

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF070518\
 Data File : BF107136.D
 Acq On : 5 Jul 2018 19:31
 Operator : JU/SJ
 Sample : J3853-12
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-11

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-BF061918.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	5.195	481	486	495	rBV	163435	226153	12.81%	1.457%
2	5.595	550	554	572	rVB	1422148	1473118	83.45%	9.493%
3	6.601	719	725	734	rBV	1337950	1548007	87.69%	9.975%
4	6.731	742	747	750	rBV	1511929	1499910	84.97%	9.665%
5	6.948	780	784	787	rBV	416909	339516	19.23%	2.188%
6	7.107	806	811	814	rBV	1288341	1238925	70.18%	7.984%
7	7.519	875	881	884	rBV	903788	1011589	57.31%	6.519%
8	8.231	998	1002	1005	rBV	480095	417796	23.67%	2.692%
9	9.307	1179	1185	1188	rBV	1802304	1765246	100.00%	11.375%
10	9.695	1245	1251	1257	rBV	385697	314468	17.81%	2.026%
11	9.989	1297	1301	1305	rBV2	522982	453520	25.69%	2.922%
12	10.789	1432	1437	1440	rBV	1096191	1021191	57.85%	6.580%
13	11.483	1552	1555	1558	rBV	464307	408013	23.11%	2.629%
14	11.689	1586	1590	1595	rBV3	20164	25267	1.43%	0.163%
15	12.936	1800	1802	1806	rVB2	27370	24103	1.37%	0.155%
16	13.071	1820	1825	1828	rBV	1514119	1492046	84.52%	9.615%
17	13.271	1853	1859	1864	rBV3	29803	40304	2.28%	0.260%
18	13.613	1914	1917	1920	rVB	37573	29728	1.68%	0.192%
19	13.795	1946	1948	1951	rBV	27936	27498	1.56%	0.177%
20	13.942	1970	1973	1979	rVB	107604	111504	6.32%	0.719%
21	14.083	1993	1997	2001	rBV	743018	660877	37.44%	4.259%
