

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111318\
 Data File : BF110729.D
 Acq On : 13 Nov 2018 19:54
 Operator : JU/SJ
 Sample : J5925-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1S

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-BF110818.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	2.275	27	32	45	rVB	112670	161120	7.20%	0.816%
2	5.193	523	528	538	rBV	60178	93592	4.18%	0.474%
3	5.569	587	592	612	rBV	2068682	2049419	91.63%	10.384%
4	6.575	758	763	780	rBV	1871724	2236560	100.00%	11.332%
5	6.716	782	787	790	rBV	2424194	2165800	96.84%	10.973%
6	6.945	822	826	832	rBV	562083	506612	22.65%	2.567%
7	7.098	848	852	863	rBV	1813413	1637898	73.23%	8.299%
8	7.510	917	922	939	rBV	1422488	1373779	61.42%	6.960%
9	8.228	1040	1044	1059	rBV	603562	653978	29.24%	3.313%
10	9.298	1221	1226	1229	rBV	2597682	2153518	96.29%	10.911%
11	9.692	1289	1293	1300	rBV	272806	269872	12.07%	1.367%
12	9.986	1339	1343	1353	rVB	686929	672012	30.05%	3.405%
13	10.780	1473	1478	1490	rBV	1145136	1193681	53.37%	6.048%
14	11.480	1593	1597	1600	rBV	556618	545123	24.37%	2.762%
15	11.504	1600	1601	1605	rVB	65955	39263	1.76%	0.199%
16	11.980	1678	1682	1686	rBV	123702	117417	5.25%	0.595%
17	12.698	1800	1804	1808	rBV	89841	78476	3.51%	0.398%
18	12.927	1836	1843	1848	rBV	92159	102822	4.60%	0.521%
19	13.057	1861	1865	1869	rBV	1511613	1343055	60.05%	6.805%
20	13.251	1892	1898	1904	rVB5	17897	36739	1.64%	0.186%
21	13.527	1940	1945	1950	rVB	138324	144505	6.46%	0.732%
22	13.933	2011	2014	2020	rBV	183014	192308	8.60%	0.974%
23	14.127	2042	2047	2050	rBV	516941	507066	22.67%	2.569%
24	14.157	2050	2052	2056	rVB	49526	44136	1.97%	0.224%
25	14.251	2063	2068	2071	rBV3	25024	34067	1.52%	0.173%
26	14.521	2108	2114	2116	rBV	19963	27733	1.24%	0.141%
27	14.557	2116	2120	2125	rBV3	47423	62423	2.79%	0.316%
28	14.868	2169	2173	2177	rBV	61374	80400	3.59%	0.407%
29	14.951	2184	2187	2192	rVB	53130	57067	2.55%	0.289%
30	15.221	2226	2233	2238	rBV2	101635	164854	7.37%	0.835%
31	15.615	2292	2300	2303	rBV2	108388	177625	7.94%	0.900%
32	15.657	2303	2307	2319	rVB	313249	438026	19.58%	2.219%
33	15.768	2324	2326	2333	rVB7	21183	27467	1.23%	0.139%
34	16.068	2372	2377	2383	rVB	96489	143131	6.40%	0.725%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.133	2384	2388	2396	rVB10	24467	51054	2.28%	0.259%
36	16.598	2462	2467	2472	rBV2	54838	90054	4.03%	0.456%
37	17.221	2568	2573	2581	rVB6	28147	64367	2.88%	0.326%

