

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
 Data File : BF108499.D
 Acq On : 27 Aug 2018 10:15
 Operator : JU/SJ
 Sample : J4629-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-038

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-BF080818.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	5.237	489	493	499	rBV	77441	93158	3.64%	0.344%
2	5.625	555	559	567	rBV	1969479	2008064	78.48%	7.425%
3	6.619	724	728	739	rBV	2046619	2147479	83.93%	7.940%
4	6.772	749	754	757	rBV	2161301	2143762	83.78%	7.927%
5	6.919	775	779	786	rVB2	20340	30369	1.19%	0.112%
6	6.995	789	792	796	rBV	808695	690173	26.97%	2.552%
7	7.154	815	819	822	rBV	2040995	1668974	65.23%	6.171%
8	7.560	883	888	891	rBV	1558959	1388012	54.25%	5.132%
9	8.284	1006	1011	1014	rBV	933078	871920	34.08%	3.224%
10	9.354	1188	1193	1196	rBV	3048359	2558777	100.00%	9.461%
11	9.748	1256	1260	1263	rBV	620544	545646	21.32%	2.018%
12	10.042	1306	1310	1316	rBV	1255143	1063265	41.55%	3.931%
13	10.219	1336	1340	1345	rBV4	25664	36086	1.41%	0.133%
14	10.442	1371	1378	1384	rBV	108445	157581	6.16%	0.583%
15	10.672	1412	1417	1420	rBV3	16783	33417	1.31%	0.124%
16	10.725	1422	1426	1433	rVB2	38956	78104	3.05%	0.289%
17	10.836	1441	1445	1457	rBV	1903673	1782231	69.65%	6.590%
18	11.536	1560	1564	1568	rBV	1336131	1139818	44.55%	4.215%
19	12.042	1644	1650	1655	rBV	327746	354158	13.84%	1.310%
20	12.783	1769	1776	1781	rBV3	77256	143281	5.60%	0.530%
21	12.830	1781	1784	1789	rVB3	46056	56097	2.19%	0.207%
22	13.124	1829	1834	1837	rBV	2820348	2556282	99.90%	9.452%
23	13.324	1862	1868	1872	rBV3	51676	98128	3.83%	0.363%
24	13.607	1909	1916	1923	rBV	186303	419300	16.39%	1.550%
25	13.671	1925	1927	1930	rVB2	50084	43641	1.71%	0.161%
26	14.001	1980	1983	1985	rBV	59005	53216	2.08%	0.197%
27	14.030	1985	1988	1999	rVB5	81037	186840	7.30%	0.691%
28	14.189	2011	2015	2019	rBV	962612	841685	32.89%	3.112%
