

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091719\
 Data File : BF117104.D
 Acq On : 17 Sep 2019 14:11
 Operator : HP/JU
 Sample : K4883-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW5-R2-1

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-BF091319.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	4.546	413	418	428	rBV	186393	217675	10.73%	1.556%
2	5.446	567	571	583	rBV	616156	673320	33.20%	4.812%
3	6.457	739	743	762	rBV	445598	502520	24.78%	3.592%
4	6.592	762	766	781	rVV	1433626	1395216	68.80%	9.972%
5	6.822	802	805	814	rBV	391337	338463	16.69%	2.419%
6	6.981	828	832	846	rBV	1521358	1301974	64.20%	9.306%
7	7.387	896	901	917	rBV	929199	1023037	50.45%	7.312%
8	8.104	1019	1023	1042	rBV	325919	418754	20.65%	2.993%
9	9.175	1201	1205	1221	rBV	2191906	2028013	100.00%	14.495%
10	9.851	1316	1320	1333	rBV	462110	511508	25.22%	3.656%
11	9.945	1333	1336	1344	rVB	150207	162908	8.03%	1.164%
12	10.639	1450	1454	1470	rBV	1167395	1234008	60.85%	8.820%
13	11.333	1568	1572	1583	rBV	430807	493735	24.35%	3.529%
14	11.827	1653	1656	1658	rBV2	31488	37076	1.83%	0.265%
15	11.857	1658	1661	1667	rVB	53460	60625	2.99%	0.433%
16	12.569	1778	1782	1788	rVB9	18566	23520	1.16%	0.168%
17	12.863	1829	1832	1836	rBV	159932	151834	7.49%	1.085%
18	12.916	1836	1841	1844	rBV	1936909	1779624	87.75%	12.720%
19	13.139	1874	1879	1882	rBV6	14717	21235	1.05%	0.152%
20	13.810	1990	1993	2004	rVB5	41554	93515	4.61%	0.668%
21	13.968	2016	2020	2029	rVB	338285	373304	18.41%	2.668%
22	14.057	2031	2035	2039	rVV	49522	58620	2.89%	0.419%
23	14.121	2043	2046	2050	rVB3	25365	28525	1.41%	0.204%
24	14.427	2095	2098	2101	rBV	42738	38221	1.88%	0.273%
25	14.727	2145	2149	2155	rVB	64845	61803	3.05%	0.442%
26	14.804	2158	2162	2164	rVB2	33877	34718	1.71%	0.248%
27	15.051	2200	2204	2209	rBV	68005	84580	4.17%	0.605%
28	15.415	2261	2266	2278	rBV2	262803	419107	20.67%	2.995%
29	15.845	2334	2339	2344	rBV2	69883	101732	5.02%	0.727%
30	16.004	2363	2366	2372	rVB2	12599	21708	1.07%	0.155%
