

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102418\
 Data File : BF110108.D
 Acq On : 24 Oct 2018 12:08
 Operator : JU/SJ
 Sample : J5610-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-1(7-9)

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-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	2.293	30	35	46	rVB	434170	590842	15.01%	1.471%
2	3.569	249	252	271	rBV	33170	95806	2.43%	0.239%
3	4.104	339	343	350	rVB	41125	48945	1.24%	0.122%
4	5.204	525	530	539	rVB	140943	180577	4.59%	0.450%
5	5.587	590	595	598	rBV	3622793	3447066	87.59%	8.582%
6	5.810	627	633	640	rBV	38600	41873	1.06%	0.104%
7	6.587	759	765	770	rBV2	3421898	3935399	100.00%	9.798%
8	6.734	785	790	793	rBV	3965959	3653499	92.84%	9.096%
9	6.793	796	800	805	rBV2	52240	64537	1.64%	0.161%
10	6.963	826	829	835	rVB	1328868	1046217	26.58%	2.605%
11	7.122	852	856	859	rBV	3436948	2779680	70.63%	6.920%
12	7.528	920	925	928	rBV	2580922	2302410	58.51%	5.732%
13	7.816	972	974	978	rBV	56207	49191	1.25%	0.122%
14	8.245	1044	1047	1053	rBV	1535982	1320093	33.54%	3.287%
15	8.457	1079	1083	1086	rBV	48145	49961	1.27%	0.124%
16	8.522	1090	1094	1097	rBV	55768	61517	1.56%	0.153%
17	8.828	1140	1146	1150	rBV	42832	46825	1.19%	0.117%
18	9.322	1226	1230	1233	rBV	4356047	3598577	91.44%	8.959%
19	9.392	1239	1242	1245	rBV2	111430	100151	2.54%	0.249%
20	9.451	1250	1252	1259	rVB2	40319	54144	1.38%	0.135%
21	9.710	1293	1296	1304	rVB	750499	666184	16.93%	1.659%
22	9.869	1319	1323	1325	rBV	94119	86151	2.19%	0.214%
23	9.922	1328	1332	1334	rVV2	111556	100770	2.56%	0.251%
24	10.004	1343	1346	1350	rVB	1443838	1304363	33.14%	3.247%
25	10.422	1411	1417	1420	rVB	119580	115054	2.92%	0.286%
26	10.557	1436	1440	1447	rVB5	21839	42593	1.08%	0.106%
27	10.639	1450	1454	1457	rBV	65780	68011	1.73%	0.169%
28	10.798	1477	1481	1484	rBV	2078825	1886856	47.95%	4.698%
29	10.910	1494	1500	1507	rVB2	139685	242159	6.15%	0.603%
30	11.345	1571	1574	1576	rBV	98819	80500	2.05%	0.200%
31	11.375	1576	1579	1581	rBV	73308	61508	1.56%	0.153%
32	11.498	1596	1600	1602	rBV	1307601	1105081	28.08%	2.751%
33	11.522	1602	1604	1609	rVV	280613	239000	6.07%	0.595%
34	11.575	1609	1613	1615	rVV	60631	65531	1.67%	0.163%

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SB-1(7-9)

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	11.769	1643	1646	1649	rBV	86919	75403	1.92%	0.188%
36	12.004	1683	1686	1688	rBV2	194300	195924	4.98%	0.488%
37	12.028	1688	1690	1695	rVB2	74906	80190	2.04%	0.200%
38	12.116	1702	1705	1707	rBV2	48985	55267	1.40%	0.138%
39	12.180	1713	1716	1718	rBV	93295	69021	1.75%	0.172%
40	12.551	1776	1779	1780	rBV	50209	47762	1.21%	0.119%
41	12.569	1780	1782	1787	rVB2	76470	69254	1.76%	0.172%
42	12.710	1803	1806	1811	rBV	473112	433005	11.00%	1.078%
43	12.945	1840	1846	1851	rBV	531441	556382	14.14%	1.385%
44	13.080	1865	1869	1877	rVB	2545606	2292914	58.26%	5.709%
45	13.298	1903	1906	1909	rBV	102716	90408	2.30%	0.225%
46	13.374	1917	1919	1921	rVB2	58200	45399	1.15%	0.113%
47	13.639	1961	1964	1967	rBV	120798	107185	2.72%	0.267%
48	13.780	1985	1988	1993	rVB	64986	75551	1.92%	0.188%
49	13.969	2017	2020	2033	rVB2	331762	460090	11.69%	1.145%
50	14.104	2041	2043	2045	rVB	135378	92793	2.36%	0.231%
51	14.145	2045	2050	2052	rBV2	1044768	1167071	29.66%	2.906%
52	14.169	2052	2054	2060	rVB	264852	208543	5.30%	0.519%
53	14.286	2071	2074	2077	rBV	271893	229747	5.84%	0.572%
54	14.592	2123	2126	2133	rVB	283454	268755	6.83%	0.669%
55	14.910	2177	2180	2186	rBV	332798	340759	8.66%	0.848%
56	15.210	2228	2231	2235	rBV	242558	378857	9.63%	0.943%
57	15.268	2238	2241	2248	rVB	454030	514618	13.08%	1.281%
58	15.533	2283	2286	2292	rVB	165688	235019	5.97%	0.585%
59	15.598	2294	2297	2303	rVB	185134	228072	5.80%	0.568%
60	15.668	2304	2309	2313	rBV	1067952	1409201	35.81%	3.508%
61	16.133	2383	2388	2393	rVB	348936	555786	14.12%	1.384%
62	16.668	2475	2479	2486	rVB	194410	352171	8.95%	0.877%

