

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111519\
 Data File : BF117810.D
 Acq On : 15 Nov 2019 18:35
 Operator : JU
 Sample : K5861-09
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP-9

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	2.181	11	16	22	rVB	686714	905097	17.29%	2.025%
2	5.128	510	517	526	rBV	776012	887481	16.96%	1.986%
3	5.528	580	585	588	rBV	3942303	3577465	68.35%	8.006%
4	6.534	751	756	761	rBV	3872225	3936471	75.21%	8.809%
5	6.686	777	782	785	rBV	4181129	3969058	75.83%	8.882%
6	6.916	818	821	825	rBV	1505155	1262406	24.12%	2.825%
7	7.075	844	848	851	rBV	3882042	3114809	59.51%	6.970%
8	7.475	912	916	920	rBV	2529254	2433347	46.49%	5.445%
9	8.204	1036	1040	1044	rBV	1993281	1657865	31.68%	3.710%
10	9.286	1219	1224	1227	rBV	5127337	4687671	89.56%	10.490%
11	9.674	1286	1290	1294	rBV	463093	353730	6.76%	0.792%
12	9.969	1336	1340	1343	rBV	2374910	1977606	37.78%	4.425%
13	10.757	1470	1474	1477	rBV	3593736	3084488	58.93%	6.902%
14	11.457	1589	1593	1597	rBV	2387134	2088193	39.90%	4.673%
15	11.980	1679	1682	1686	rBV	264146	246522	4.71%	0.552%
16	12.768	1813	1816	1828	rBV2	81773	109684	2.10%	0.245%
17	12.933	1840	1844	1854	rVB	58259	99489	1.90%	0.223%
18	13.051	1859	1864	1867	rBV	5865112	5233913	100.00%	11.712%
19	13.957	2014	2018	2038	rBV4	164676	552207	10.55%	1.236%
20	14.109	2038	2044	2047	rBV	1866018	1829599	34.96%	4.094%
21	14.580	2121	2124	2127	rBV	84511	70785	1.35%	0.158%
22	14.898	2175	2178	2184	rVB	105446	108297	2.07%	0.242%
23	14.980	2188	2192	2197	rBV	204853	203799	3.89%	0.456%
24	15.256	2234	2239	2244	rBV	104347	134944	2.58%	0.302%
25	15.615	2294	2300	2305	rBV	1345958	1785559	34.12%	3.996%
26	15.656	2305	2307	2318	rVB	123546	150122	2.87%	0.336%
27	16.115	2380	2385	2393	rVB	84451	136720	2.61%	0.306%
