

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101518\
 Data File : BF109892.D
 Acq On : 15 Oct 2018 21:14
 Operator : JU/SJ
 Sample : J5198-15
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CL-02-101218-C

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-BF101518.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	2.316	33	39	44	rVB	629139	820587	18.63%	1.973%
2	5.210	527	531	539	rVB	162995	201198	4.57%	0.484%
3	5.598	591	597	600	rBV	4371796	4329589	98.29%	10.411%
4	6.592	760	766	770	rBV	4562689	4405131	100.00%	10.593%
5	6.745	787	792	795	rBV	4886932	4381521	99.46%	10.536%
6	6.975	828	831	835	rVB	1686299	1460555	33.16%	3.512%
7	7.134	854	858	861	rBV	4093870	3386843	76.88%	8.144%
8	7.539	922	927	930	rBV	2737463	2661818	60.43%	6.401%
9	8.257	1045	1049	1053	rBV	1922910	1721826	39.09%	4.140%
10	9.333	1227	1232	1235	rBV	4769668	3837301	87.11%	9.227%
11	9.722	1295	1298	1302	rBV	505418	391012	8.88%	0.940%
12	10.016	1344	1348	1352	rVB	1641895	1514988	34.39%	3.643%
13	10.433	1413	1419	1422	rVB2	35332	56183	1.28%	0.135%
14	10.804	1478	1482	1486	rBV	2234198	1896713	43.06%	4.561%
15	11.386	1579	1581	1587	rVB2	34376	47088	1.07%	0.113%
16	11.510	1598	1602	1604	rBV	1534423	1359018	30.85%	3.268%
17	11.533	1604	1606	1609	rVB	155319	127802	2.90%	0.307%
18	11.886	1663	1666	1669	rBV	78624	64923	1.47%	0.156%