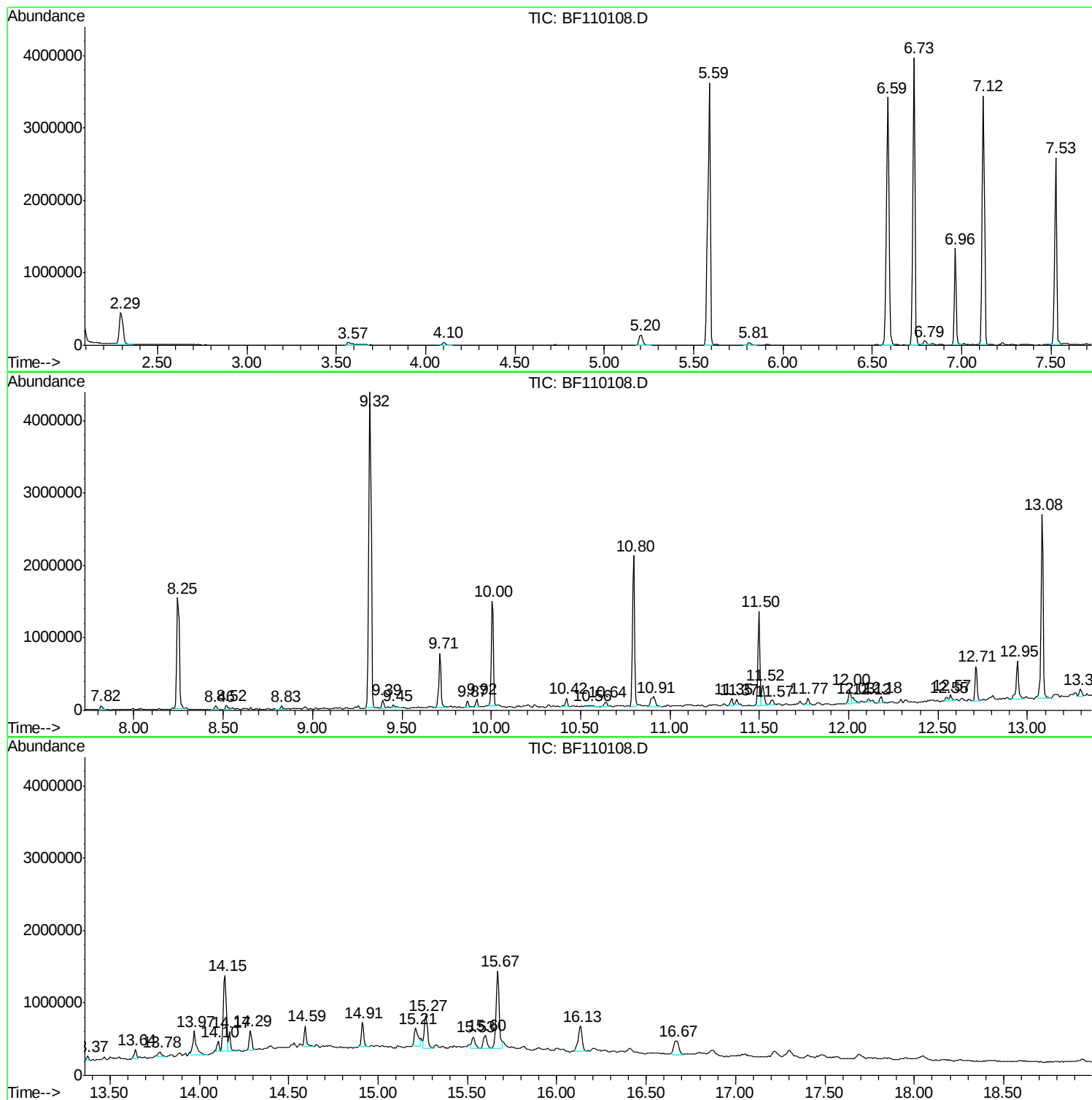
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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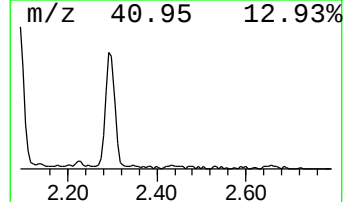
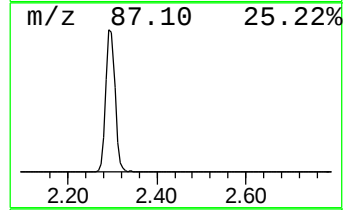
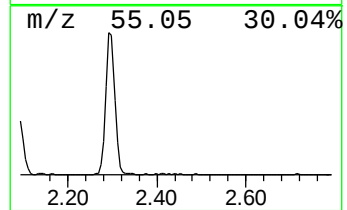
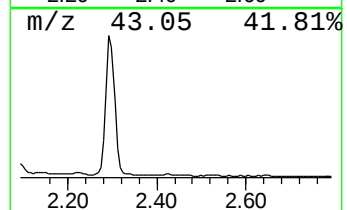
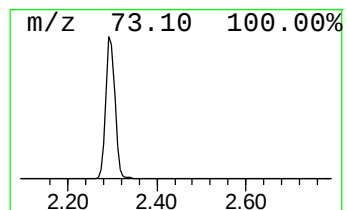
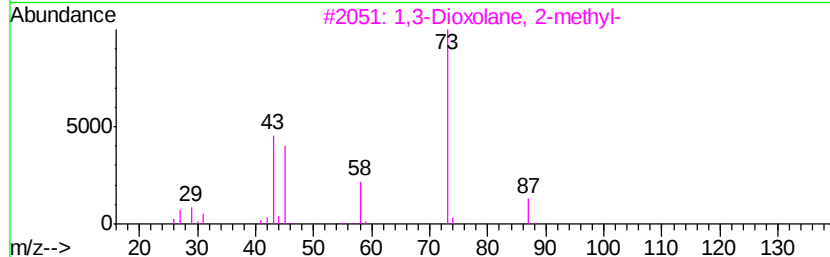
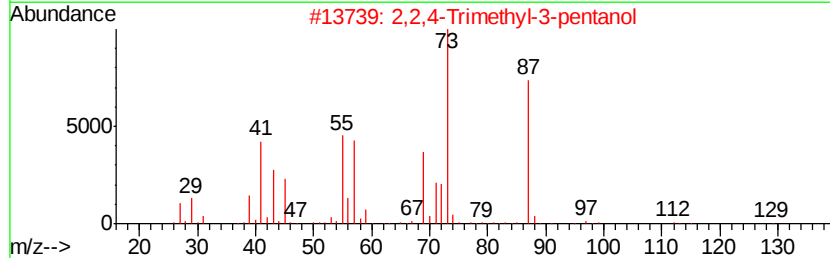
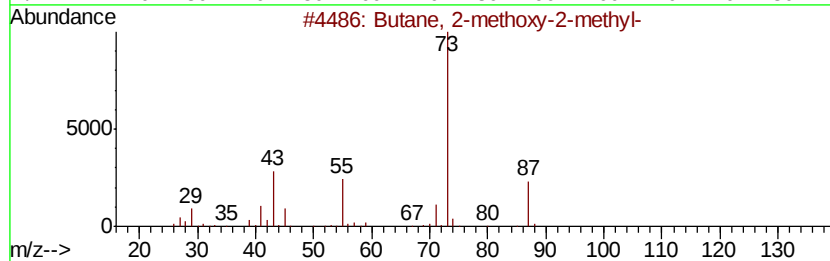
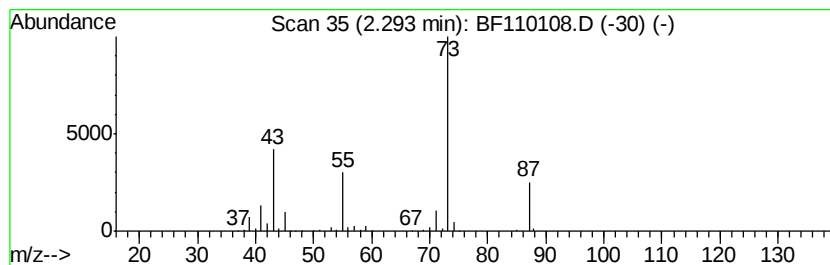
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.29	11.29 ng	590842	1,4-Dichlorobenzene-d4	6.96