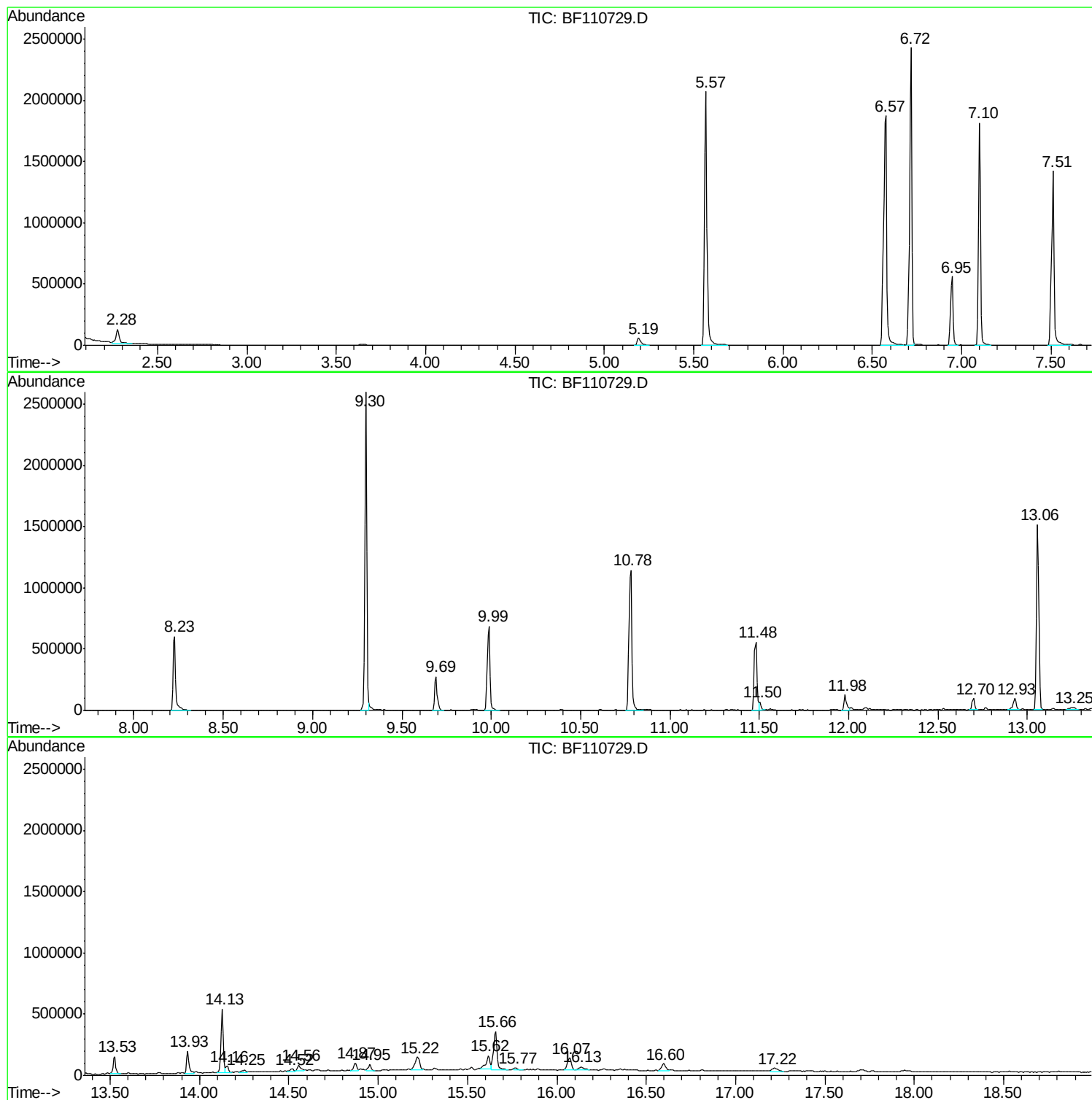
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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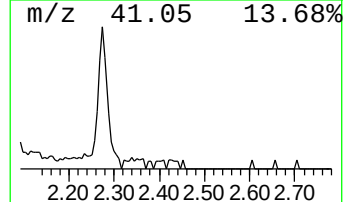
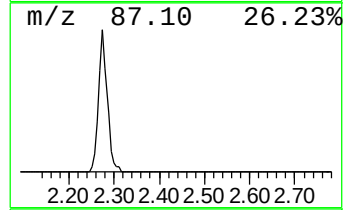
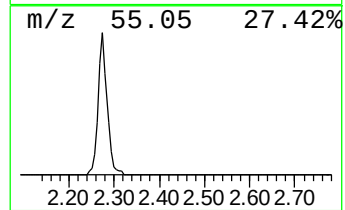
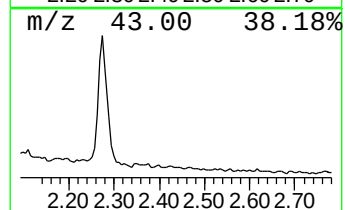
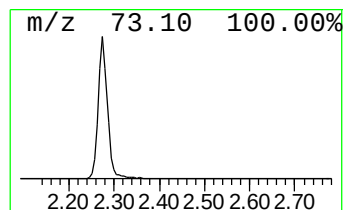
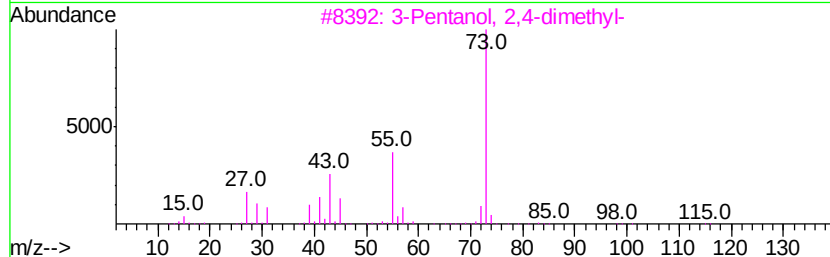
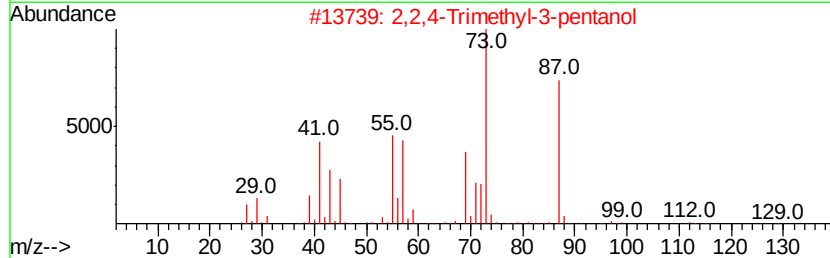
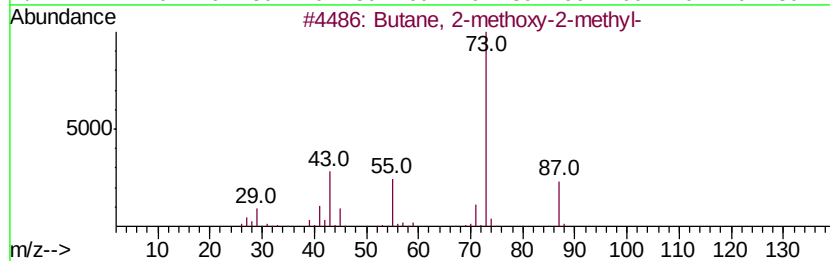
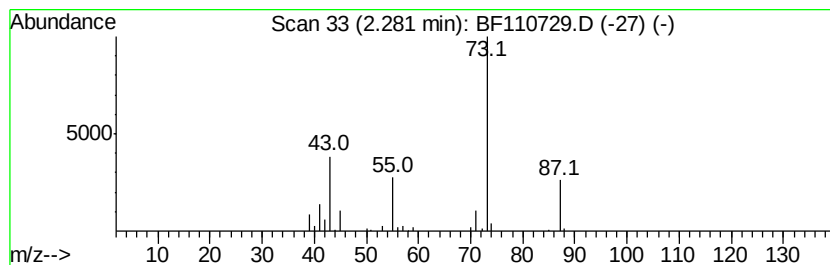
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.28	6.36 ng	161120	1,4-Dichlorobenzene-d4	6.95

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	39
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35



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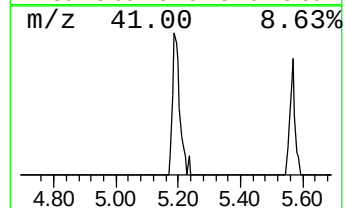
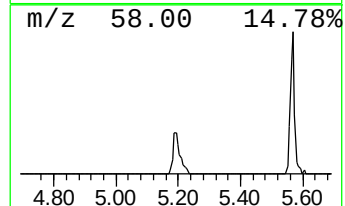
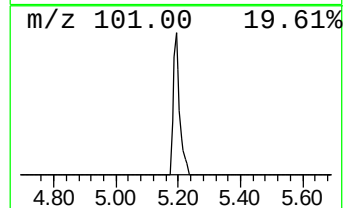
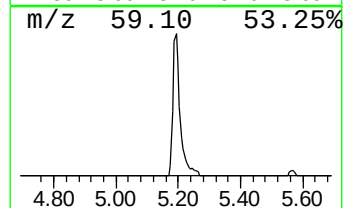
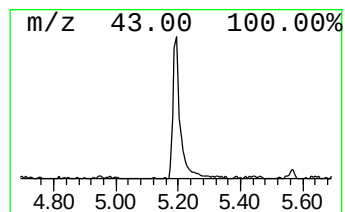
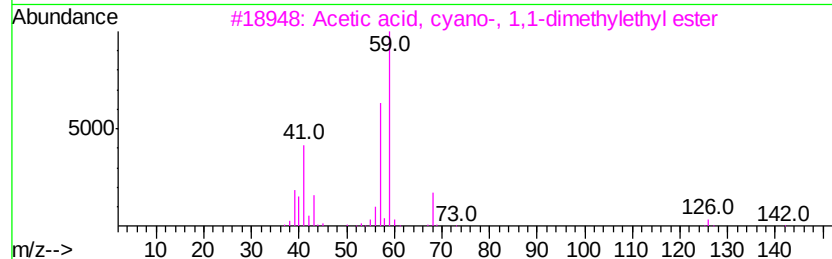
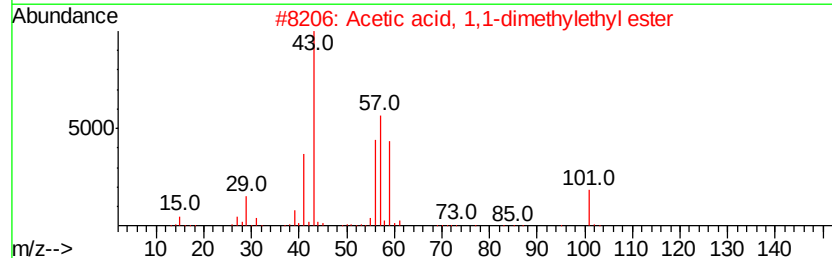
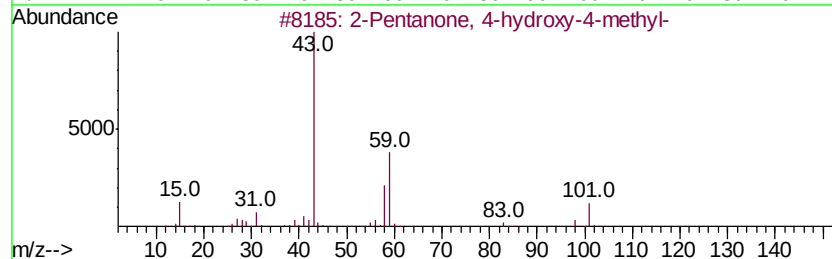
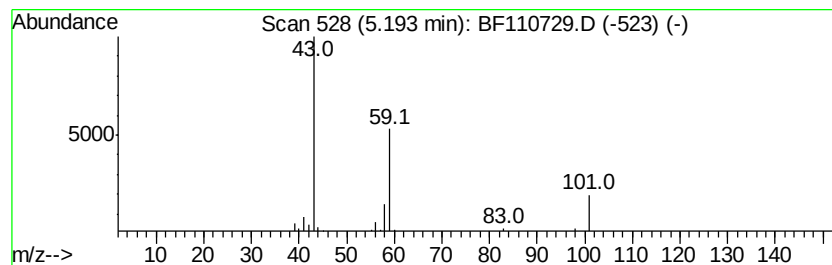
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	3.69 ng	93592	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		Acetamide	59	C2H5NO	000060-35-5	9
5		Propylamine	59	C3H9N	000107-10-8	9