29	14.242	2019	2024	2034	rVV	348085	575693	22.50%	2.129%
30	14.318	2034	2037	2041	rVV	76651	66456	2.60%	0.246%
31	14.624	2086	2089	2094	rBV	108241	108157	4.23%	0.400%
32	14.789	2111	2117	2128	rVB	389973	639910	25.01%	2.366%
33	14.948	2140	2144	2150	rVB	125716	142376	5.56%	0.526%
34	15.030	2155	2158	2162	rVB	27769	32702	1.28%	0.121%

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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.313	2201	2206	2212	rVB	183762	235967	9.22%	0.872%
36	15.389	2213	2219	2227	rVB	248138	481252	18.81%	1.779%
37	15.742	2270	2279	2286	rBV2	575703	942380	36.83%	3.484%
38	16.077	2330	2336	2346	rVB	106202	246476	9.63%	0.911%
39	16.195	2350	2356	2363	rVB	143815	240466	9.40%	0.889%
40	16.742	2445	2449	2455	rVB2	58587	94251	3.68%	0.348%
41	18.018	2662	2666	2669	rBV6	23626	49584	1.94%	0.183%

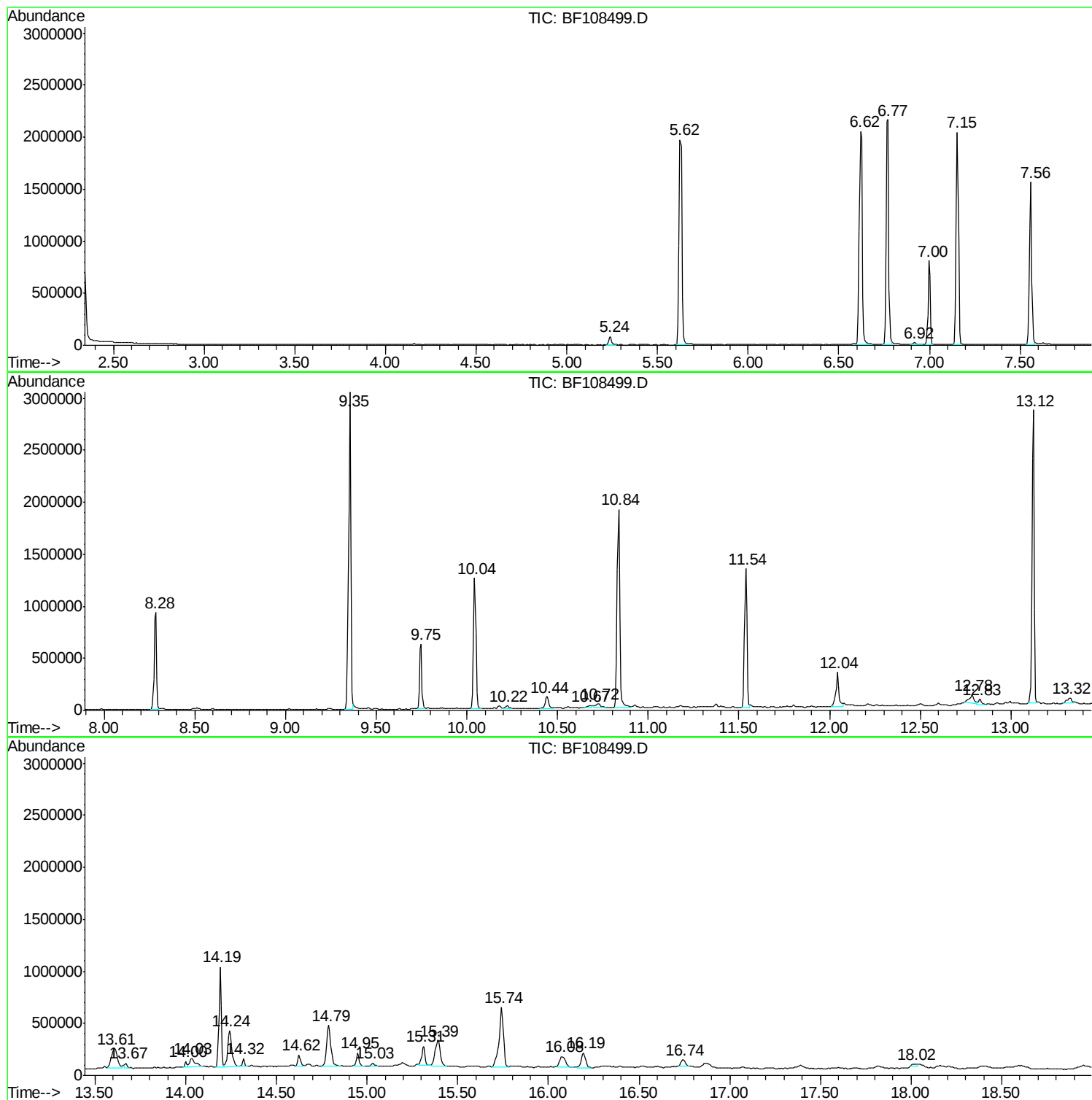
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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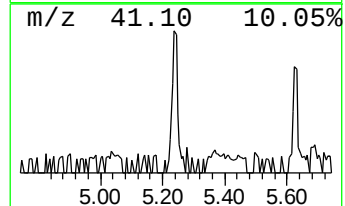
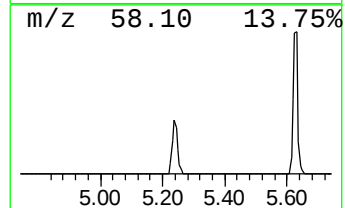
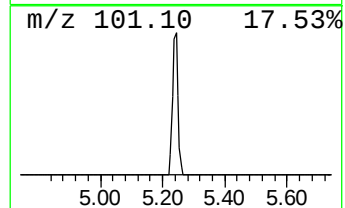
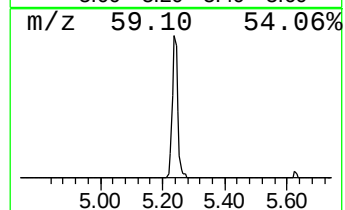
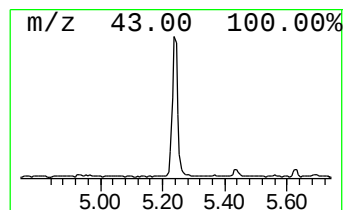
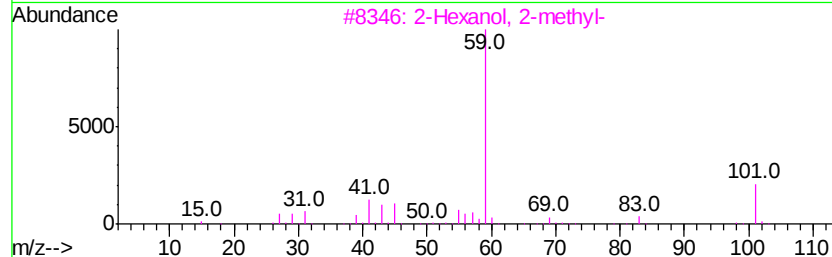
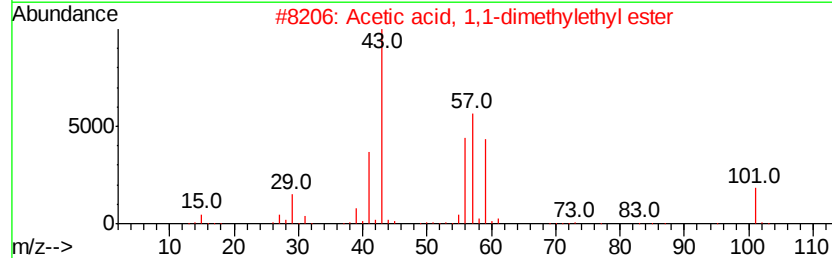
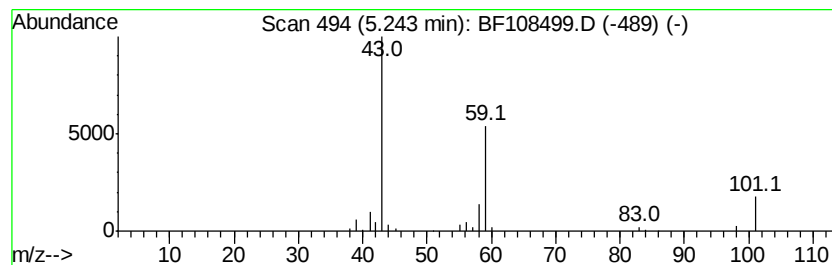
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	2.70 ng	93158	1,4-Dichlorobenzene-d4	7.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28	
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23	



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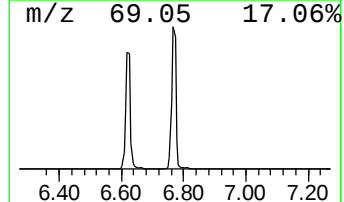
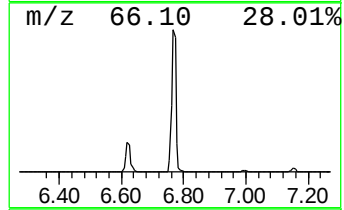
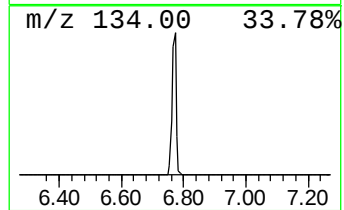
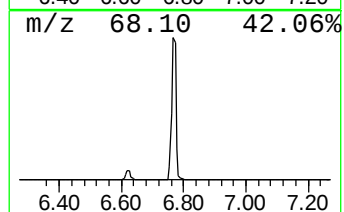
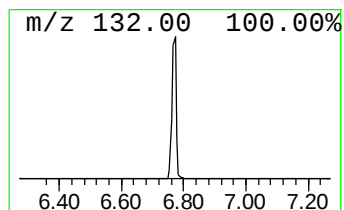
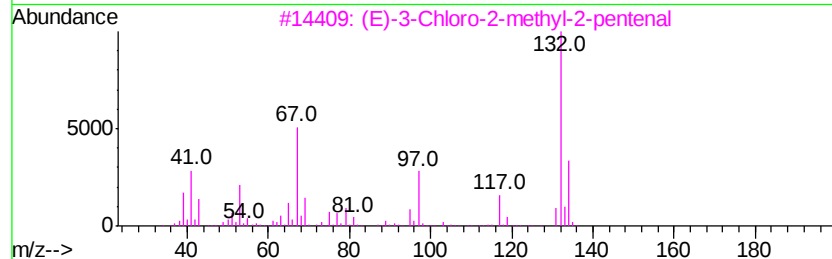
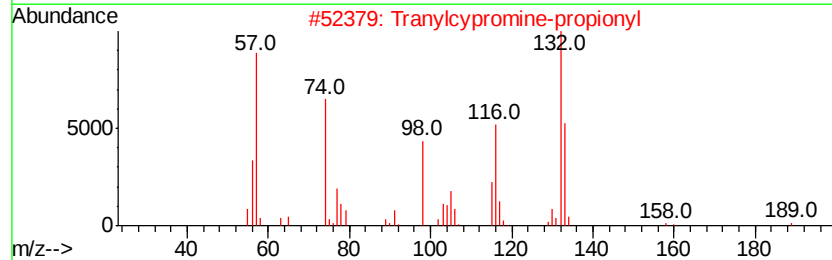
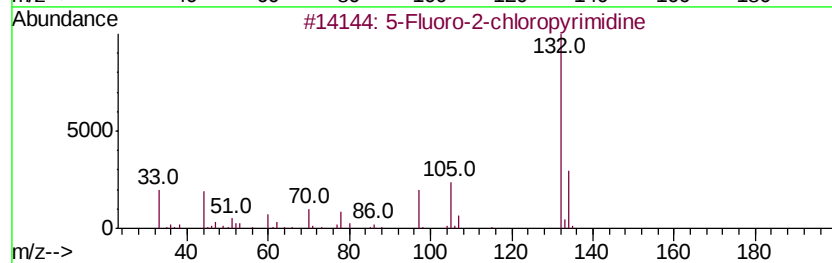