31	16.327	2414	2421	2427	rBV2	44671	85649	4.22%	0.612%
32	16.904	2513	2519	2524	rBV3	18882	36426	1.80%	0.260%
33	17.051	2537	2544	2553	rVB3	40900	88936	4.39%	0.636%
34	17.574	2625	2633	2639	rVB10	9523	21687	1.07%	0.155%

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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 >
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.474	2779	2786	2795	rVB5	25011	67715	3.34%	0.484%
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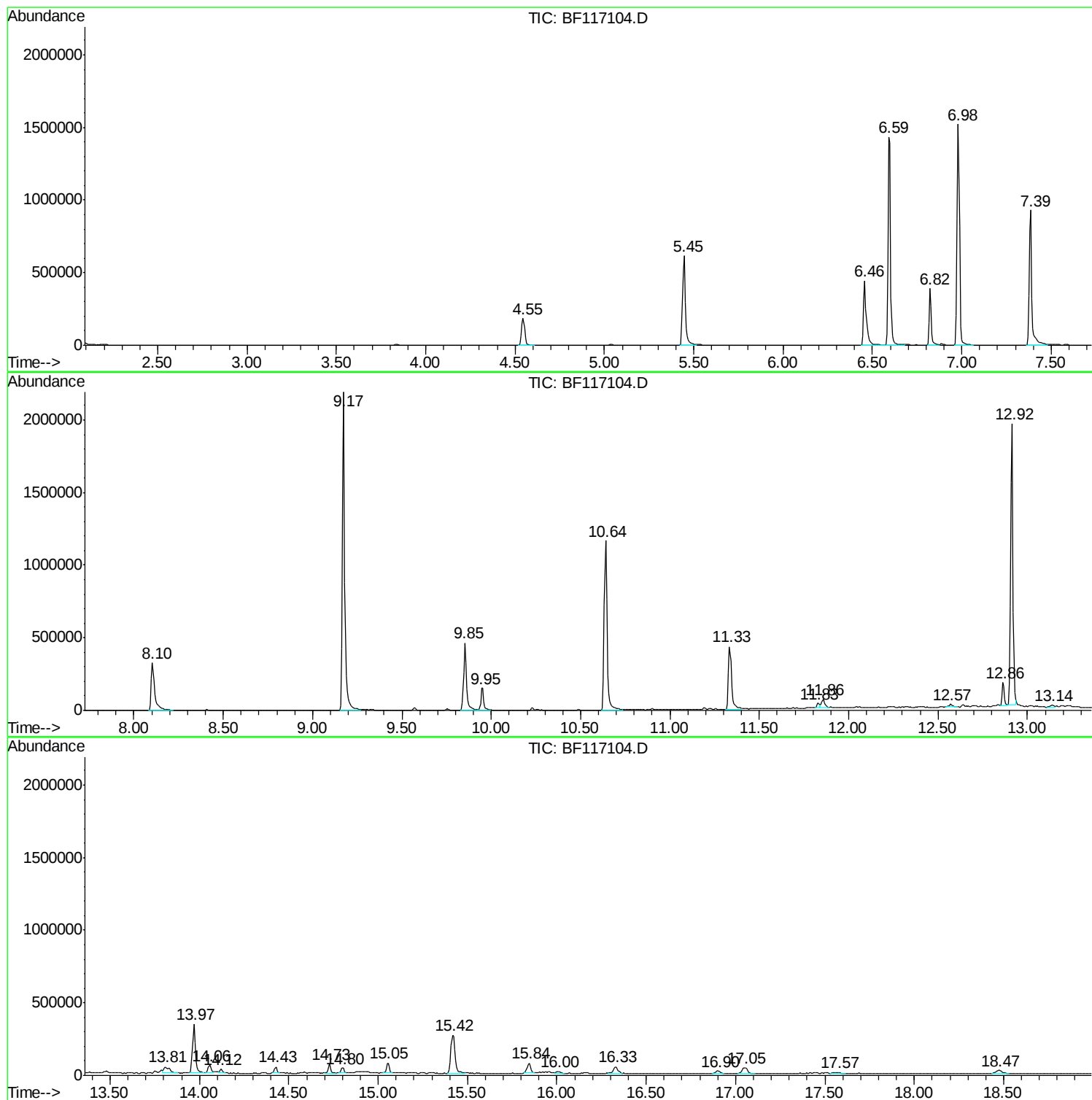
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091319.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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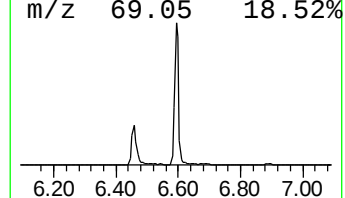
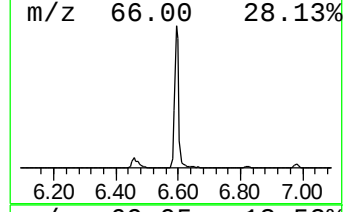
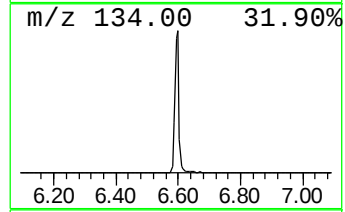
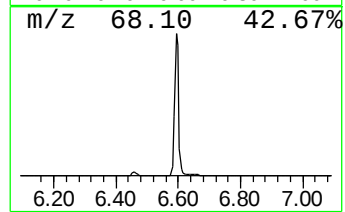
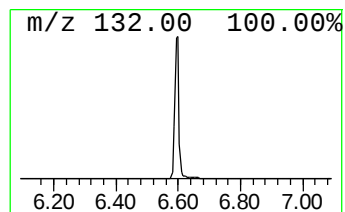
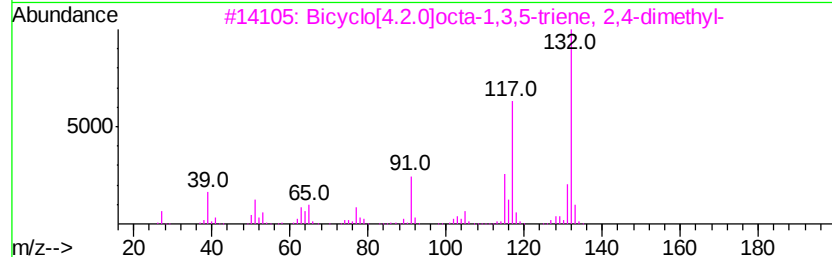
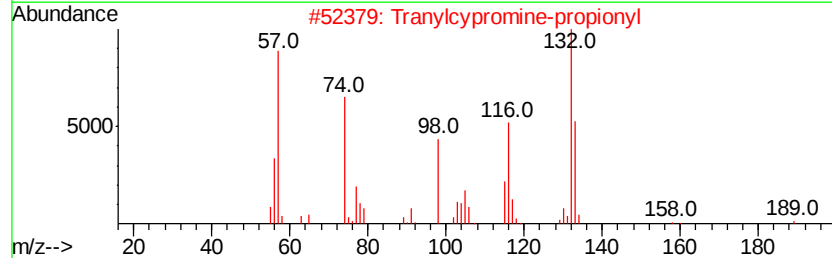
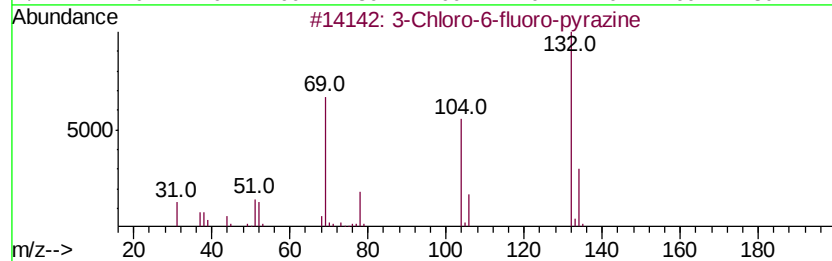
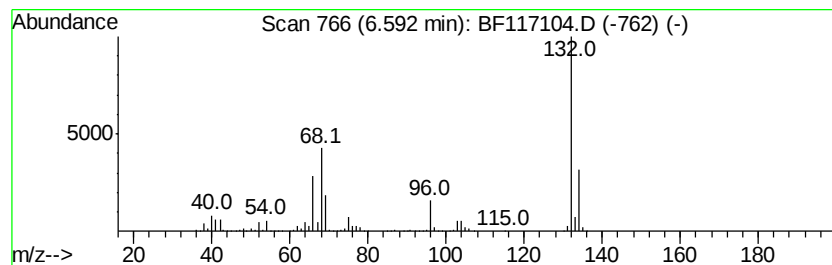
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	82.44 ng	1395220	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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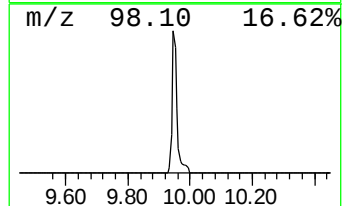
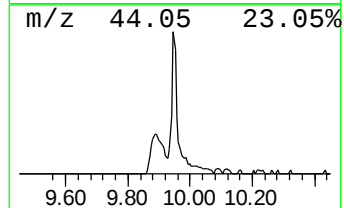
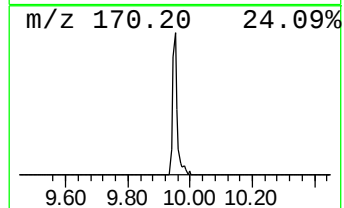
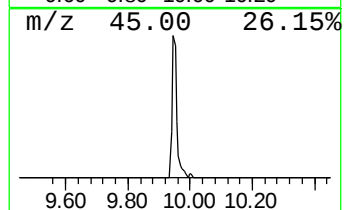
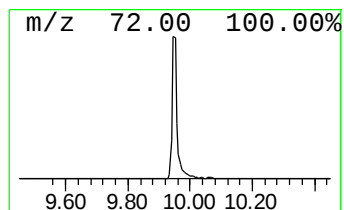
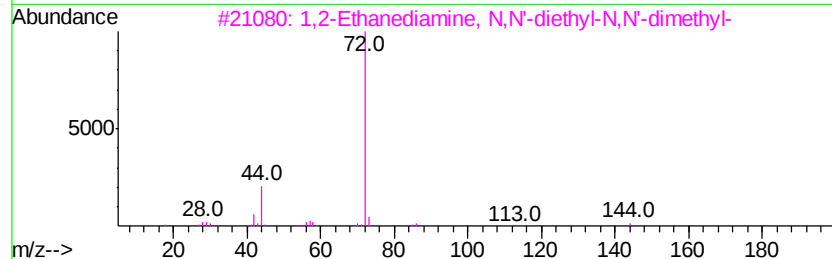
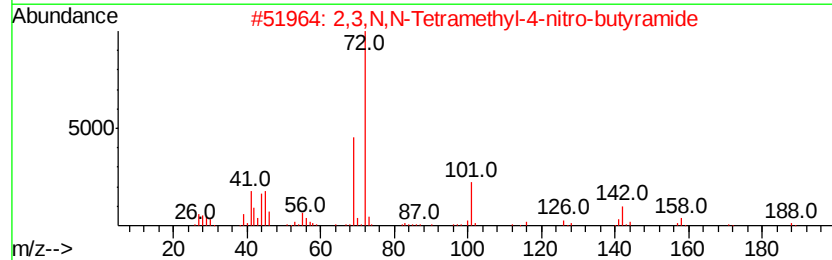
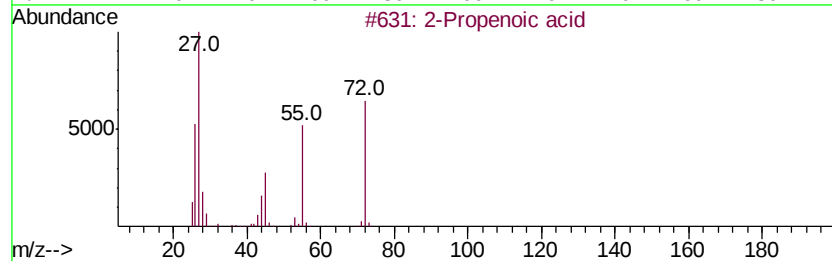
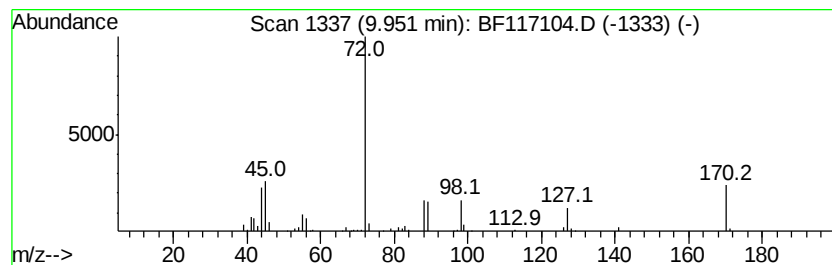
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown9.95 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.95	6.37 ng	162908	Acenaphthene-d10	9.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propenoic acid	72	C3H4O2	000079-10-7	43
2		2,3,N,N-Tetramethyl-4-nitro-buty...	188	C8H16N2O3	1000187-66-9	43
