

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111519\
 Data File : BF117813.D
 Acq On : 15 Nov 2019 19:57
 Operator : JU
 Sample : K5861-15
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP-12

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-BF111319.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	2.193	13	18	24	rVB	823016	1095339	17.23%	1.972%
2	5.134	511	518	527	rBV	968328	1177128	18.52%	2.119%
3	5.534	580	586	589	rBV	5154525	5135841	80.80%	9.246%
4	6.539	751	757	761	rBV	5265792	5603377	88.16%	10.088%
5	6.686	777	782	785	rBV	5908204	5539100	87.14%	9.972%
6	6.916	818	821	825	rBV	1477200	1287407	20.25%	2.318%
7	7.075	844	848	852	rBV	4807090	4239755	66.70%	7.633%
8	7.481	912	917	920	rBV	3817887	3425469	53.89%	6.167%
9	8.204	1036	1040	1044	rBV	2034315	1654225	26.03%	2.978%
10	9.286	1219	1224	1227	rBV	6801844	6212963	97.75%	11.185%
11	9.675	1286	1290	1294	rBV	834834	681378	10.72%	1.227%
12	9.969	1336	1340	1343	rBV	2402851	1894050	29.80%	3.410%
13	10.757	1469	1474	1478	rBV	4731130	4255753	66.95%	7.661%
14	11.457	1590	1593	1597	rBV	2203133	1958265	30.81%	3.525%
15	11.980	1679	1682	1687	rBV	424954	399207	6.28%	0.719%
16	12.768	1813	1816	1830	rBV	103924	135689	2.13%	0.244%
17	12.927	1836	1843	1859	rBV	161265	275532	4.33%	0.496%
18	13.051	1859	1864	1867	rBV	7017163	6356207	100.00%	11.443%
19	13.951	2013	2017	2032	rBV3	167970	540175	8.50%	0.972%
20	14.104	2039	2043	2047	rVB	1799598	1635712	25.73%	2.945%
21	14.574	2120	2123	2126	rBV	72379	76460	1.20%	0.138%
22	14.892	2175	2177	2182	rVB	75555	77953	1.23%	0.140%
23	15.251	2234	2238	2242	rBV	96738	107084	1.68%	0.193%
24	15.615	2294	2300	2304	rBV	1256626	1587550	24.98%	2.858%
25	15.651	2304	2306	2313	rVB	77252	95216	1.50%	0.171%
26	16.109	2380	2384	2391	rVB	62844	100426	1.58%	0.181%

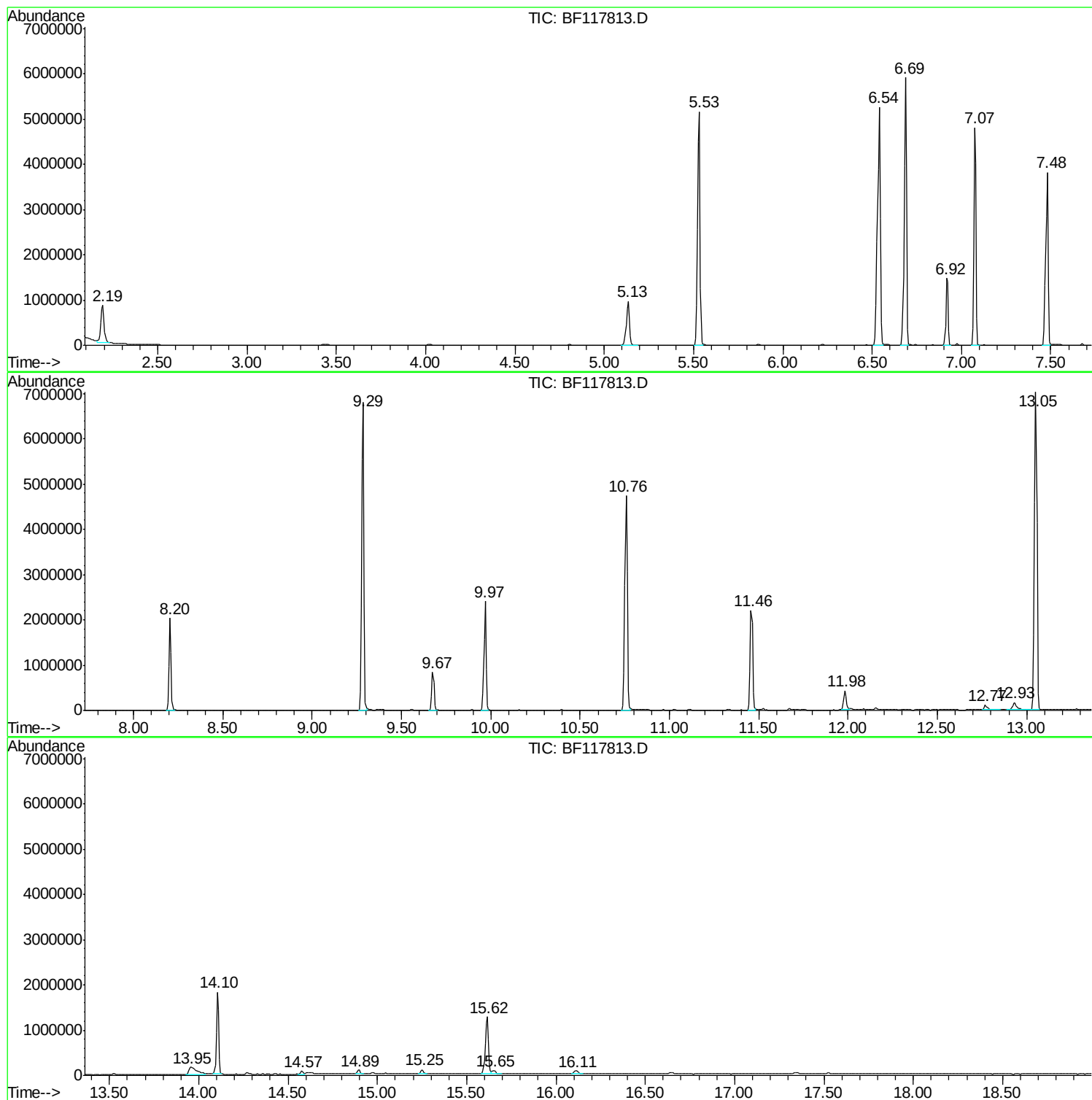