22	14.136	2002	2006	2010	rBV	461689	445488	25.24%	2.871%
23	14.260	2024	2027	2031	rBV	45066	47007	2.66%	0.303%
24	14.583	2077	2082	2086	rBV2	64460	133084	7.54%	0.858%
25	14.801	2116	2119	2124	rVB4	27719	25491	1.44%	0.164%
26	14.889	2131	2134	2140	rVB2	37207	47035	2.66%	0.303%
27	15.042	2157	2160	2166	rVB	58395	67697	3.83%	0.436%
28	15.236	2191	2193	2197	rVB	47114	55177	3.13%	0.356%
29	15.277	2197	2200	2206	rVB4	27213	36259	2.05%	0.234%
30	15.677	2263	2268	2274	rVB	234068	306335	17.35%	1.974%
31	16.095	2336	2339	2343	rVB2	37003	47442	2.69%	0.306%
32	17.548	2581	2586	2594	rVB3	87317	178687	10.12%	1.151%

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Misc :
ALS Vial : 22 Sample Multiplier: 1

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

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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

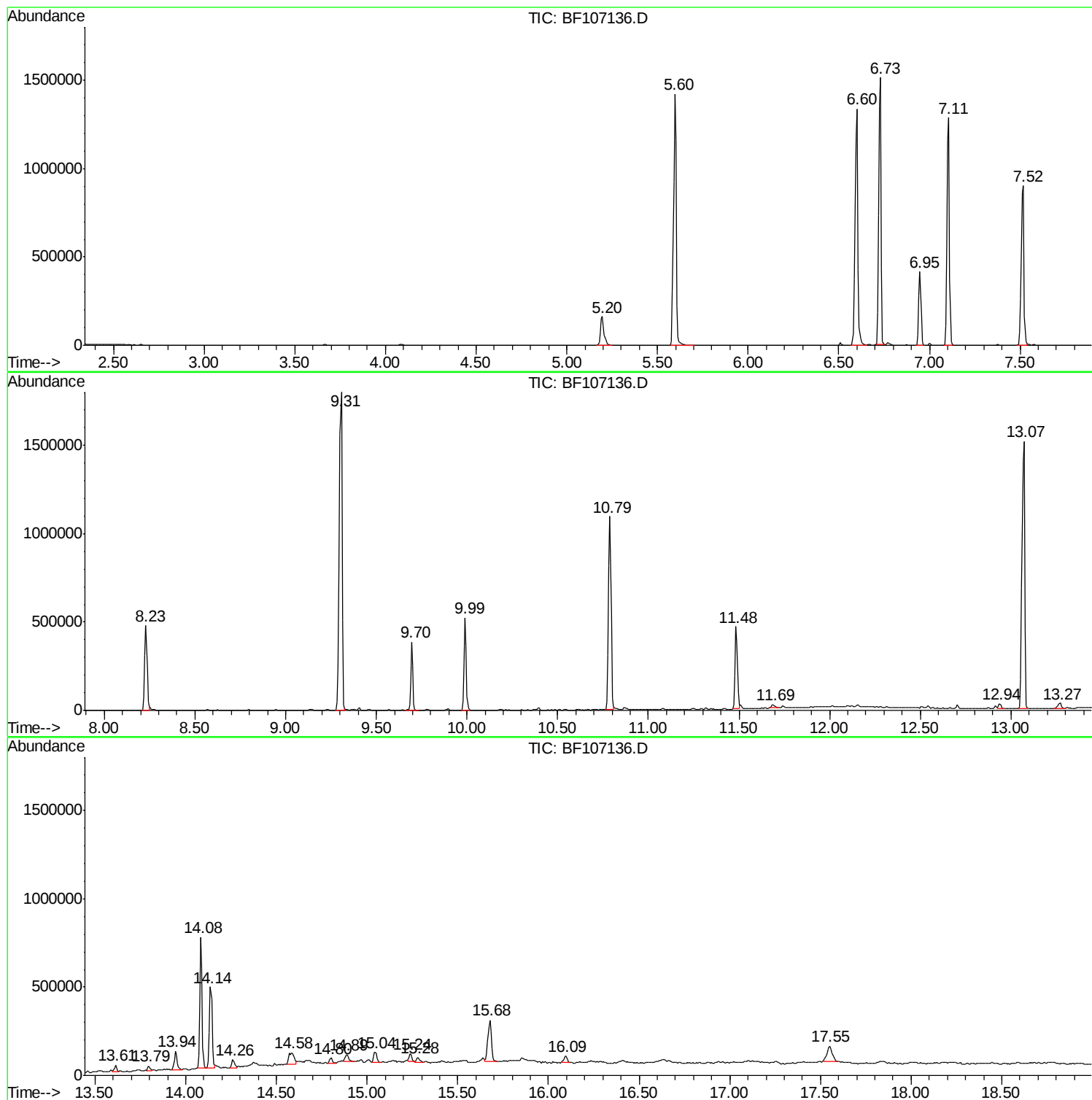
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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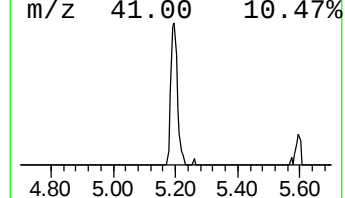
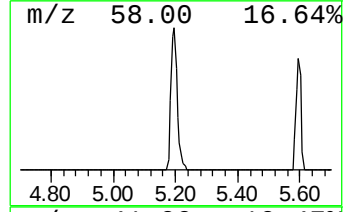
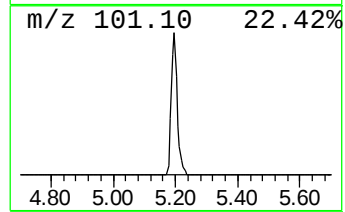
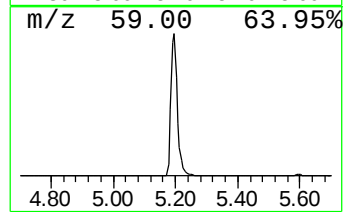
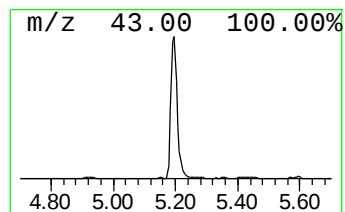
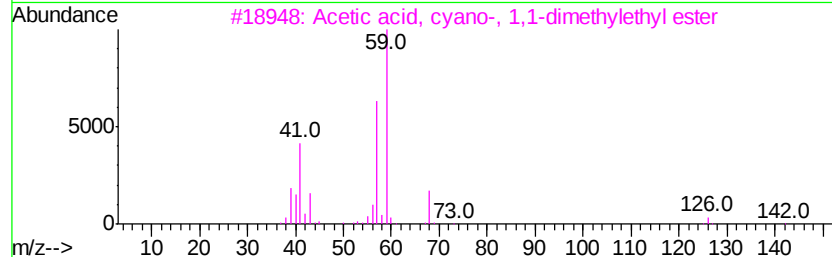
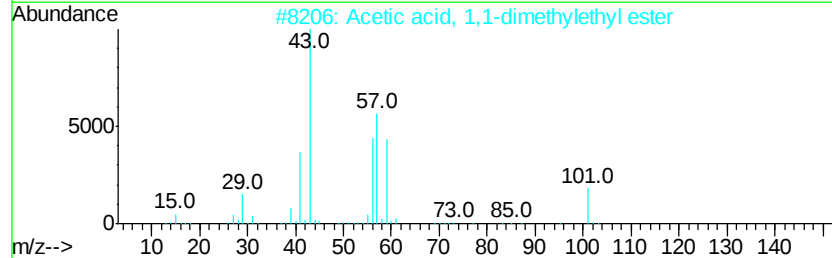
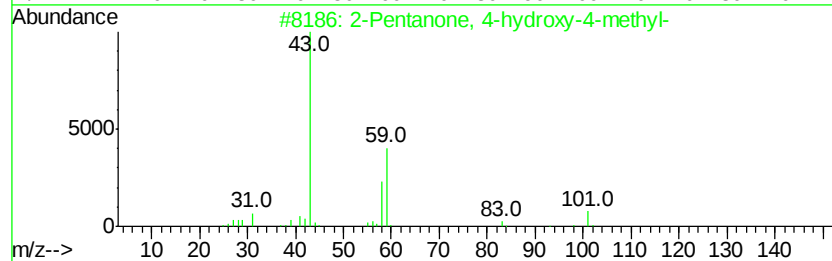
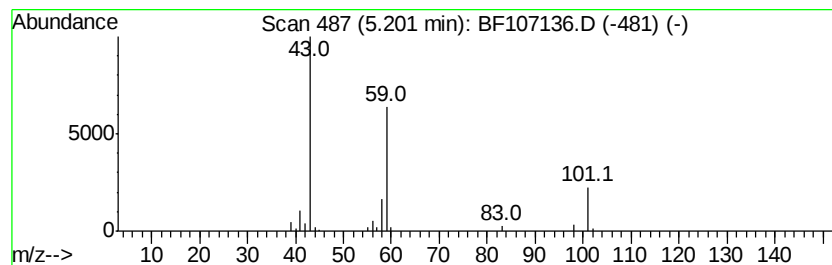