3		1,2-Ethanediamine, N,N'-diethyl-...	144	C8H20N2	000106-66-1	37
4		1-Dimethylcarbamidovl-3,3-dimeth...	143	C6H13N3O	054897-21-1	33
5		DL-Norvaline	117	C5H11NO2	000760-78-1	32



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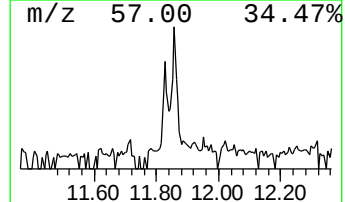
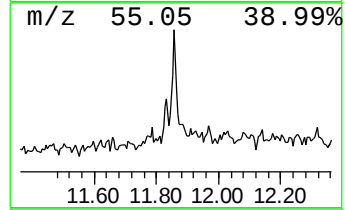
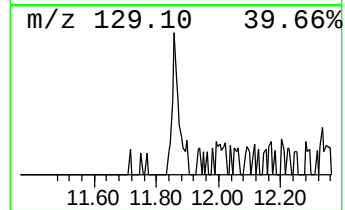
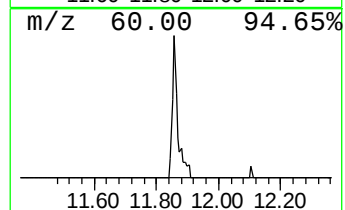
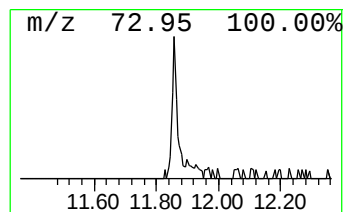
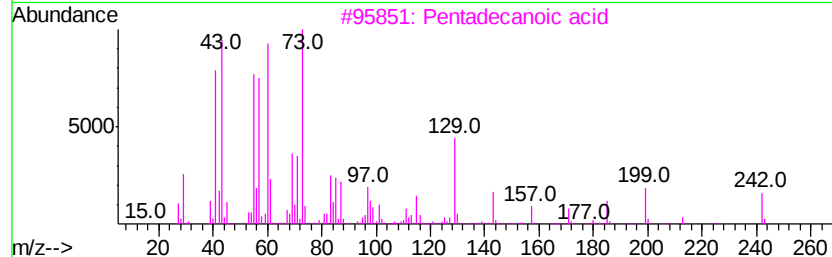
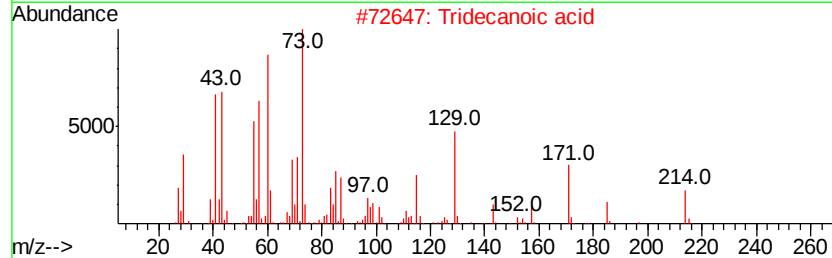
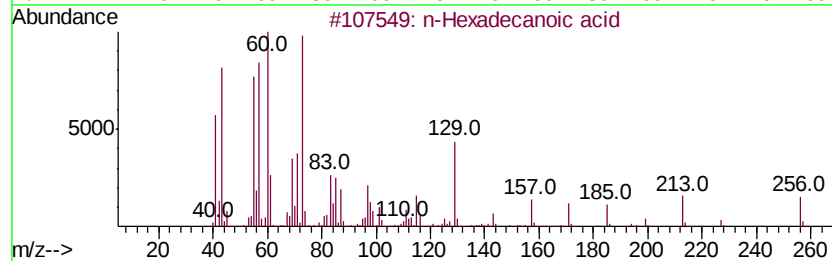
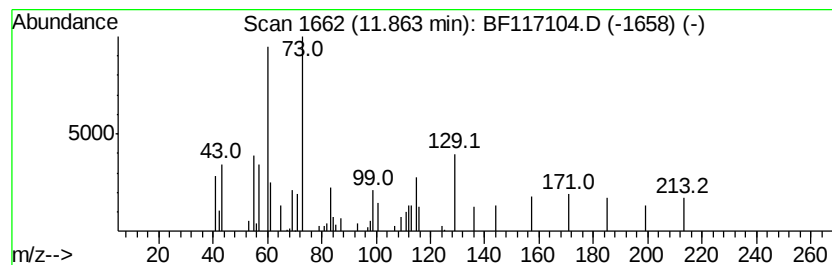
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.46 ng	60625	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
2		Tridecanoic acid	214	C13H26O2	000638-53-9	64
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4		Dodecanoic acid	200	C12H24O2	000143-07-7	53
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	52



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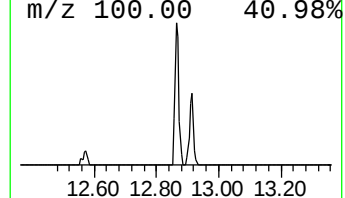
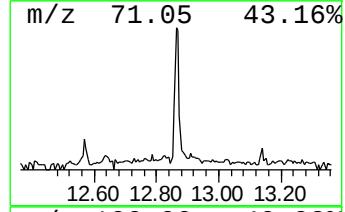
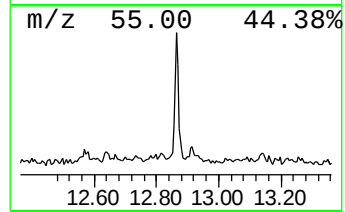
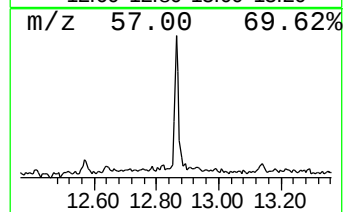
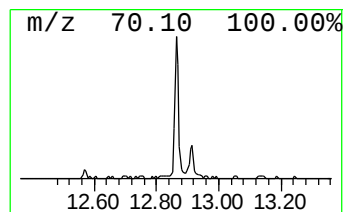
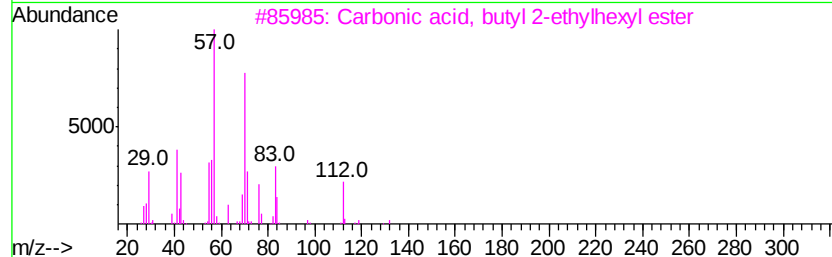
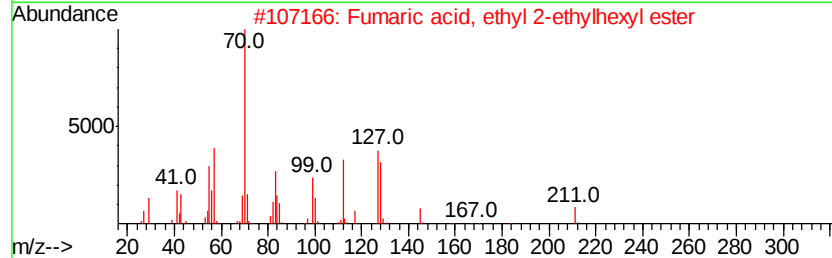
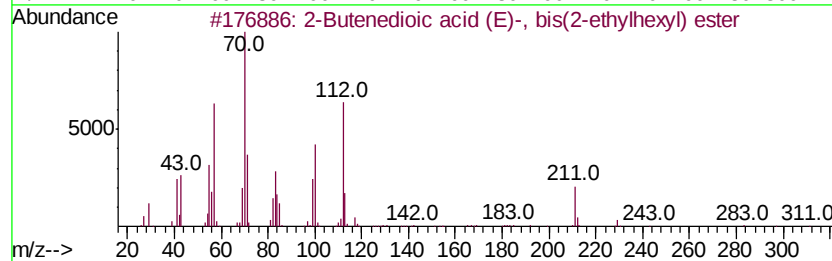
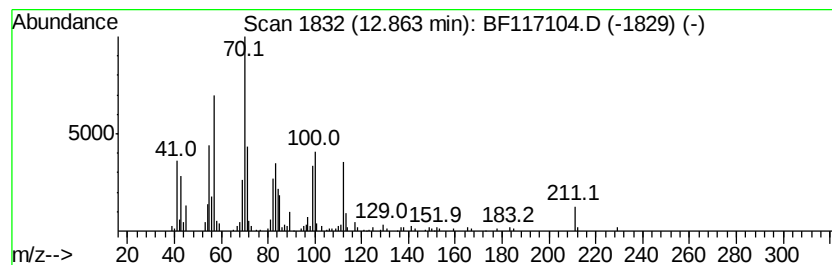
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Butenedioic acid (E)-, bi... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.86	8.13 ng	151834	Chrysene-d12	13.97		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenedioic acid (E)-, bis(2-e...	340	C20H36O4	000141-02-6	72	
2	Fumaric acid, ethyl 2-ethylhexyl...	256	C14H24O4	1000339-13-5	53	
3	Carbonic acid, butyl 2-ethylhexv...	230	C13H26O3	1000357-84-4	43	
4	2-Methylpyrrolidine	85	C5H11N	000765-38-8	38	
5	Cyclopentane, 1,2,4-trimethyl-	112	C8H16	002815-58-9	38	



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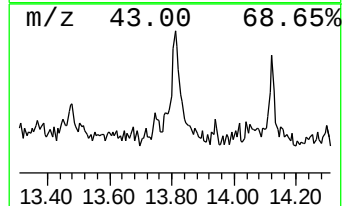