19	12.016	1684	1688	1691	rBV2	220919	261127	5.93%	0.628%
20	12.121	1703	1706	1708	rBV2	62813	61824	1.40%	0.149%
21	12.574	1777	1783	1785	rBV3	179270	213554	4.85%	0.514%
22	12.592	1785	1786	1789	rVB2	207421	160632	3.65%	0.386%
23	12.680	1798	1801	1804	rBV2	53638	50267	1.14%	0.121%
24	12.721	1805	1808	1812	rBV	418171	355428	8.07%	0.855%
25	12.804	1820	1822	1826	rBV3	66261	95353	2.16%	0.229%
26	12.951	1842	1847	1854	rVB	445210	449451	10.20%	1.081%
27	13.092	1867	1871	1874	rBV	3676543	3076081	69.83%	7.397%
28	13.280	1900	1903	1906	rVB	80150	71277	1.62%	0.171%
29	13.310	1906	1908	1910	rBV	57869	46491	1.06%	0.112%
30	13.345	1912	1914	1917	rVB2	70248	56488	1.28%	0.136%
31	13.974	2018	2021	2026	rBV2	436490	432202	9.81%	1.039%
32	14.151	2047	2051	2054	rBV	1819300	1725975	39.18%	4.150%
33	14.610	2126	2129	2135	rVB2	216161	266420	6.05%	0.641%
34	15.286	2241	2244	2247	rBV	218186	218647	4.96%	0.526%

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ClientSampleId :
CL-02-101218-C

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-BF101518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.674	2306	2310	2319	rVB	903069	1381013	31.35%	3.321%
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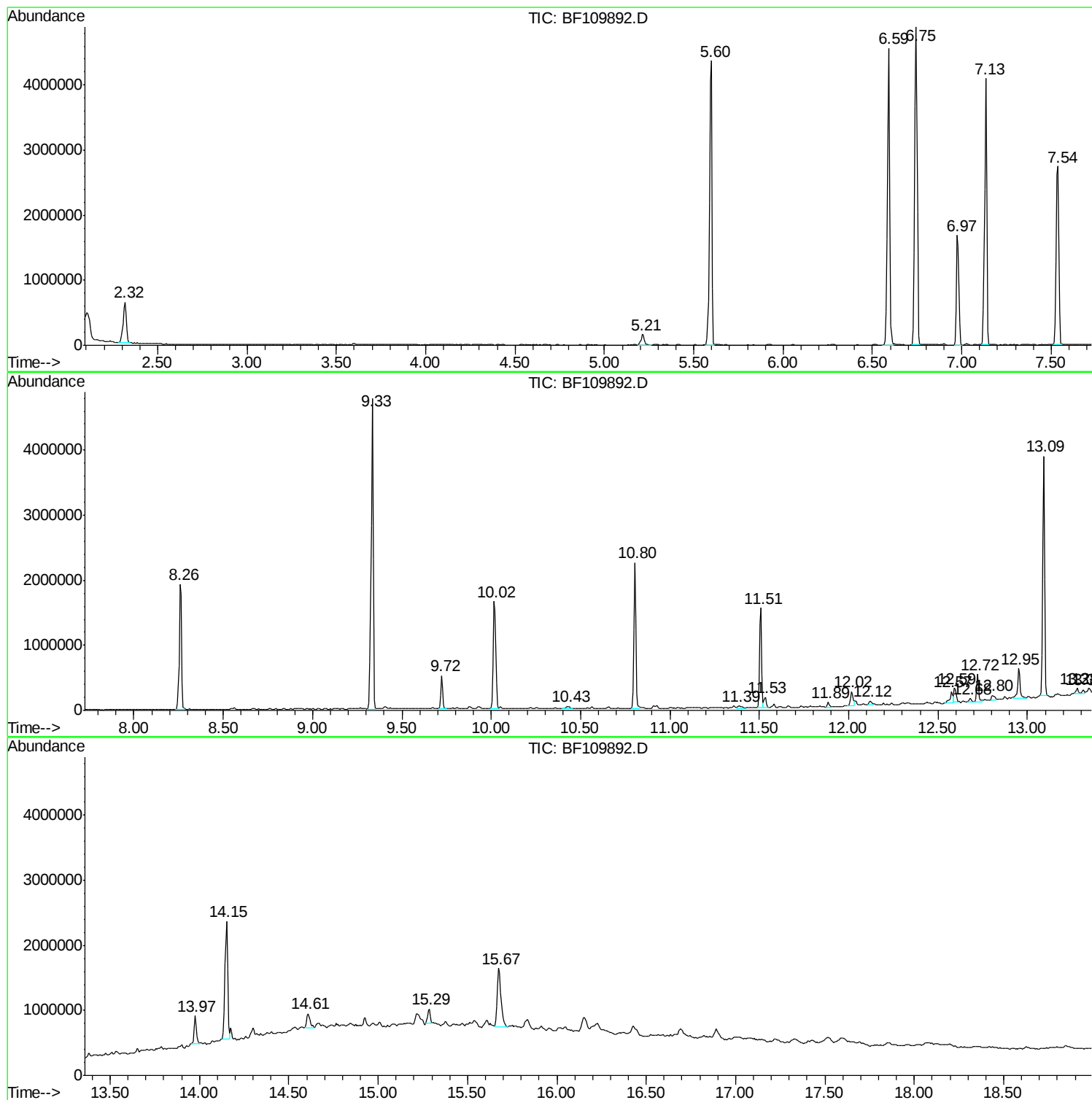
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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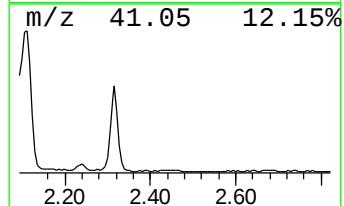