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	13.32 ng	226153	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
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	25
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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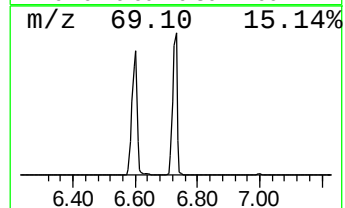
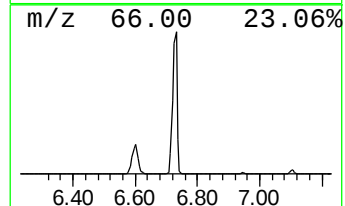
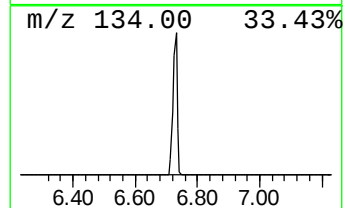
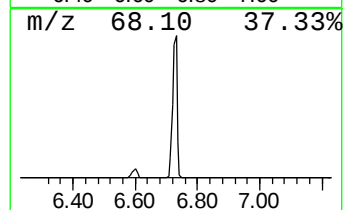
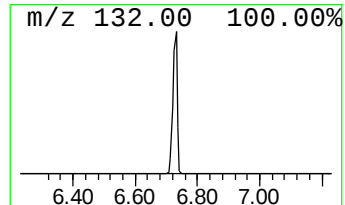
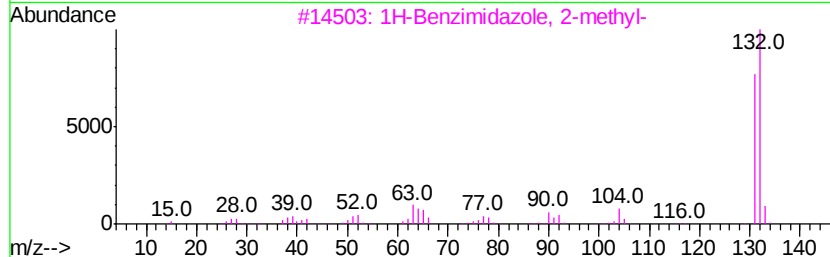
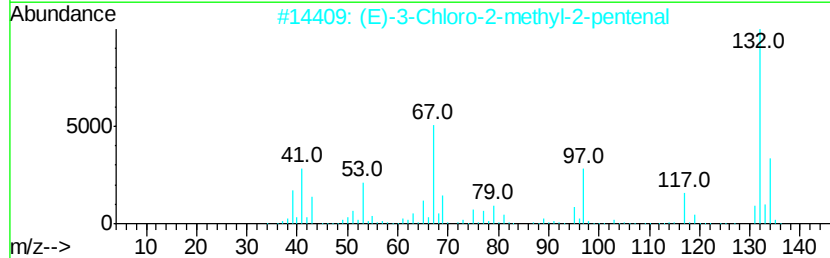
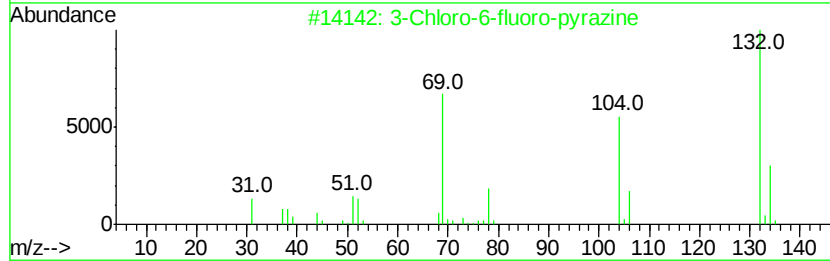
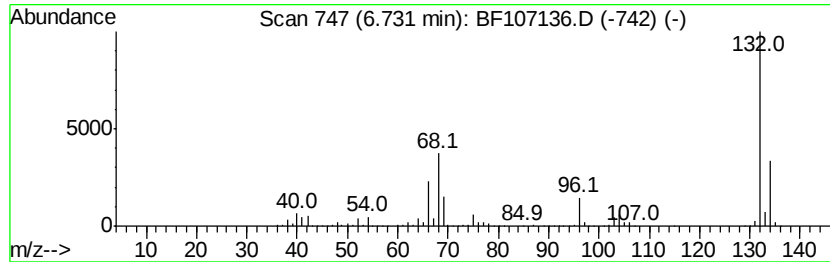
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	88.36 ng	1499910	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	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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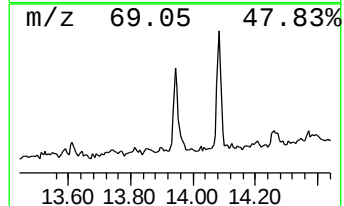
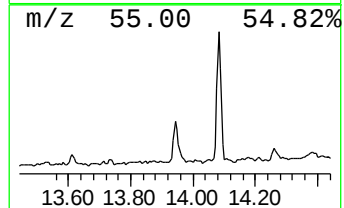
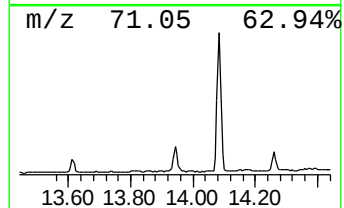
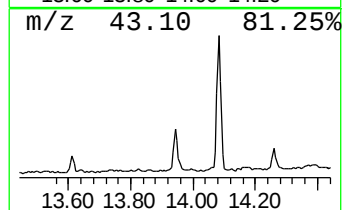
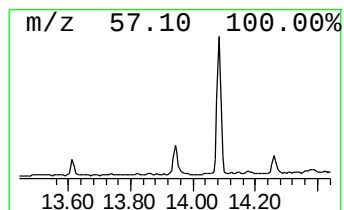
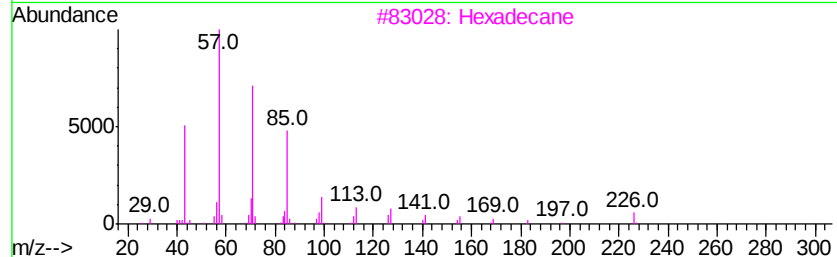
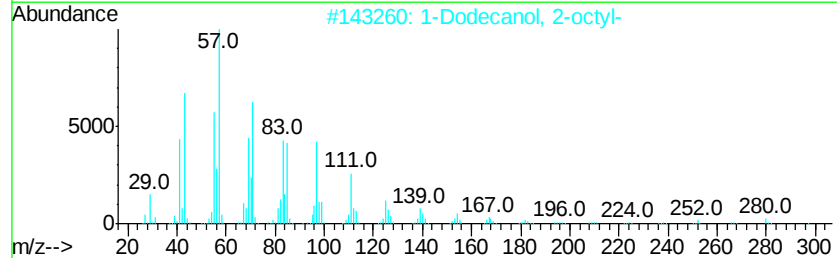
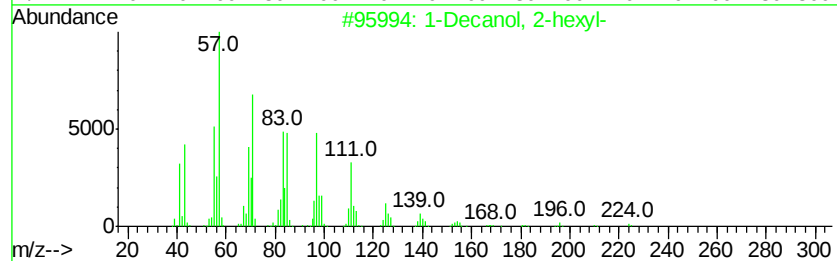
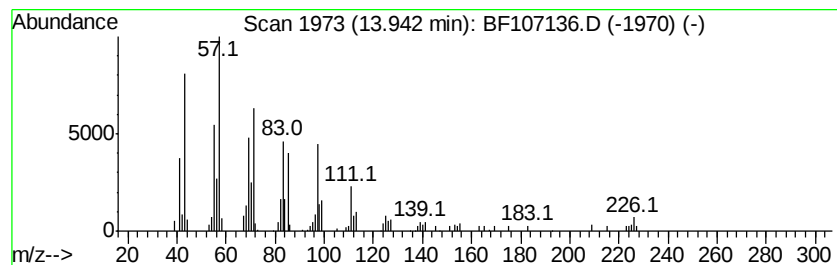
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Decanol, 2-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	5.01 ng	111504	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
2		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