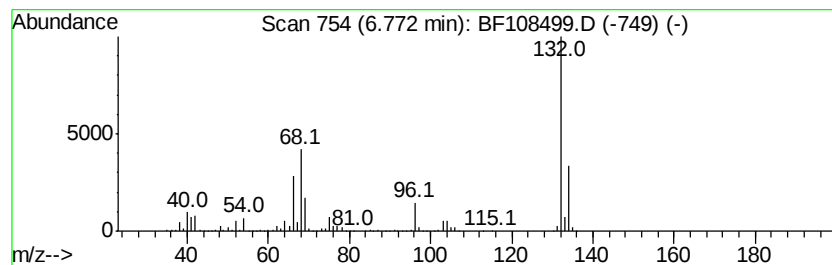
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	62.12 ng	2143760	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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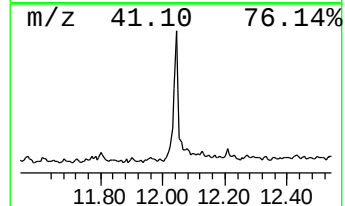
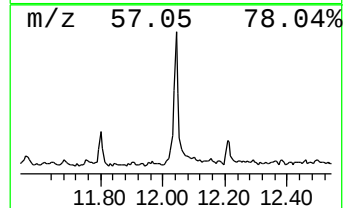
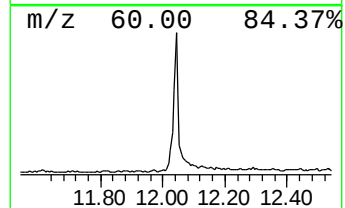
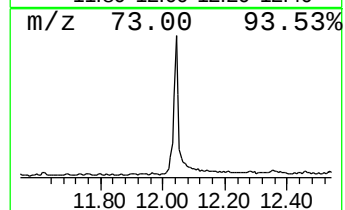
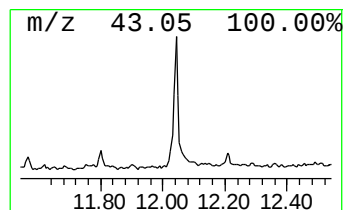
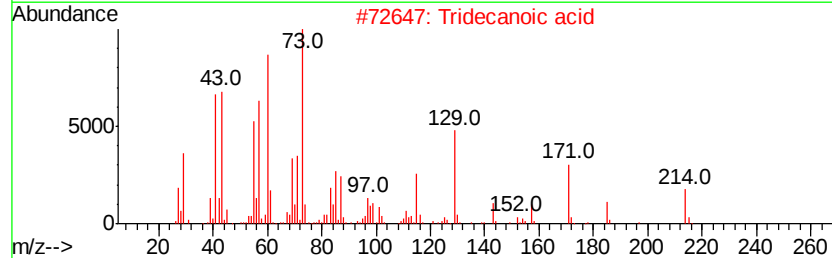
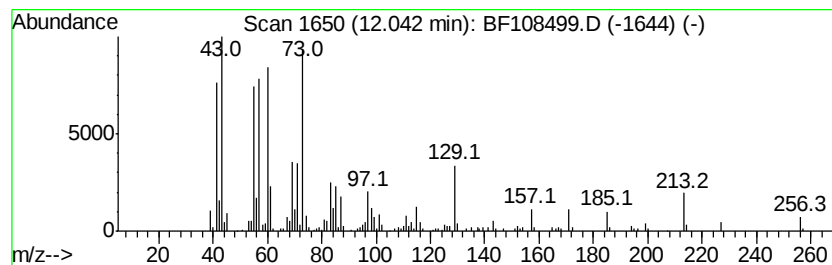
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	6.21 ng	354158	Phenanthrene-d10	11.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
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	64
5		Dodecanoic acid	200	C12H24O2	000143-07-7	53



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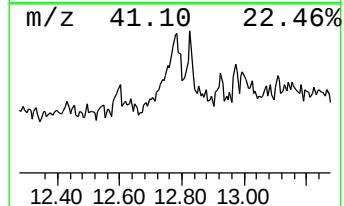
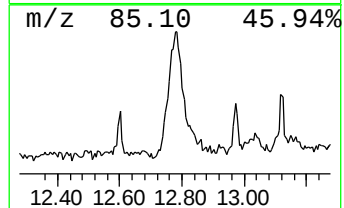
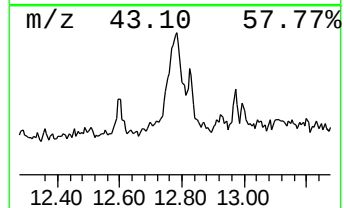
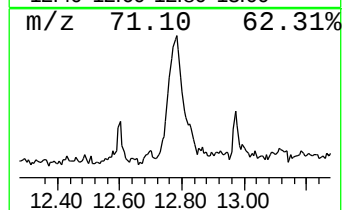
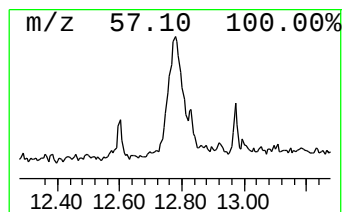
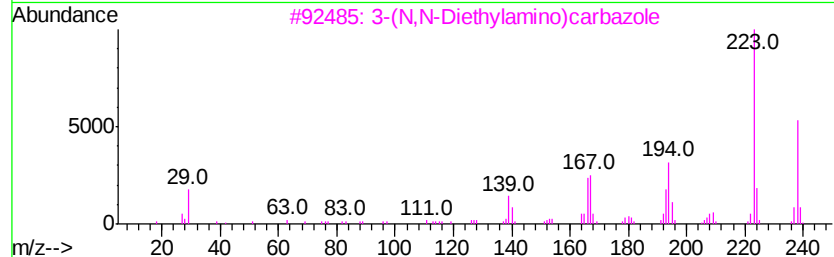
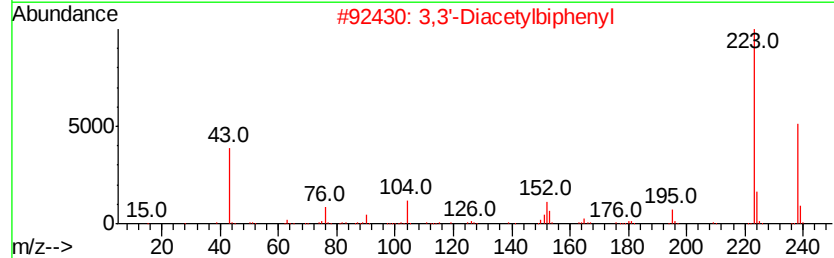
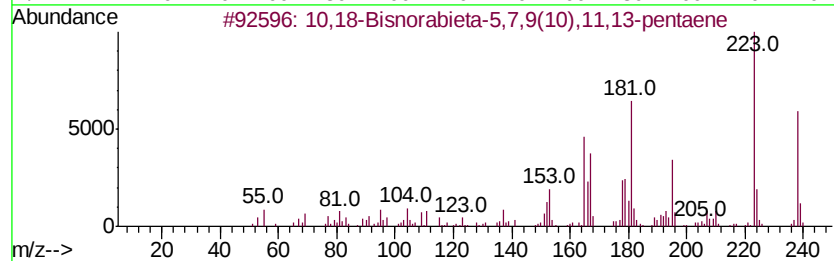
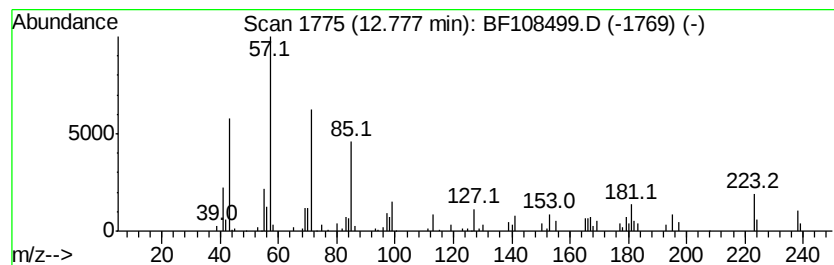
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 10,18-Bisnorabieta-5,7,9(10... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.78	2.51 ng	143281	Phenanthrene-d10	11.54	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	97
2	3,3'-Diacetylbiiphenyl	238	C16H14O2	094113-07-2	30
3	3-(N,N-Diethylamino)carbazole	238	C16H18N2	054994-31-9	30
4	Hexacosane	366	C26H54	000630-01-3	25
5	4,4'-Diacetyl biphenyl	238	C16H14O2	000787-69-9	25



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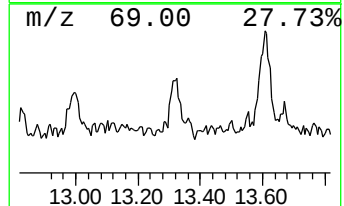
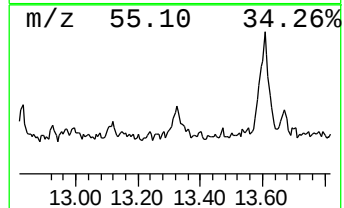
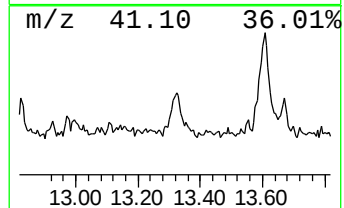
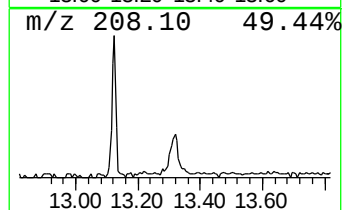
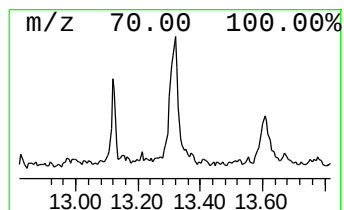