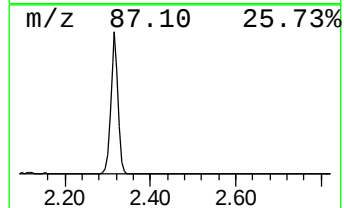
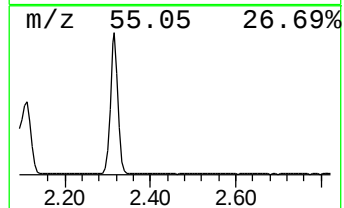
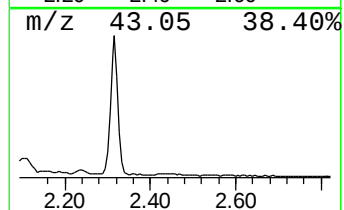
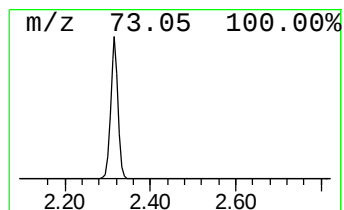
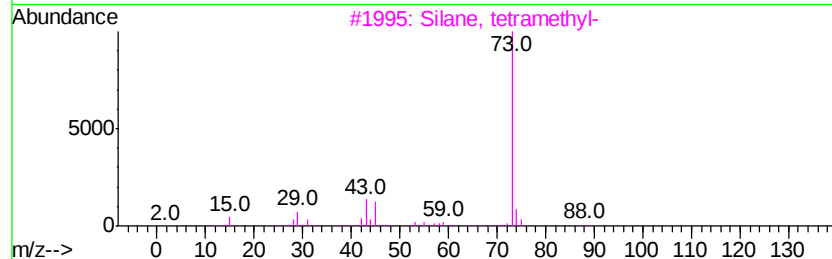
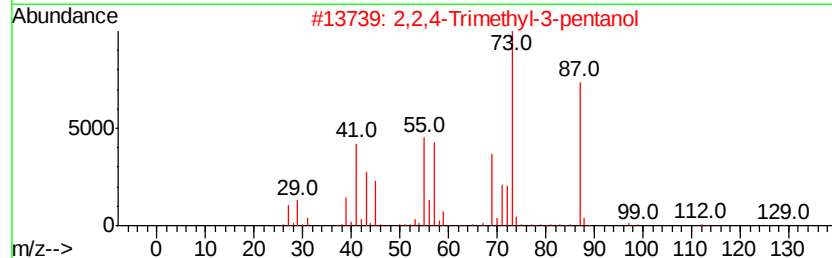
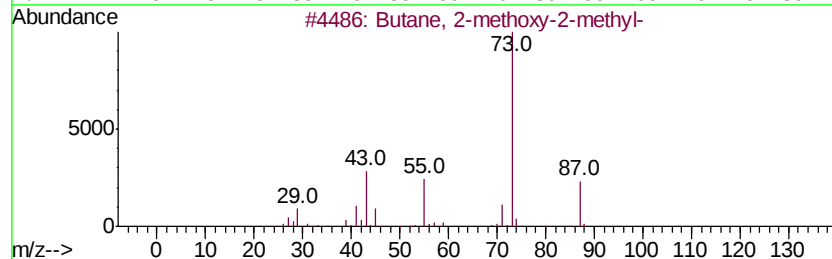
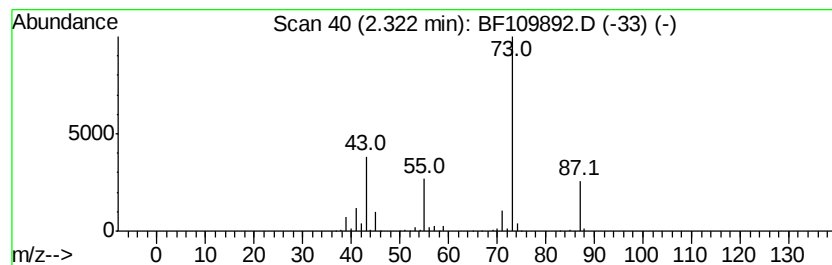
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.32	11.24 ng	820587	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		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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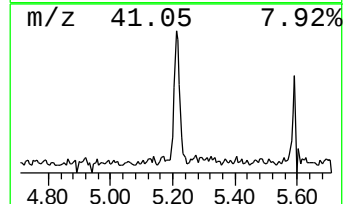
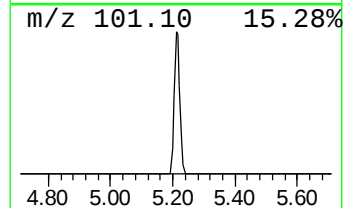
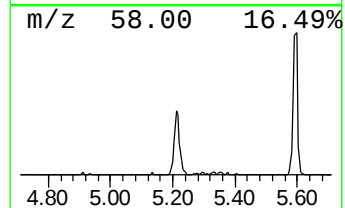
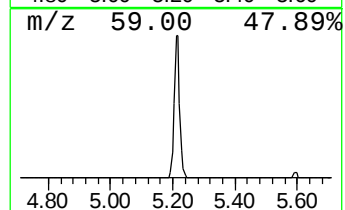
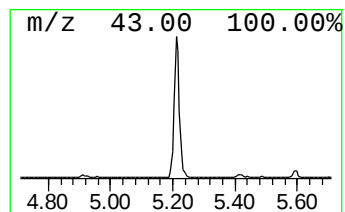
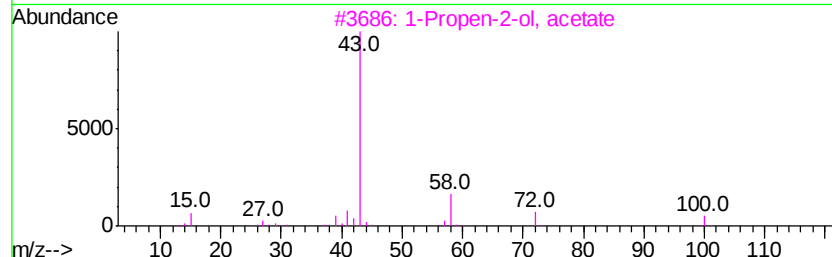
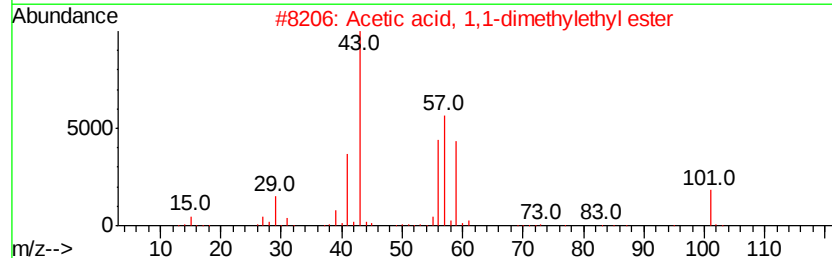
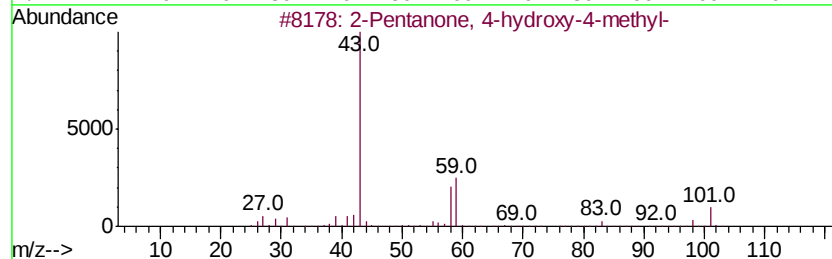
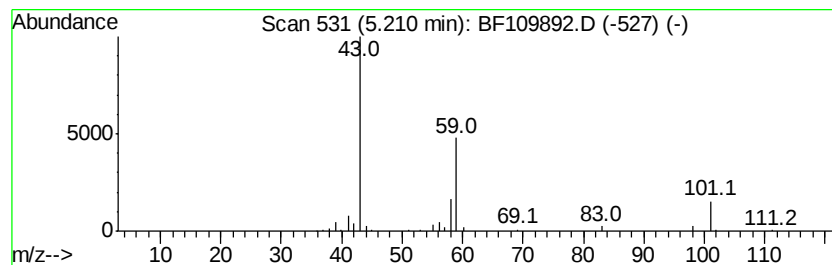
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	2.76 ng	201198	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	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10



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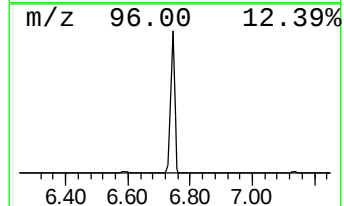
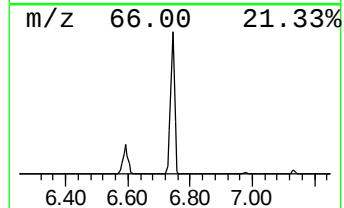
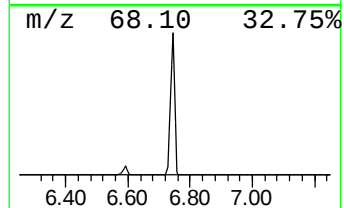