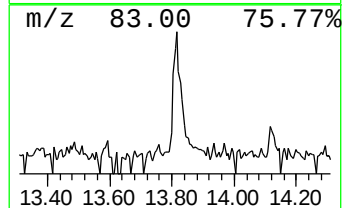
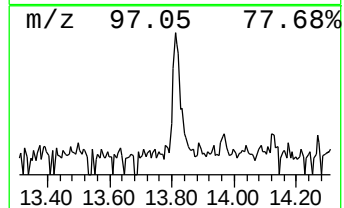
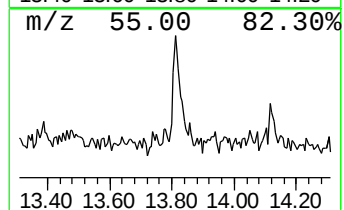
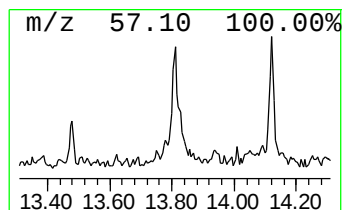
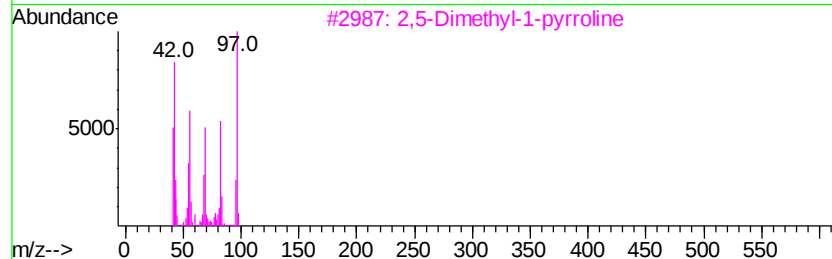
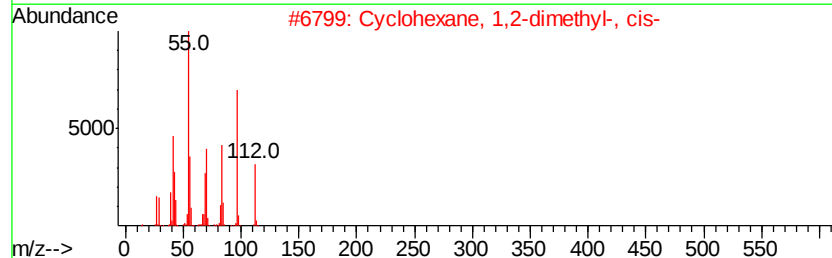
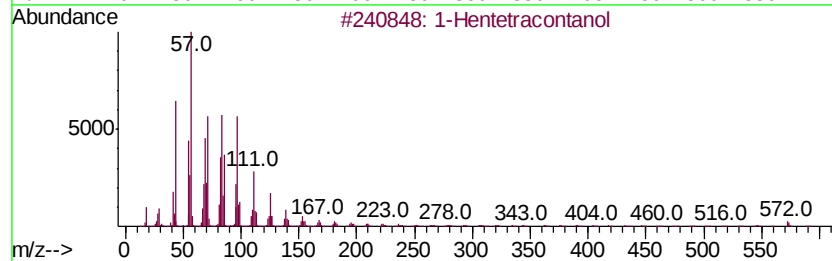
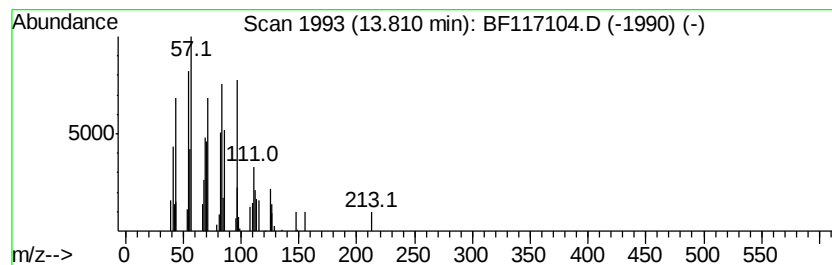
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Hentetracontanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	5.01 ng	93515	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hentetracontanol	593	C41H84O	040710-42-7	86
2	Cyclohexane, 1,2-dimethyl-, cis-	112	C8H16	002207-01-4	53
3	2,5-Dimethyl-1-pyrroline	97	C6H11N	000822-64-0	47
4	Cyclohexane, ethyl-	112	C8H16	001678-91-7	38
5	Cyclohexanone, 2,3-dimethyl-	126	C8H14O	013395-76-1	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091719\
Data File : BF117104.D
Acq On : 17 Sep 2019 14:11
Operator : HP/JU
Sample : K4883-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

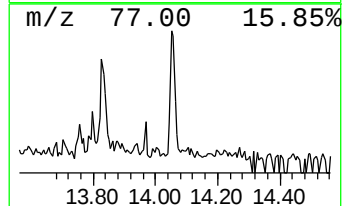
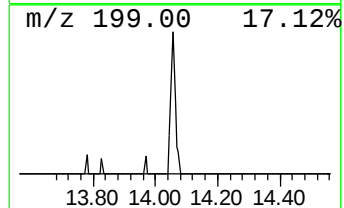
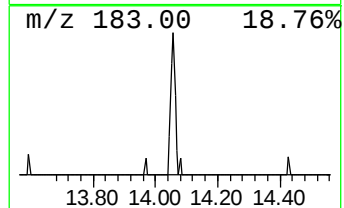
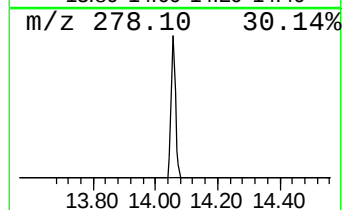
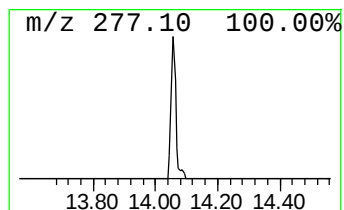
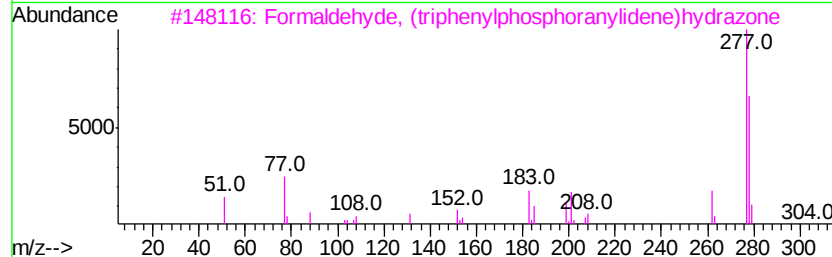
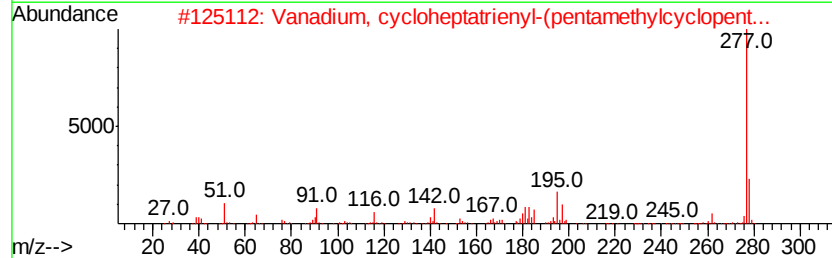
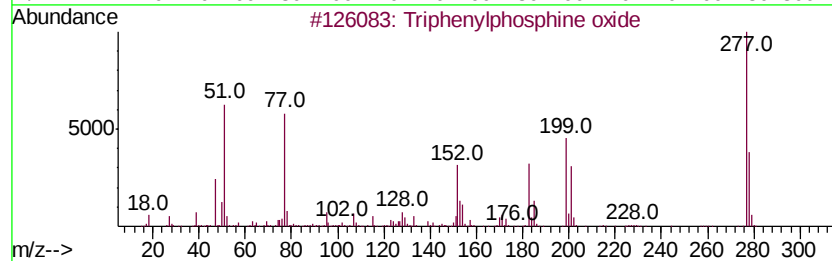
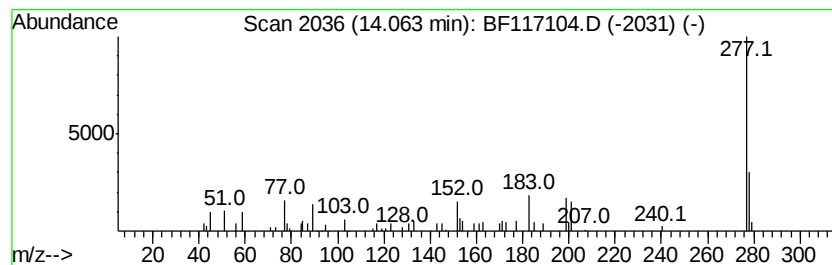
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.06	3.14 ng	58620	Chrysene-d12	13.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	81
2	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	49
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4	2-Propenoic acid, 2-cyano-3-(3-p...	277	C18H15NO2	1000080-00-3	37
5	Cobalt, (.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091719\
Data File : BF117104.D
Acq On : 17 Sep 2019 14:11
Operator : HP/JU
Sample : K4883-01
Misc :
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Instrument :
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ClientSampleId :