3		Hexadecane	226	C16H34	000544-76-3	90
4		Cyclohexadecane	224	C16H32	000295-65-8	89
5		Cetene	224	C16H32	000629-73-2	86



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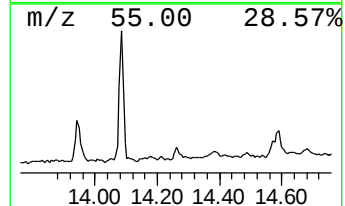
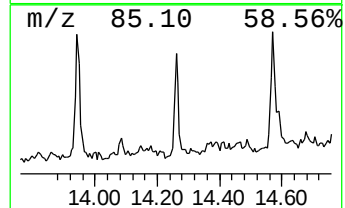
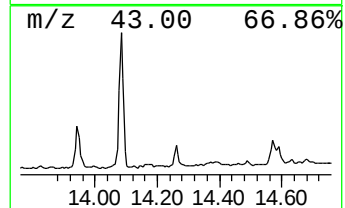
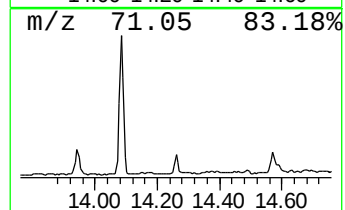
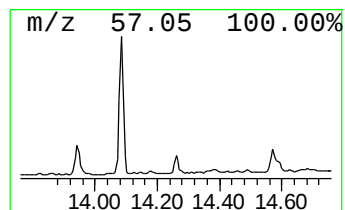
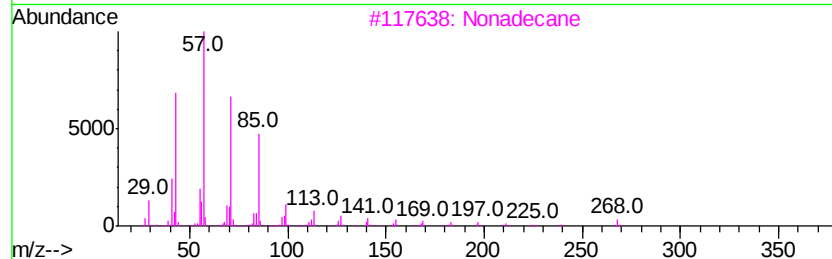
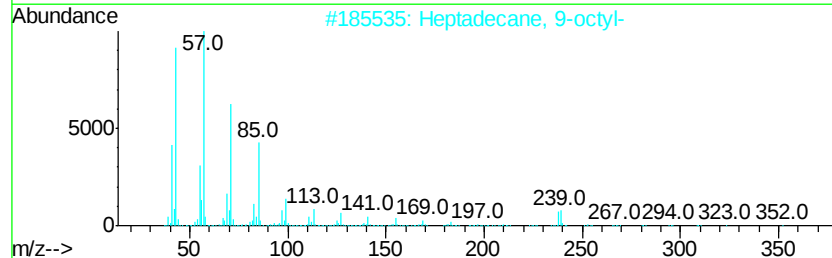
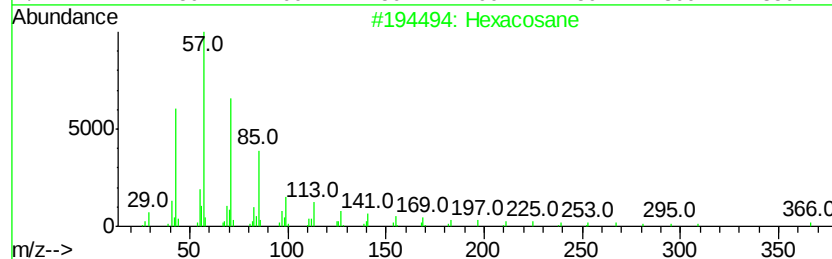
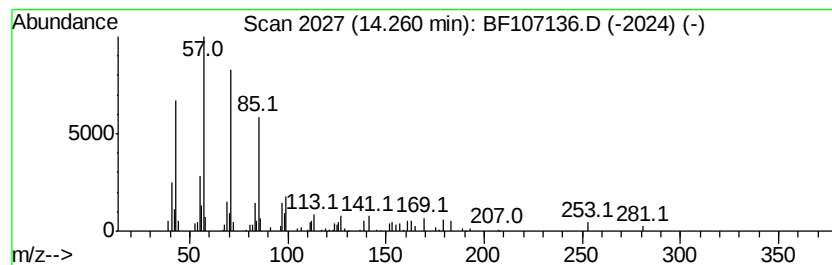
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	2.11 ng	47007	Chrysene-d12	14.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	80
3	Nonadecane		268	C19H40	000629-92-5	80
4	Heptadecane		240	C17H36	000629-78-7	80
5	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	72



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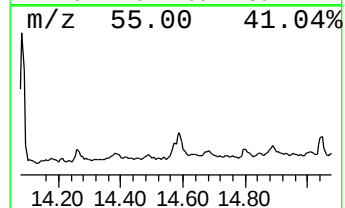
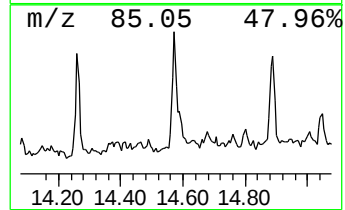
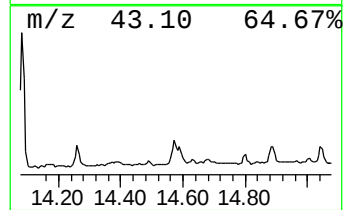
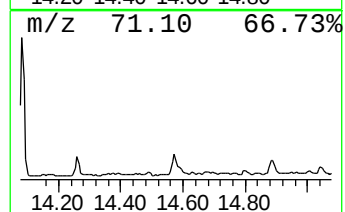
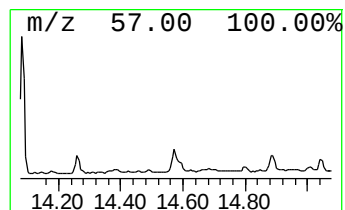
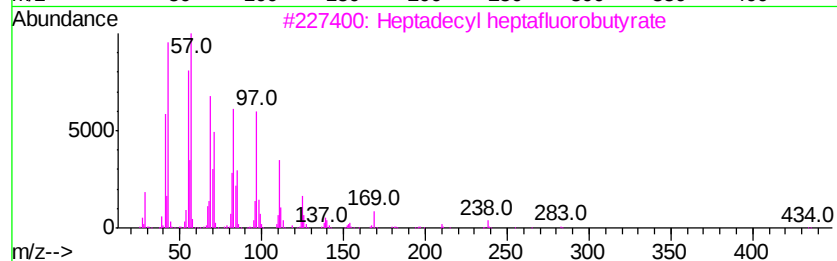
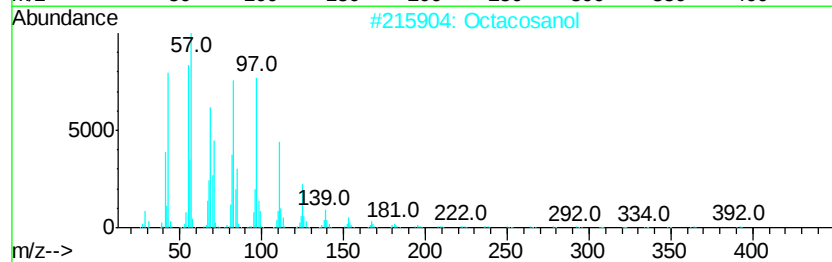
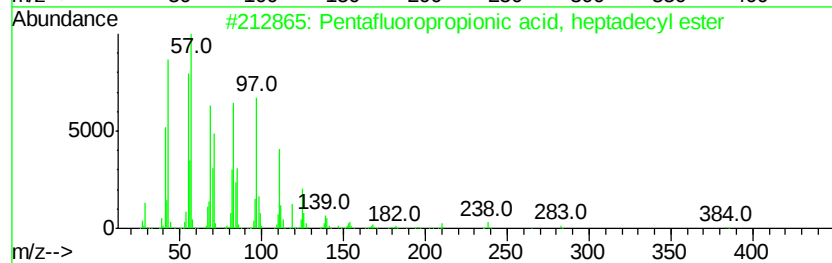
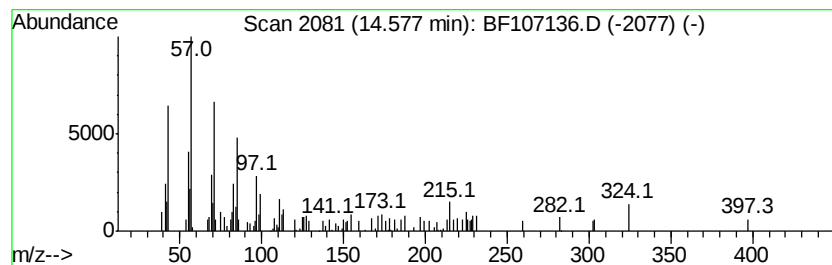
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Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	5.97 ng	133084	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	81
2		Octacosanol	410	C28H58O	000557-61-9	81