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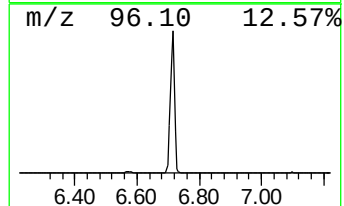
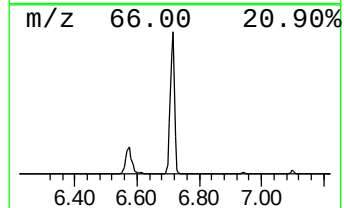
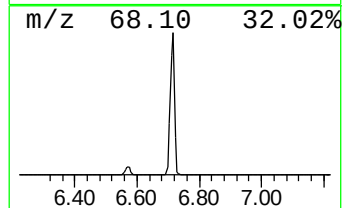
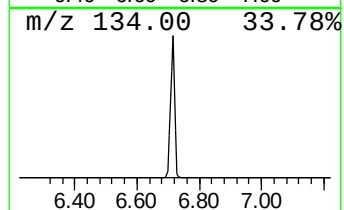
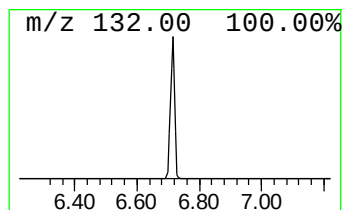
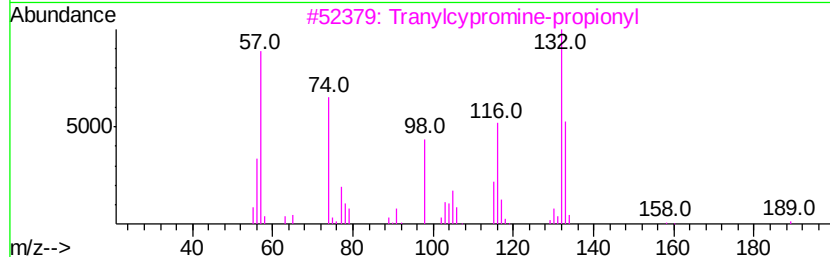
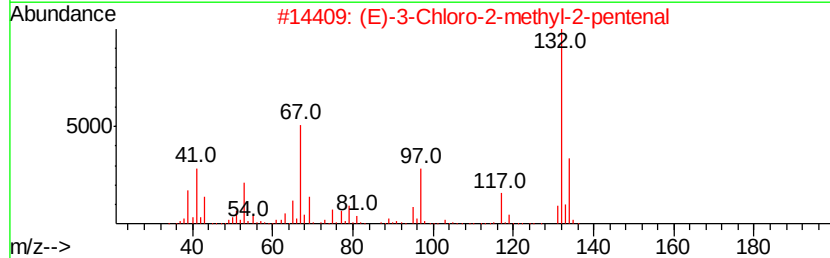
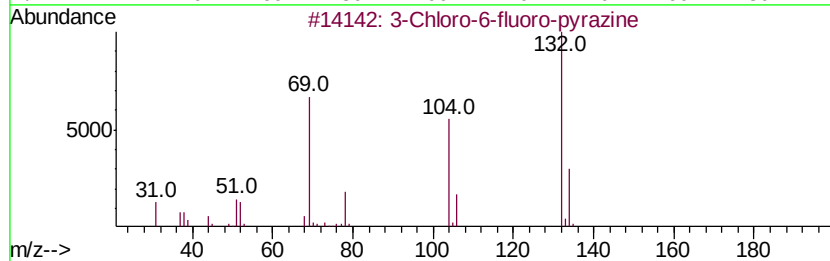
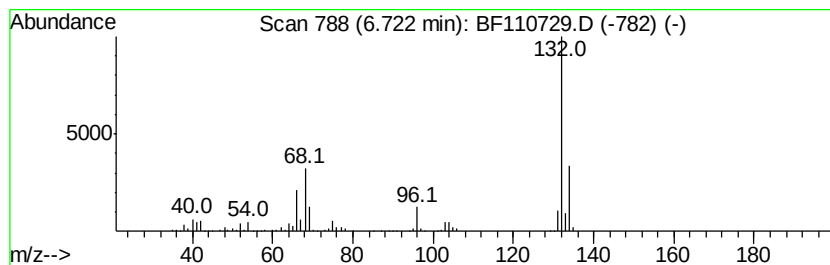
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	85.50 ng	2165800	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9