Sum of corrected areas: 55547261

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111519\
Data File : BF117813.D
Acq On : 15 Nov 2019 19:57
Operator : JU
Sample : K5861-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111519\
Data File : BF117813.D
Acq On : 15 Nov 2019 19:57
Operator : JU
Sample : K5861-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-12

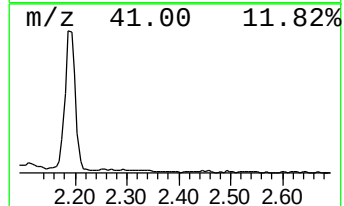
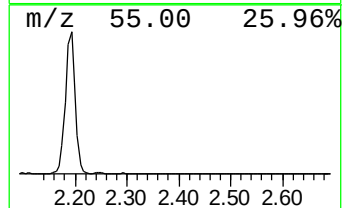
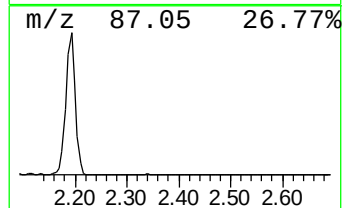
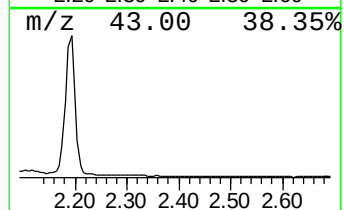
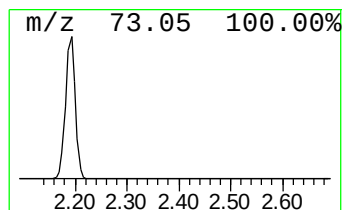
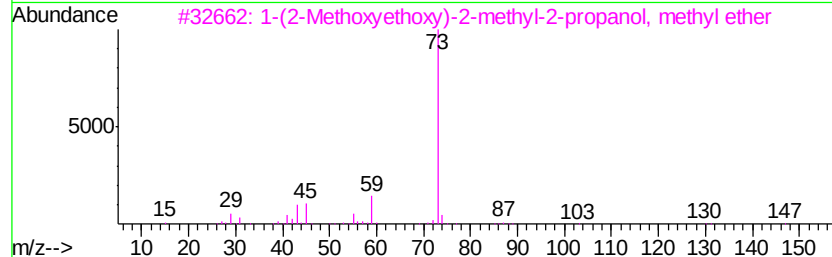
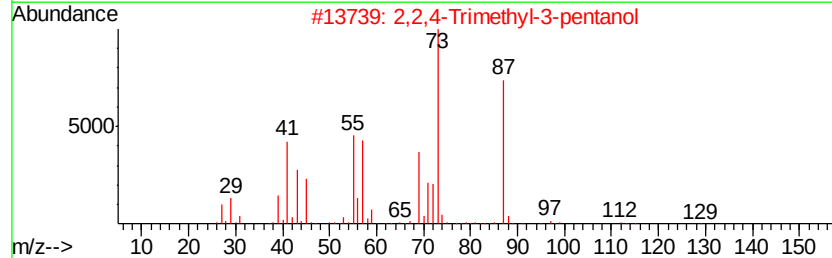
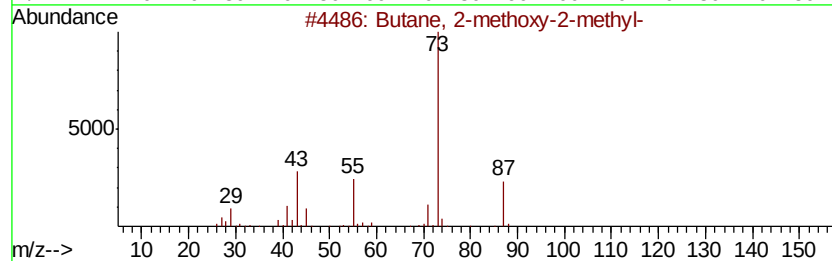
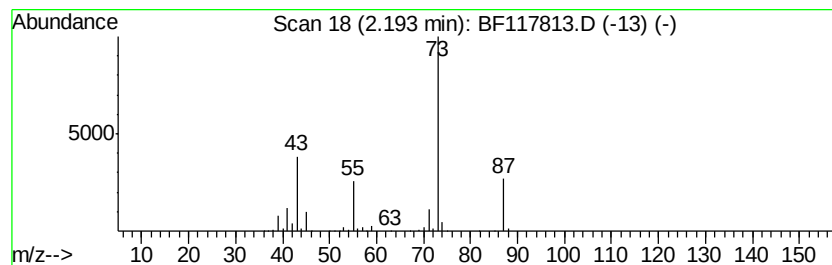
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	17.02 ng	1095340	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1-(2-Methoxyethoxy)-2-methyl-2-propanol	162	C8H18O3	1000364-24-4	23