3		Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	81
4		1-Heptacosanol	396	C27H56O	002004-39-9	81
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	81



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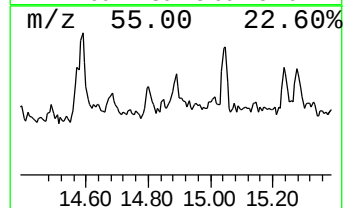
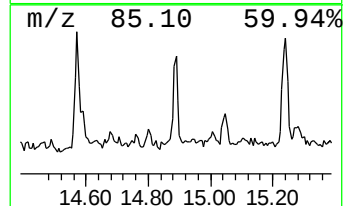
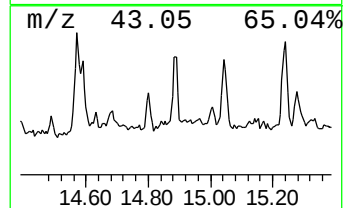
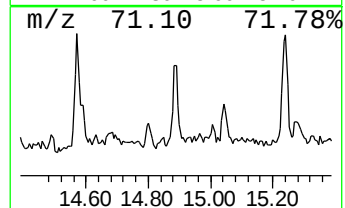
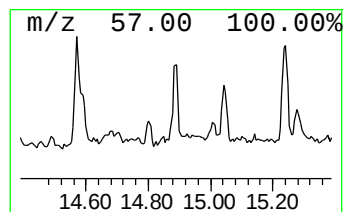
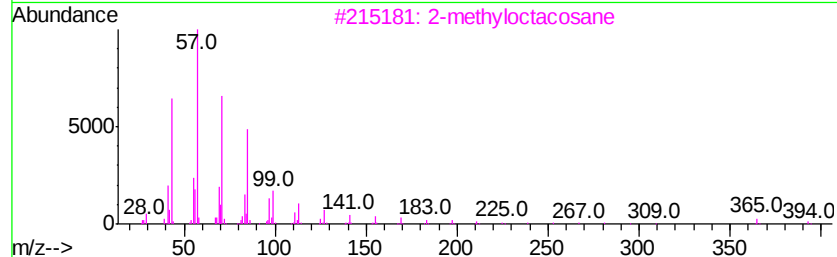
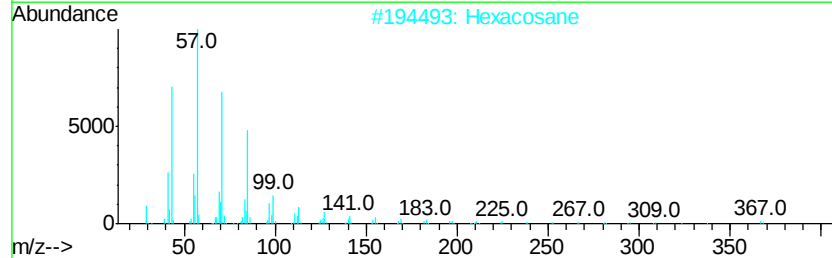
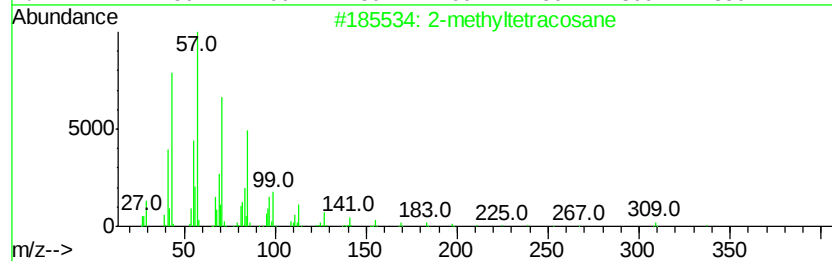
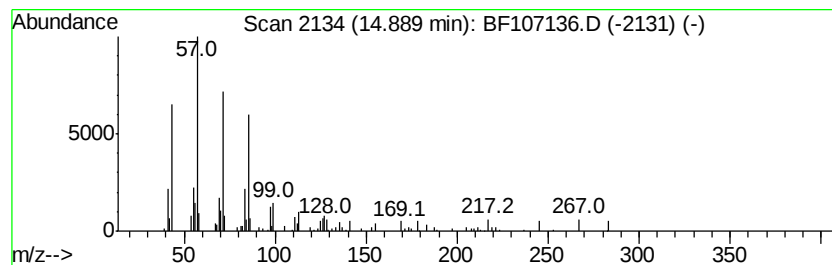
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-methyltetracosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	2.11 ng	47035	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyltetracosane	352	C25H52	1000376-72-6	86
2		Hexacosane	366	C26H54	000630-01-3	83
3		2-methyloctacosane	408	C29H60	1000376-72-8	83
4		Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	80
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070518\
Data File : BF107136.D
Acq On : 5 Jul 2018 19:31
Operator : JU/SJ
Sample : J3853-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

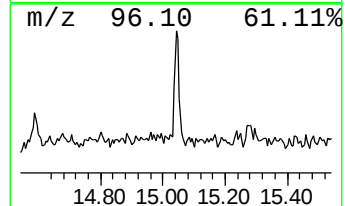
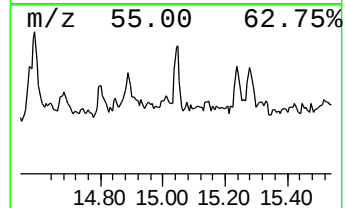
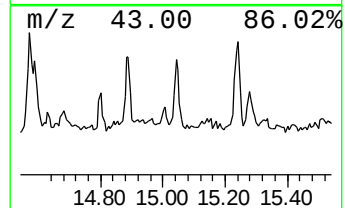
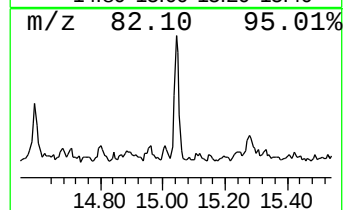
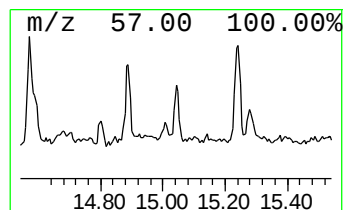
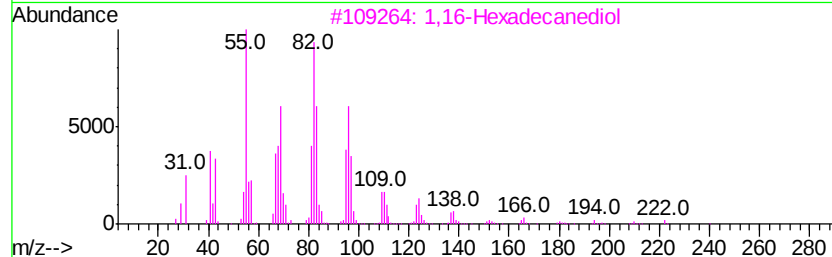
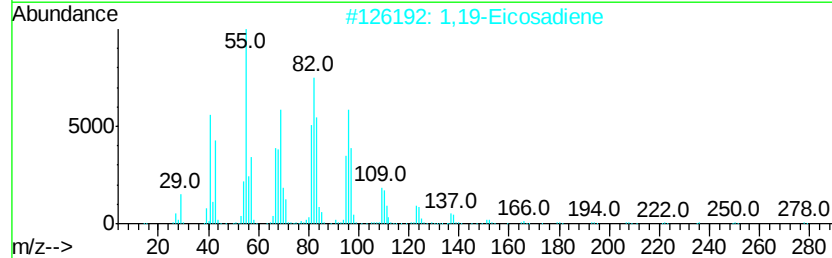