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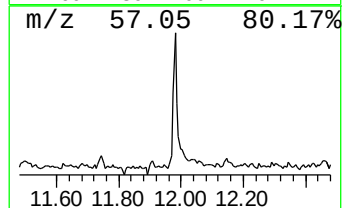
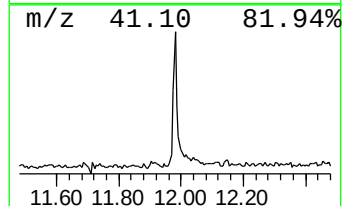
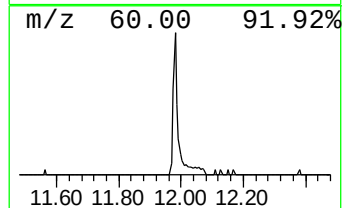
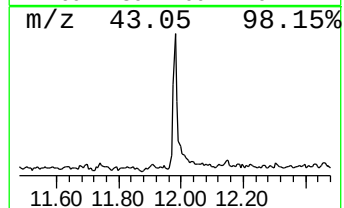
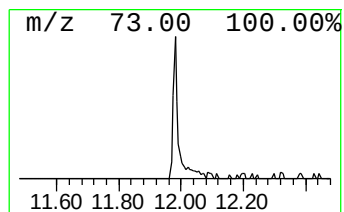
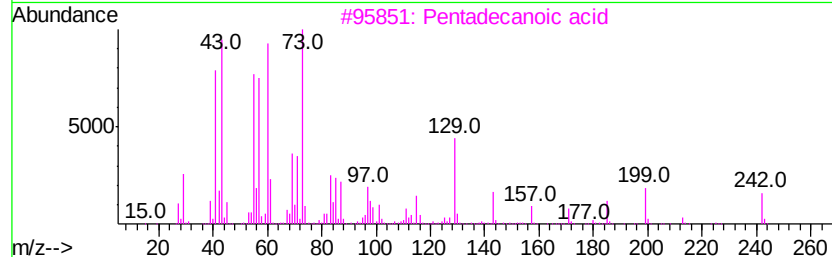
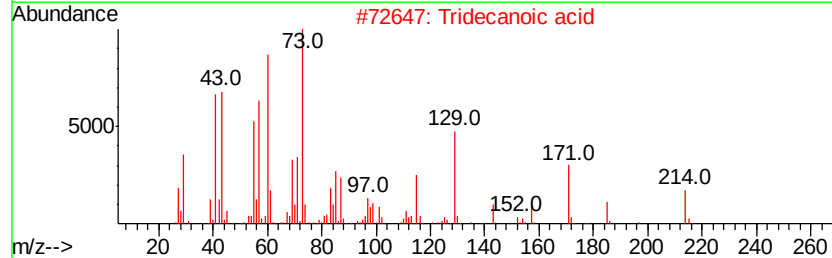
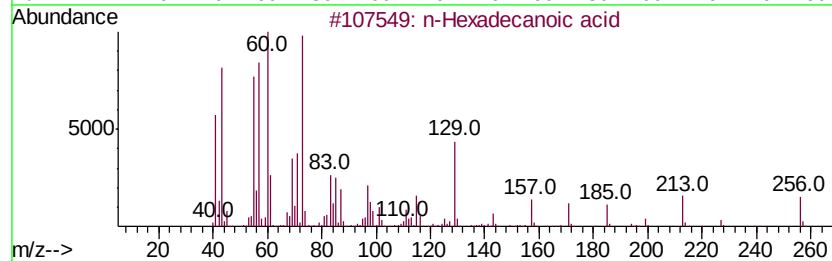
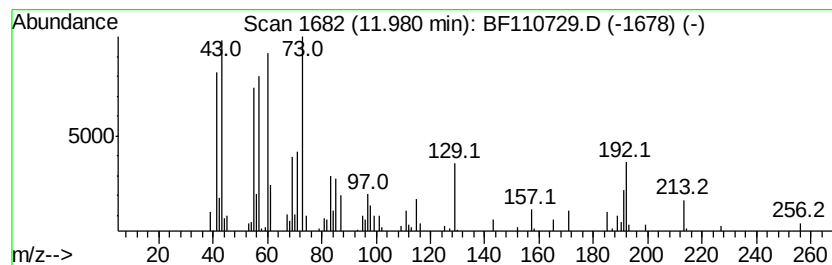
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	4.31 ng	117417	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58



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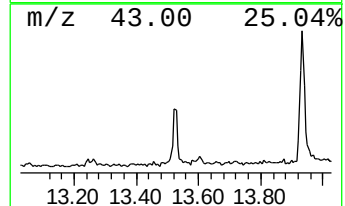
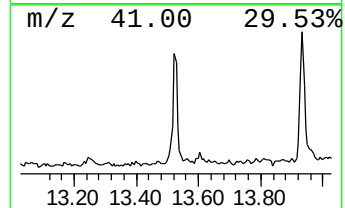
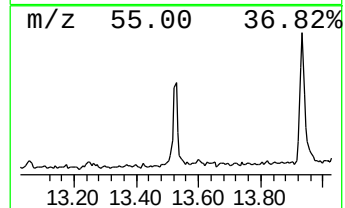
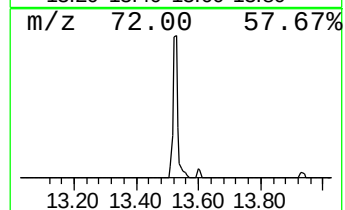
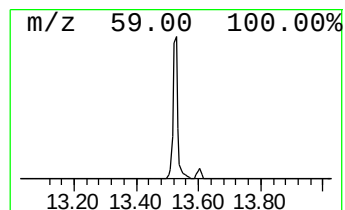
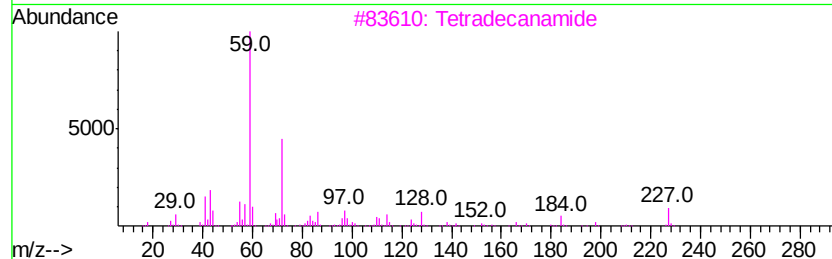
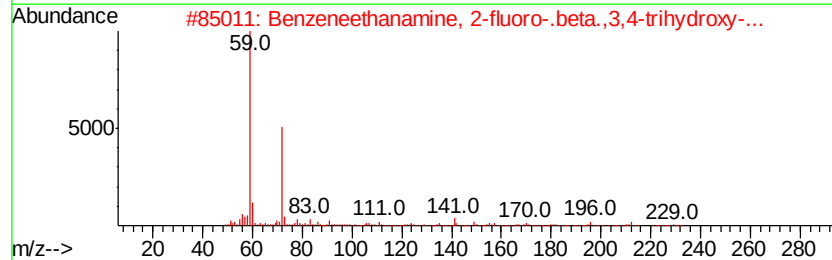
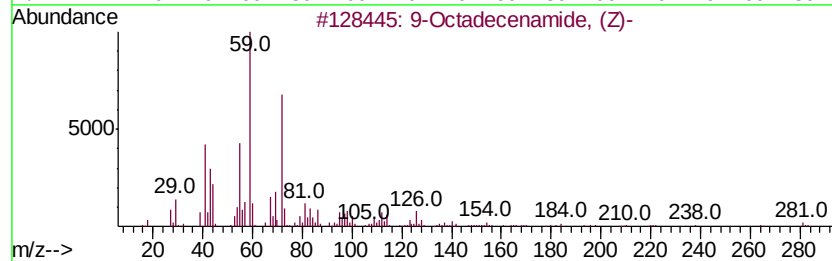
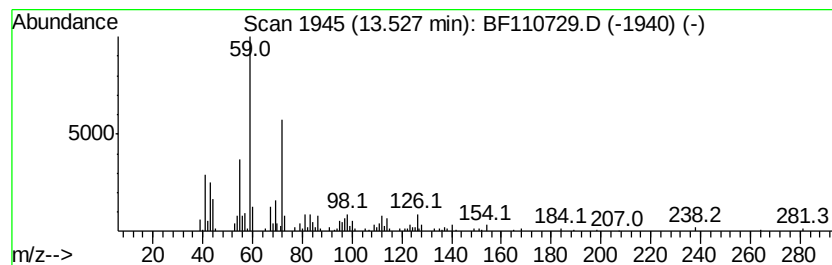
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	5.70 ng	144505	Chrysene-d12	14.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
3		Tetradecanamide	227	C14H29NO	000638-58-4	56
4		Dodecanamide	199	C12H25NO	001120-16-7	53
5		Hexadecanamide	255	C16H33NO	000629-54-9	53