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111519\
Data File : BF117813.D
Acq On : 15 Nov 2019 19:57
Operator : JU
Sample : K5861-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-12

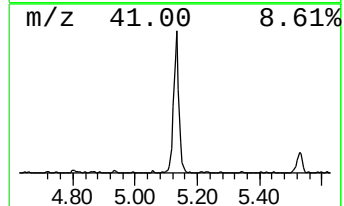
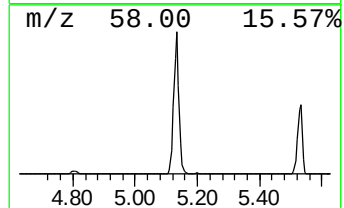
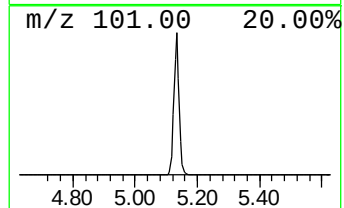
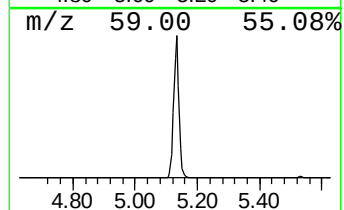
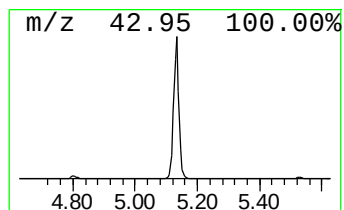
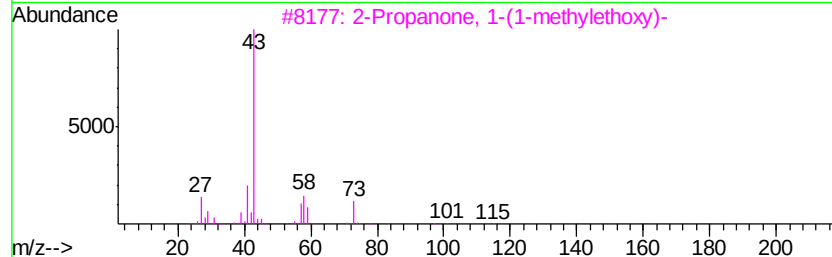
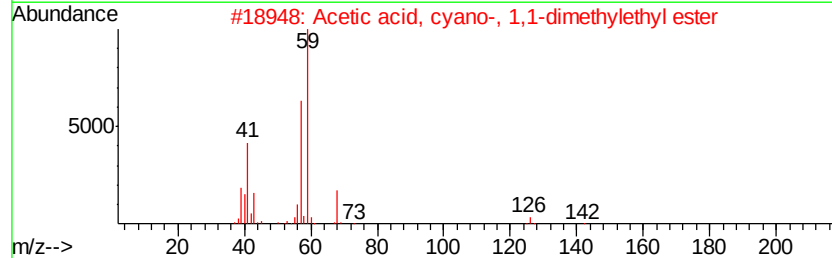
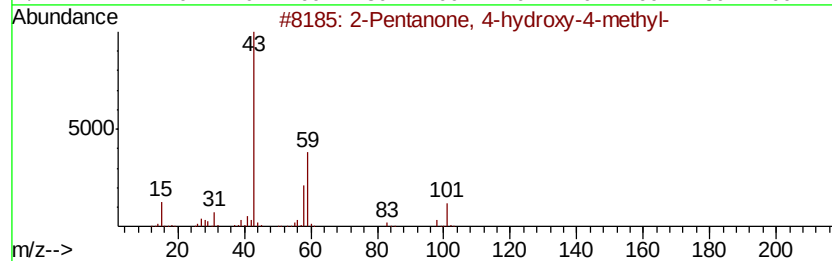
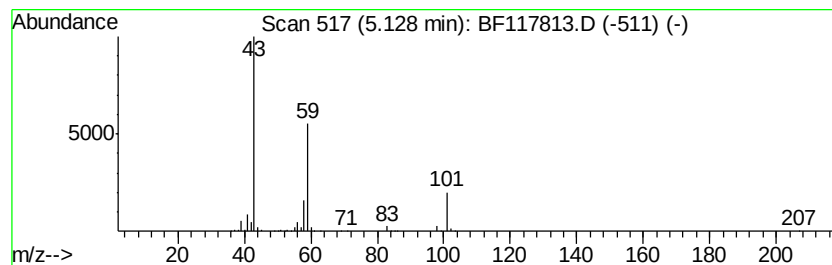
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	18.29 ng	1177130	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
4		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111519\
Data File : BF117813.D
Acq On : 15 Nov 2019 19:57
Operator : JU