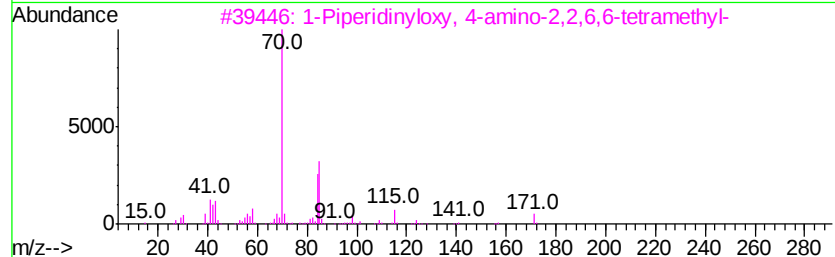
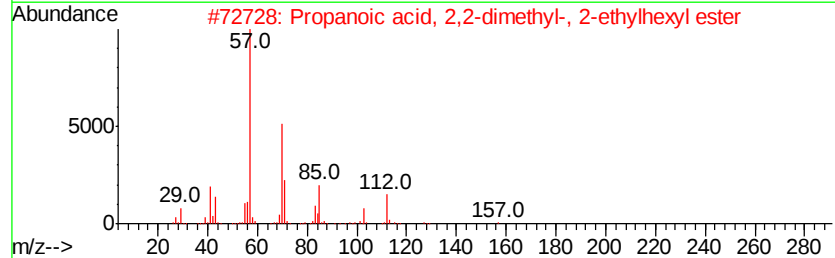
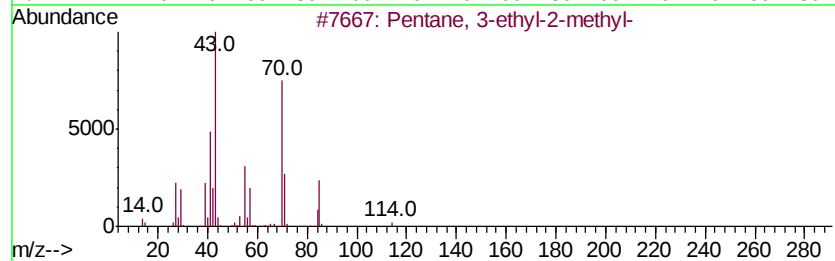
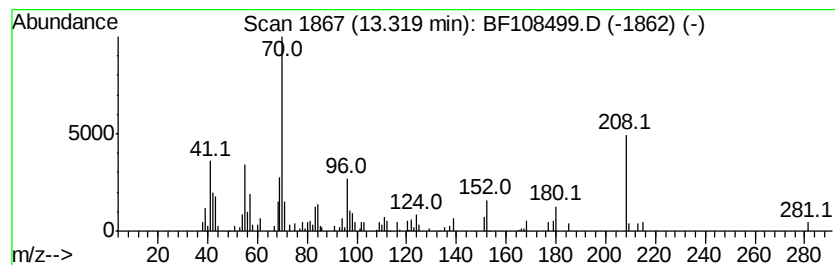
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 unknown13.32 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.32	2.33 ng	98128	Chrysene-d12	14.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	43
2		Propanoic acid, 2,2-dimethyl-, 2...	214	C13H26O2	016387-18-1	43
3		1-Piperidinylloxv, 4-amino-2,2,6,...	171	C9H19N2O	014691-88-4	38
4		5-Undecene, 9-methyl-, (Z)-	168	C12H24	074630-65-2	30
5		2-Propen-1-amine, N-ethyl-	85	C5H11N	002424-02-4	30



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Acq On : 27 Aug 2018 10:15
Operator : JU/SJ
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Misc :
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ClientSampleId :
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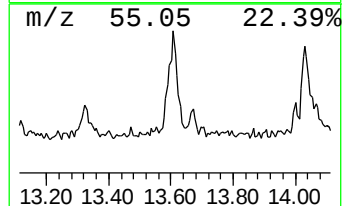
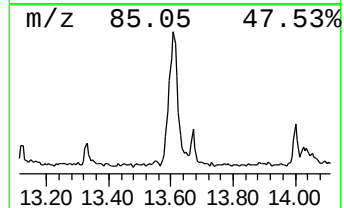
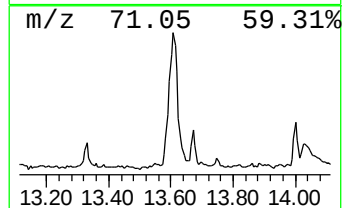
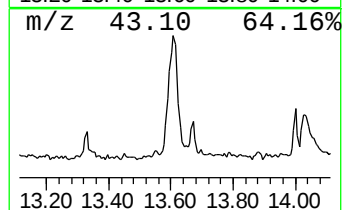
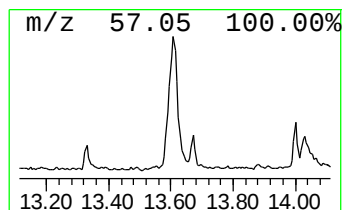
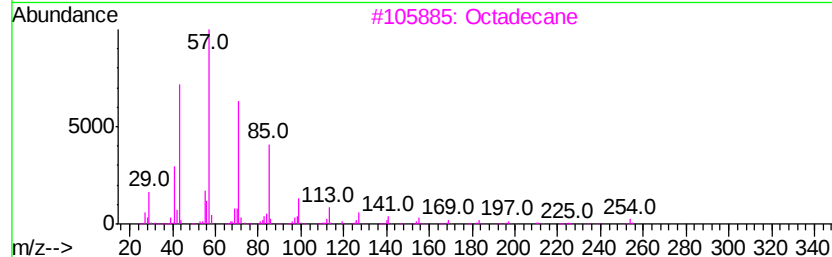
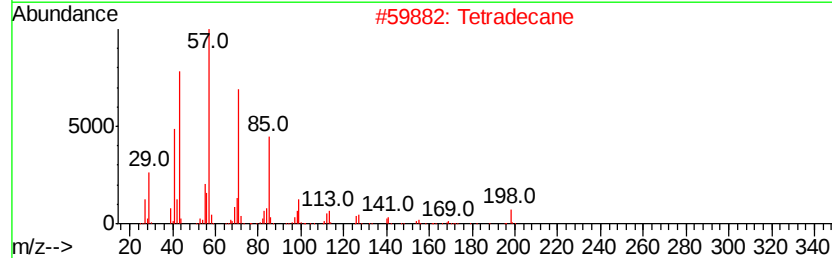
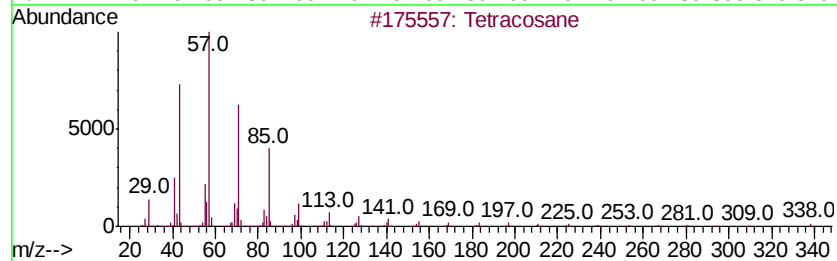
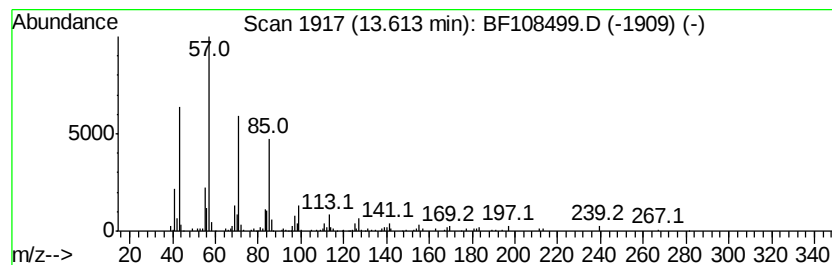
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	9.96 ng	419300	Chrysene-d12	14.19

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Tetradecane	198	C14H30	000629-59-4	91
3			Octadecane	254	C18H38	000593-45-3	91
4			Eicosane	282	C20H42	000112-95-8	91
5			Pentadecane	212	C15H32	000629-62-9	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
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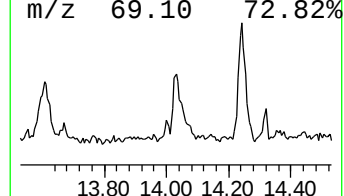
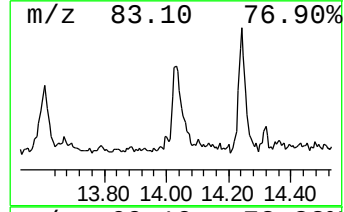
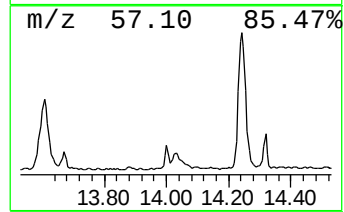
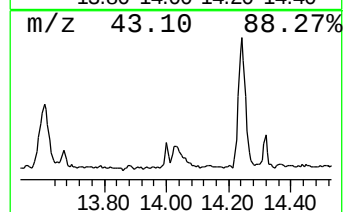
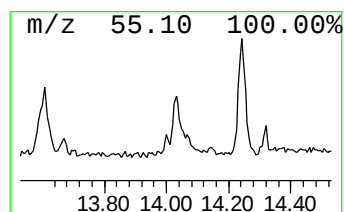