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Operator : JU/SJ
Sample : J5925-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1S

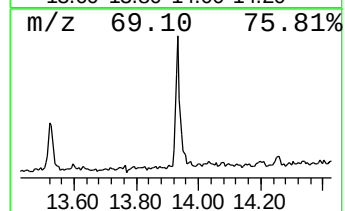
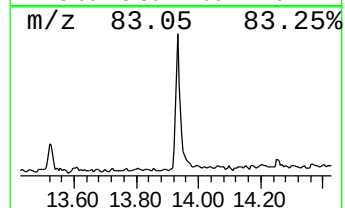
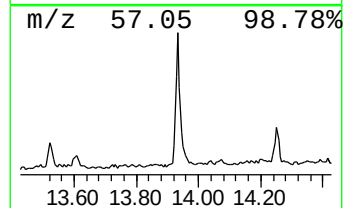
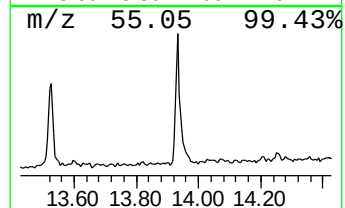
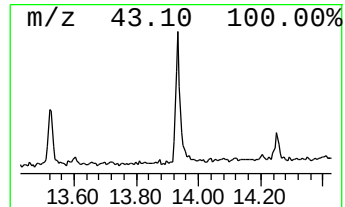
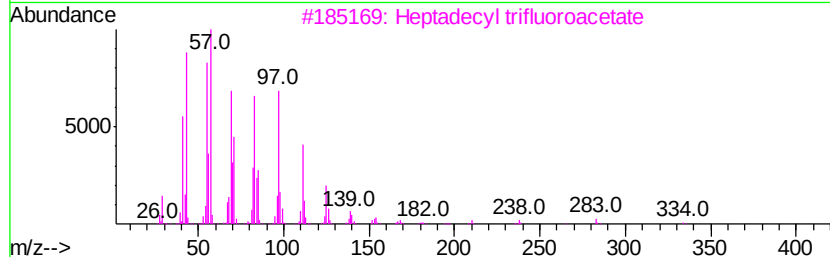
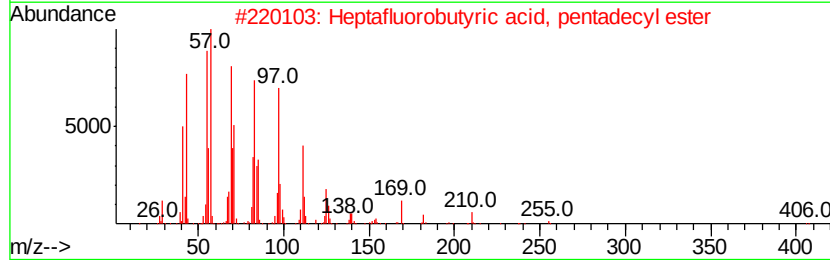
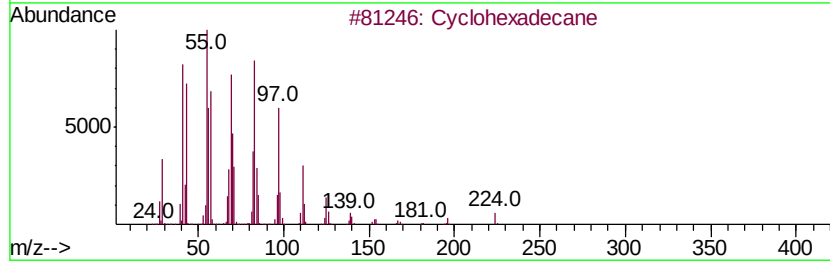
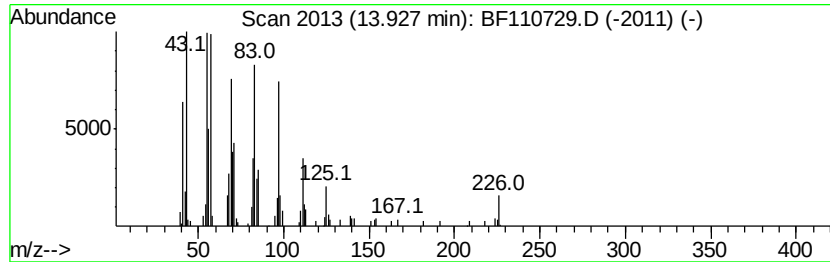
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	7.59 ng	192308	Chrysene-d12	14.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexadecane	224	C16H32	000295-65-8	97
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111318\
Data File : BF110729.D
Acq On : 13 Nov 2018 19:54
Operator : JU/SJ
Sample : J5925-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