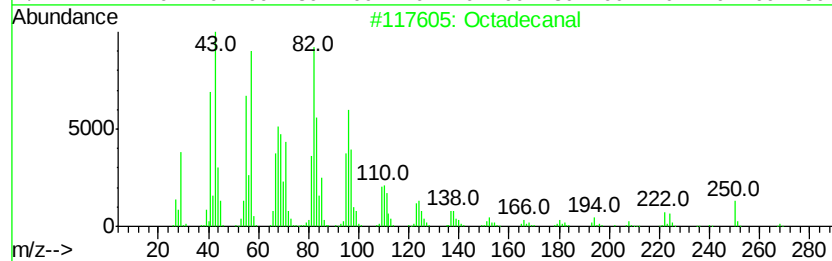
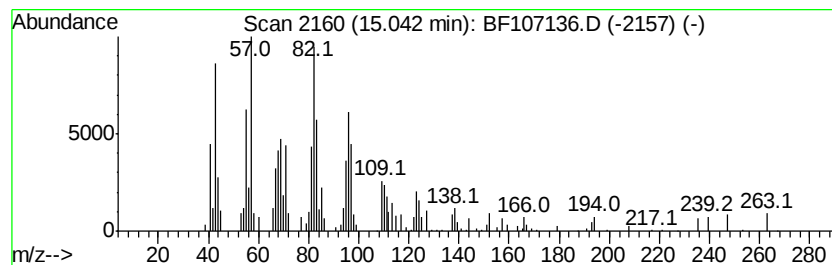
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.04	4.42 ng	67697	Perylene-d12	15.68	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	90
2	1,19-Eicosadiene	278	C20H38	014811-95-1	80
3	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	72
4	E-6-Octadecen-1-ol acetate	310	C20H38O2	1000130-94-7	72
5	1,13-Tridecanediol, diacetate	300	C17H32O4	042236-70-4	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070518\
Data File : BF107136.D
Acq On : 5 Jul 2018 19:31
Operator : JU/SJ
Sample : J3853-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

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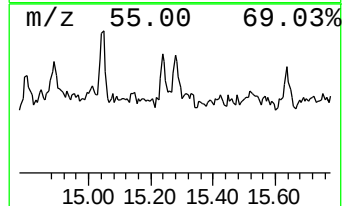
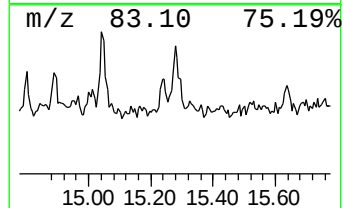
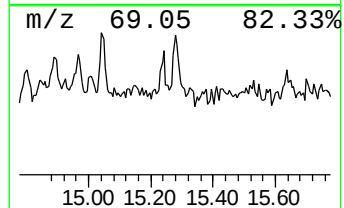
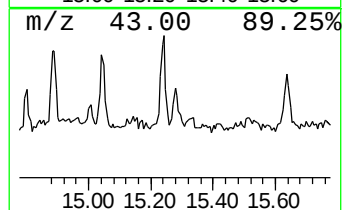
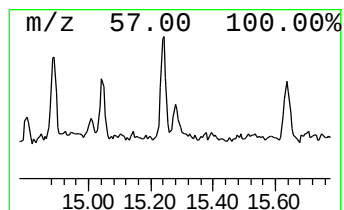
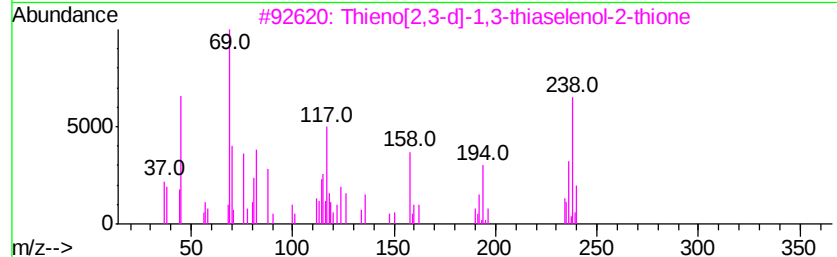
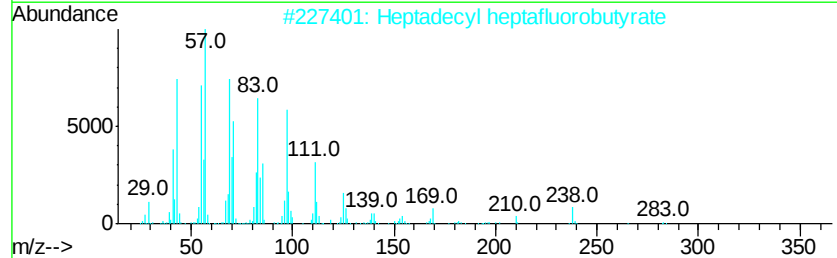
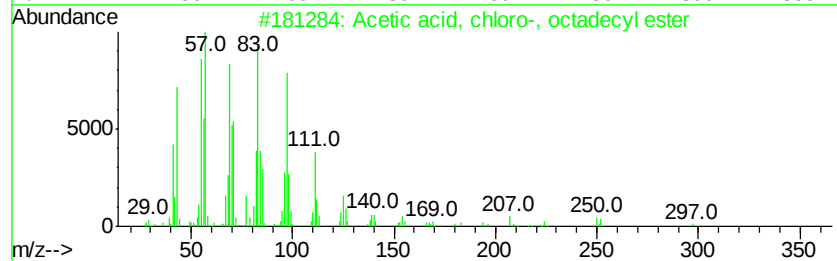
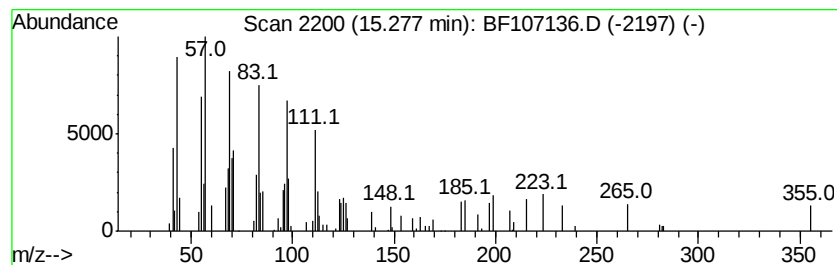
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Acetic acid, chloro-, octad... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	2.37 ng	36259	Perylene-d12	15.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	64
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	58
3			Thieno[2,3-d]-1,3-thiaselenol-2-...	238	C5H2S3Se	081803-09-0	56
4			Ethyl .alpha.-hydroxymyristate	272	C16H32O3	129086-73-3	52