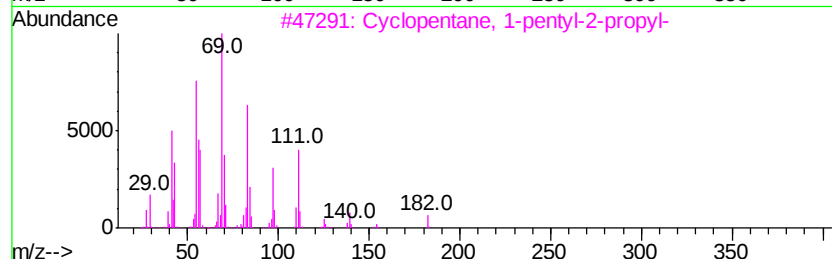
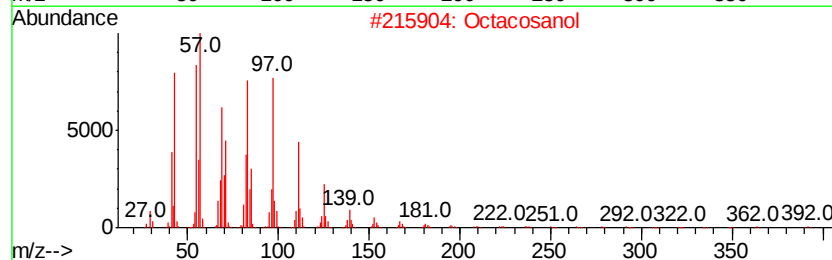
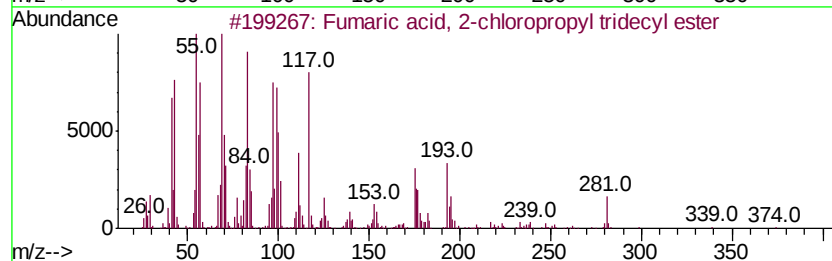
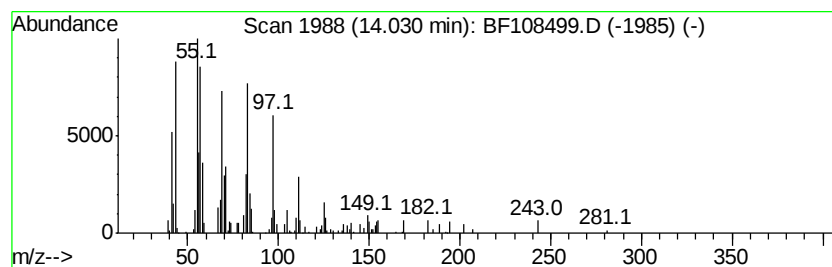
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Fumaric acid, 2-chloropropyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.03	4.44 ng	186840	Chrysene-d12	14.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1000348-57-1	86
2		Octacosanol	410	C28H58O	000557-61-9	86
3		Cyclopentane, 1-pentyl-2-propyl-	182	C13H26	062199-51-3	64
4		Cyclopentane, 1,2-dibutyl-	182	C13H26	062199-52-4	62
5		Cycloeicosane	280	C20H40	000296-56-0	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108499.D
Acq On : 27 Aug 2018 10:15
Operator : JU/SJ
Sample : J4629-01
Misc :
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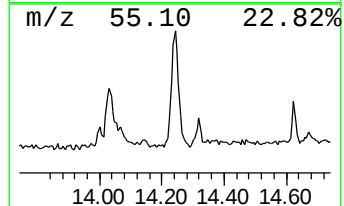
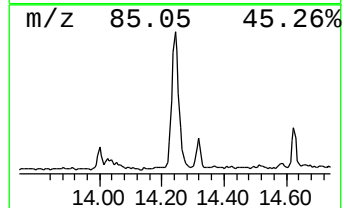
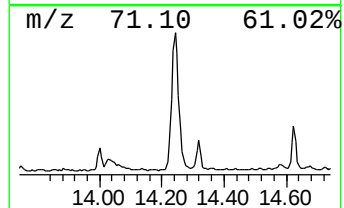
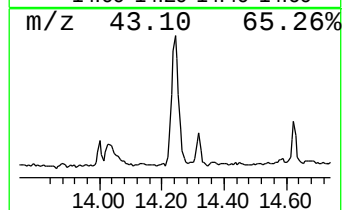
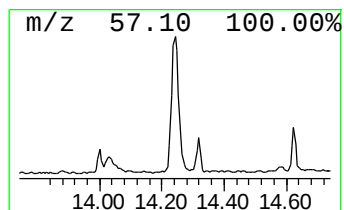
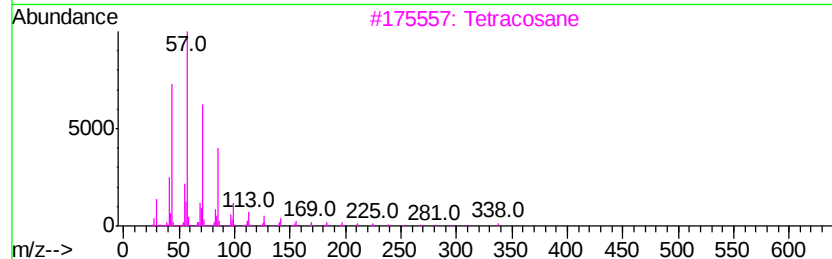
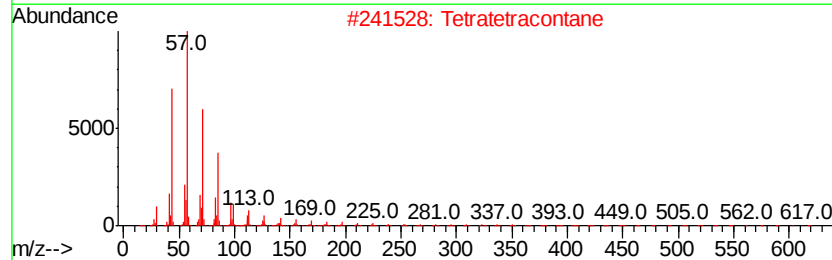
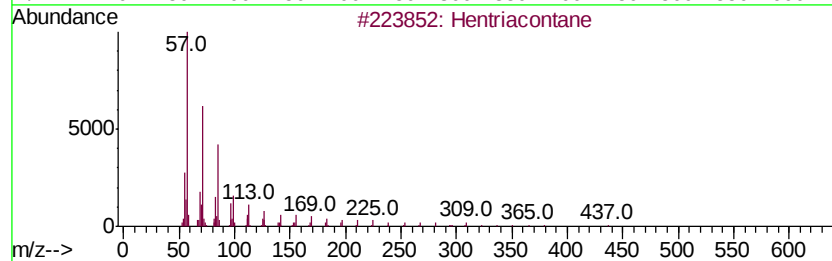
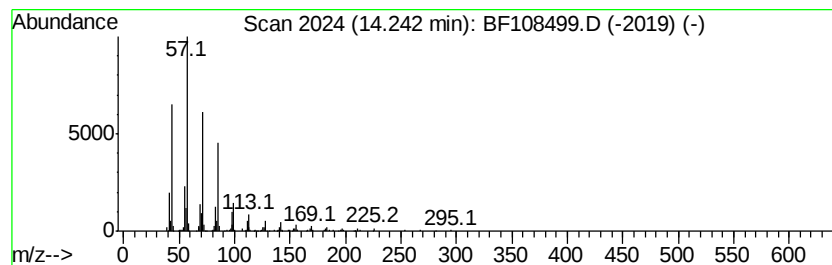
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hentriacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.24	13.68 ng	575693	Chrysene-d12	14.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	91
2	Tetratetracontane		619	C44H90	007098-22-8	91
3	Tetracosane		338	C24H50	000646-31-1	91
4	Octacosane		394	C28H58	000630-02-4	91
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108499.D
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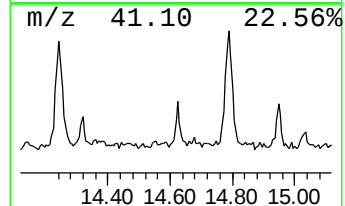
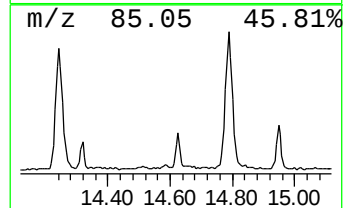
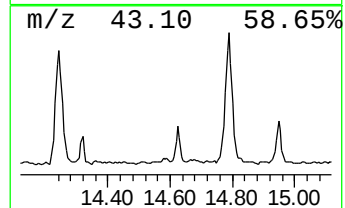
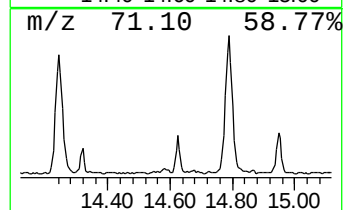
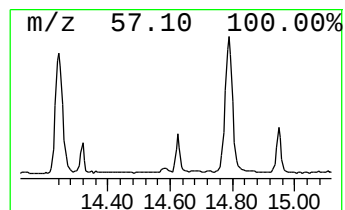
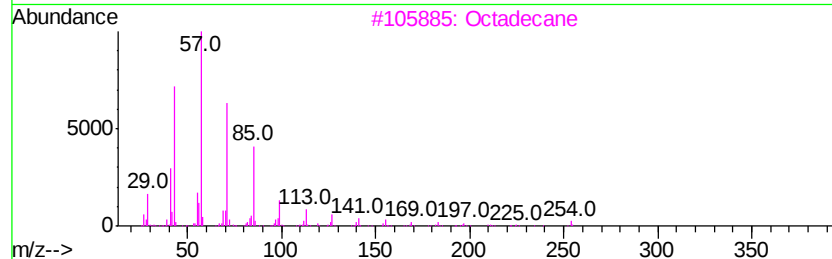
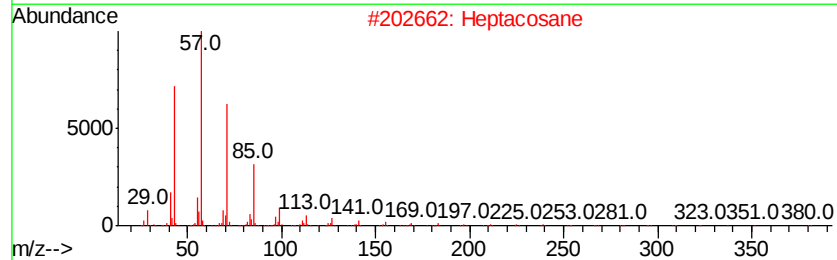