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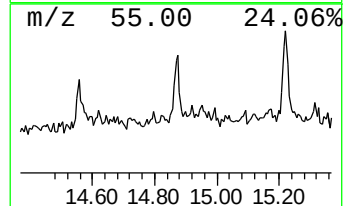
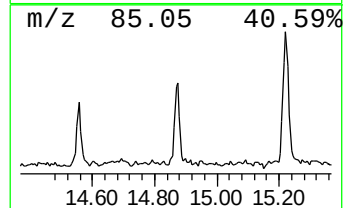
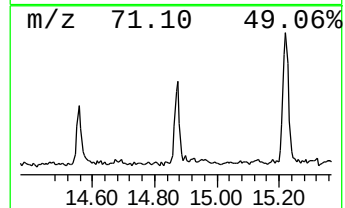
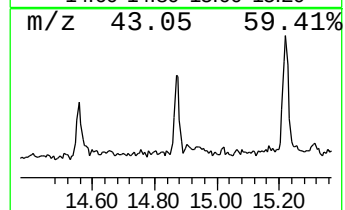
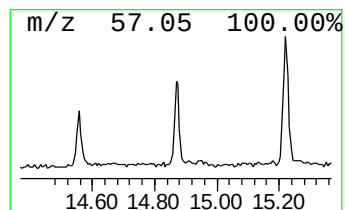
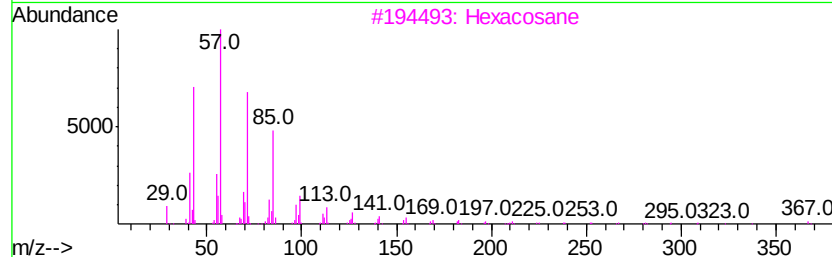
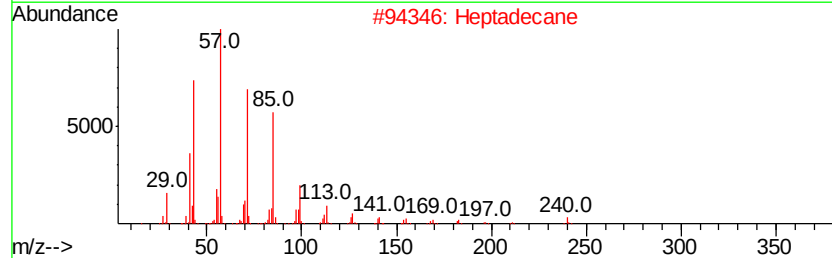
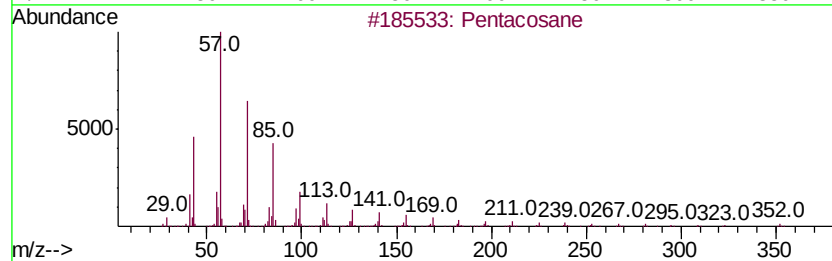
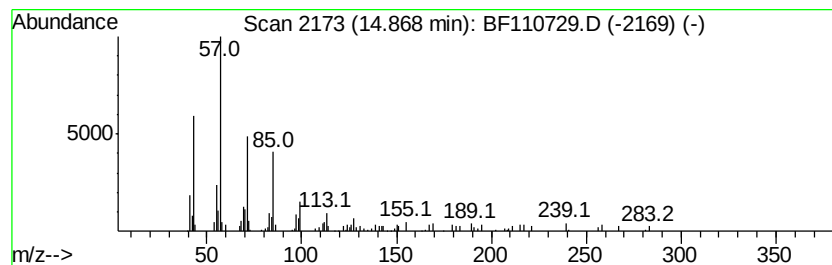
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	3.17 ng	80400	Chrysene-d12	14.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	87
2	Heptadecane		240	C17H36	000629-78-7	87
3	Hexacosane		366	C26H54	000630-01-3	87
4	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	83
5	Octacosane		394	C28H58	000630-02-4	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111318\
Data File : BF110729.D
Acq On : 13 Nov 2018 19:54
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Sample : J5925-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

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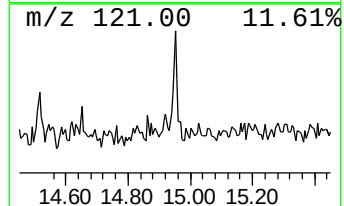
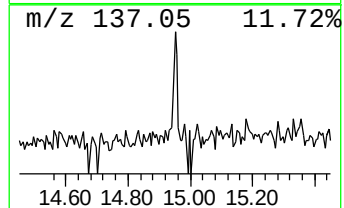
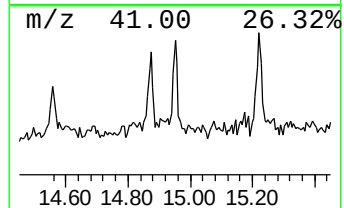
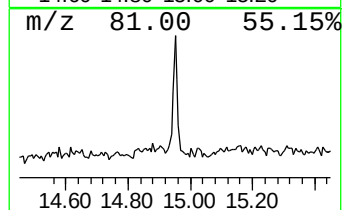
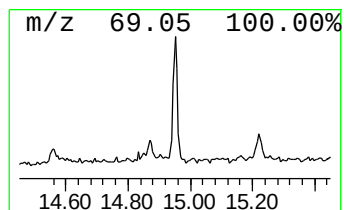
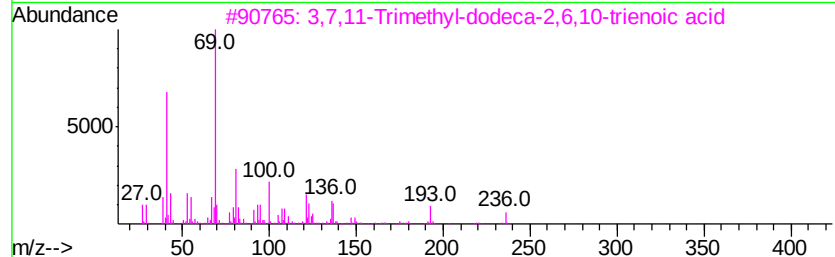
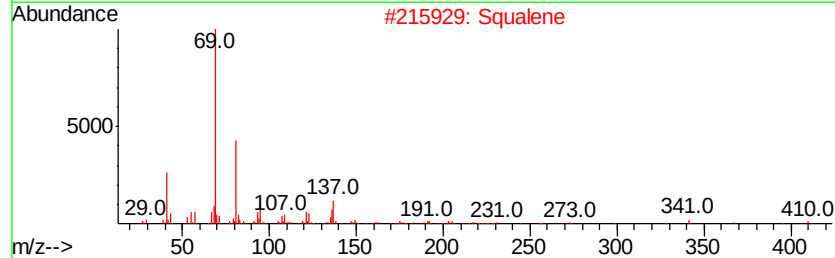
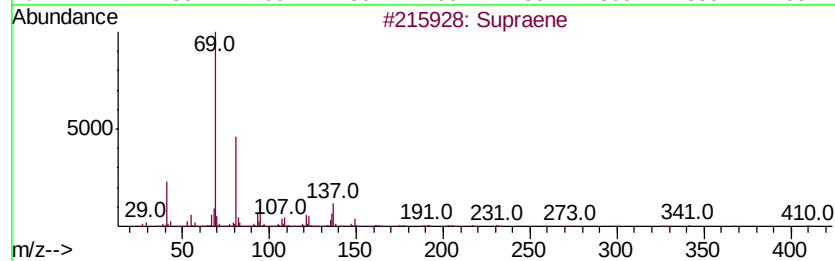
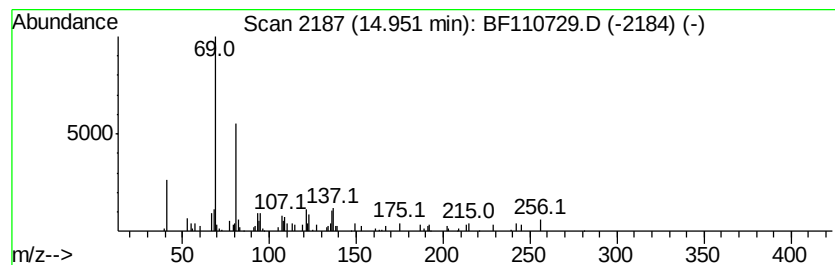
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Supraene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	2.61 ng	57067	Perylene-d12	15.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	80
2		Squalene	410	C30H50	000111-02-4	80
3		3,7,11-Trimethyl-dodeca-2,6,10-t...	236	C15H24O2	007548-13-2	72
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5		trans-Farnesol	222	C15H26O	000106-28-5	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111318\
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Sample : J5925-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