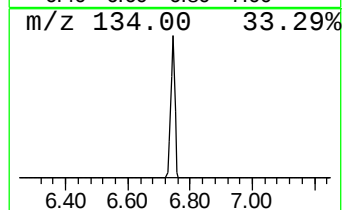
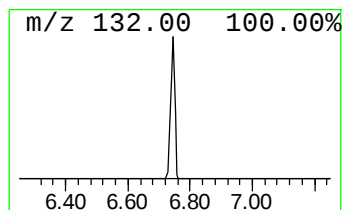
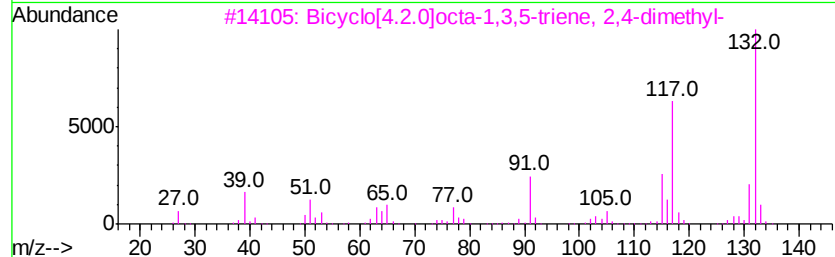
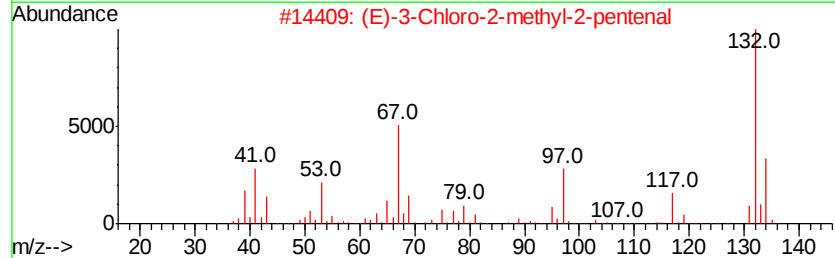
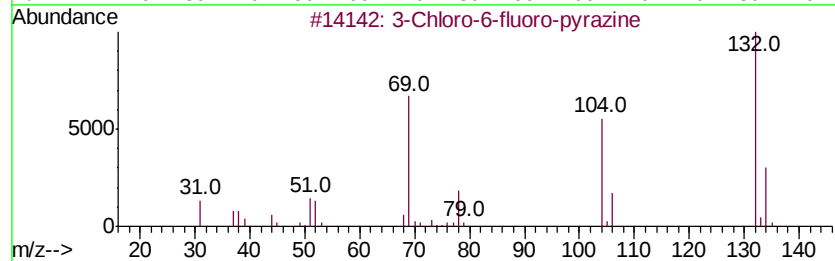
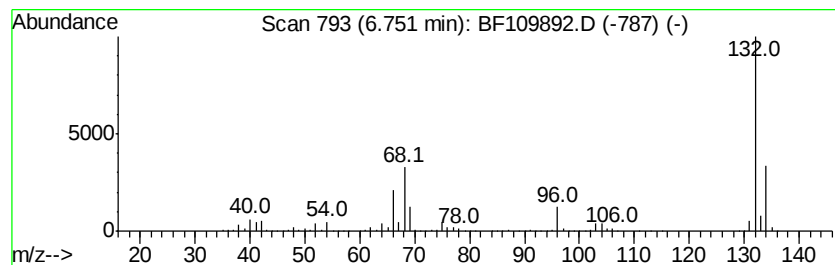
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	60.00 ng	4381520	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12	
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9	
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9	



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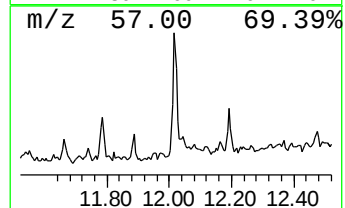
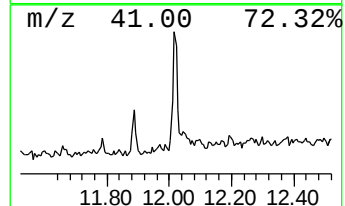
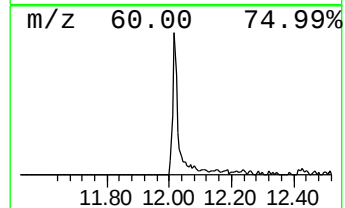
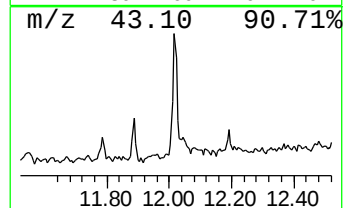
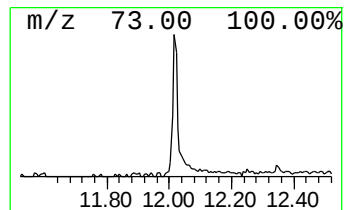
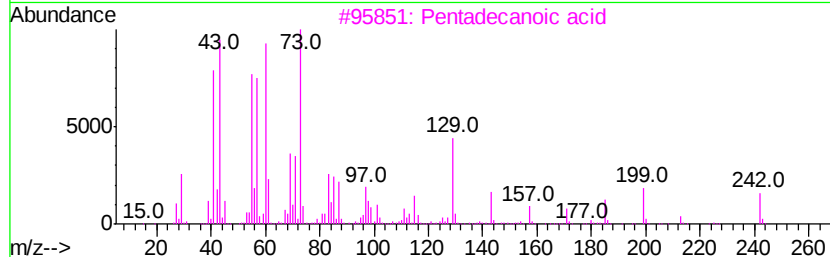
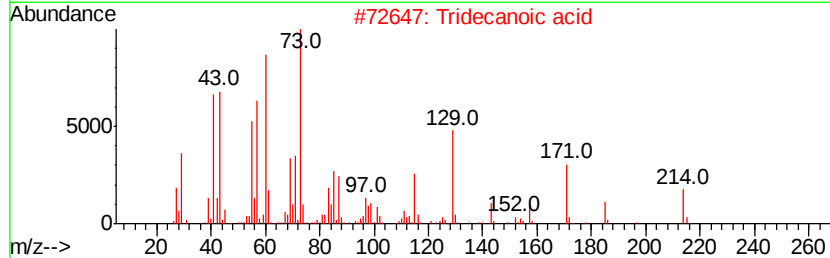
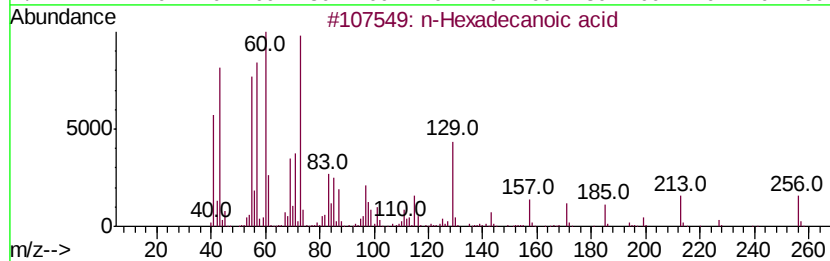
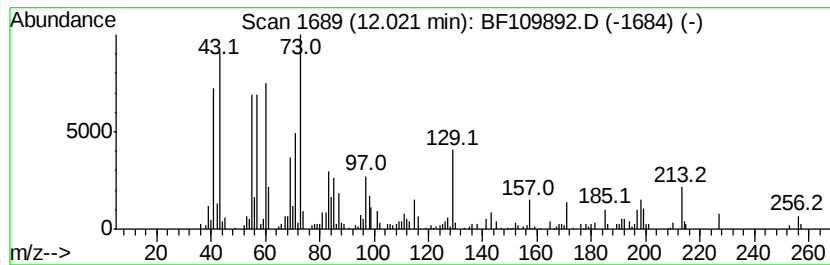
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	3.84 ng	261127	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Tetradecane	198	C14H30	000629-59-4	53



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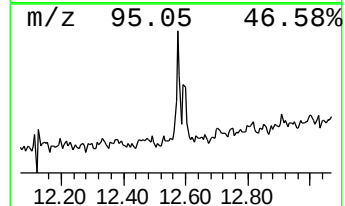
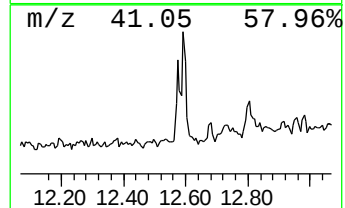
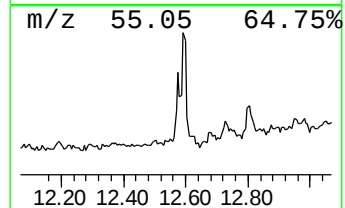
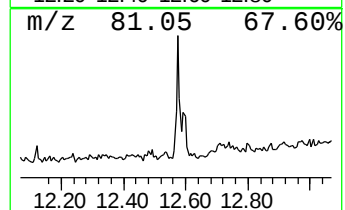
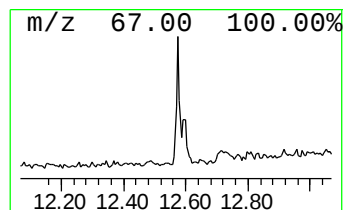