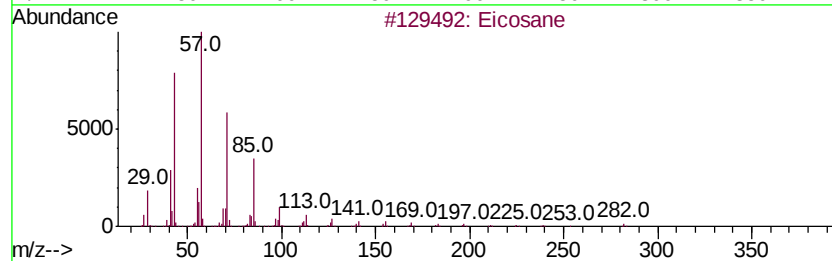
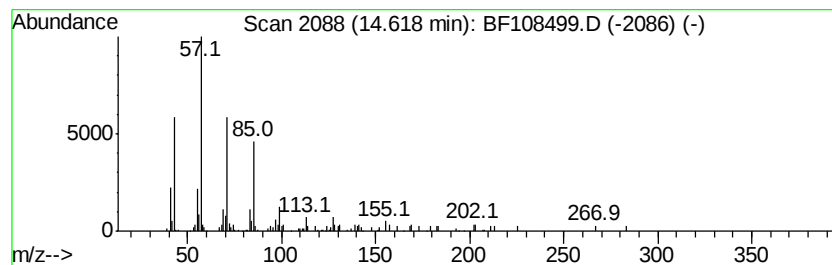
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.57 ng	108157	Chrysene-d12	14.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	96
2		Heptacosane	380	C27H56	000593-49-7	91
3		Octadecane	254	C18H38	000593-45-3	91
4		Docosane	310	C22H46	000629-97-0	91
5		Tetracosane	338	C24H50	000646-31-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108499.D
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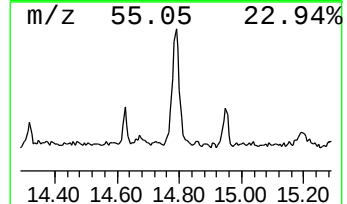
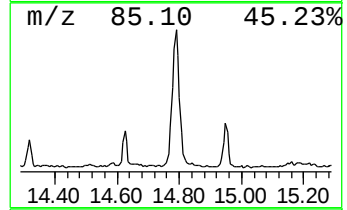
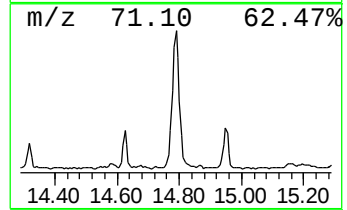
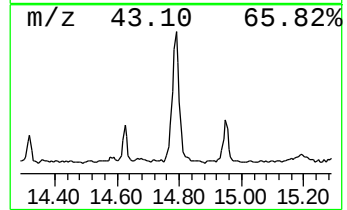
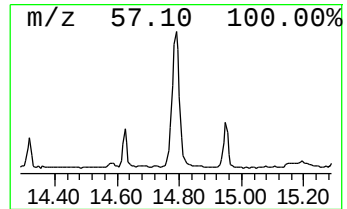
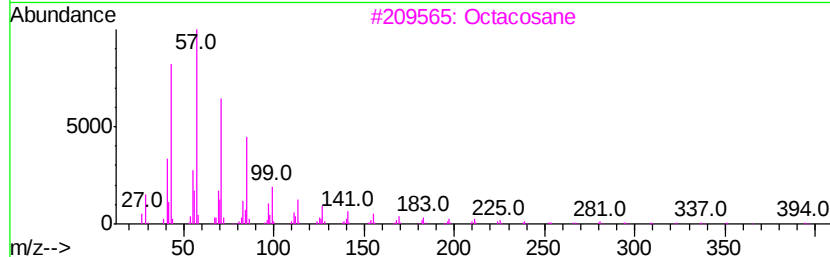
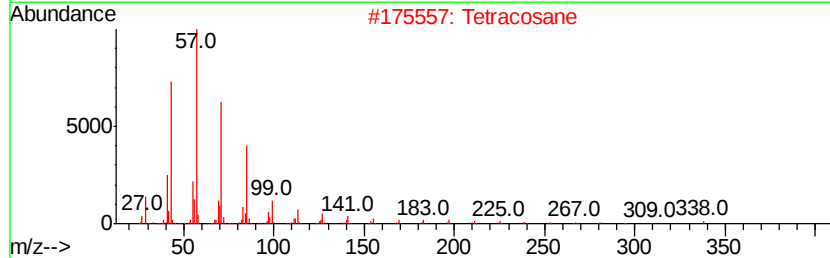
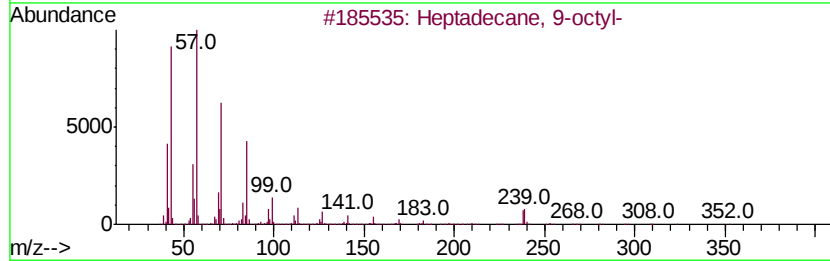
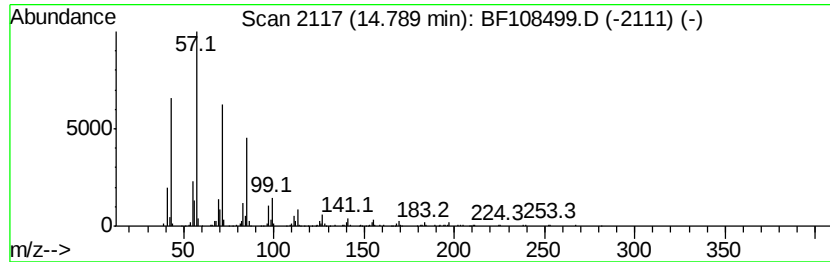
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Heptadecane, 9-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	15.21 ng	639910	Chrysene-d12	14.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heptacosane	380	C27H56	000593-49-7	91
5		Tetratetracontane	619	C44H90	007098-22-8	91



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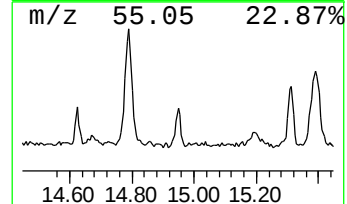
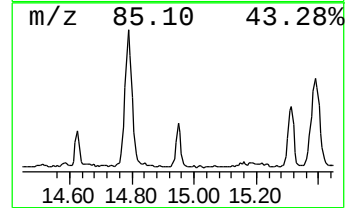
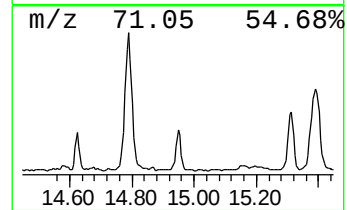
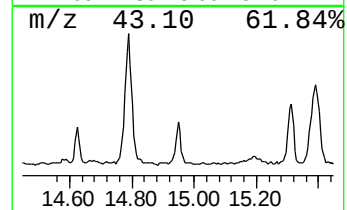
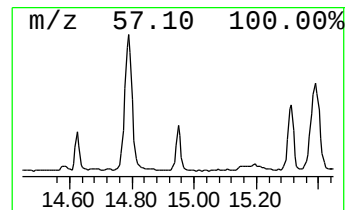
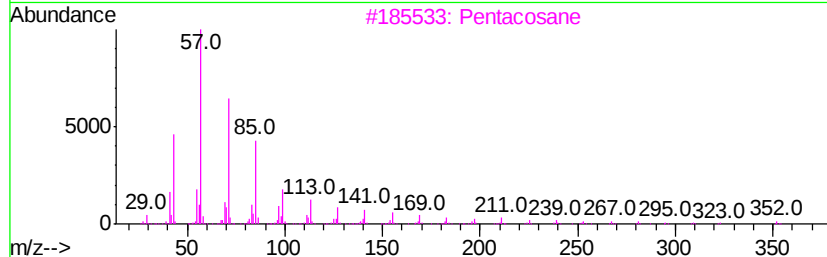
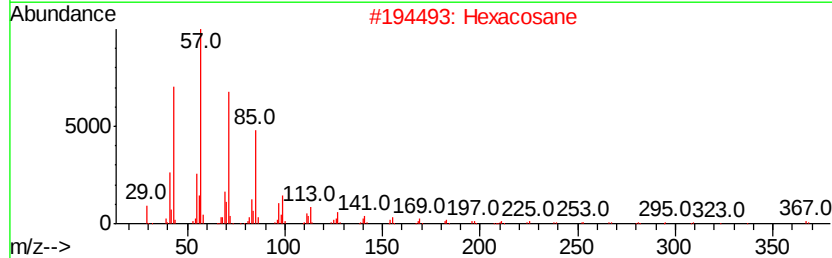
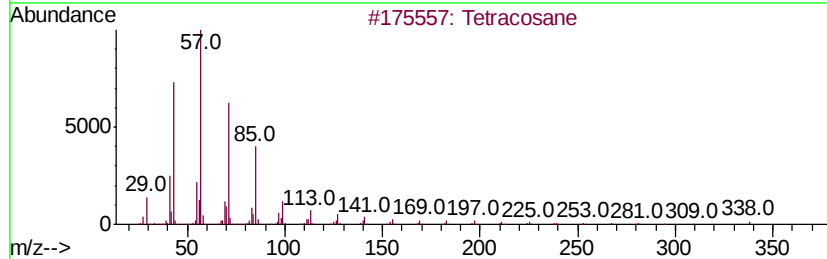
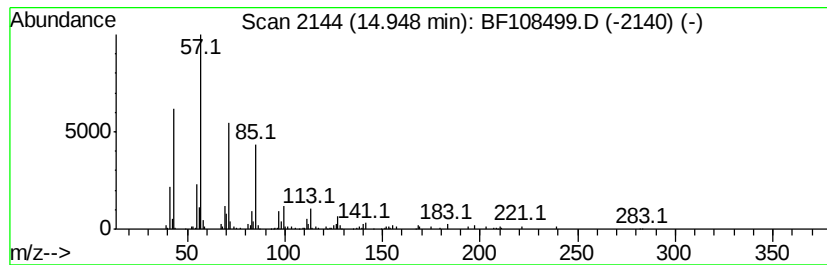
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Pentacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	3.38 ng	142376	Chrysene-d12	14.19

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	90
2			Hexacosane	366	C26H54	000630-01-3	90
3			Pentacosane	352	C25H52	000629-99-2	90