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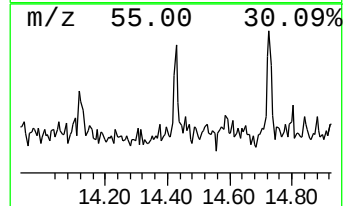
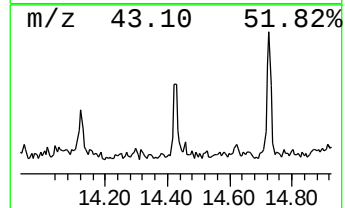
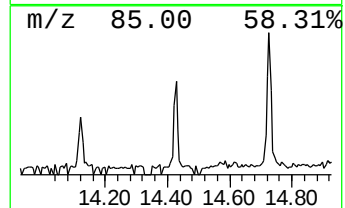
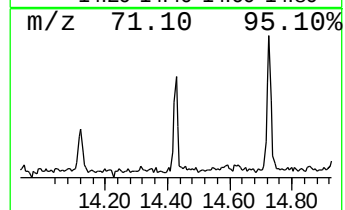
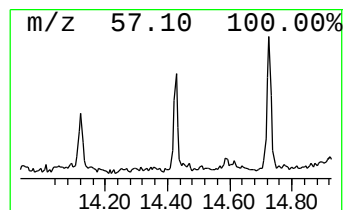
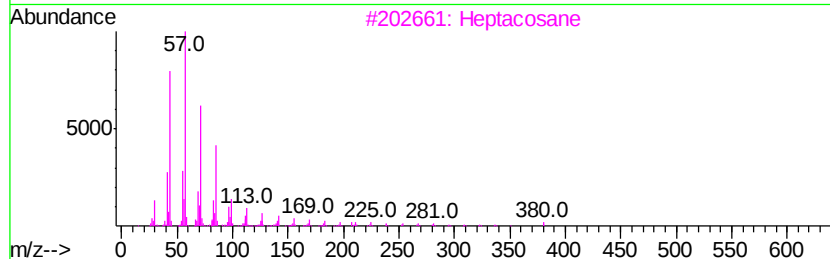
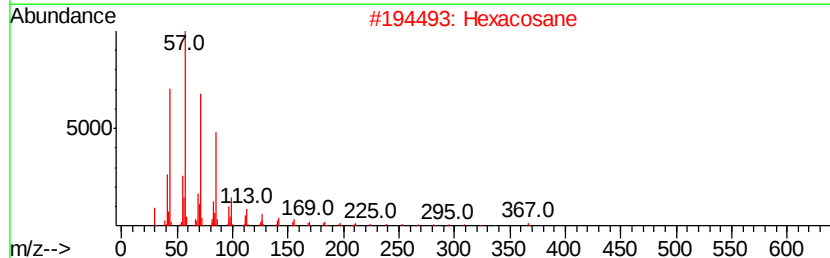
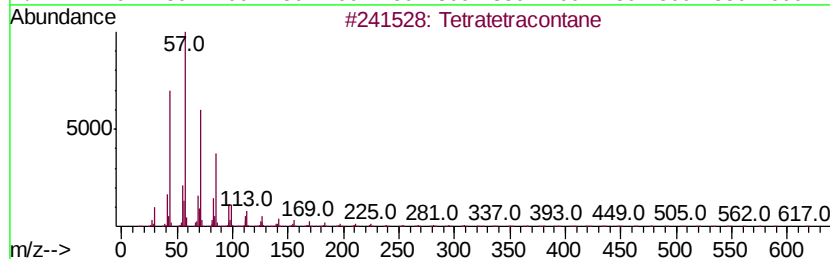
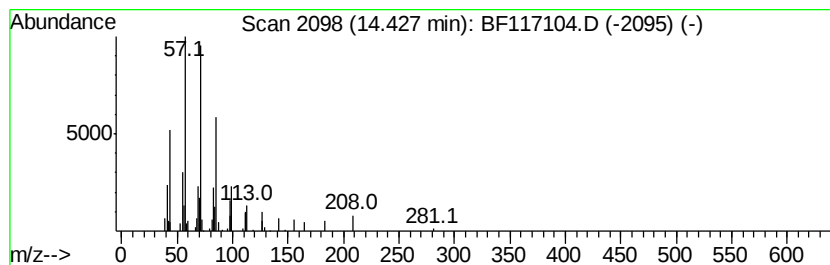
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetratetracontane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	2.05 ng	38221	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Octacosane	394	C28H58	000630-02-4	90
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091719\
Data File : BF117104.D
Acq On : 17 Sep 2019 14:11
Operator : HP/JU
Sample : K4883-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW5-R2-1

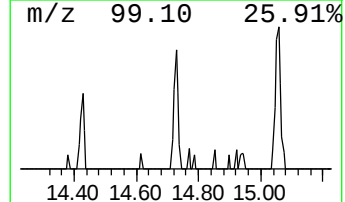
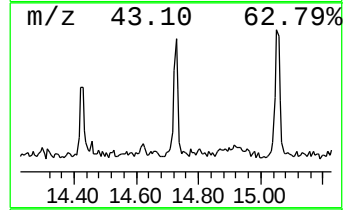
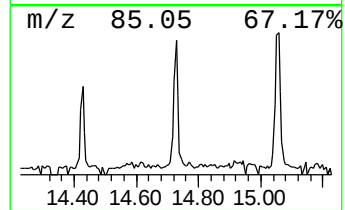
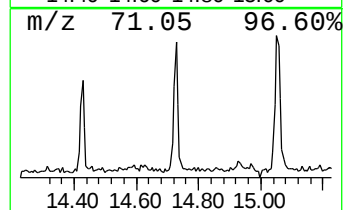
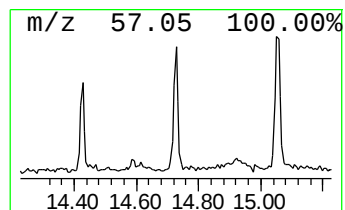
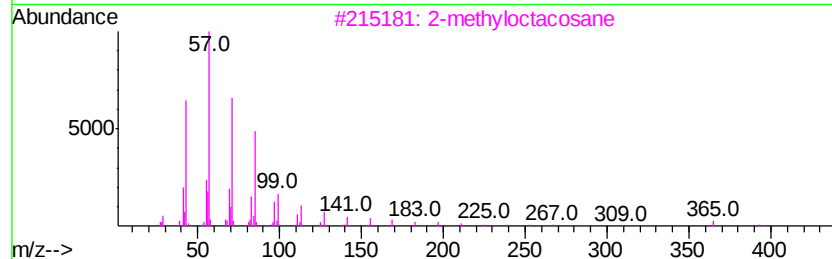
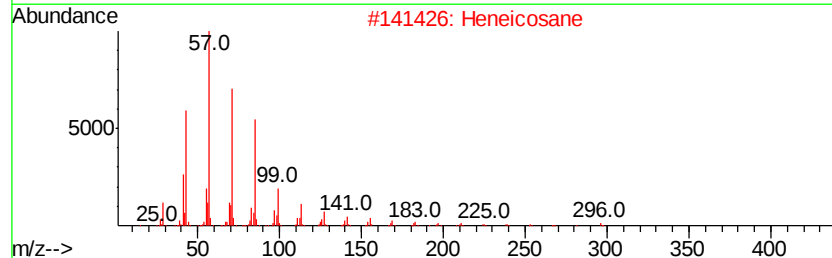
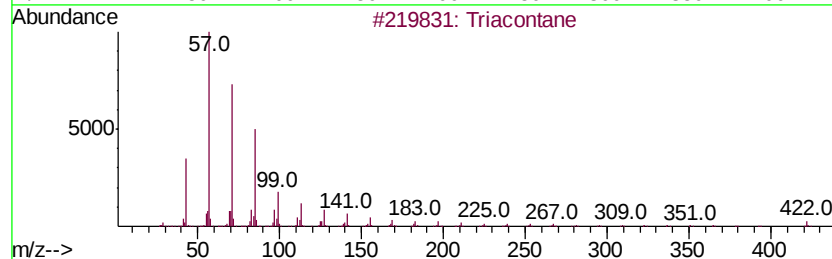
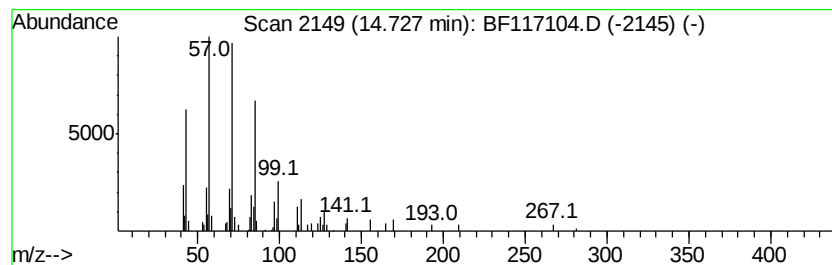
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Triacontane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	2.95 ng	61803	Perylene-d12	15.42

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	90
2			Heneicosane	296	C21H44	000629-94-7	90
3			2-methyloctacosane	408	C29H60	1000376-72-8	86
4			Octadecane	254	C18H38	000593-45-3	86
5			5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091719\
Data File : BF117104.D
Acq On : 17 Sep 2019 14:11
Operator : HP/JU
Sample : K4883-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

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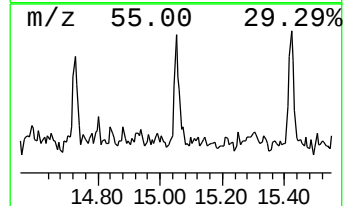
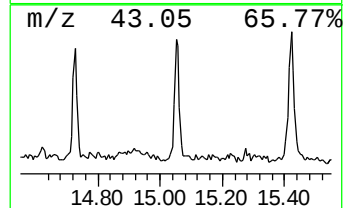
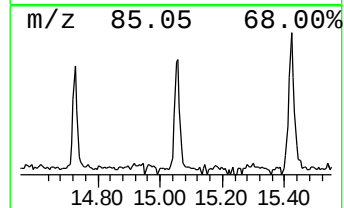