28	16.650	2471	2476	2483	rVB3	47165	89715	1.71%	0.201%

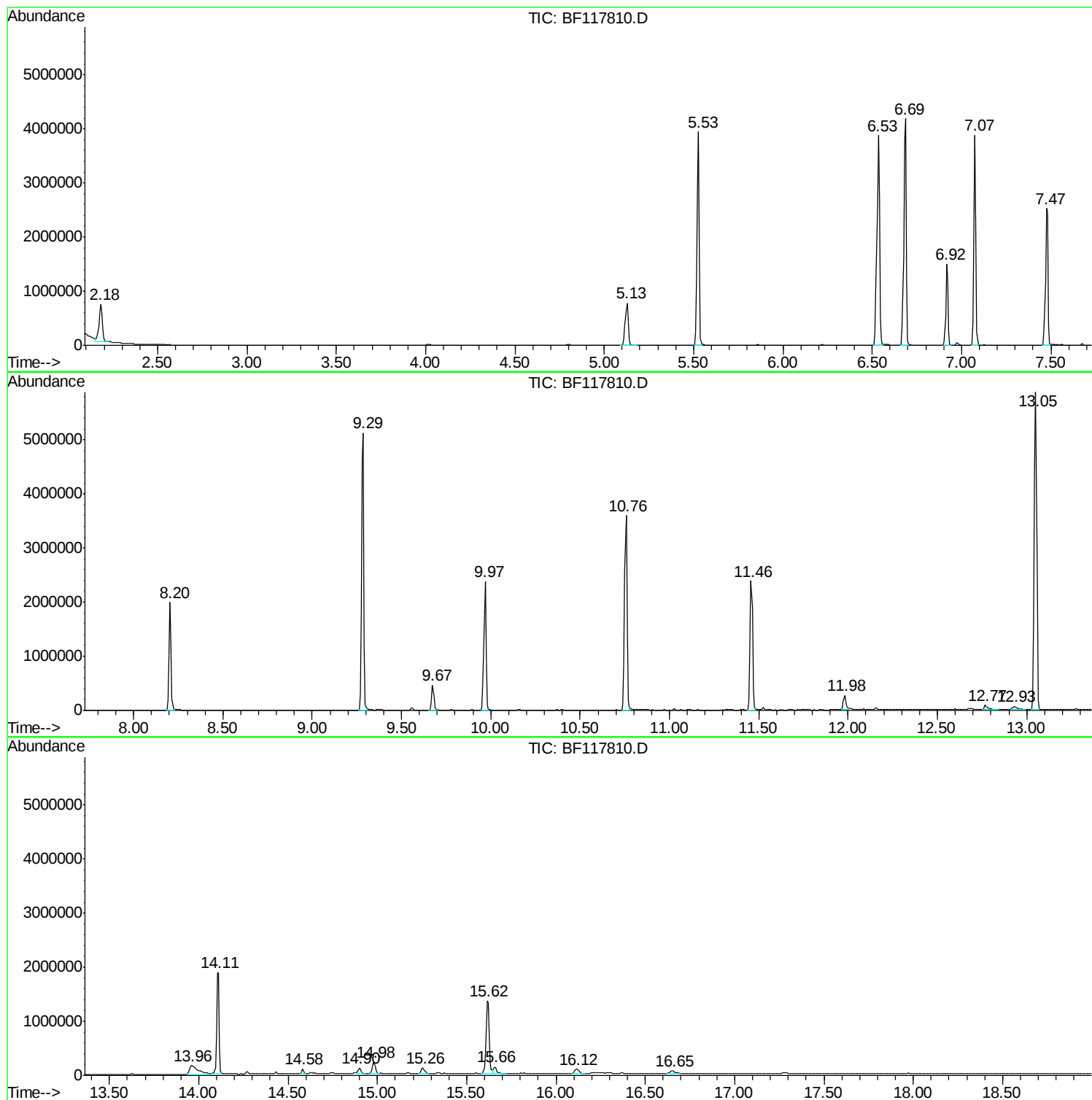
Sum of corrected areas: 44687042

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111519\
Data File : BF117810.D
Acq On : 15 Nov 2019 18:35
Operator : JU
Sample : K5861-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-9

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 : BF117810.D
Acq On : 15 Nov 2019 18:35
Operator : JU
Sample : K5861-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-9

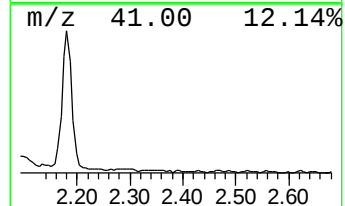
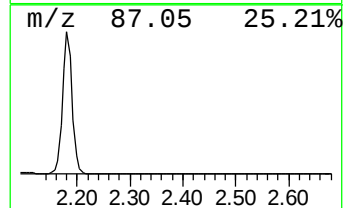
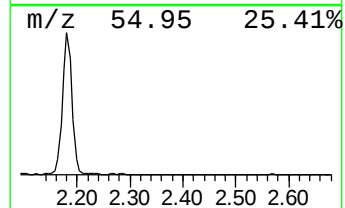
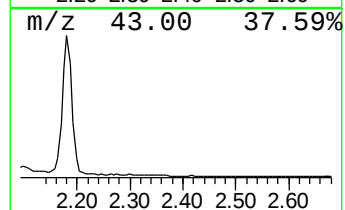
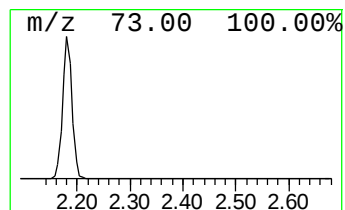
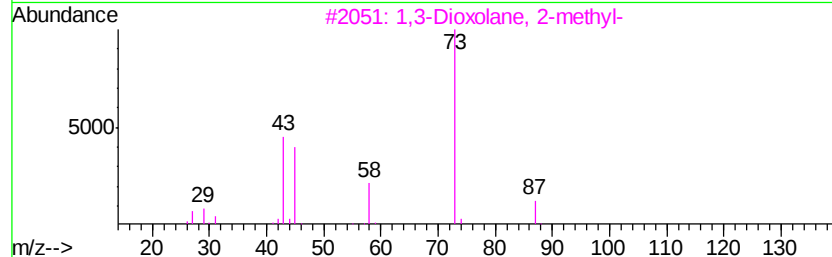
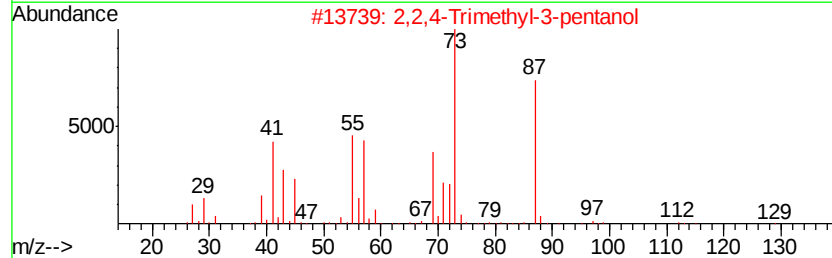
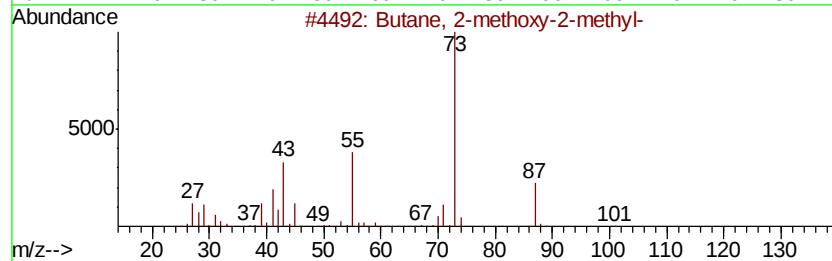
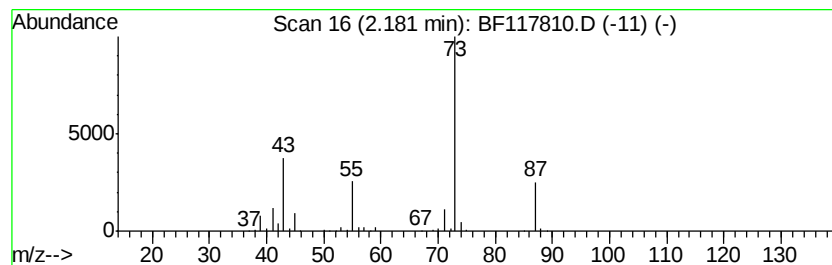