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		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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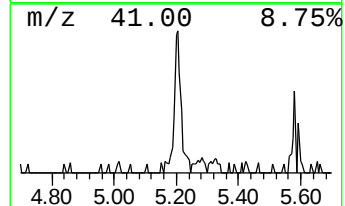
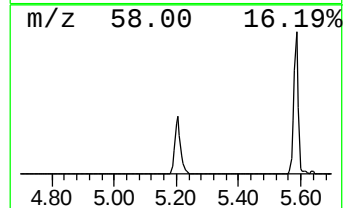
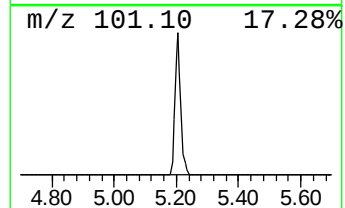
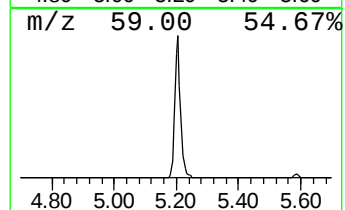
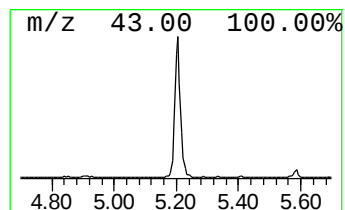
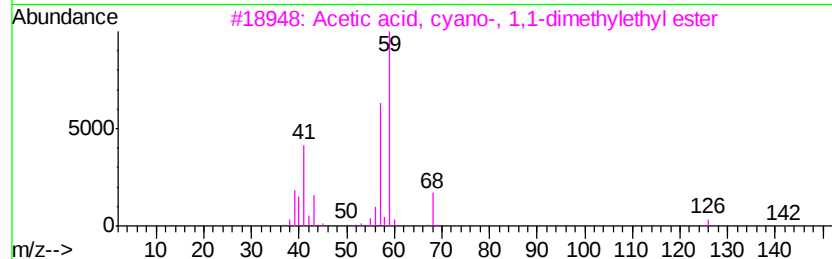
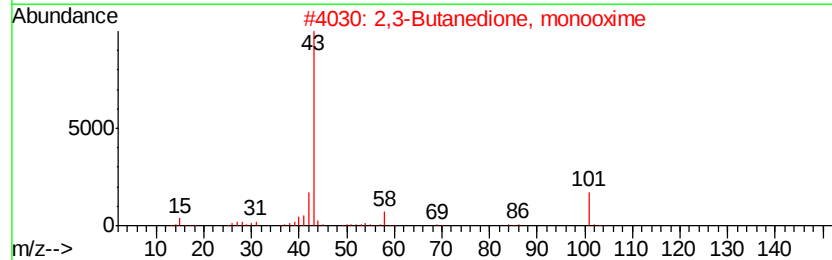
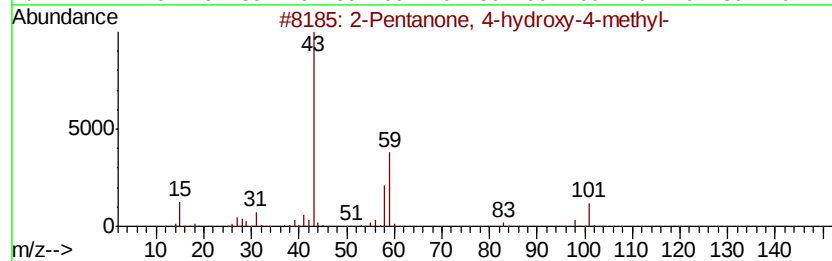
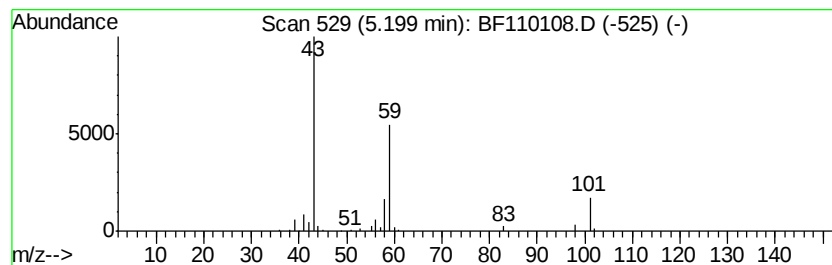
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	3.45 ng	180577	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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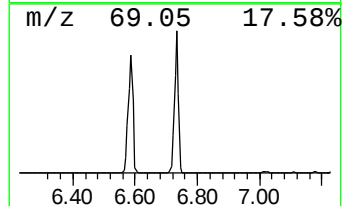
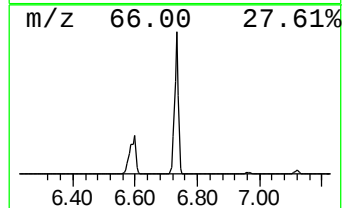
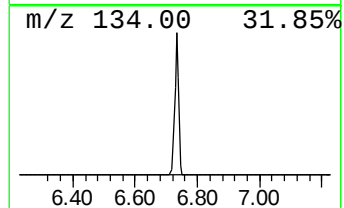
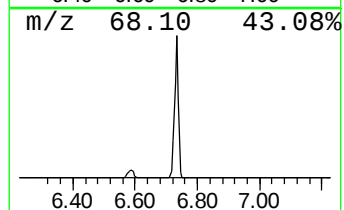
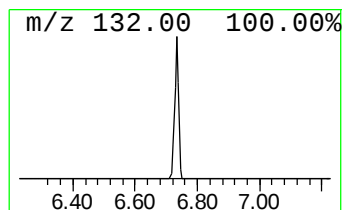
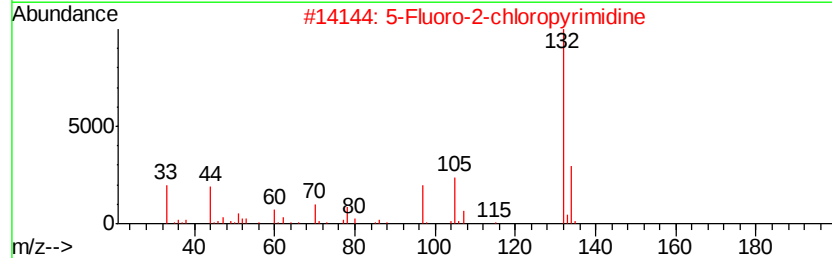
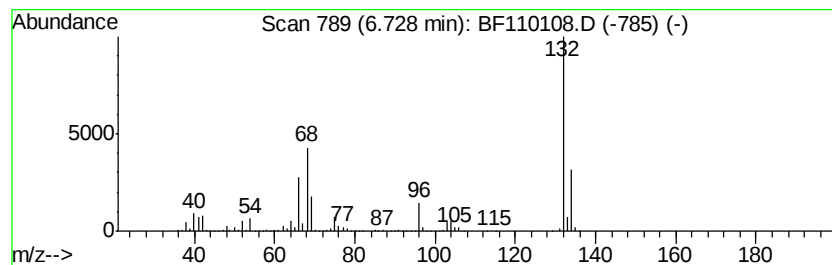
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	69.84 ng	3653500	1,4-Dichlorobenzene-d4	6.96