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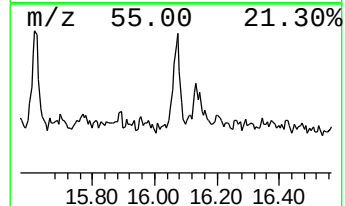
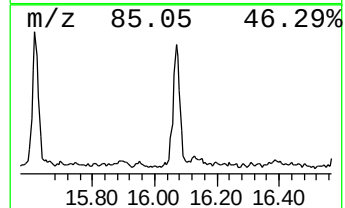
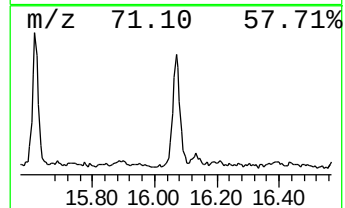
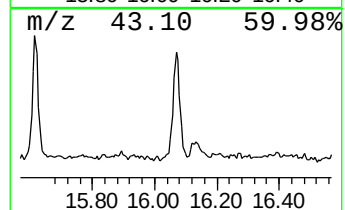
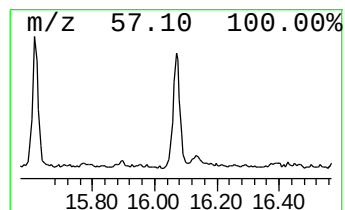
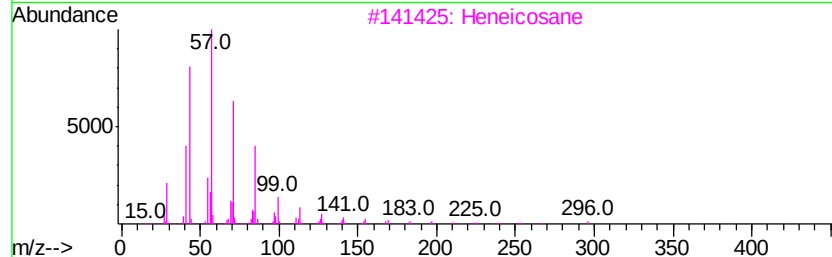
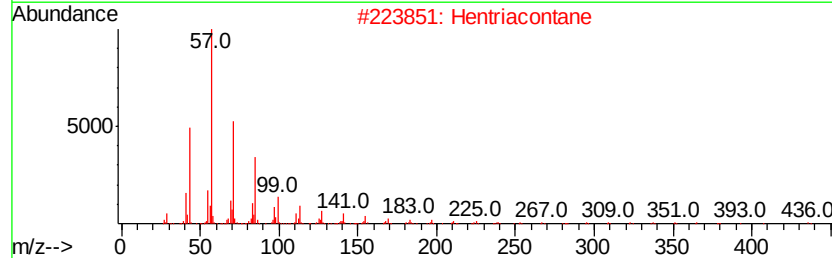
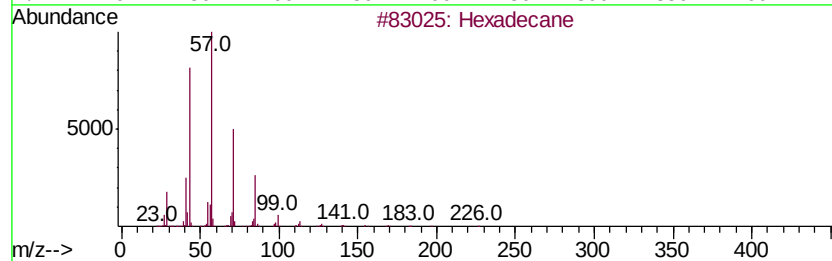
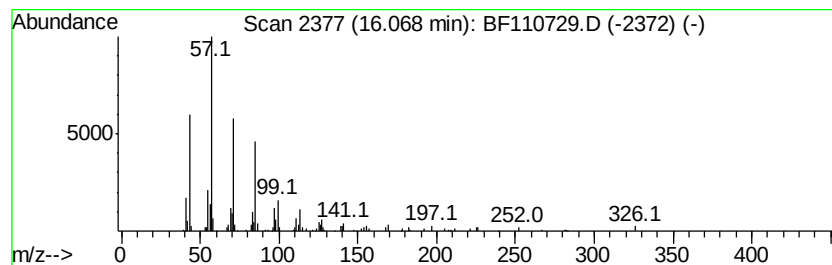
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	6.54 ng	143131	Perylene-d12	15.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	91
2			Hentriacontane	437	C31H64	000630-04-6	91
3			Heneicosane	296	C21H44	000629-94-7	86
4			2-methyloctacosane	408	C29H60	1000376-72-8	83
5			Nonadecane	268	C19H40	000629-92-5	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111318\
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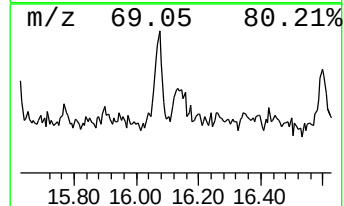
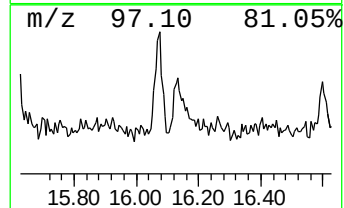
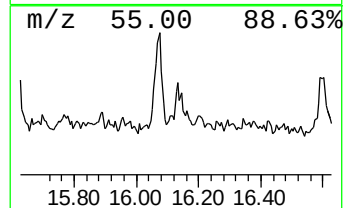
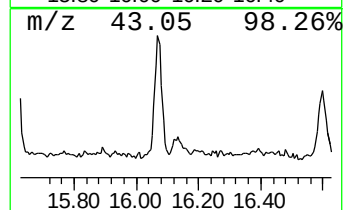
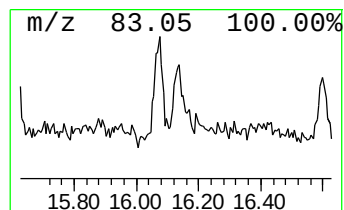
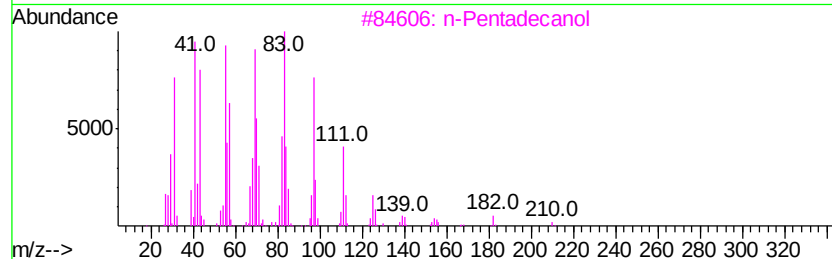
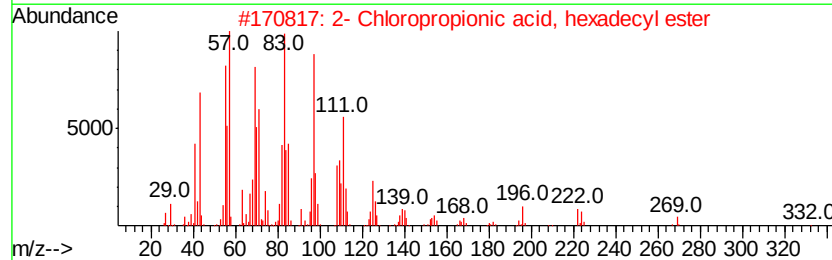
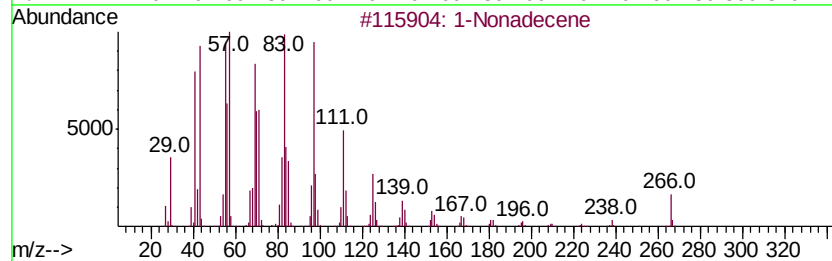
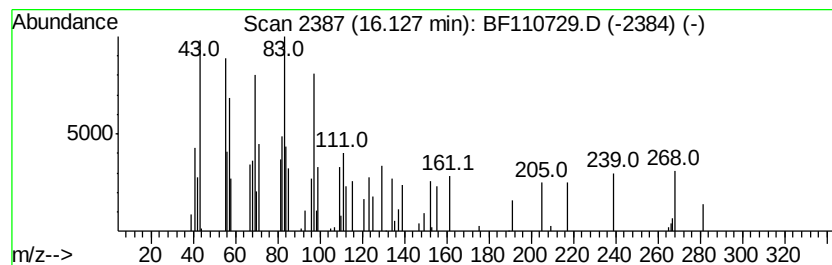
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Nonadecene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	2.33 ng	51054	Perylene-d12	15.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonadecene	266	C19H38	018435-45-5	62
2			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	50
3			n-Pentadecanol	228	C15H32O	000629-76-5	49
4			Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	47
5			Octacosyl acetate	452	C30H60O2	018206-97-8	43