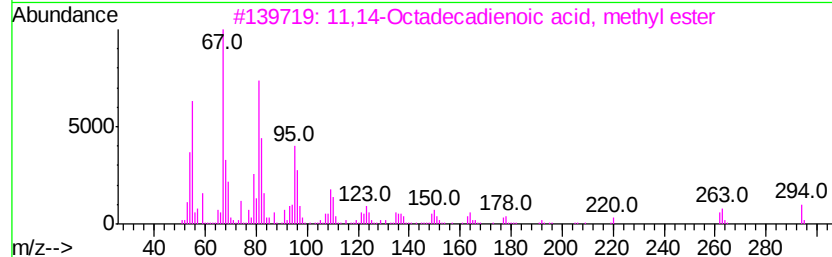
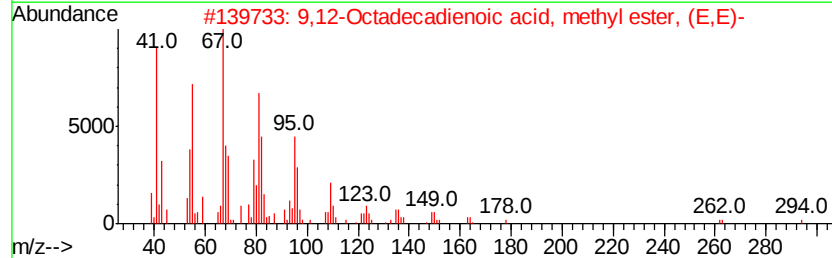
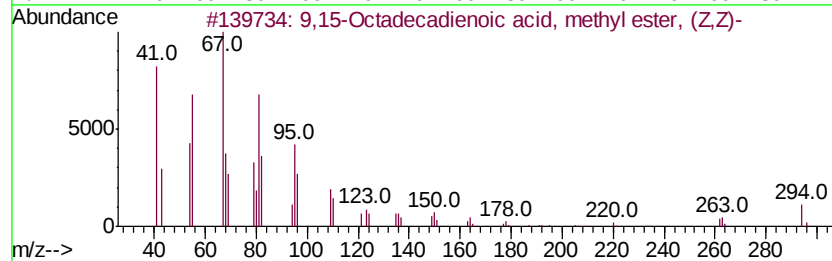
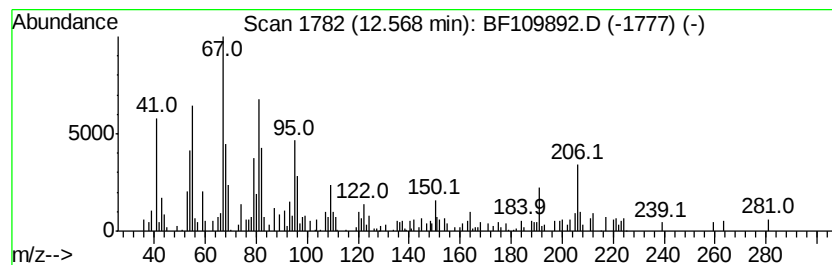
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TIC Integration Parameters: LSCINT.P

Peak Number 6 9,15-Octadecadienoic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	3.14 ng	213554	Phenanthrene-d10	11.51

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98		
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	94		
3	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	93		
4	8-Octadecvnoic acid, methyl ester	294	C19H34O2	018545-05-6	91		
5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	91		



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101518\
Data File : BF109892.D
Acq On : 15 Oct 2018 21:14
Operator : JU/SJ
Sample : J5198-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-101218-C

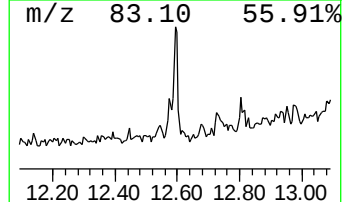
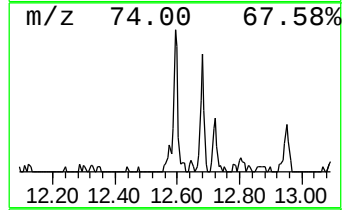
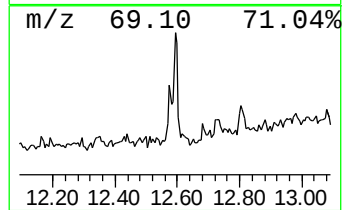
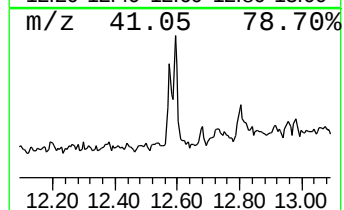
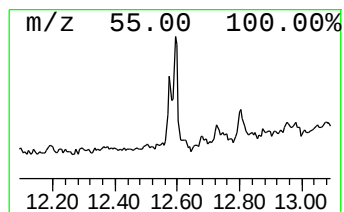
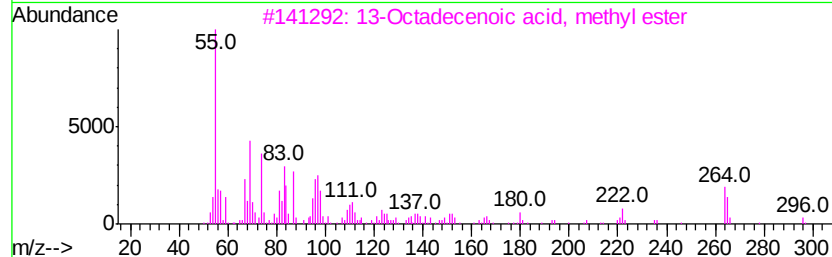
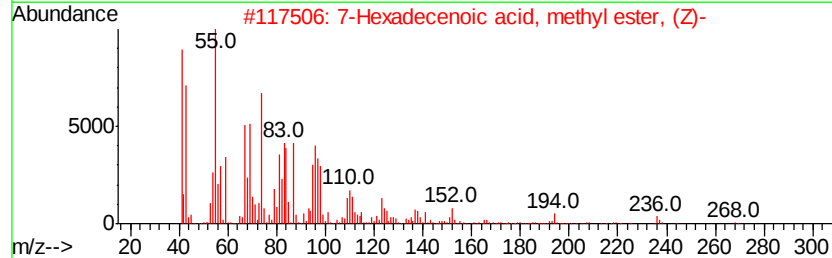
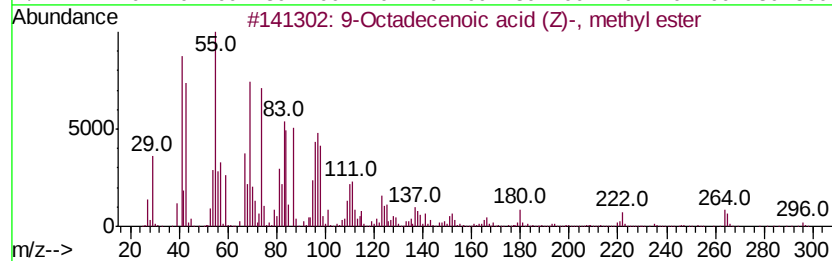
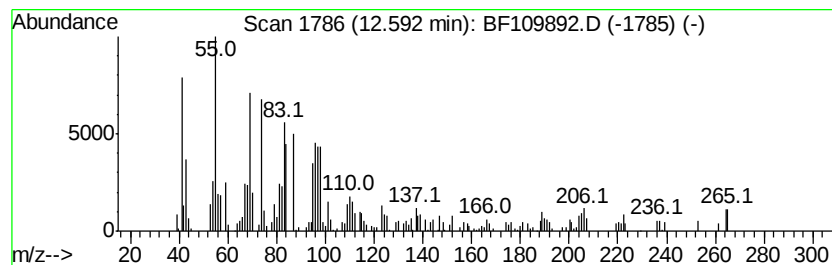