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	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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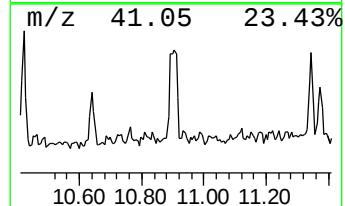
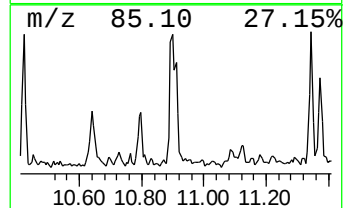
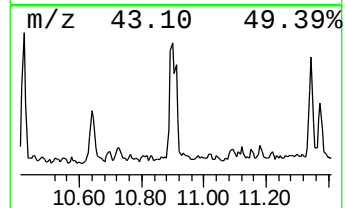
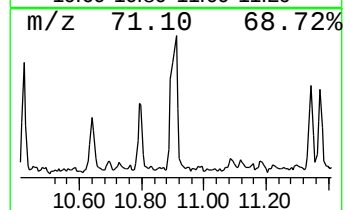
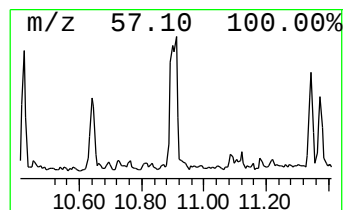
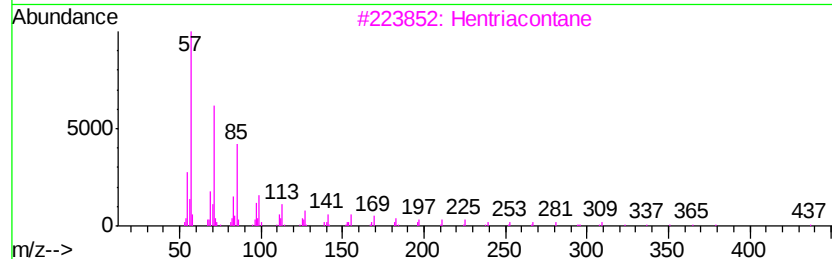
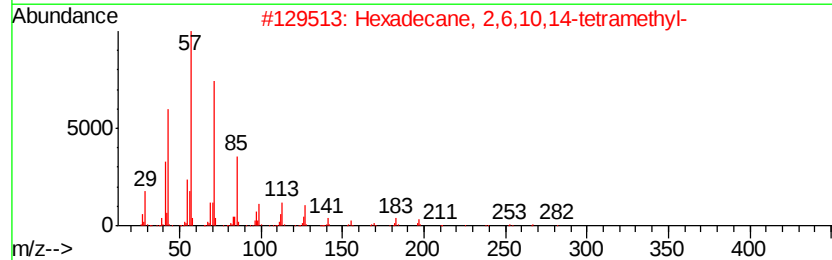
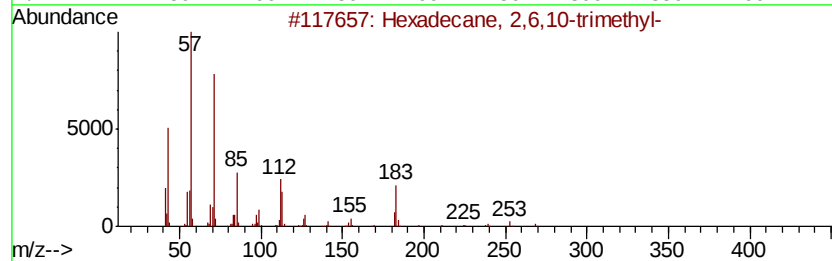
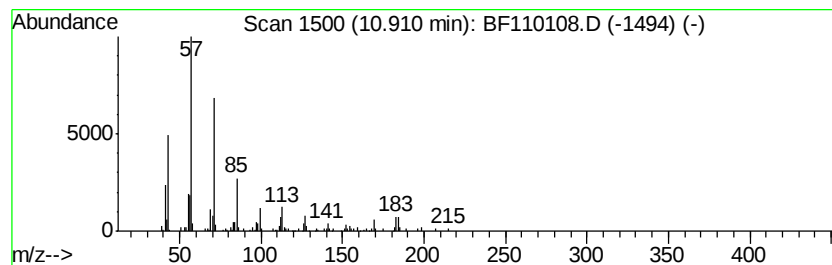
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane, 2,6,10-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	4.38 ng	242159	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	80
2		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	74
3		Hentriacontane	437	C31H64	000630-04-6	72
4		Pentadecane	212	C15H32	000629-62-9	72
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	64



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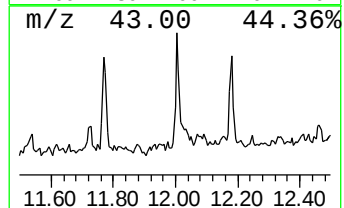
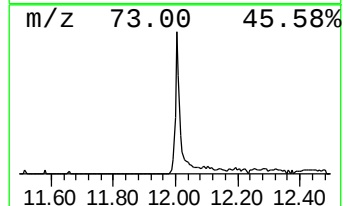
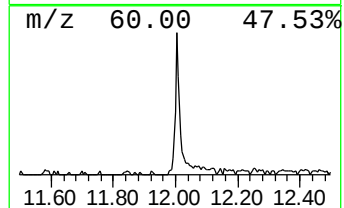
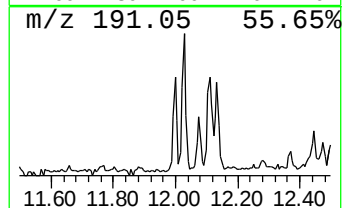
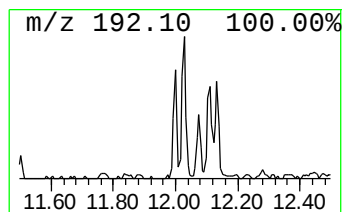
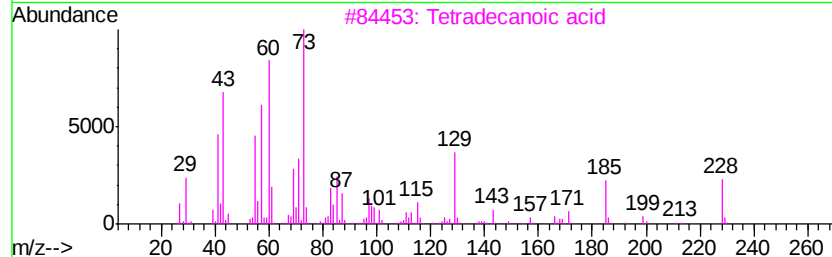
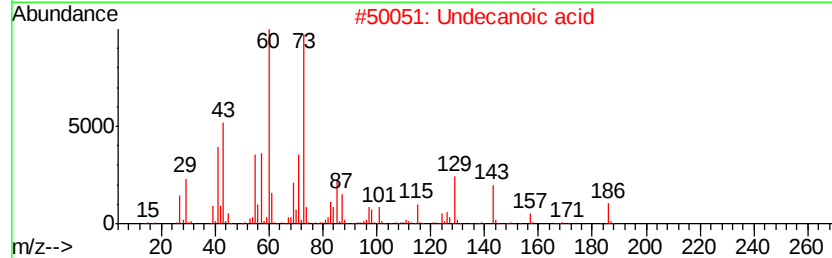
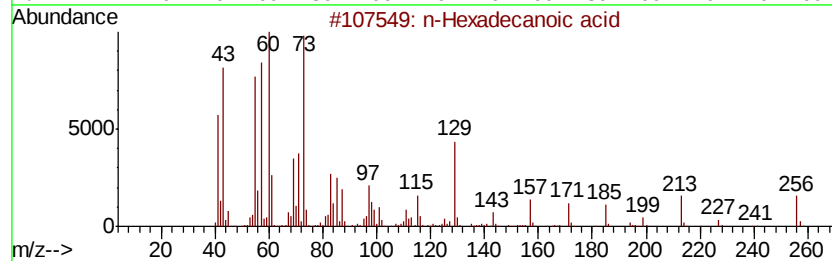
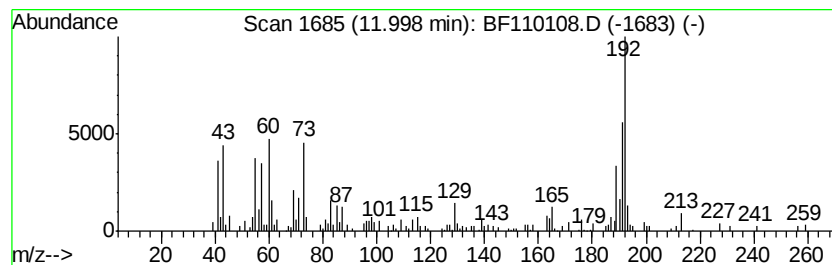
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	3.55 ng	195924	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Undecanoic acid	186	C11H22O2	000112-37-8	70
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5		Tridecanoic acid	214	C13H26O2	000638-53-9	60