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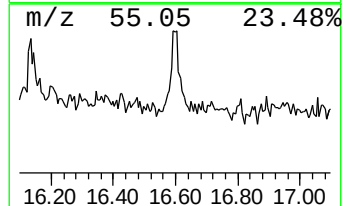
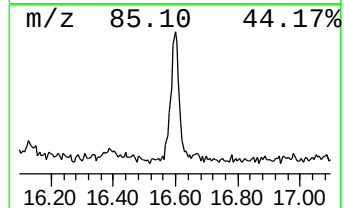
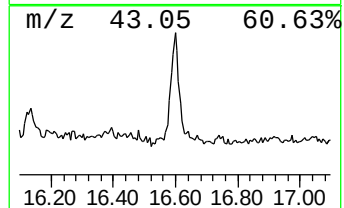
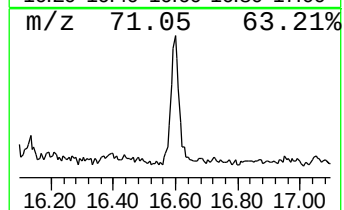
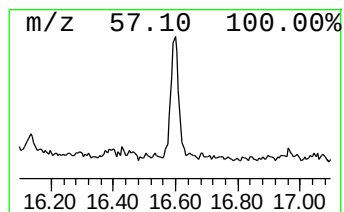
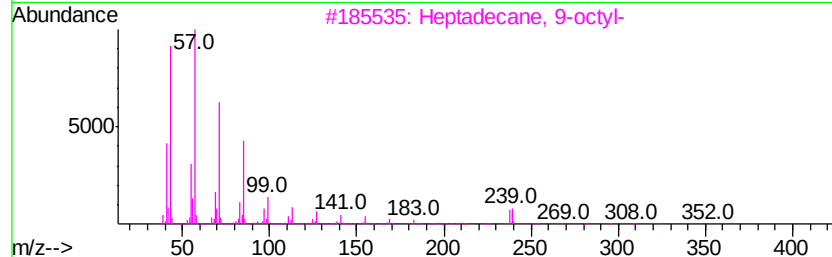
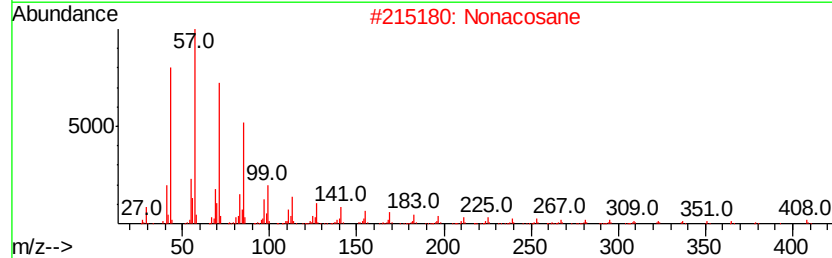
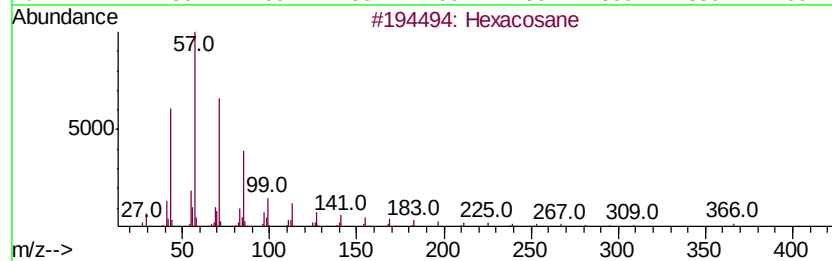
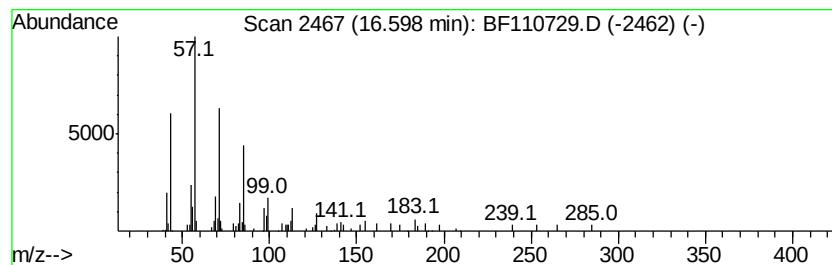
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.60	4.11 ng	90054	Perylene-d12	15.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Nonacosane	408	C29H60	000630-03-5	90
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4			Docosane	310	C22H46	000629-97-0	86
5			Hentriacontane	437	C31H64	000630-04-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111318\
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Misc :
ALS Vial : 12 Sample Multiplier: 1

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.19	3.7	ng	93592	1	6.95	506612	20.0
unknown6.72	6.72	85.5	ng	2165800	1	6.95	506612	20.0
n-Hexadecanoic acid	11.98	4.3	ng	117417	4	11.48	545123	20.0
9-Octadecenamide,...	13.53	5.7	ng	144505	5	14.13	507066	20.0
Cyclohexadecane	13.93	7.6	ng	192308	5	14.13	507066	20.0
Pentacosane	14.87	3.2	ng	80400	5	14.13	507066	20.0
Supraene	14.95	2.6	ng	57067	6	15.66	438026	20.0
Hexadecane	16.07	6.5	ng	143131	6	15.66	438026	20.0
1-Nonadecene	16.13	2.3	ng	51054	6	15.66	438026	20.0
Hexacosane	16.60	4.1	ng	90054	6	15.66	438026	20.0