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenoic acid (Z)-, m... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	2.36 ng	160632	Phenanthrene-d10	11.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
2		7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	87
3		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	80
4		6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	64
5		trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101518\
Data File : BF109892.D
Acq On : 15 Oct 2018 21:14
Operator : JU/SJ
Sample : J5198-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

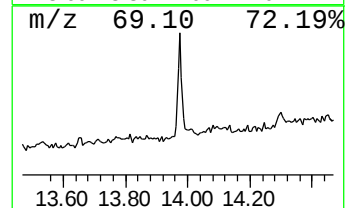
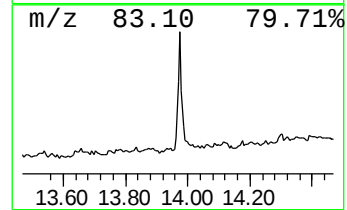
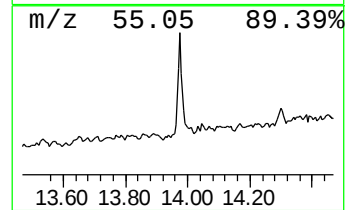
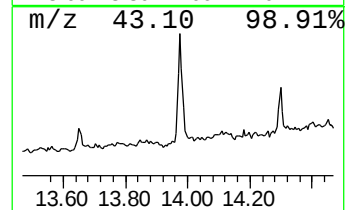
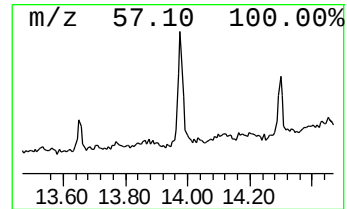
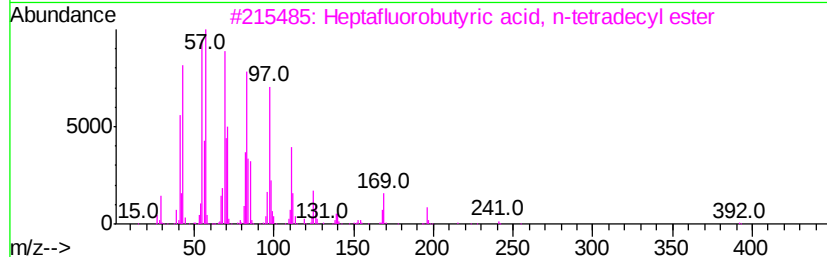
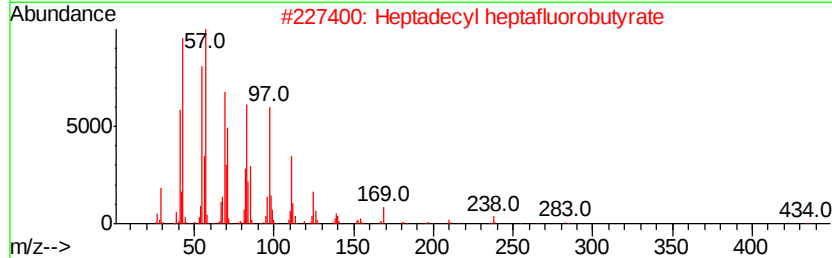
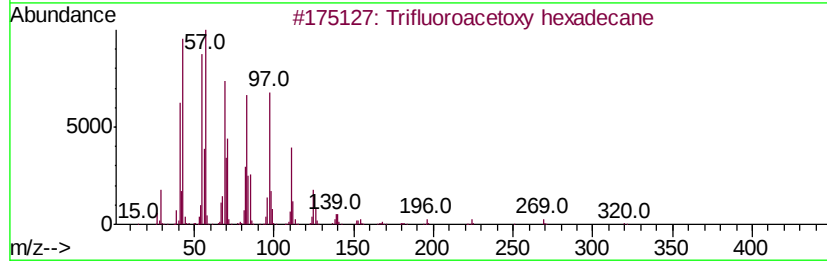
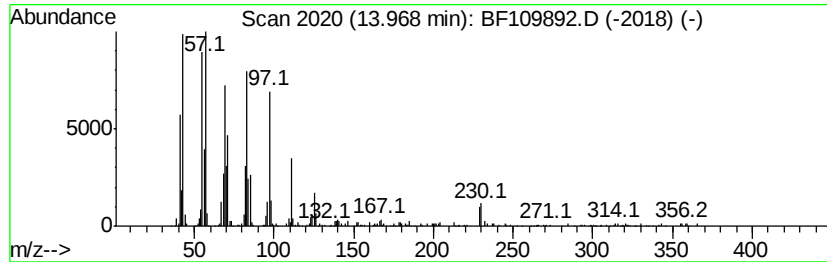
Instrument :
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ClientSampleId :
CL-02-101218-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.97	5.01 ng	432202	Chrysene-d12		14.15	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3		Heptafluorobutvric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
4		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101518\
Data File : BF109892.D
Acq On : 15 Oct 2018 21:14