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102418\
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Acq On : 24 Oct 2018 12:08
Operator : JU/SJ
Sample : J5610-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1(7-9)

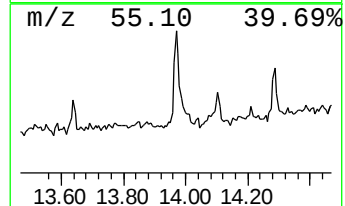
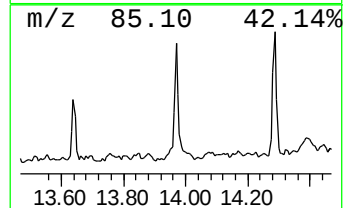
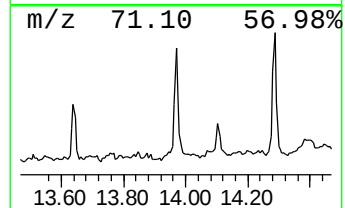
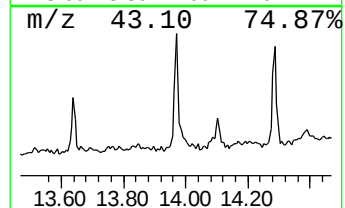
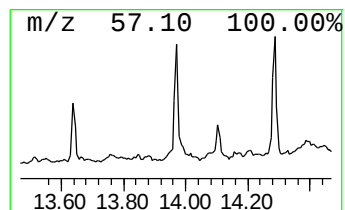
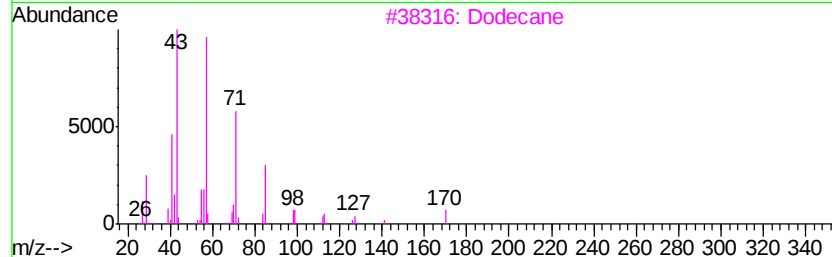
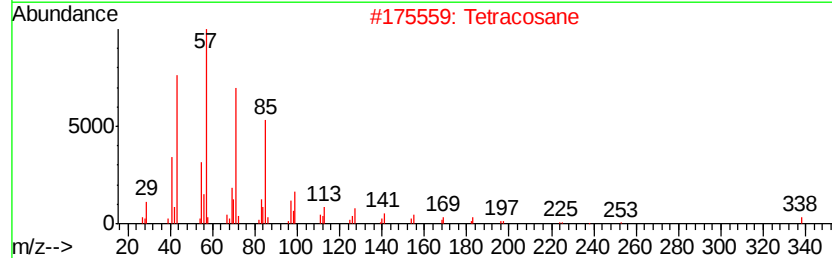
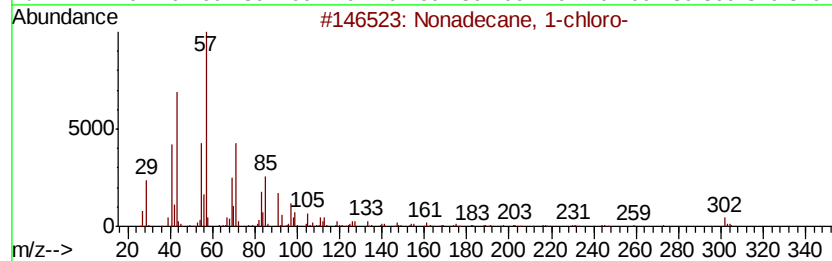
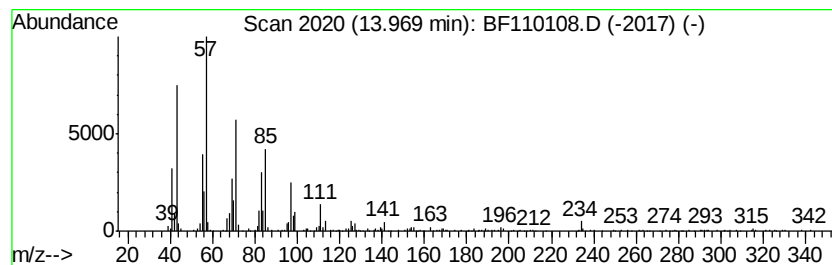
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane, 1-chloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	7.88 ng	460090	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	94
2		Tetracosane	338	C24H50	000646-31-1	93
3		Dodecane	170	C12H26	000112-40-3	70
4		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	68
5		1-Heptadecene	238	C17H34	006765-39-5	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102418\
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Operator : JU/SJ
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SB-1(7-9)