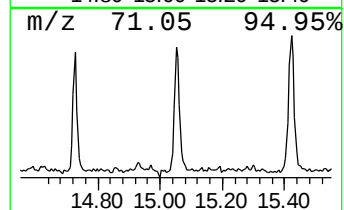
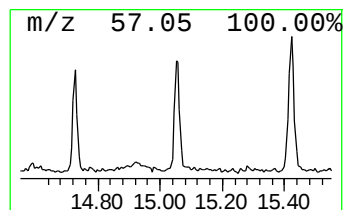
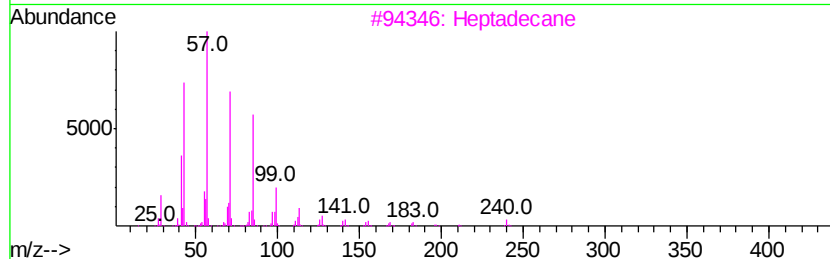
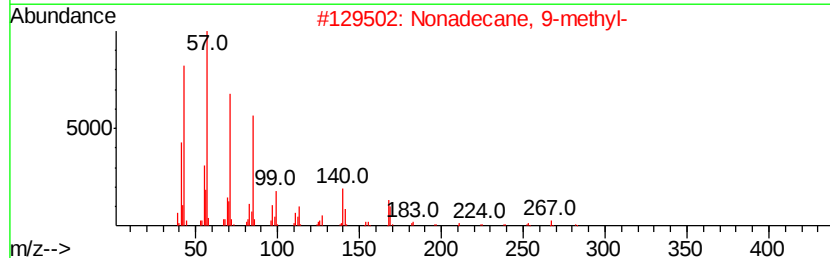
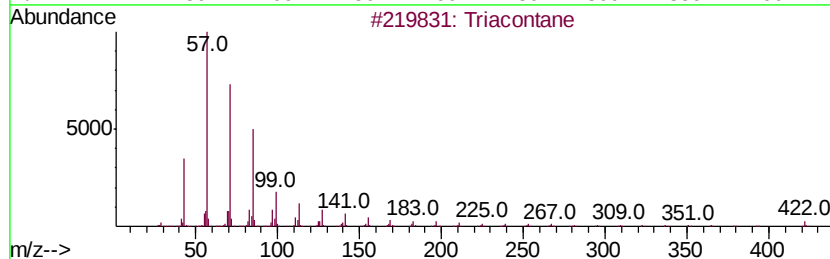
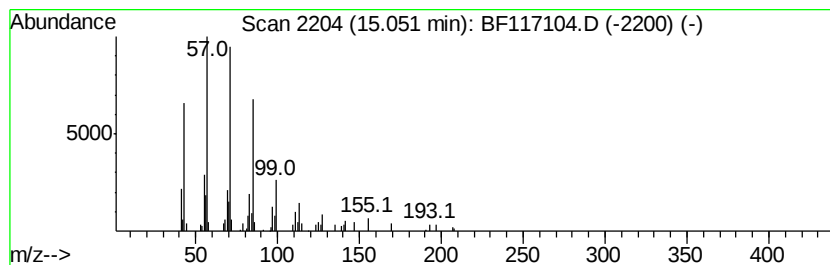
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonadecane, 9-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.05	4.04 ng	84580	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	91
2		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	91
3		Heptadecane	240	C17H36	000629-78-7	87
4		Hexacosane	366	C26H54	000630-01-3	87
5		Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091719\
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Acq On : 17 Sep 2019 14:11
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Sample : K4883-01
Misc :
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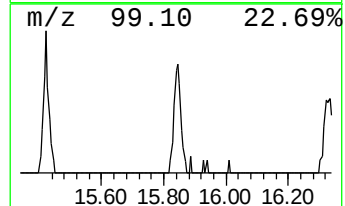
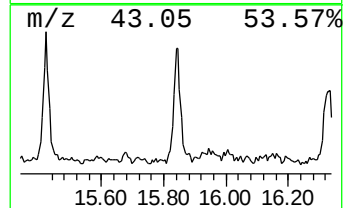
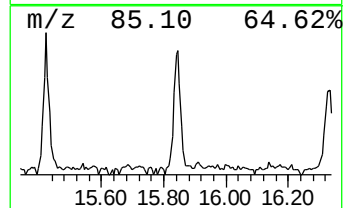
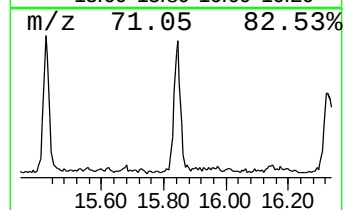
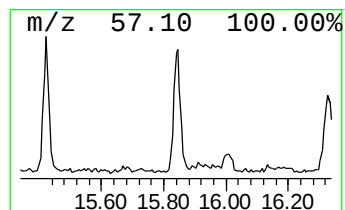
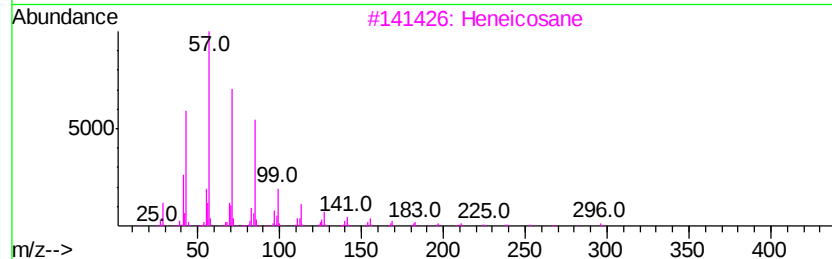
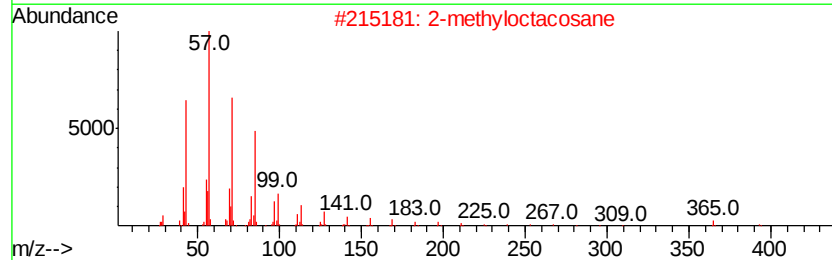
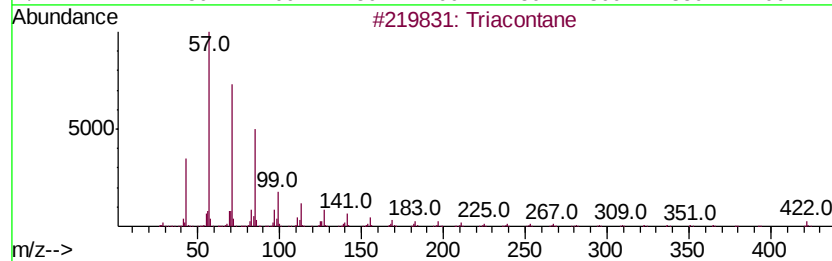
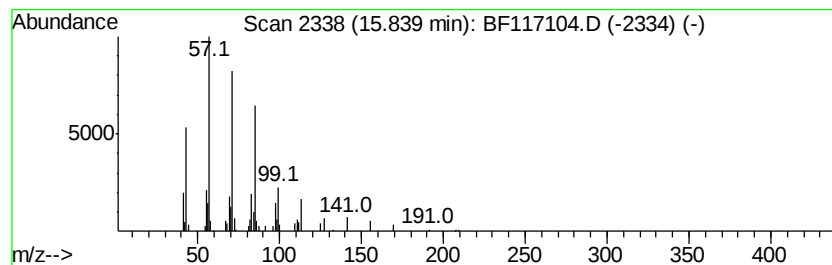
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.84	4.85 ng	101732	Perylene-d12	15.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Tetracosane	338	C24H50	000646-31-1	86
5	Octacosane	394	C28H58	000630-02-4	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091719\
Data File : BF117104.D
Acq On : 17 Sep 2019 14:11
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Misc :
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ClientSampleId :
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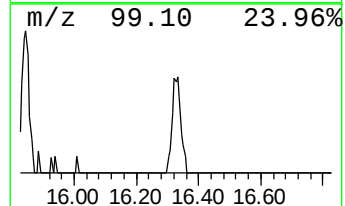
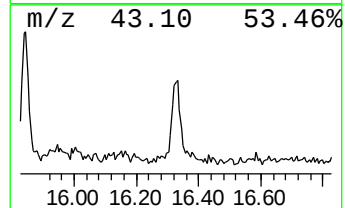
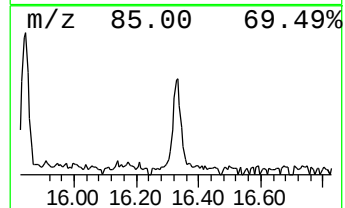
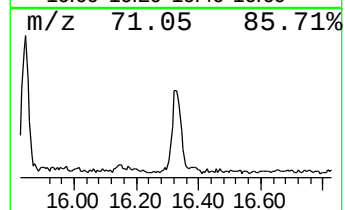
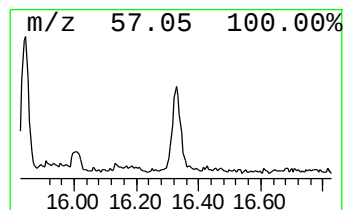