4			2-methyloctacosane	408	C29H60	1000376-72-8	86
5			2-Bromotetradecane	276	C14H29Br	074036-95-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
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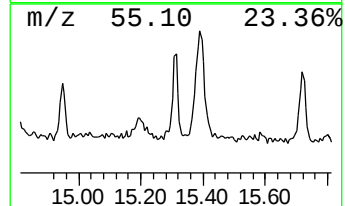
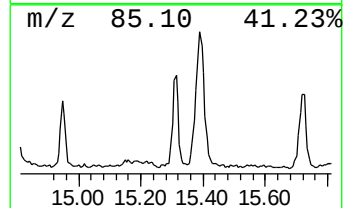
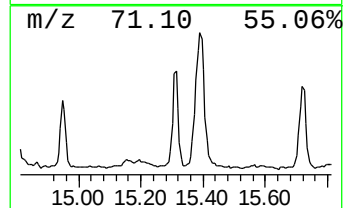
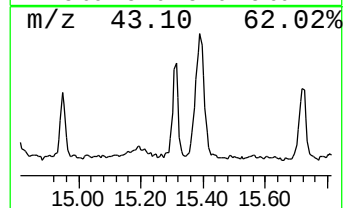
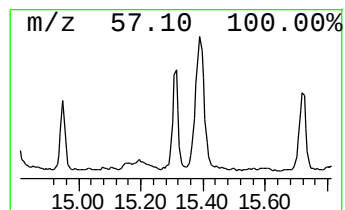
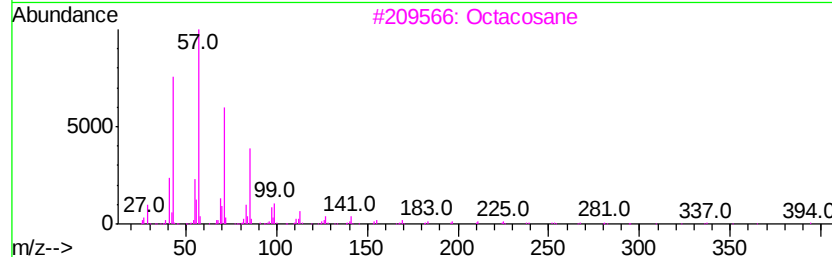
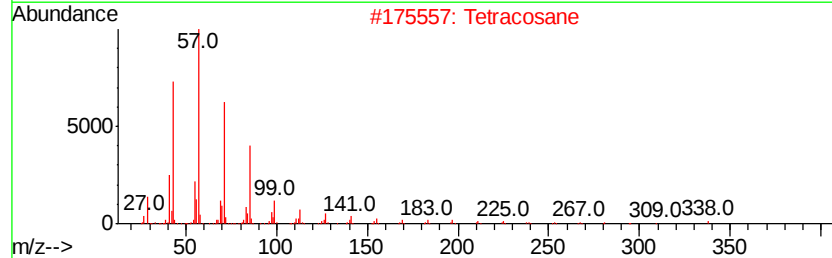
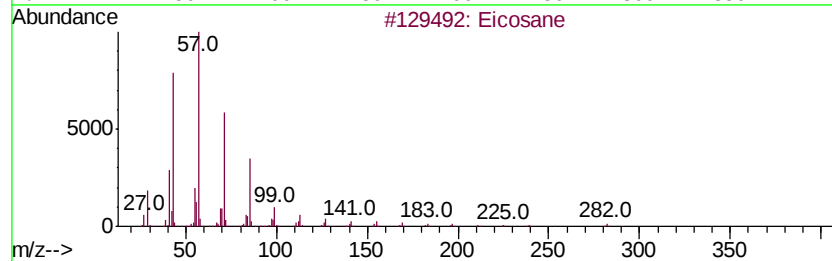
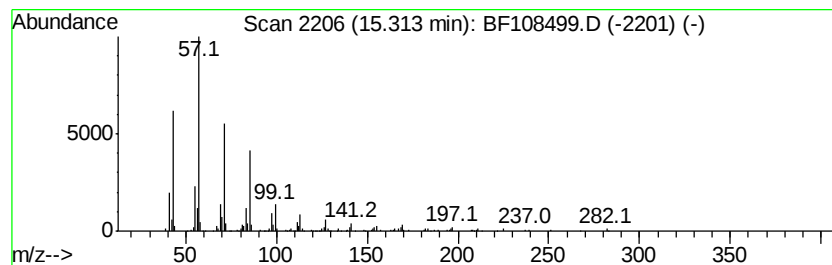
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	5.01 ng	235967	Perylene-d12	15.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Tetracosane	338	C24H50	000646-31-1	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Heptacosane	380	C27H56	000593-49-7	87
5			Docosane	310	C22H46	000629-97-0	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108499.D
Acq On : 27 Aug 2018 10:15
Operator : JU/SJ
Sample : J4629-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-038

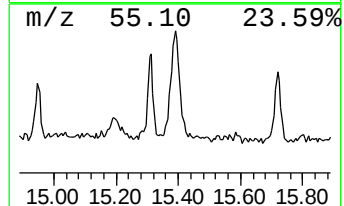
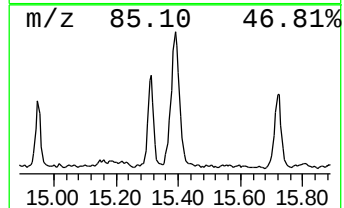
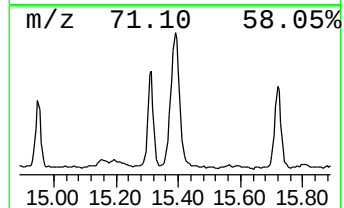
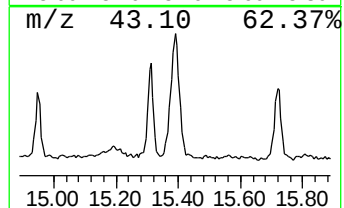
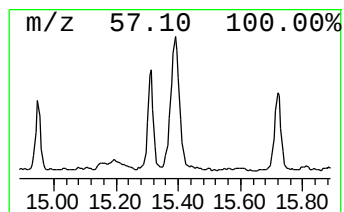
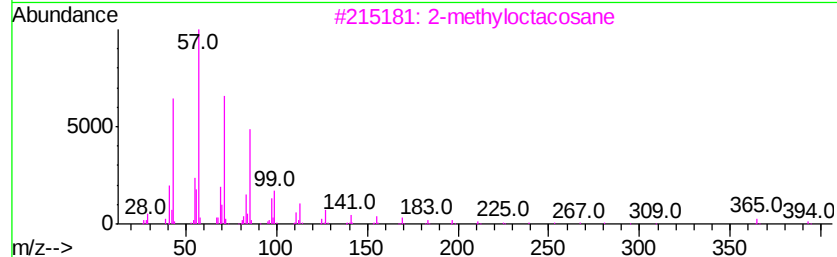
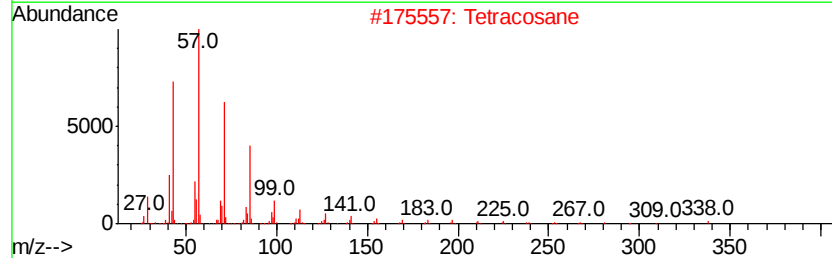
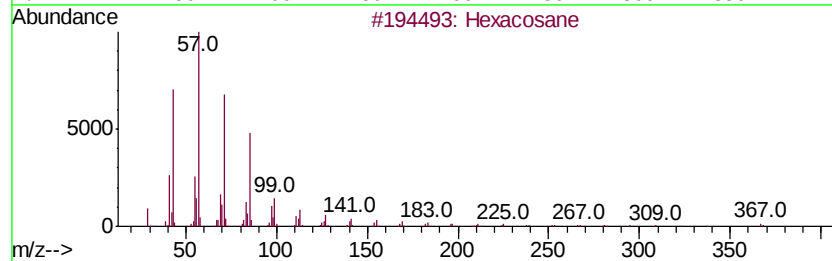
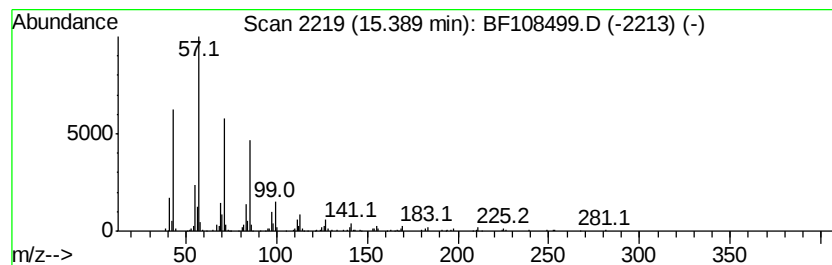
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.39	10.21 ng	481252	Perylene-d12	15.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	94
2		Tetracosane	338	C24H50	000646-31-1	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Tetratetracontane	619	C44H90	007098-22-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108499.D
Acq On : 27 Aug 2018 10:15
Operator : JU/SJ
Sample : J4629-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-038