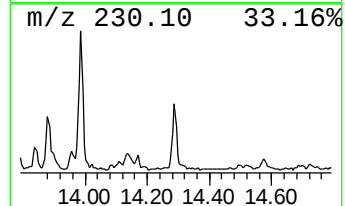
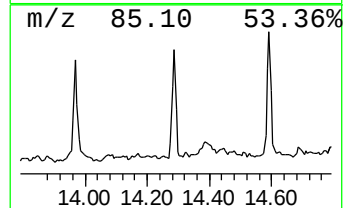
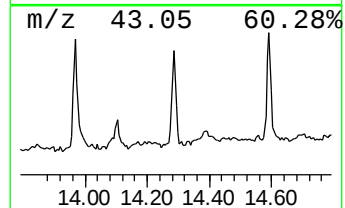
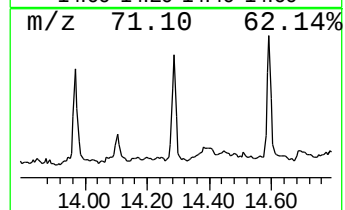
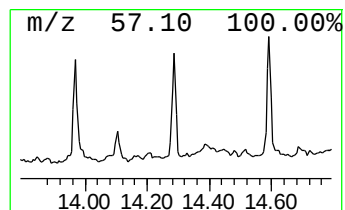
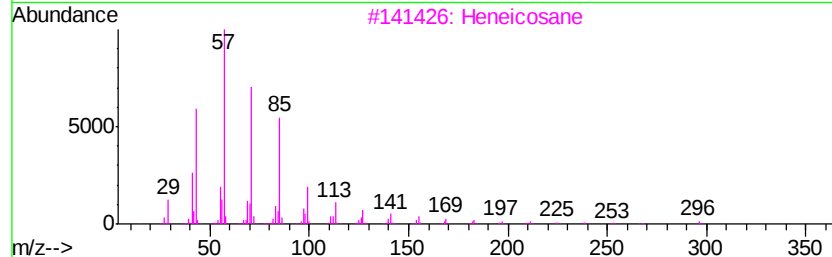
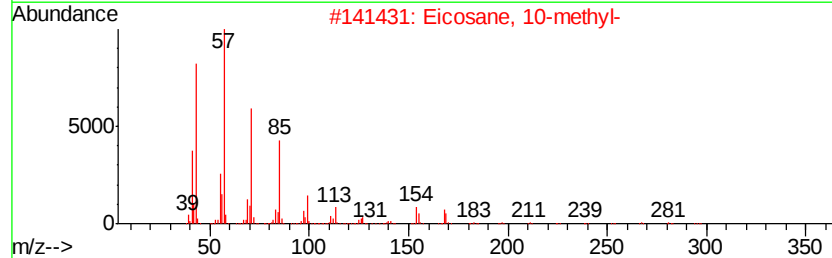
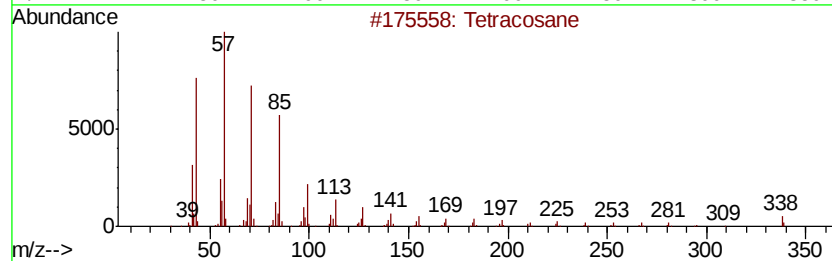
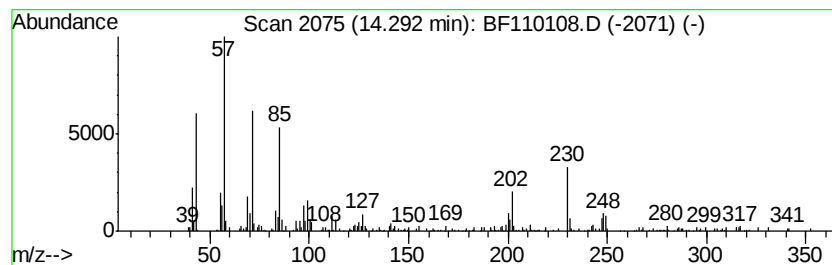
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	3.94 ng	229747	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	96
2		Eicosane, 10-methyl-	296	C21H44	054833-23-7	68
3		Heneicosane	296	C21H44	000629-94-7	64
4		Eicosane	282	C20H42	000112-95-8	62
5		Octacosane	394	C28H58	000630-02-4	60



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102418\
 Data File : BF110108.D
 Acq On : 24 Oct 2018 12:08
 Operator : JU/SJ
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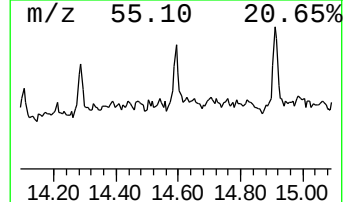
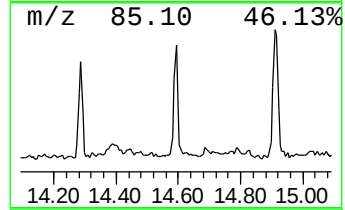
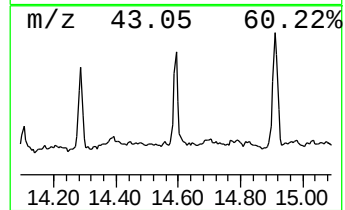
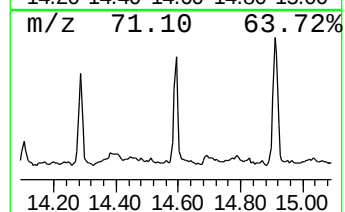
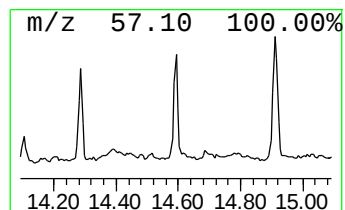
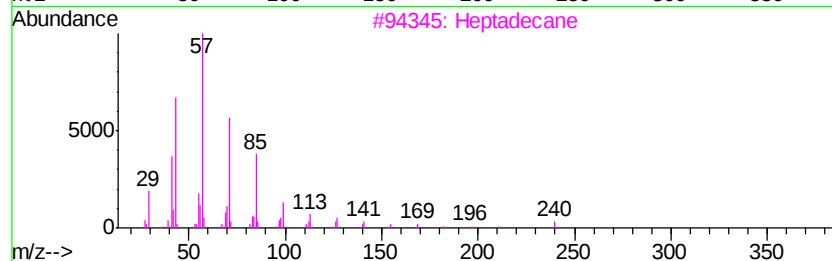
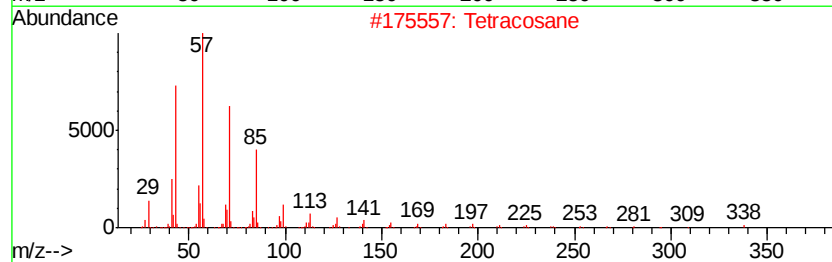
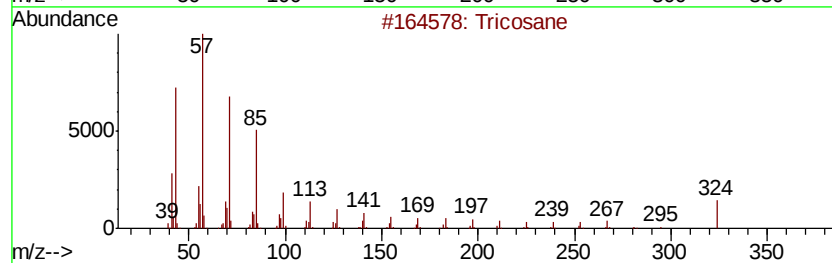