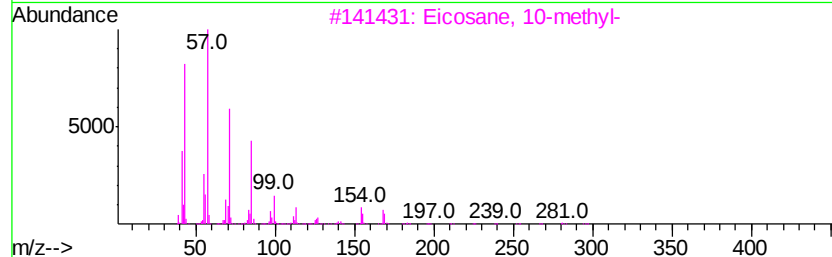
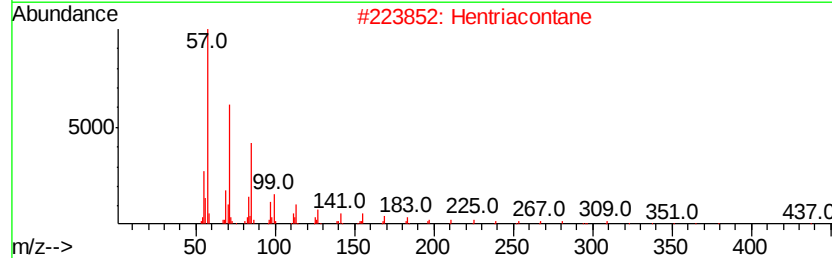
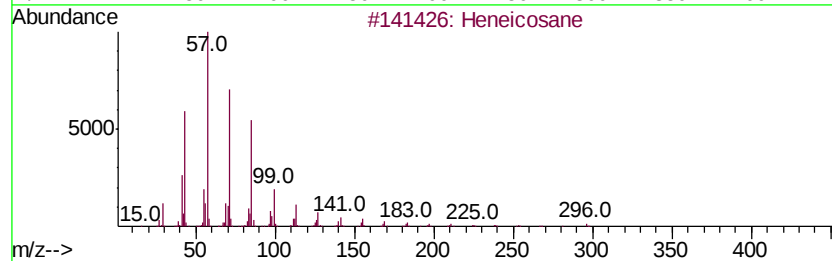
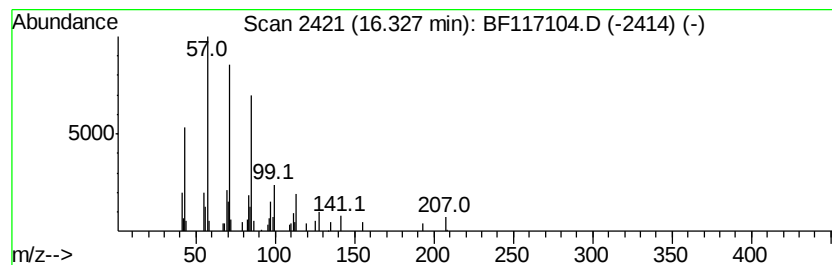
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Eicosane, 10-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.33	4.09 ng	85649	Perylene-d12	15.42

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	87
2			Hentriacontane	437	C31H64	000630-04-6	87
3			Eicosane, 10-methyl-	296	C21H44	054833-23-7	86
4			Triacontane	422	C30H62	000638-68-6	86
5			Octacosane	394	C28H58	000630-02-4	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091719\
Data File : BF117104.D
Acq On : 17 Sep 2019 14:11
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Misc :
ALS Vial : 12 Sample Multiplier: 1

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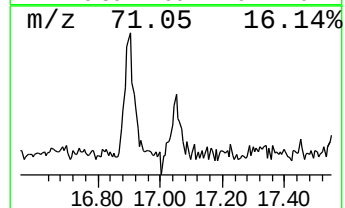
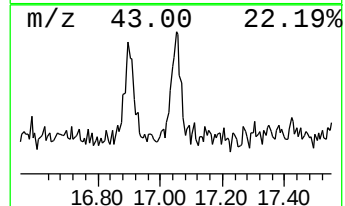
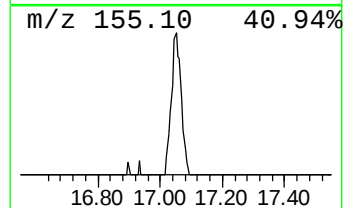
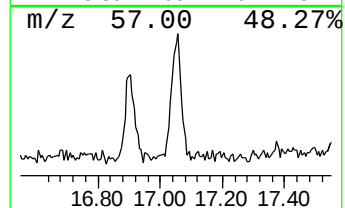
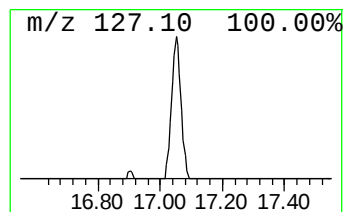
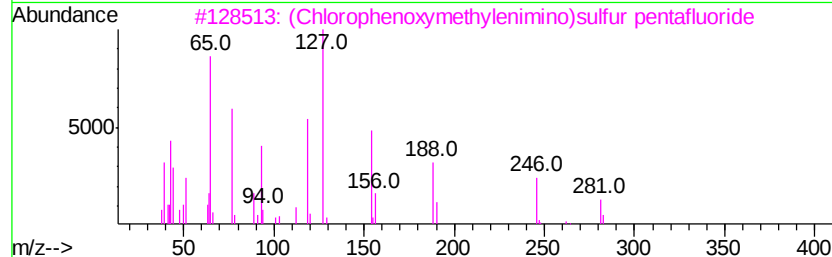
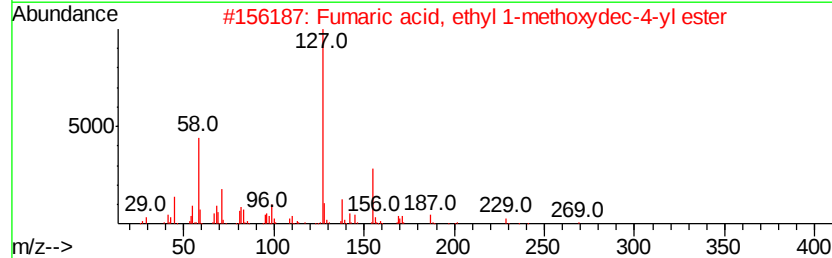
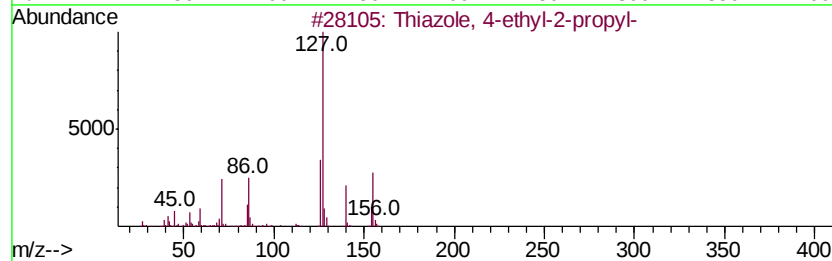
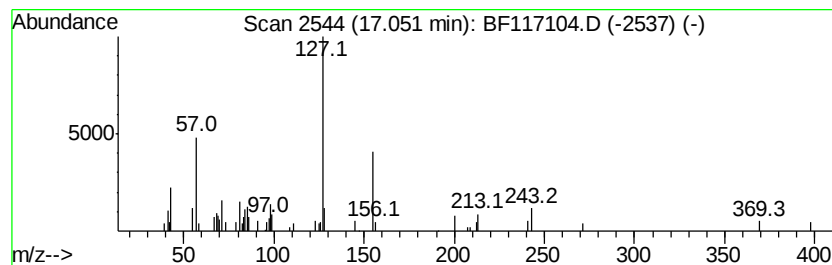
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Thiazole, 4-ethyl-2-propyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.05	4.24 ng	88936	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiazole, 4-ethyl-2-propyl-	155	C8H13NS	041981-68-4	50
2		Fumaric acid, ethyl 1-methoxydec...	314	C17H30O5	1000339-18-8	47
3		(Chlorophenoxy)methylenimino)sulf...	281	C7H5ClF5NOS	081439-21-6	46
4		3,5-Heptanedione, 2,2,6,6-tetram...	184	C11H20O2	001118-71-4	43
5		Urea, 1-(4-chlorophenyl)-3-propyl-	212	C10H13ClN2O	013208-64-5	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091719\
Data File : BF117104.D
Acq On : 17 Sep 2019 14:11
Operator : HP/JU
Sample : K4883-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

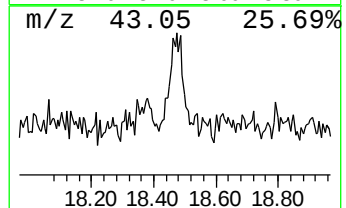