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	14.34 ng	905097	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	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111519\
Data File : BF117810.D
Acq On : 15 Nov 2019 18:35
Operator : JU
Sample : K5861-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-9

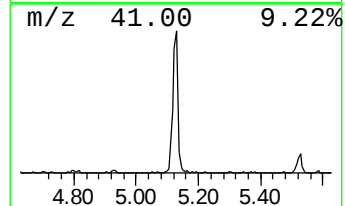
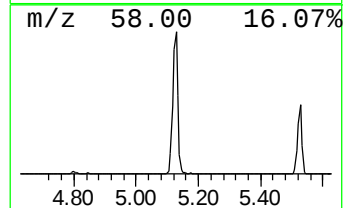
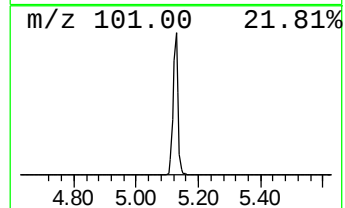
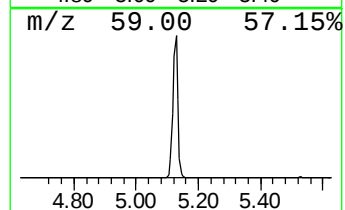
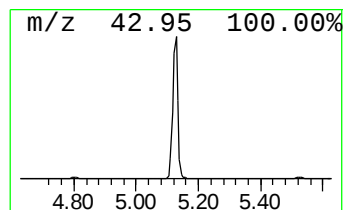
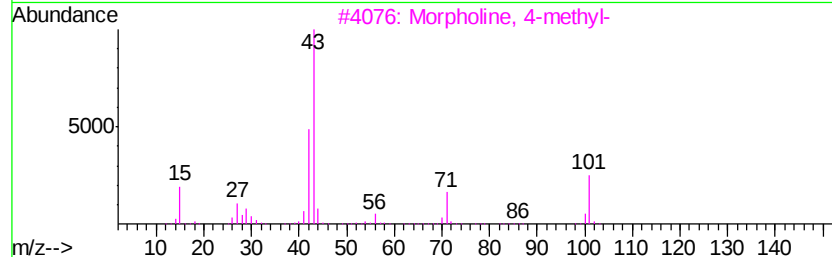
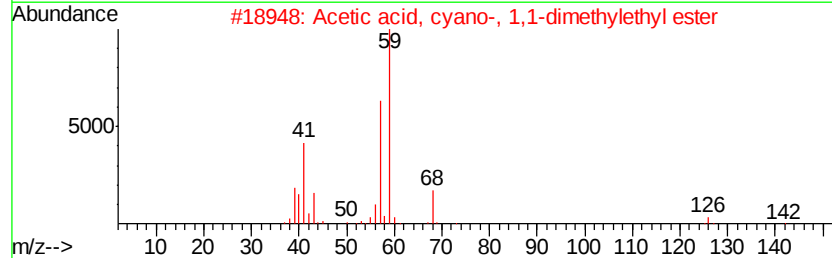
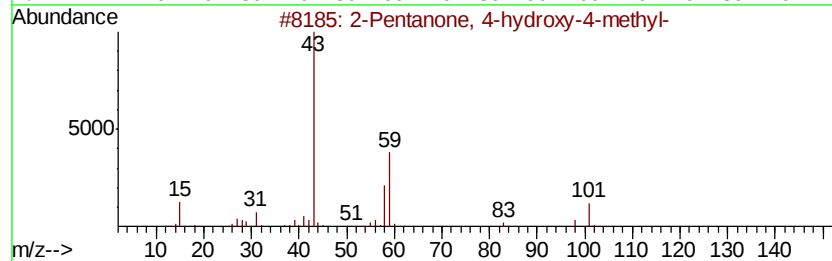
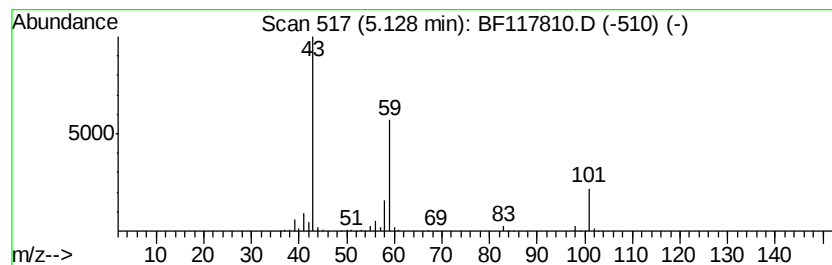
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	14.06 ng	887481	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	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	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 : BF117810.D