Sample : K5861-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-12

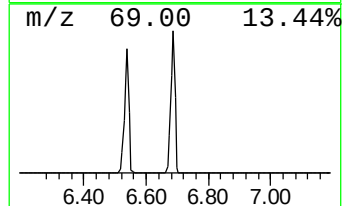
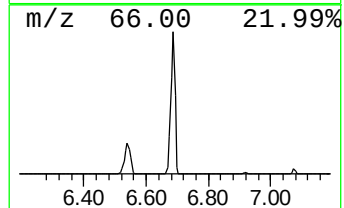
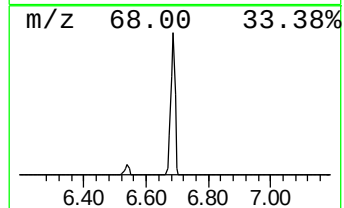
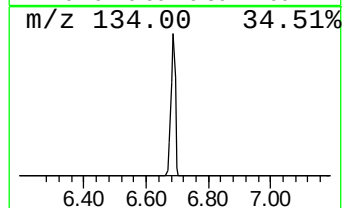
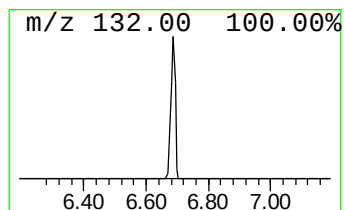
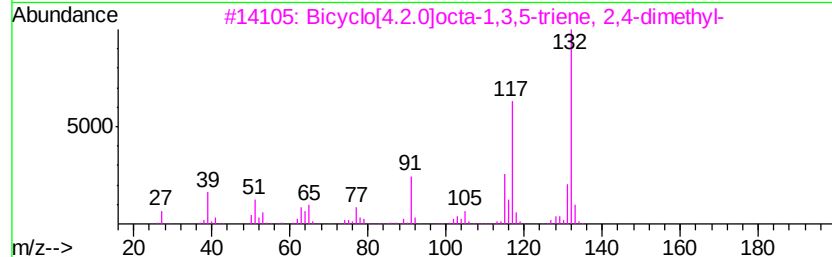
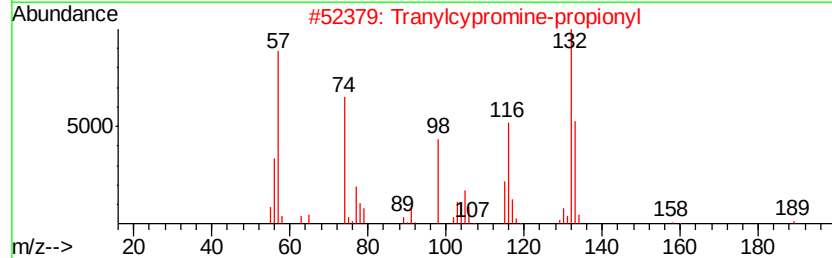
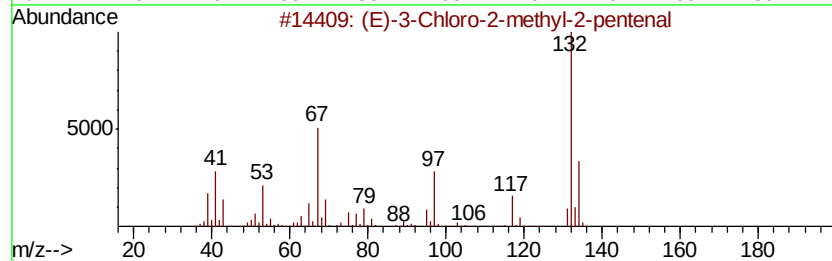
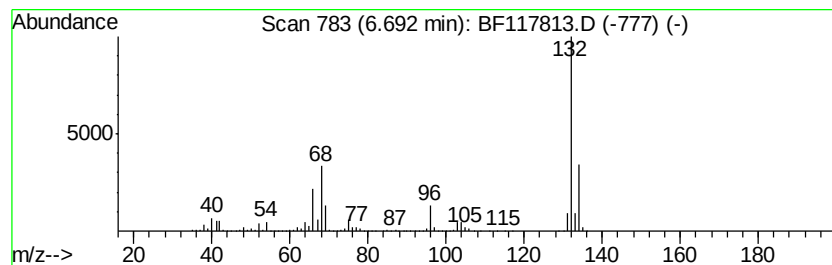
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	86.05 ng	5539100	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
2		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111519\
Data File : BF117813.D
Acq On : 15 Nov 2019 19:57
Operator : JU
Sample : K5861-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-12

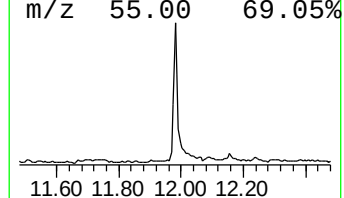
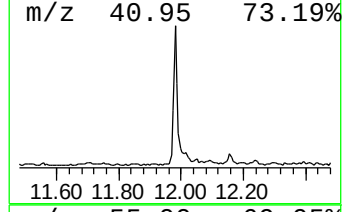
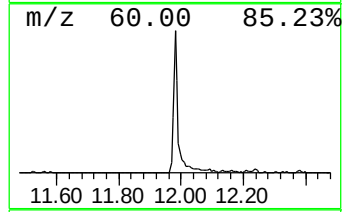
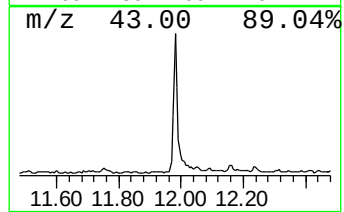