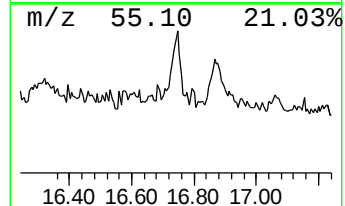
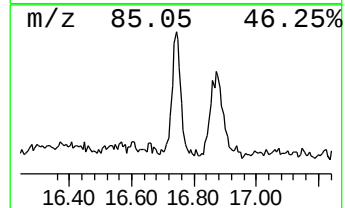
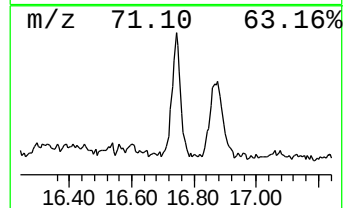
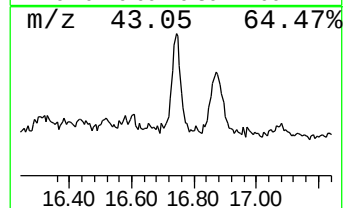
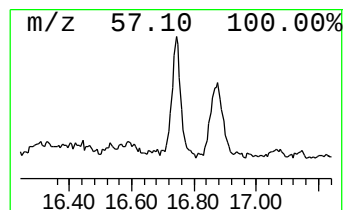
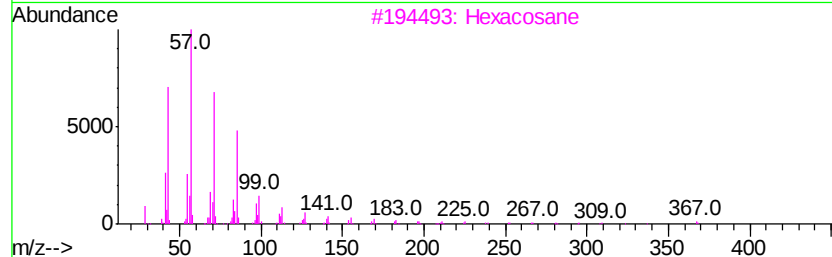
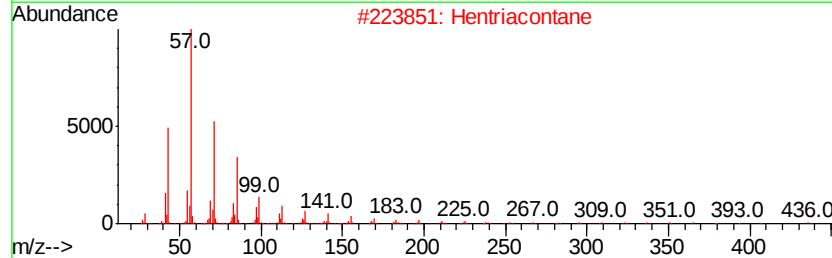
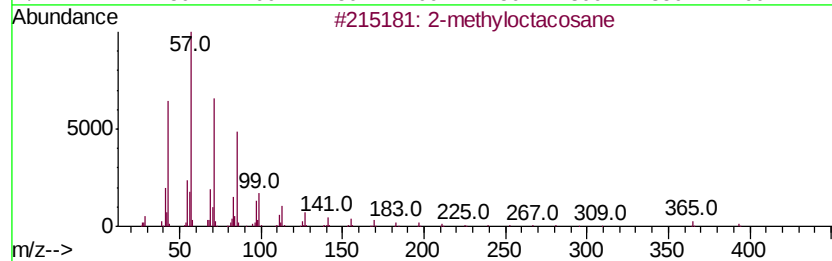
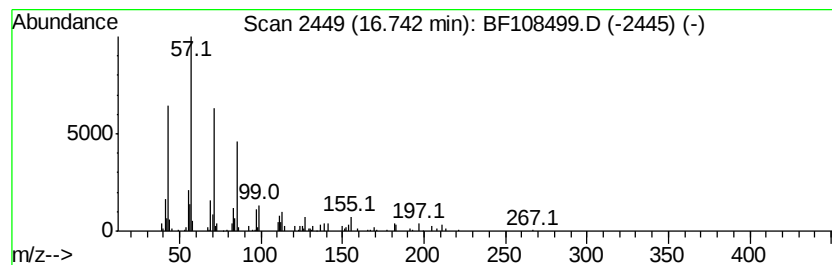
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 2-methyloctacosane Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.74	2.00 ng	94251	Perylene-d12	15.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyloctacosane	408	C29H60	1000376-72-8	87
2			Hentriacontane	437	C31H64	000630-04-6	87
3			Hexacosane	366	C26H54	000630-01-3	87
4			Octacosane	394	C28H58	000630-02-4	87
5			Octadecane	254	C18H38	000593-45-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082718\
 Data File : BF108499.D
 Acq On : 27 Aug 2018 10:15
 Operator : JU/SJ
 Sample : J4629-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-038

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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
2-Pentanone, 4-hy...	5.24	2.7	ng	93158	1	7.00	690173	20.0
unknown6.77	6.77	62.1	ng	2143760	1	7.00	690173	20.0
n-Hexadecanoic acid	12.04	6.2	ng	354158	4	11.54	1139820	20.0
10,18-Bisnorabiet...	12.78	2.5	ng	143281	4	11.54	1139820	20.0
unknown13.32	13.32	2.3	ng	98128	5	14.19	841685	20.0
Tetracosane	13.61	10.0	ng	419300	5	14.19	841685	20.0
Fumaric acid, 2-c...	14.03	4.4	ng	186840	5	14.19	841685	20.0
Hentriacontane	14.24	13.7	ng	575693	5	14.19	841685	20.0
Eicosane	14.62	2.6	ng	108157	5	14.19	841685	20.0
Heptadecane, 9-oc...	14.79	15.2	ng	639910	5	14.19	841685	20.0
Pentacosane	14.95	3.4	ng	142376	5	14.19	841685	20.0
Octacosane	15.31	5.0	ng	235967	6	15.74	942380	20.0
Hexacosane	15.39	10.2	ng	481252	6	15.74	942380	20.0
2-methyloctacosane	16.74	2.0	ng	94251	6	15.74	942380	20.0