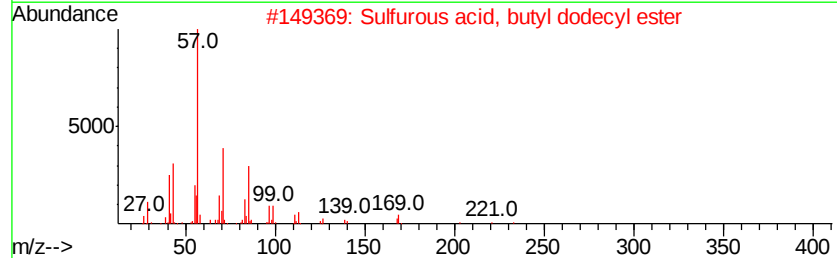
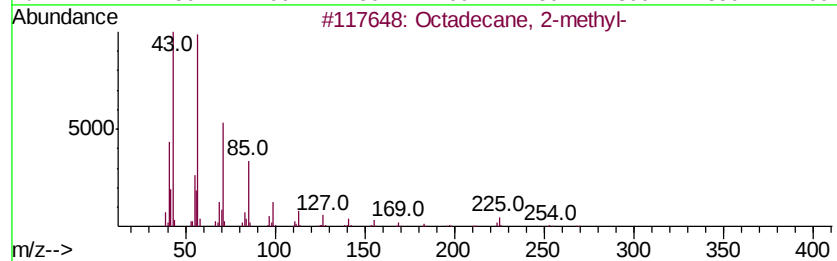
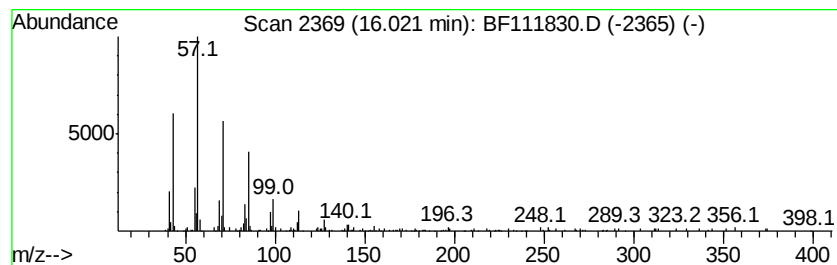
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 10 Octadecane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	2.53 ng	181108	Perylene-d12	15.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	86
2		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86
3		Heptacosane	380	C27H56	000593-49-7	86
4		Heptadecane	240	C17H36	000629-78-7	80
5		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF010319\
Data File : BF111830.D
Acq On : 3 Jan 2019 19:27
Operator : JU/SJ
Sample : K1017-21
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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...	2.20	2.6	ng	223760	1	6.90	1705240	20.0
(S)-(+)-1,2-Propa...	3.45	2.3	ng	195306	1	6.90	1705240	20.0
2-Pentanone, 4-hy...	5.13	4.6	ng	393844	1	6.90	1705240	20.0
unknown6.68	6.68	72.5	ng	6180260	1	6.90	1705240	20.0
1-Eicosene	13.90	4.7	ng	428289	5	14.06	1815640	20.0
Octadecane	14.53	2.7	ng	246545	5	14.06	1815640	20.0
Heptadecane, 2,6,...	14.84	2.7	ng	193540	6	15.55	1432560	20.0
Nonadecane	15.19	3.3	ng	233601	6	15.55	1432560	20.0
Octadecane, 2-met...	16.02	2.5	ng	181108	6	15.55	1432560	20.0