Acq On : 15 Nov 2019 18:35
Operator : JU
Sample : K5861-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-9

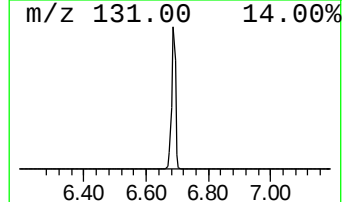
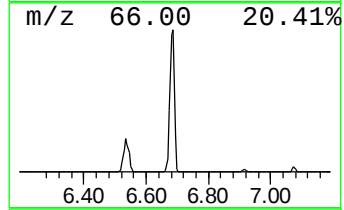
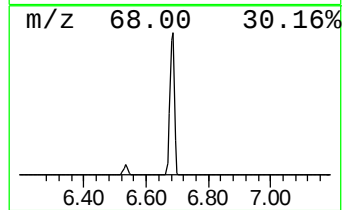
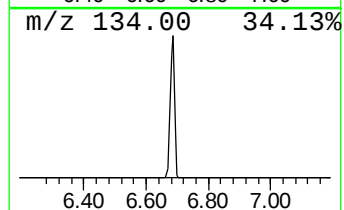
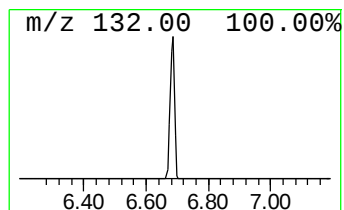
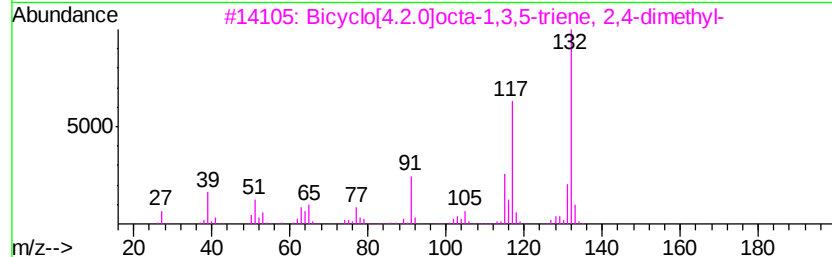
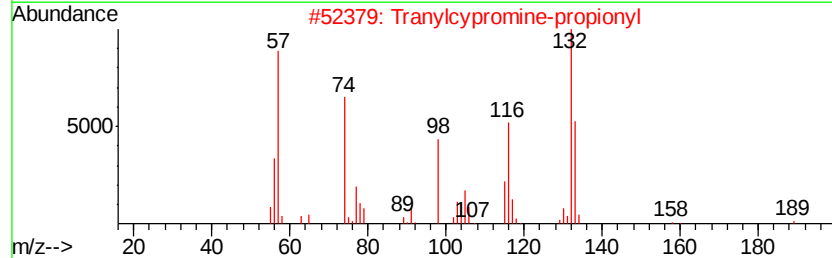
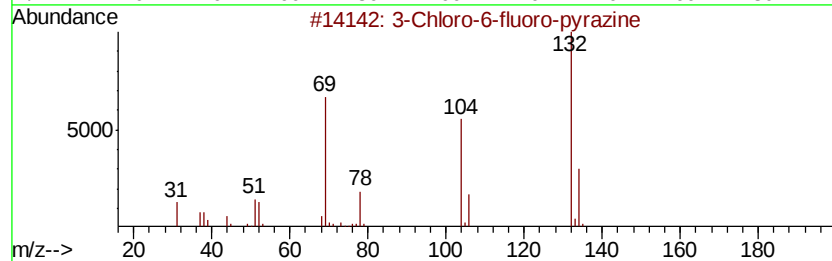
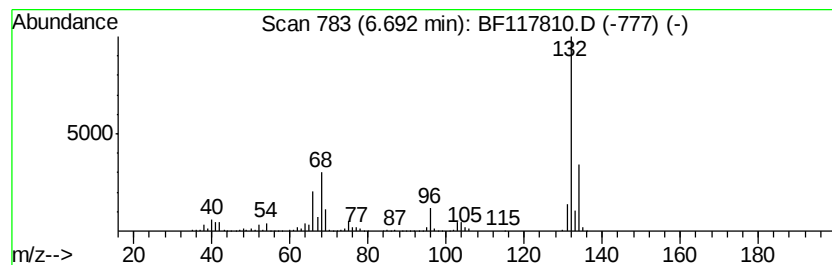
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	62.88 ng	3969060	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111519\
Data File : BF117810.D
Acq On : 15 Nov 2019 18:35
Operator : JU
Sample : K5861-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-9

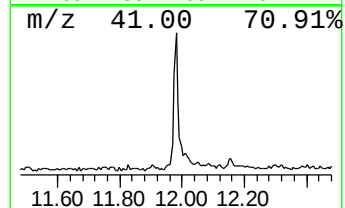
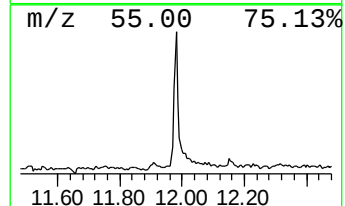
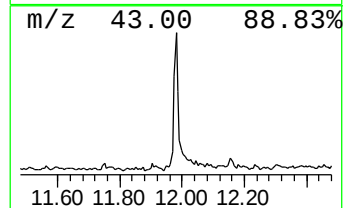