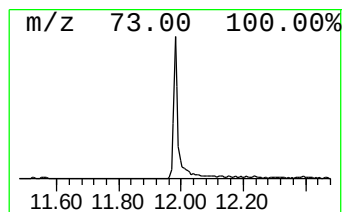
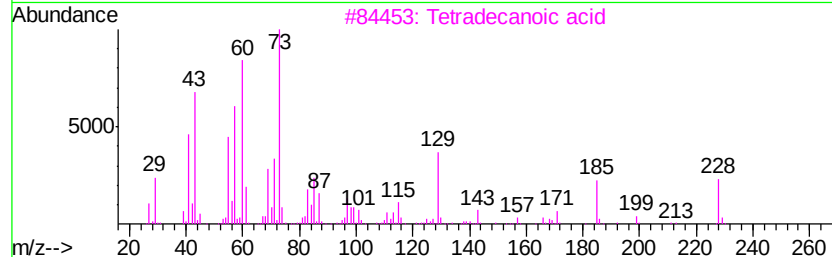
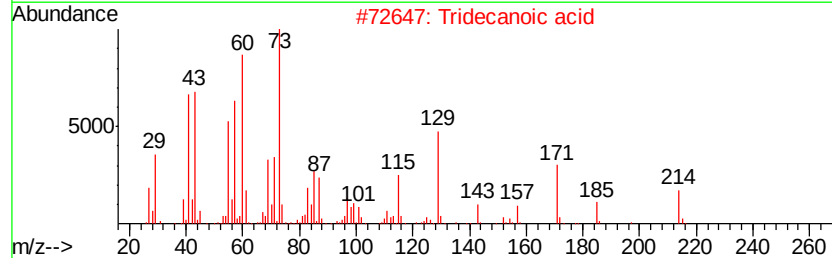
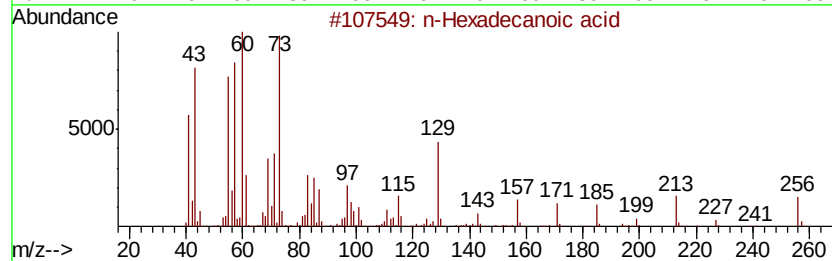
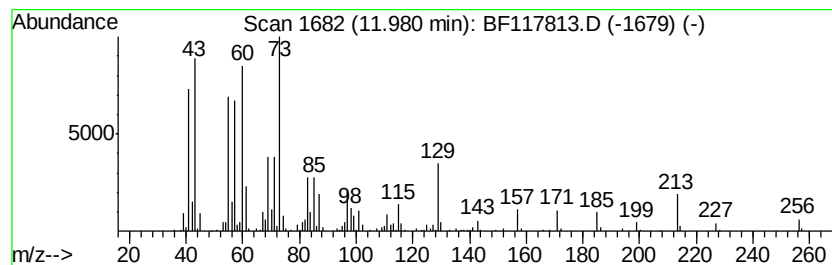
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	4.08 ng	399207	Phenanthrene-d10	11.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5		Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111519\
Data File : BF117813.D
Acq On : 15 Nov 2019 19:57
Operator : JU
Sample : K5861-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

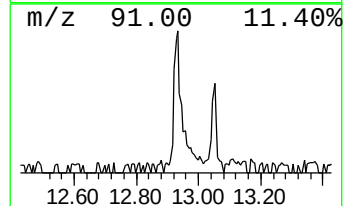
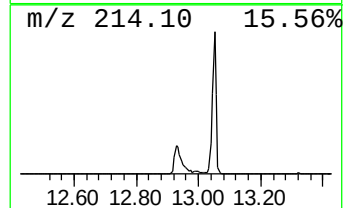
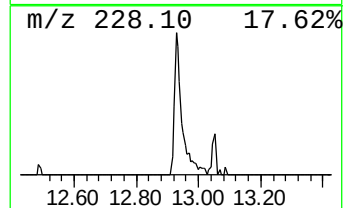
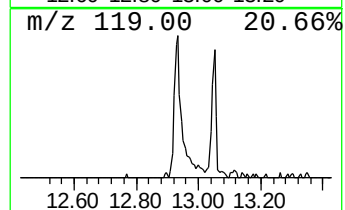
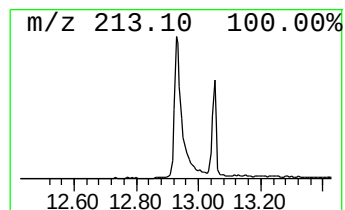
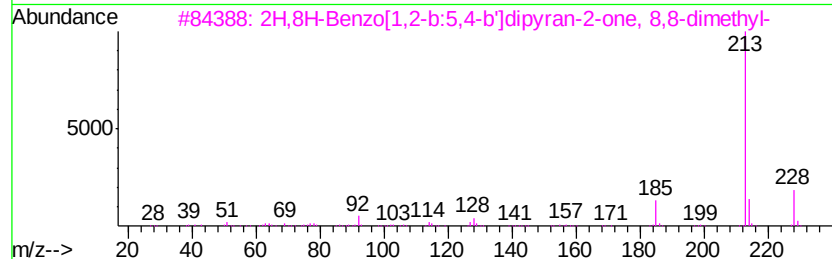
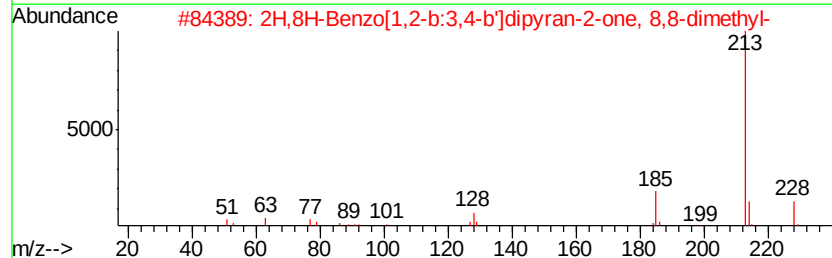
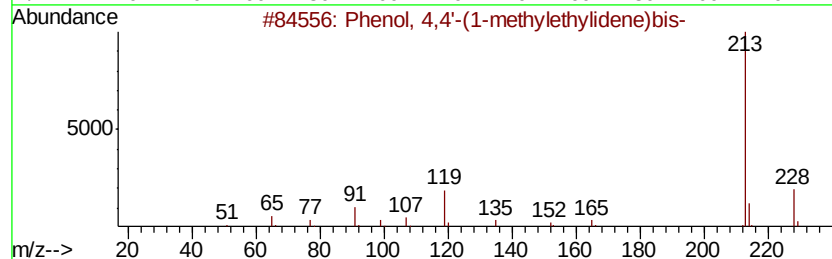
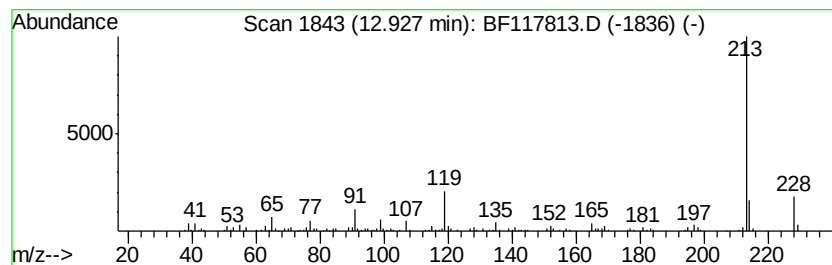