5			Acetic acid n-octadecyl ester	312	C20H40O2	000822-23-1	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070518\
Data File : BF107136.D
Acq On : 5 Jul 2018 19:31
Operator : JU/SJ
Sample : J3853-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-11

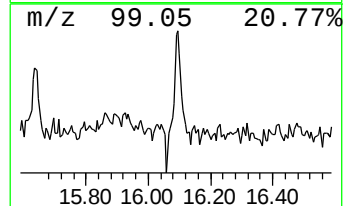
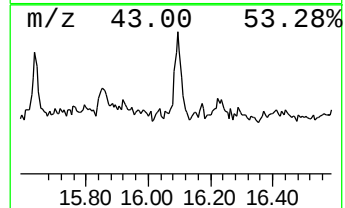
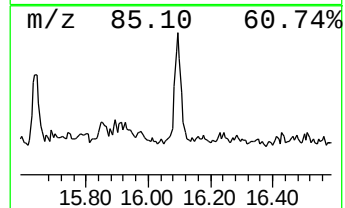
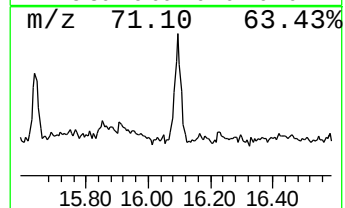
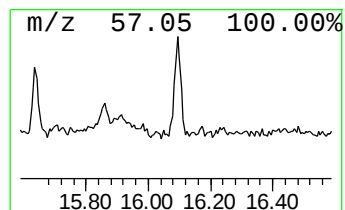
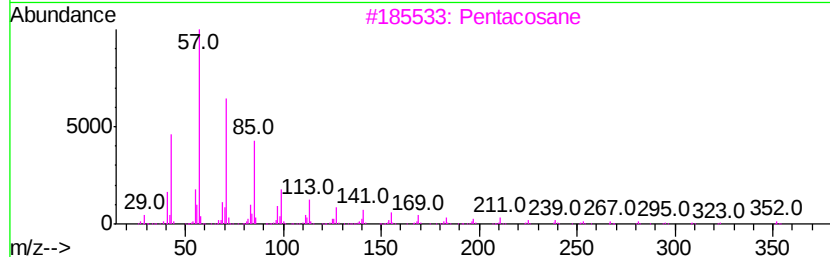
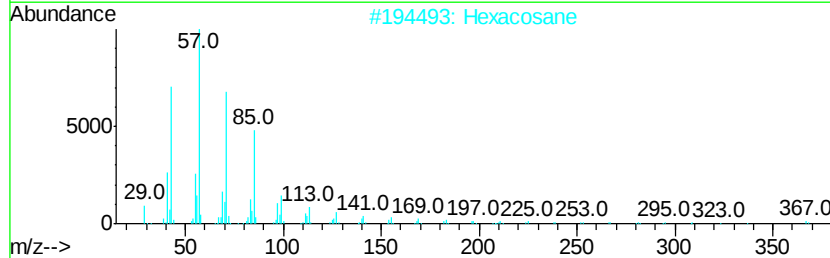
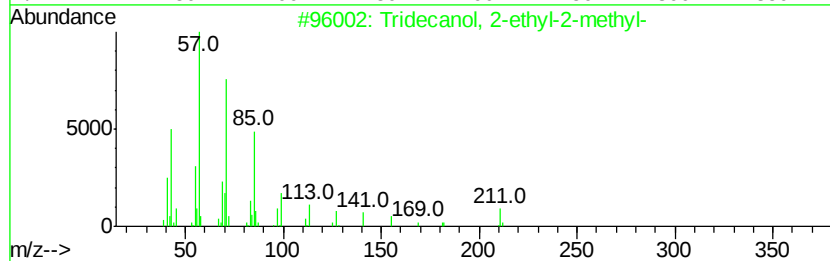
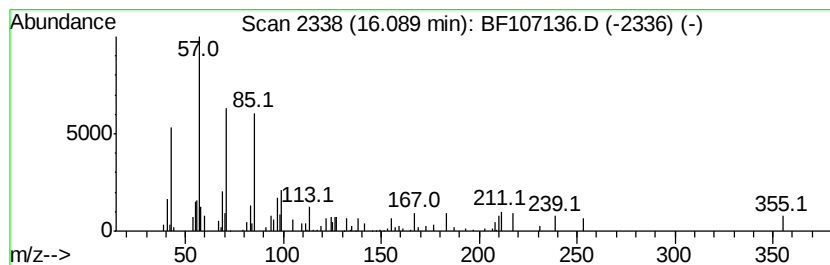
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tridecanol, 2-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	3.10 ng	47442	Perylene-d12	15.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	87
2			Hexacosane	366	C26H54	000630-01-3	86
3			Pentacosane	352	C25H52	000629-99-2	86
4			2-methyloctacosane	408	C29H60	1000376-72-8	86
5			Triacontane	422	C30H62	000638-68-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070518\
Data File : BF107136.D
Acq On : 5 Jul 2018 19:31
Operator : JU/SJ
Sample : J3853-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampled :
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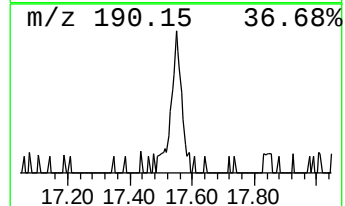
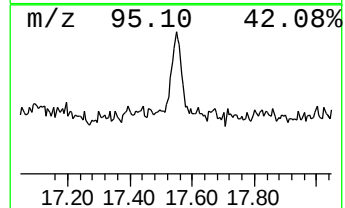
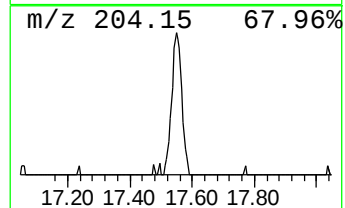
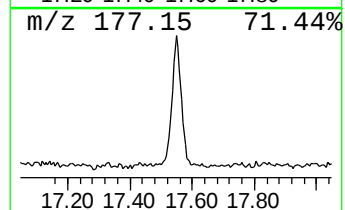
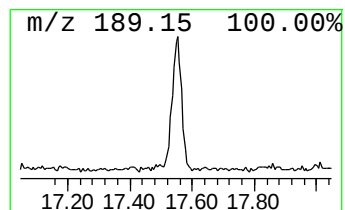