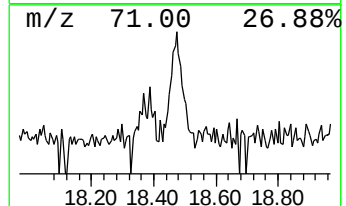
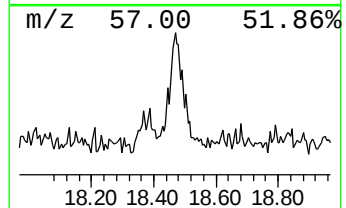
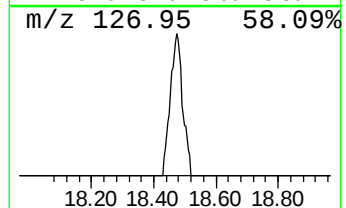
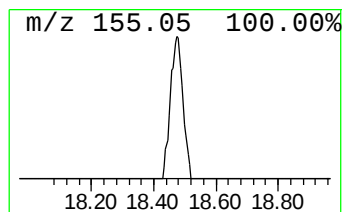
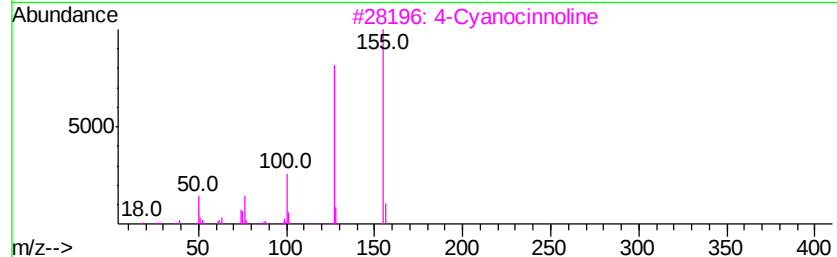
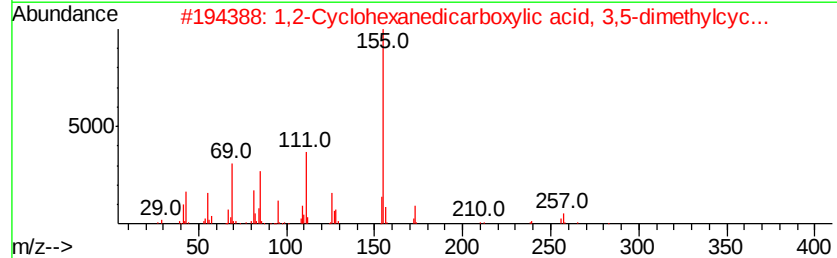
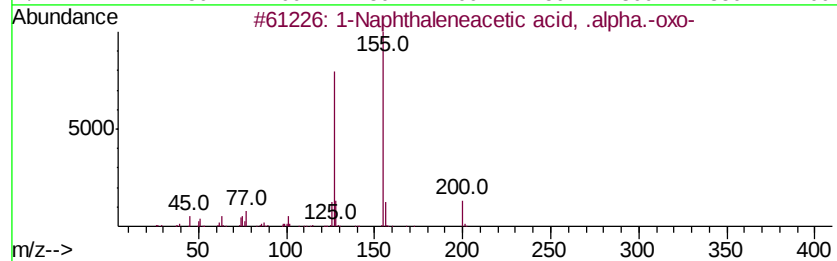
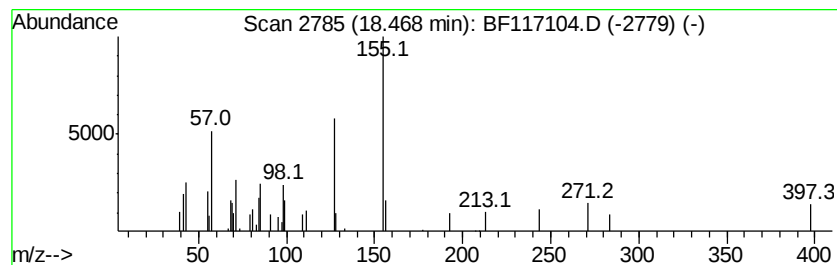
Instrument :
BNA_F
ClientSampleId :
MW5-R2-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 1-Naphthaleneacetic acid, Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.47	3.23 ng	67715	Perylene-d12	15.42		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Naphthaleneacetic acid, .alpha...	200	C12H8O3	026153-26-4	58
2		1,2-Cyclohexanedicarboxylic acid...	366	C22H38O4	1000339-84-9	50
3		4-Cvanocinnoline	155	C9H5N3	016470-90-9	50
4		Benzene, 2,4-difluoro-1-isocvanato-	155	C7H3F2N0	059025-55-7	50
5		1,3,5-Triazin-2(1H)-one, 4-amino...	155	C5H9N5O	007313-54-4	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091719\
 Data File : BF117104.D
 Acq On : 17 Sep 2019 14:11
 Operator : HP/JU
 Sample : K4883-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW5-R2-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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
unknown6.59	6.59	82.4	ng	1395220	1	6.82	338463	20.0
unknown9.95	9.95	6.4	ng	162908	3	9.85	511508	20.0
n-Hexadecanoic acid	11.86	2.5	ng	60625	4	11.33	493735	20.0
2-Butenedioic aci...	12.86	8.1	ng	151834	5	13.97	373304	20.0
1-Hentetracontanol	13.81	5.0	ng	93515	5	13.97	373304	20.0
Triphenylphosphin...	14.06	3.1	ng	58620	5	13.97	373304	20.0
Tetratetracontane	14.43	2.0	ng	38221	5	13.97	373304	20.0
Triacontane	14.73	3.0	ng	61803	6	15.42	419107	20.0
Nonadecane, 9-met...	15.05	4.0	ng	84580	6	15.42	419107	20.0
2-methyloctacosane	15.84	4.8	ng	101732	6	15.42	419107	20.0
Eicosane, 10-methyl-	16.33	4.1	ng	85649	6	15.42	419107	20.0
Thiazole, 4-ethyl...	17.05	4.2	ng	88936	6	15.42	419107	20.0
1-Naphthaleneacet...	18.47	3.2	ng	67715	6	15.42	419107	20.0