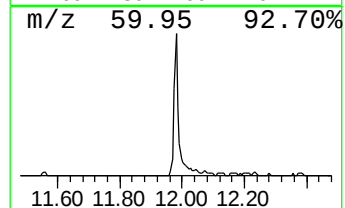
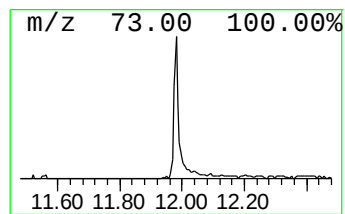
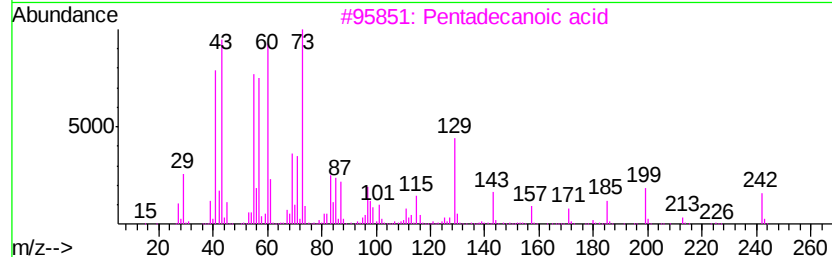
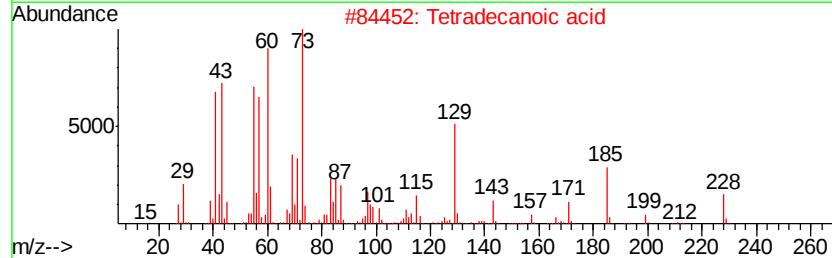
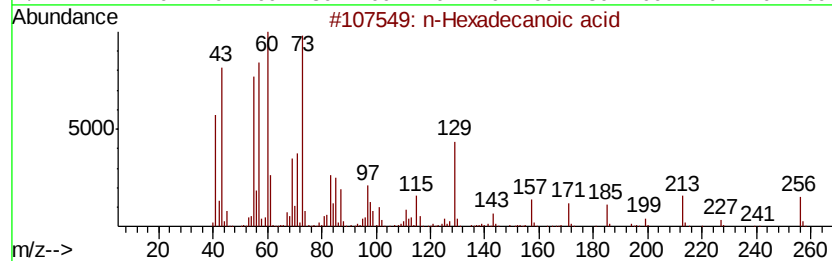
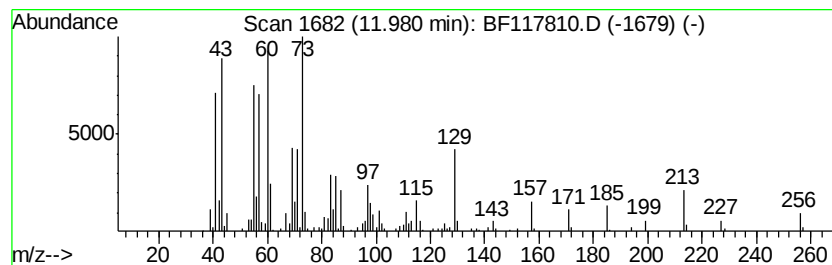
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	2.36 ng	246522	Phenanthrene-d10	11.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tridecanoic acid	214	C13H26O2	000638-53-9	90
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111519\
Data File : BF117810.D
Acq On : 15 Nov 2019 18:35
Operator : JU
Sample : K5861-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-9

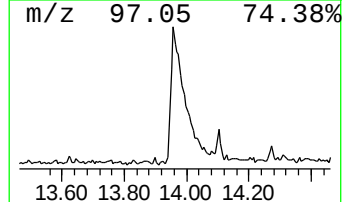
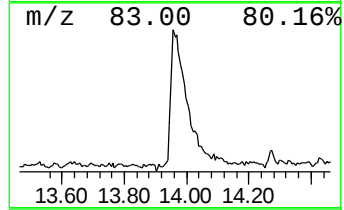
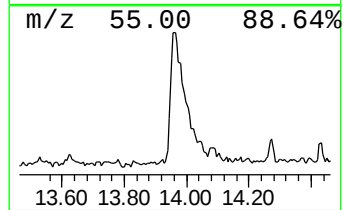
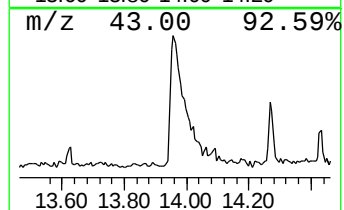
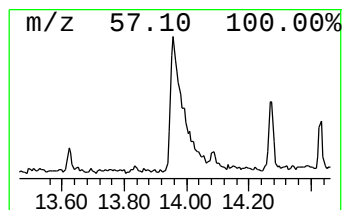
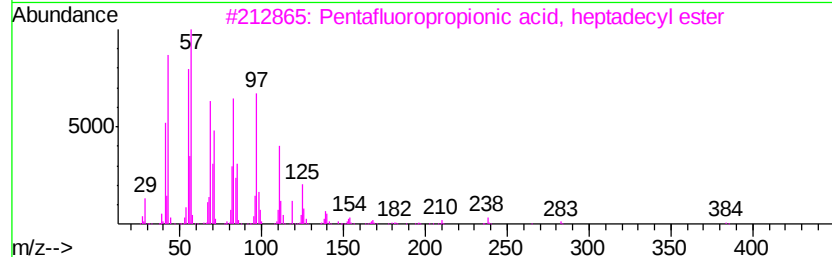