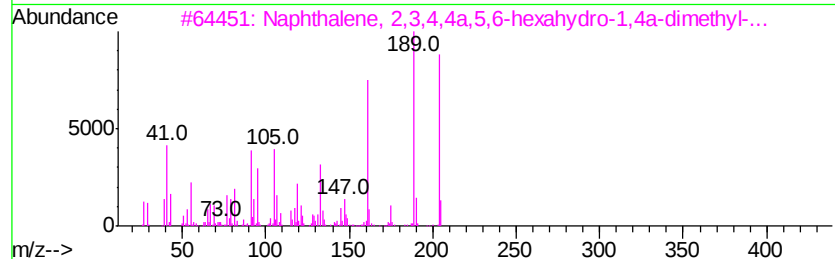
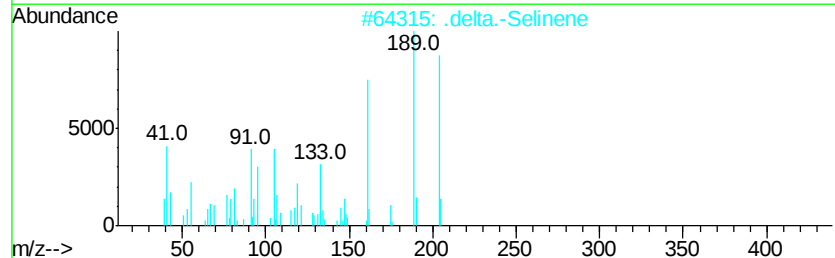
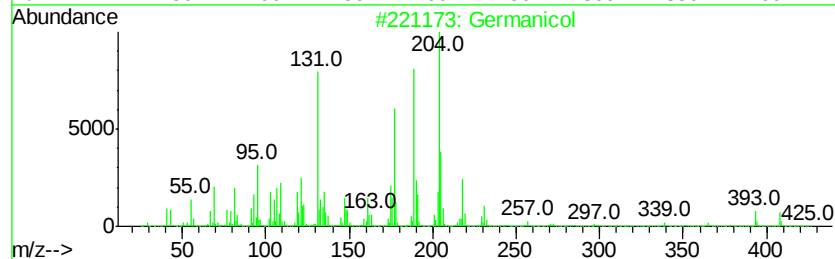
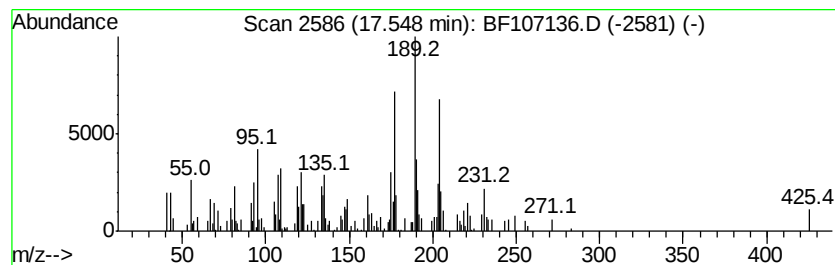
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Germanicol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.55	11.67 ng	178687	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Germanicol	426	C30H500	000465-02-1	53
2		.delta.-Selinene	204	C15H24	028624-23-9	45
3		Naphthalene, 2,3,4,4a,5,6-hexahv...	204	C15H24	000473-14-3	45
4		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	44
5		Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	005951-61-1	41



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF070518\
 Data File : BF107136.D
 Acq On : 5 Jul 2018 19:31
 Operator : JU/SJ
 Sample : J3853-12
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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...	5.20	13.3	ng	226153	1	6.95	339516	20.0
unknown6.73	6.73	88.4	ng	1499910	1	6.95	339516	20.0
1-Decanol, 2-hexyl-	13.94	5.0	ng	111504	5	14.14	445488	20.0
Hexacosane	14.26	2.1	ng	47007	5	14.14	445488	20.0
Pentafluoropropio...	14.58	6.0	ng	133084	5	14.14	445488	20.0
2-methyltetracosane	14.89	2.1	ng	47035	5	14.14	445488	20.0
Octadecanal	15.04	4.4	ng	67697	6	15.68	306335	20.0
Acetic acid, chlo...	15.28	2.4	ng	36259	6	15.68	306335	20.0
Tridecanol, 2-eth...	16.09	3.1	ng	47442	6	15.68	306335	20.0
Germanicol	17.55	11.7	ng	178687	6	15.68	306335	20.0