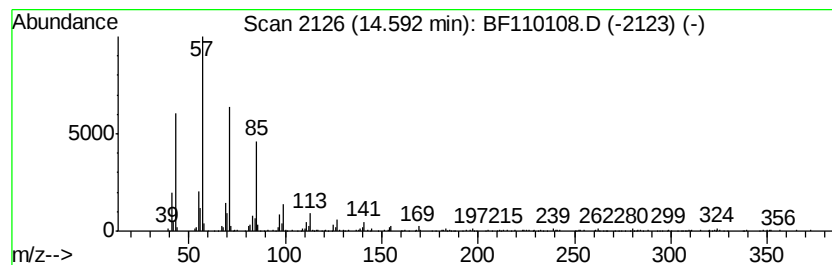
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Tricosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	4.61 ng	268755	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane		324	C23H48	000638-67-5	97
2	Tetracosane		338	C24H50	000646-31-1	94
3	Heptadecane		240	C17H36	000629-78-7	94
4	Heneicosane		296	C21H44	000629-94-7	91
5	Hexadecane		226	C16H34	000544-76-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102418\
Data File : BF110108.D
Acq On : 24 Oct 2018 12:08
Operator : JU/SJ
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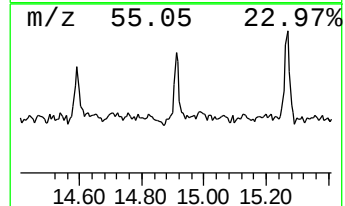
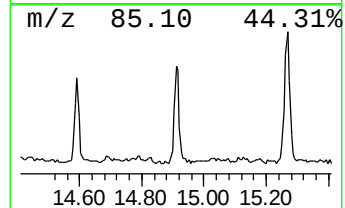
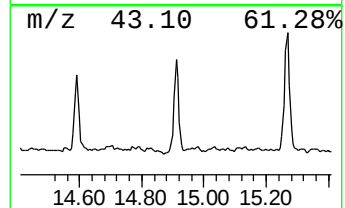
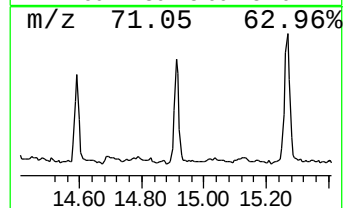
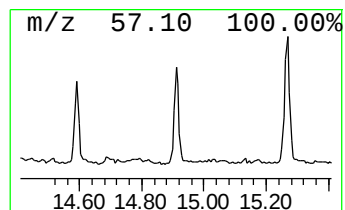
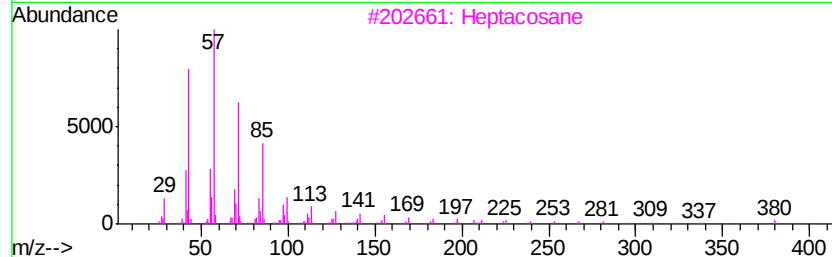
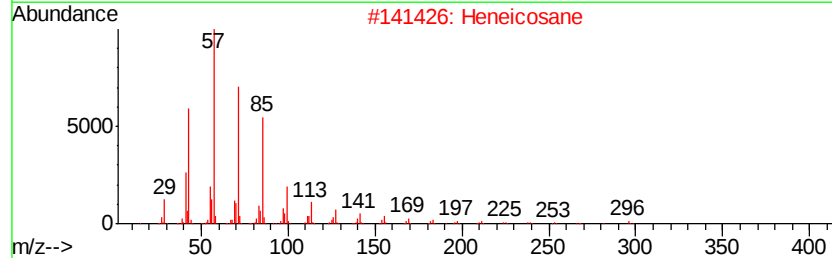
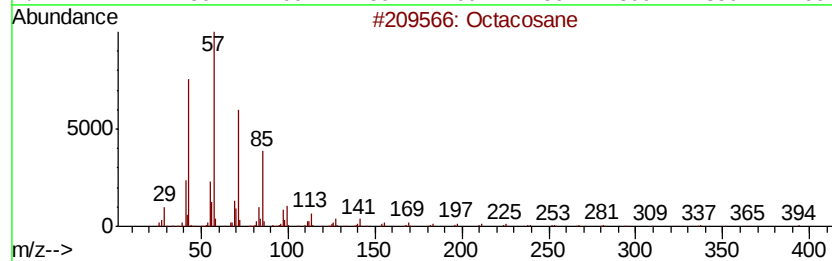
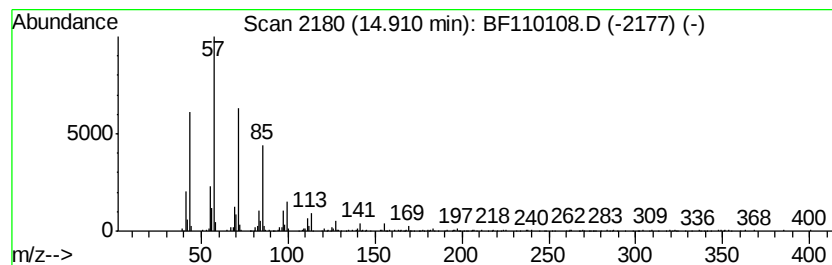
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	4.84 ng	340759	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Pentacosane	352	C25H52	000629-99-2	91
5		Hexacosane	366	C26H54	000630-01-3	91