Instrument :
BNA_F
ClientSampleId :
EP-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phenol, 4,4'-(1-methylethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.93	3.37 ng	275532	Chrysene-d12	14.10	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	98
2	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	53
3	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	53
4	6-Bromo-2-(methylamino)tropone	213	C8H8BrNO	1000241-43-1	50
5	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111519\
Data File : BF117813.D
Acq On : 15 Nov 2019 19:57
Operator : JU
Sample : K5861-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-12

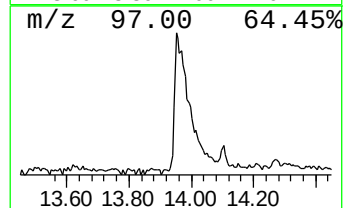
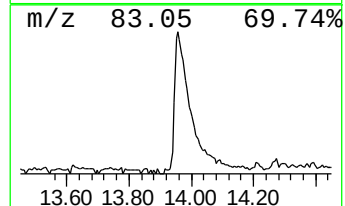
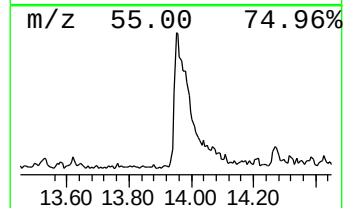
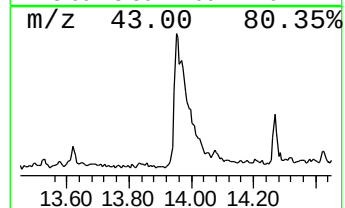
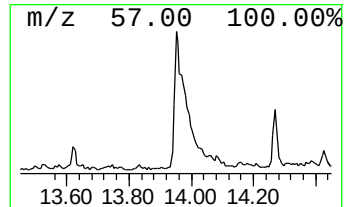
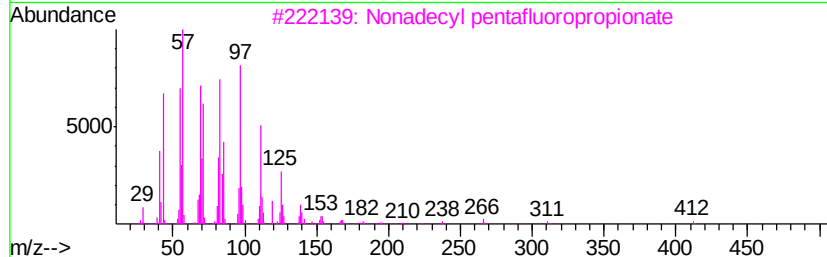