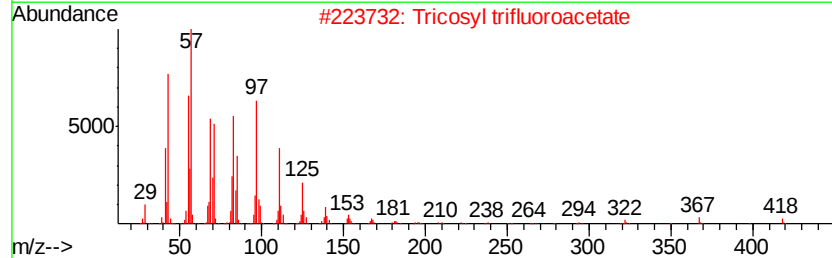
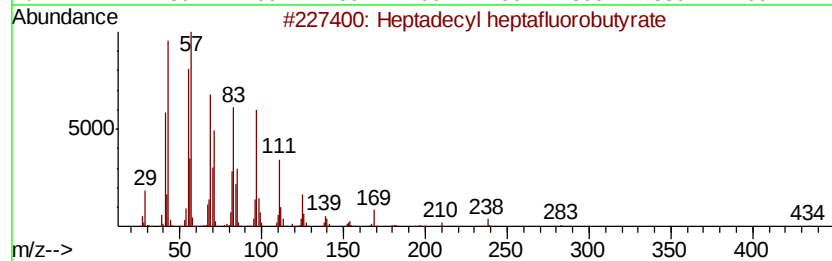
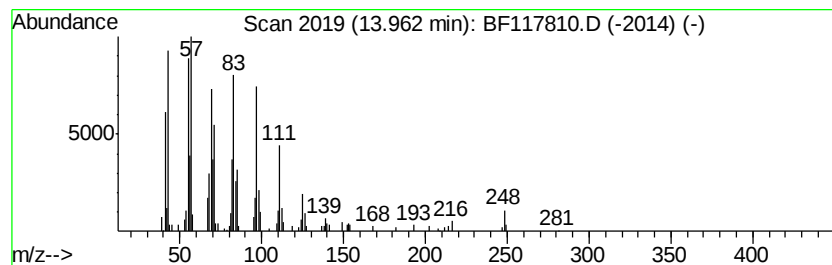
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	6.04 ng	552207	Chrysene-d12	14.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	94
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111519\
Data File : BF117810.D
Acq On : 15 Nov 2019 18:35
Operator : JU
Sample : K5861-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-9

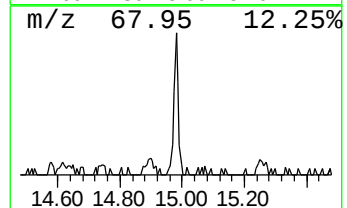
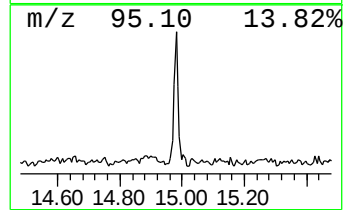
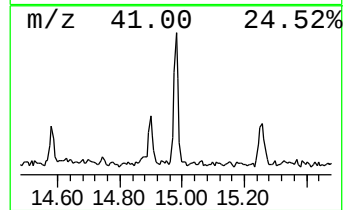
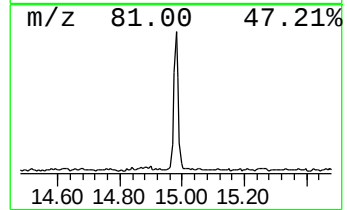
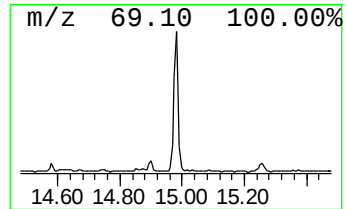
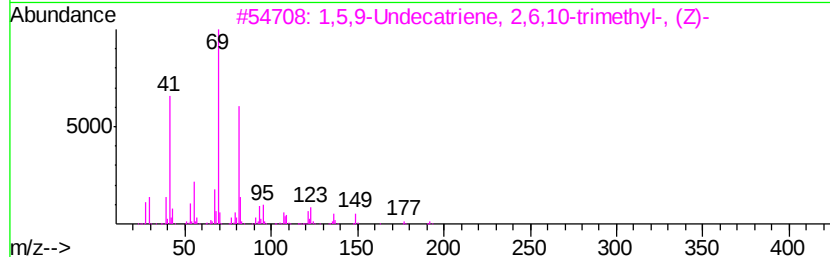
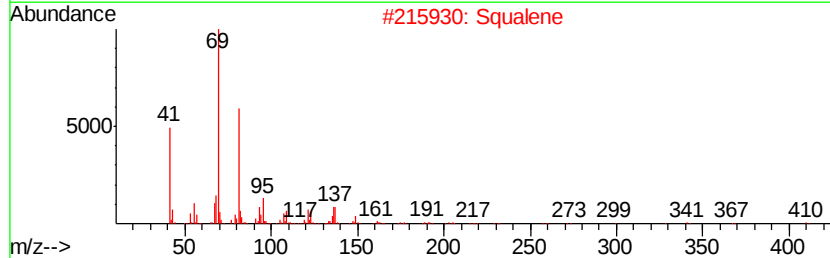
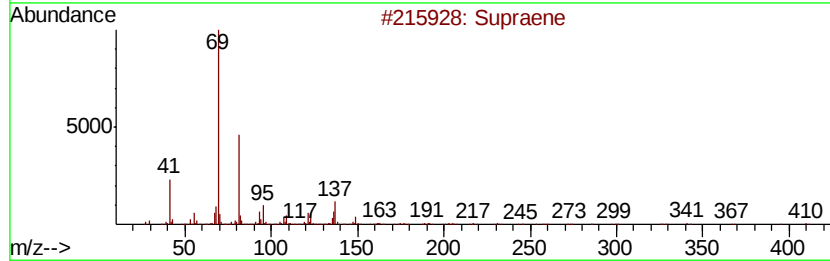
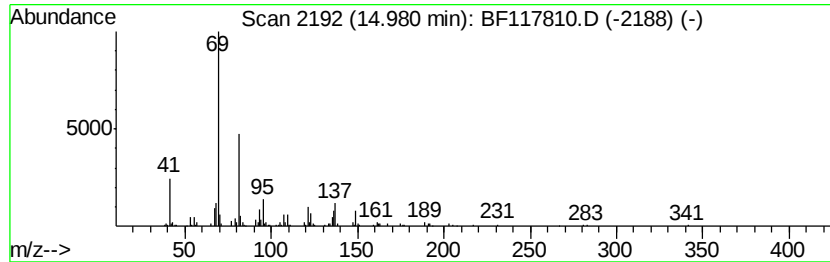
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.28 ng	203799	Perylene-d12	15.62

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene		410	C30H50	007683-64-9	91
2	Squalene		410	C30H50	000111-02-4	91
3	1,5,9-Undecatriene, 2,6,10-trime...		192	C14H24	062951-96-6	87
4	2,6-Octadiene, 4-methyl-		124	C9H16	074498-94-5	50
5	1,5-Heptadiene, 3,4-dimethyl-		124	C9H16	1000061-77-9	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111519\
Data File : BF117810.D
Acq On : 15 Nov 2019 18:35
Operator : JU
Sample : K5861-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-9

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...	2.18	14.3	ng	905097	1	6.92	1262410	20.0
2-Pentanone, 4-hy...	5.13	14.1	ng	887481	1	6.92	1262410	20.0
unknown6.69	6.69	62.9	ng	3969060	1	6.92	1262410	20.0
n-Hexadecanoic acid	11.98	2.4	ng	246522	4	11.46	2088190	20.0
Heptadecyl hepta...	13.96	6.0	ng	552207	5	14.11	1829600	20.0
Supraene	14.98	2.3	ng	203799	6	15.62	1785560	20.0