Operator : JU/SJ
Sample : J5198-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

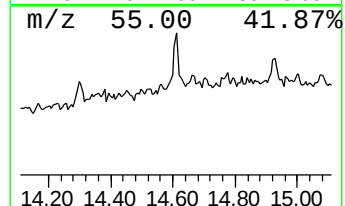
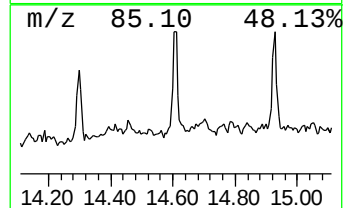
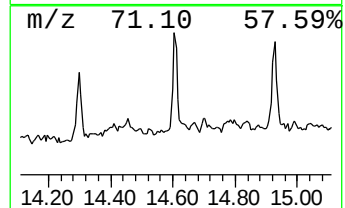
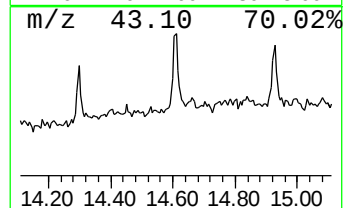
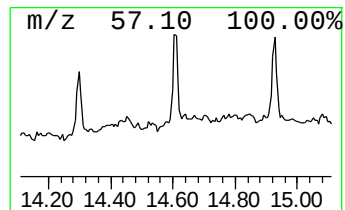
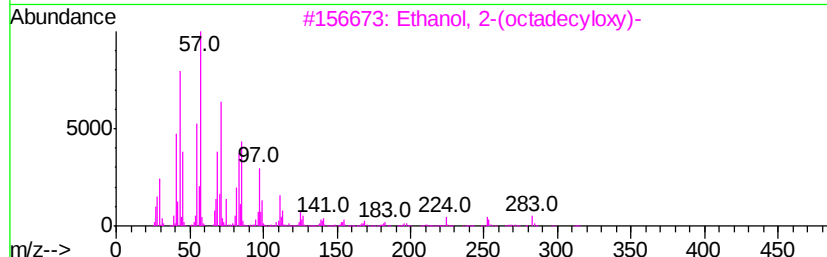
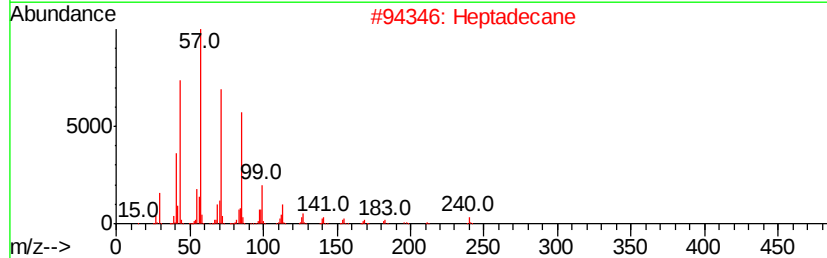
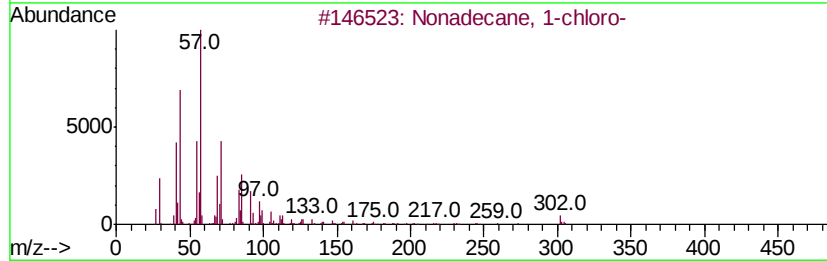
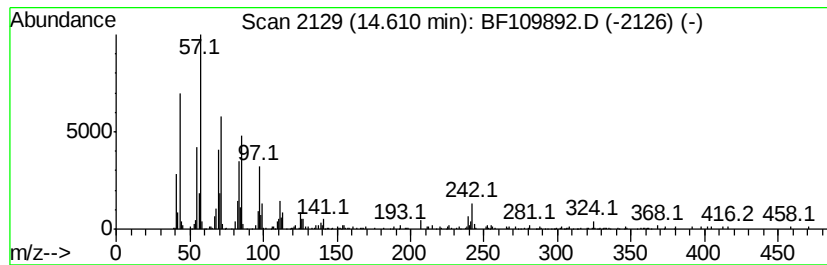
Instrument :
BNA_F
ClientSampleId :
CL-02-101218-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane, 1-chloro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.61	3.09 ng	266420	Chrysene-d12	14.15	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	94
2	Heptadecane	240	C17H36	000629-78-7	92
3	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	91
4	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	89
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101518\
Data File : BF109892.D
Acq On : 15 Oct 2018 21:14
Operator : JU/SJ
Sample : J5198-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CL-02-101218-C

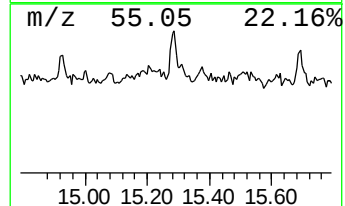
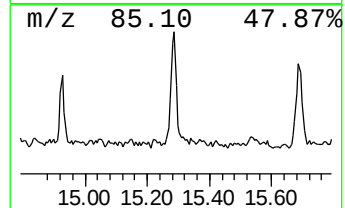
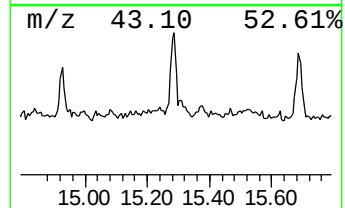
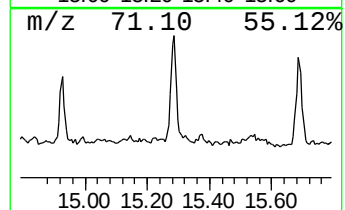
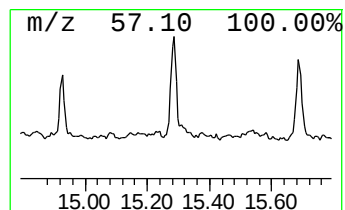
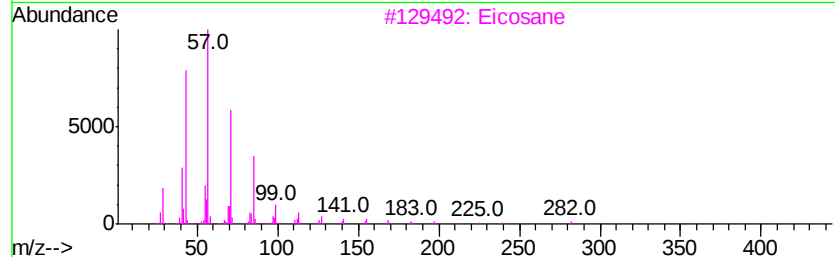