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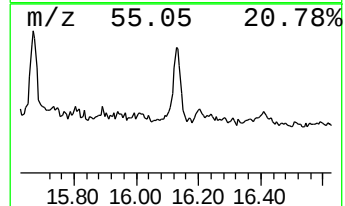
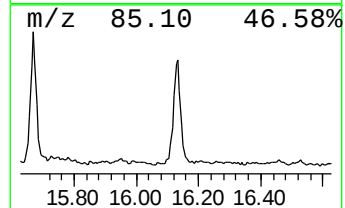
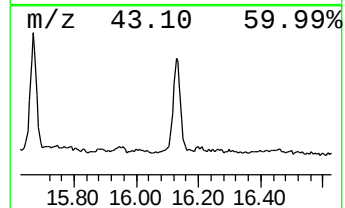
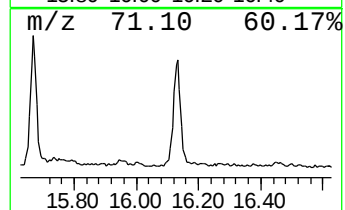
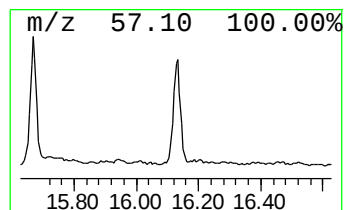
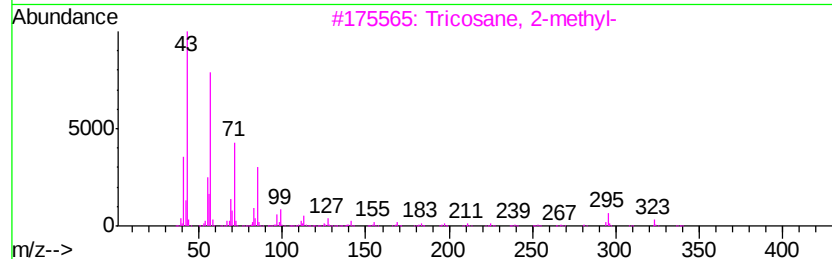
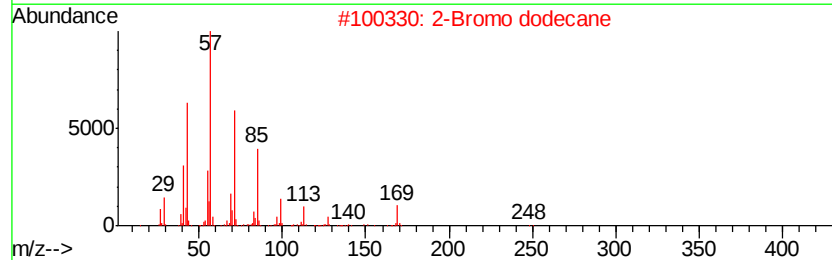
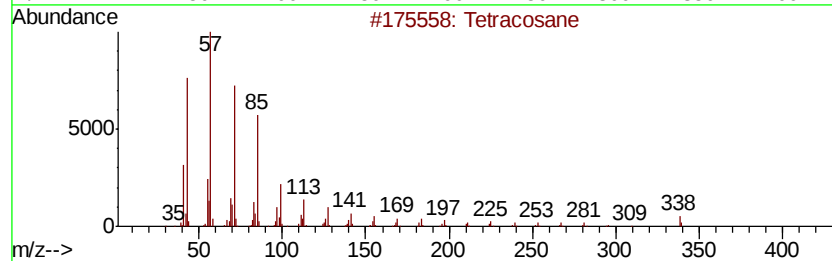
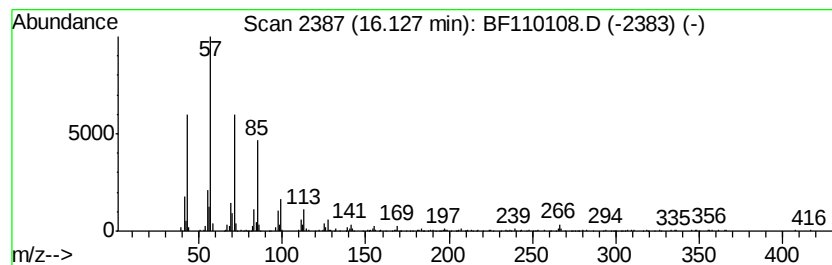
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2-Bromo dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	7.89 ng	555786	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	94
2			2-Bromo dodecane	248	C12H25Br	013187-99-0	93
3			Tricosane, 2-methyl-	338	C24H50	001928-30-9	91
4			Hentriacontane	437	C31H64	000630-04-6	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102418\
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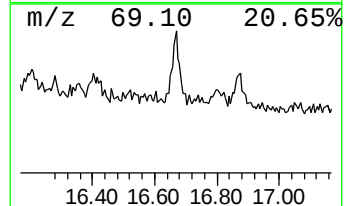
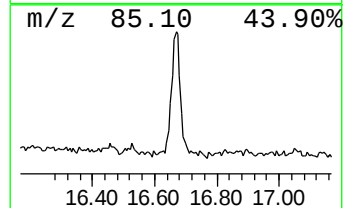
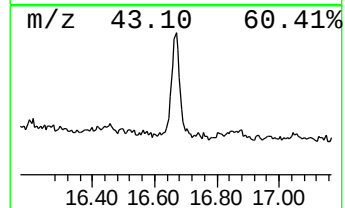
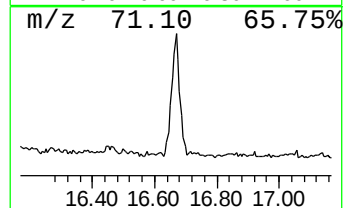
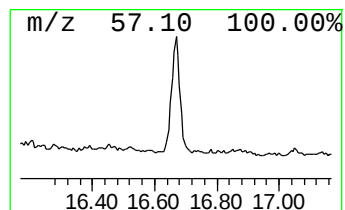
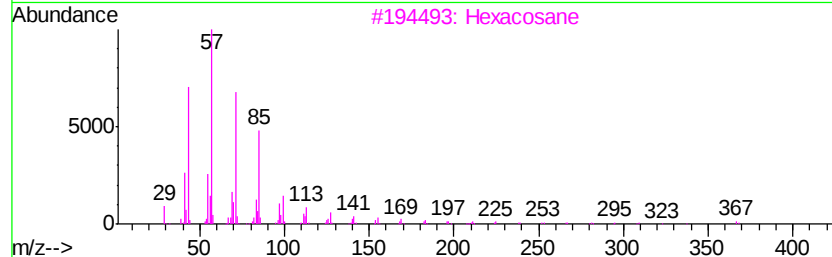
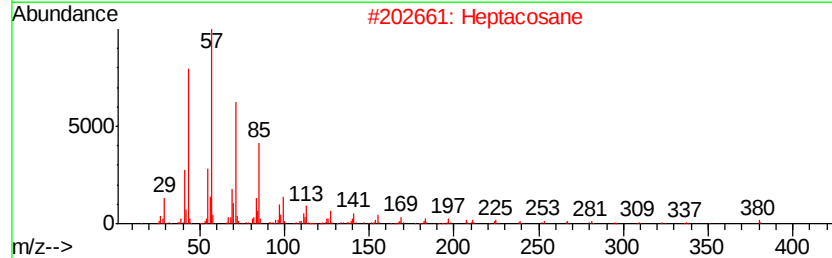
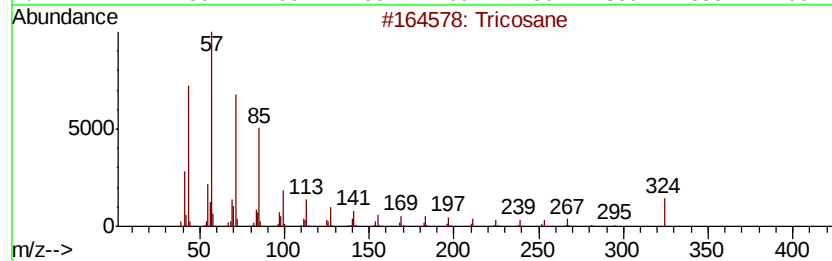
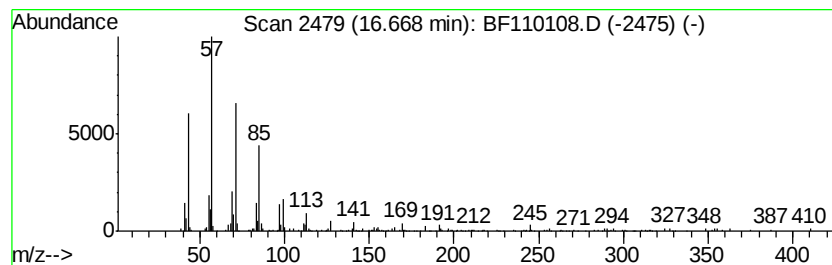
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.67	5.00 ng	352171	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosane	324	C23H48	000638-67-5	87
2			Heptacosane	380	C27H56	000593-49-7	87
3			Hexacosane	366	C26H54	000630-01-3	87
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5			Hentriacontane	437	C31H64	000630-04-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102418\
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Misc :
ALS Vial : 7 Sample Multiplier: 1

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ClientSampleId :
SB-1(7-9)

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
Butane, 2-methoxy...	2.29	11.3	ng	590842	1	6.96	1046220	20.0
2-Pentanone, 4-hy...	5.20	3.5	ng	180577	1	6.96	1046220	20.0
unknown6.73	6.73	69.8	ng	3653500	1	6.96	1046220	20.0
Hexadecane, 2,6,1...	10.91	4.4	ng	242159	4	11.50	1105080	20.0
n-Hexadecanoic acid	12.00	3.5	ng	195924	4	11.50	1105080	20.0
Nonadecane, 1-chl...	13.97	7.9	ng	460090	5	14.15	1167070	20.0
Tetracosane	14.29	3.9	ng	229747	5	14.15	1167070	20.0
Tricosane	14.59	4.6	ng	268755	5	14.15	1167070	20.0
Octacosane	14.91	4.8	ng	340759	6	15.67	1409200	20.0
2-Bromo dodecane	16.13	7.9	ng	555786	6	15.67	1409200	20.0
Heptacosane	16.67	5.0	ng	352171	6	15.67	1409200	20.0