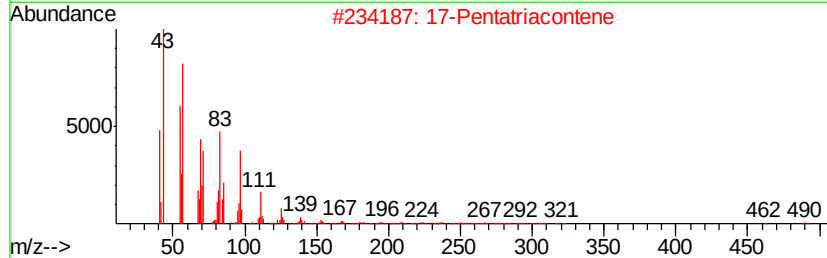
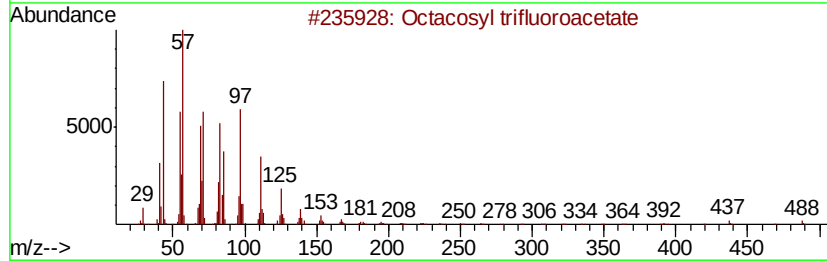
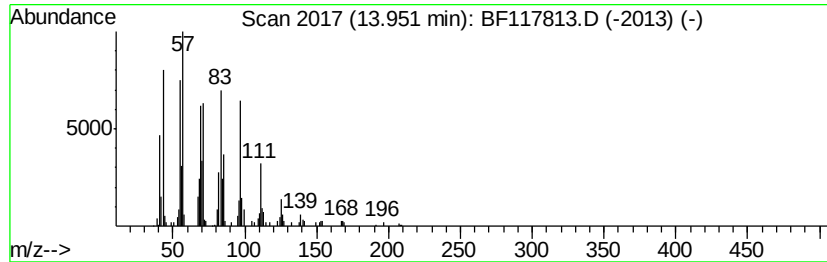
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	6.60 ng	540175	Chrysene-d12	14.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2		17-Pentatriacontene	491	C35H70	006971-40-0	91
3		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5		Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111519\
Data File : BF117813.D
Acq On : 15 Nov 2019 19:57
Operator : JU
Sample : K5861-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.19	17.0	ng	1095340	1	6.92	1287410	20.0
2-Pentanone, 4-hy...	5.13	18.3	ng	1177130	1	6.92	1287410	20.0
unknown6.69	6.69	86.0	ng	5539100	1	6.92	1287410	20.0
n-Hexadecanoic acid	11.98	4.1	ng	399207	4	11.46	1958270	20.0
Phenol, 4,4'-(1-m...	12.93	3.4	ng	275532	5	14.10	1635710	20.0
Octacosyl trifluo...	13.95	6.6	ng	540175	5	14.10	1635710	20.0