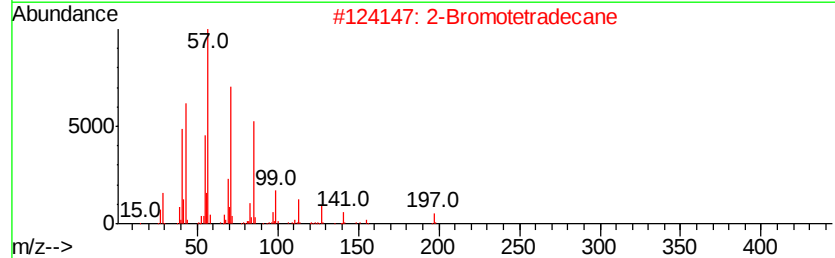
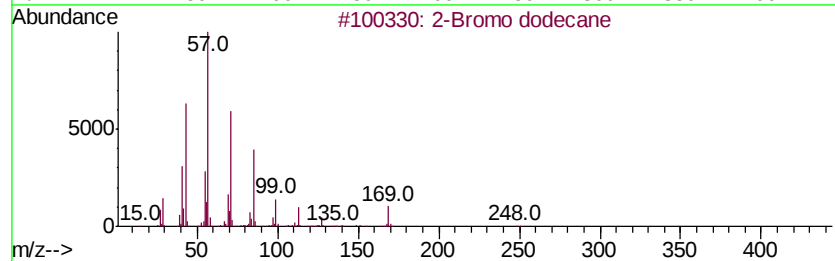
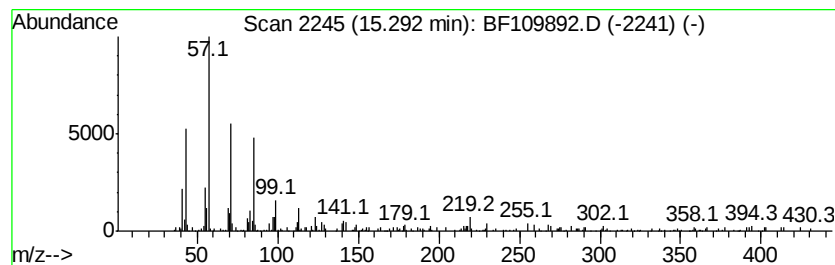
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-Bromo dodecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	3.17 ng	218647	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Bromo dodecane	248	C12H25Br	013187-99-0	93
2			2-Bromotetradecane	276	C14H29Br	074036-95-6	87
3			Eicosane	282	C20H42	000112-95-8	87
4			Octadecane	254	C18H38	000593-45-3	86
5			1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101518\
Data File : BF109892.D
Acq On : 15 Oct 2018 21:14
Operator : JU/SJ
Sample : J5198-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CL-02-101218-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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...	2.32	11.2	ng	820587	1	6.97	1460560	20.0
2-Pentanone, 4-hy...	5.21	2.8	ng	201198	1	6.97	1460560	20.0
unknown6.75	6.75	60.0	ng	4381520	1	6.97	1460560	20.0
n-Hexadecanoic acid	12.02	3.8	ng	261127	4	11.51	1359020	20.0
9,15-Octadecadien...	12.57	3.1	ng	213554	4	11.51	1359020	20.0
9-Octadecenoic ac...	12.59	2.4	ng	160632	4	11.51	1359020	20.0
Trifluoroacetoxy ...	13.97	5.0	ng	432202	5	14.15	1725980	20.0
Nonadecane, 1-chl...	14.61	3.1	ng	266420	5	14.15	1725980	20.0
2-Bromo dodecane	15.29	3.2	ng	218647	6	15.67	1381010	20.0