

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100820\
 Data File : BF121890.D
 Acq On : 8 Oct 2020 15:43
 Operator : JU/CG
 Sample : L4297-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-RBR-200034

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-BF091020.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	2.475	62	66	79	rVB	51690	104433	4.90%	0.538%
2	3.199	186	189	210	rBV	84632	245592	11.51%	1.264%
3	4.963	486	489	496	rBV	27175	34889	1.64%	0.180%
4	5.381	556	560	578	rBV	1986685	1981366	92.88%	10.200%
5	6.404	730	734	752	rBV	1983049	1960697	91.91%	10.094%
6	6.604	763	768	780	rBV2	11530	26179	1.23%	0.135%
7	6.757	790	794	798	rBV	887020	683642	32.05%	3.519%
8	7.322	886	890	911	rBV	1408343	1378750	64.63%	7.098%
9	8.039	1008	1012	1029	rBV	924616	921449	43.19%	4.744%
10	8.163	1029	1033	1045	rVB	30260	52435	2.46%	0.270%
11	9.116	1191	1195	1206	rBV	2430696	2133297	100.00%	10.982%
12	9.298	1221	1226	1243	rBV	12724	34007	1.59%	0.175%
13	9.516	1259	1263	1270	rBV	236837	231220	10.84%	1.190%
14	9.792	1306	1310	1320	rVB	1126308	1105728	51.83%	5.692%
15	10.586	1441	1445	1460	rBV	1691397	1561170	73.18%	8.037%
16	11.280	1559	1563	1571	rBV	1293248	1193393	55.94%	6.144%
17	11.716	1634	1637	1645	rBV	18975	23832	1.12%	0.123%
18	11.810	1651	1653	1658	rBV2	26342	28299	1.33%	0.146%
19	12.492	1766	1769	1773	rVB	158821	135450	6.35%	0.697%
20	12.721	1803	1808	1813	rVB	140419	139635	6.55%	0.719%
21	12.780	1813	1818	1823	rBV2	40869	50128	2.35%	0.258%
22	12.863	1828	1832	1836	rVV	2162581	1947051	91.27%	10.023%
23	13.092	1867	1871	1874	rBV2	21736	32862	1.54%	0.169%
24	13.721	1975	1978	1982	rBV2	46923	53433	2.50%	0.275%
25	13.768	1982	1986	1996	rVB	389436	574442	26.93%	2.957%
26	13.921	2004	2012	2015	rBV	1116904	1052987	49.36%	5.421%
27	13.945	2015	2016	2019	rVB	74691	46969	2.20%	0.242%
28	14.080	2036	2039	2041	rBV	26784	35626	1.67%	0.183%
29	14.386	2088	2091	2092	rBV2	32722	31200	1.46%	0.161%
30	14.433	2097	2099	2106	rVB	72089	82876	3.88%	0.427%
31	14.568	2118	2122	2129	rBV	44341	69842	3.27%	0.360%
32	14.680	2138	2141	2145	rVB	44682	44755	2.10%	0.230%
33	14.951	2183	2187	2194	rBV	70007	130028	6.10%	0.669%
34	15.010	2194	2197	2200	rBV	55657	64838	3.04%	0.334%

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100820\
Data File : BF121890.D
Acq On : 8 Oct 2020 15:43
Operator : JU/CG
Sample : L4297-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-RBR-200034

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-BF091020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.239	2233	2236	2242	rVB	47373	67924	3.18%	0.350%
36	15.298	2243	2246	2252	rVV	51014	71119	3.33%	0.366%
37	15.362	2252	2257	2267	rVV	716222	933443	43.76%	4.805%
38	15.786	2325	2329	2333	rBV	45334	62808	2.94%	0.323%
39	15.862	2338	2342	2348	rBV2	44743	97210	4.56%	0.500%

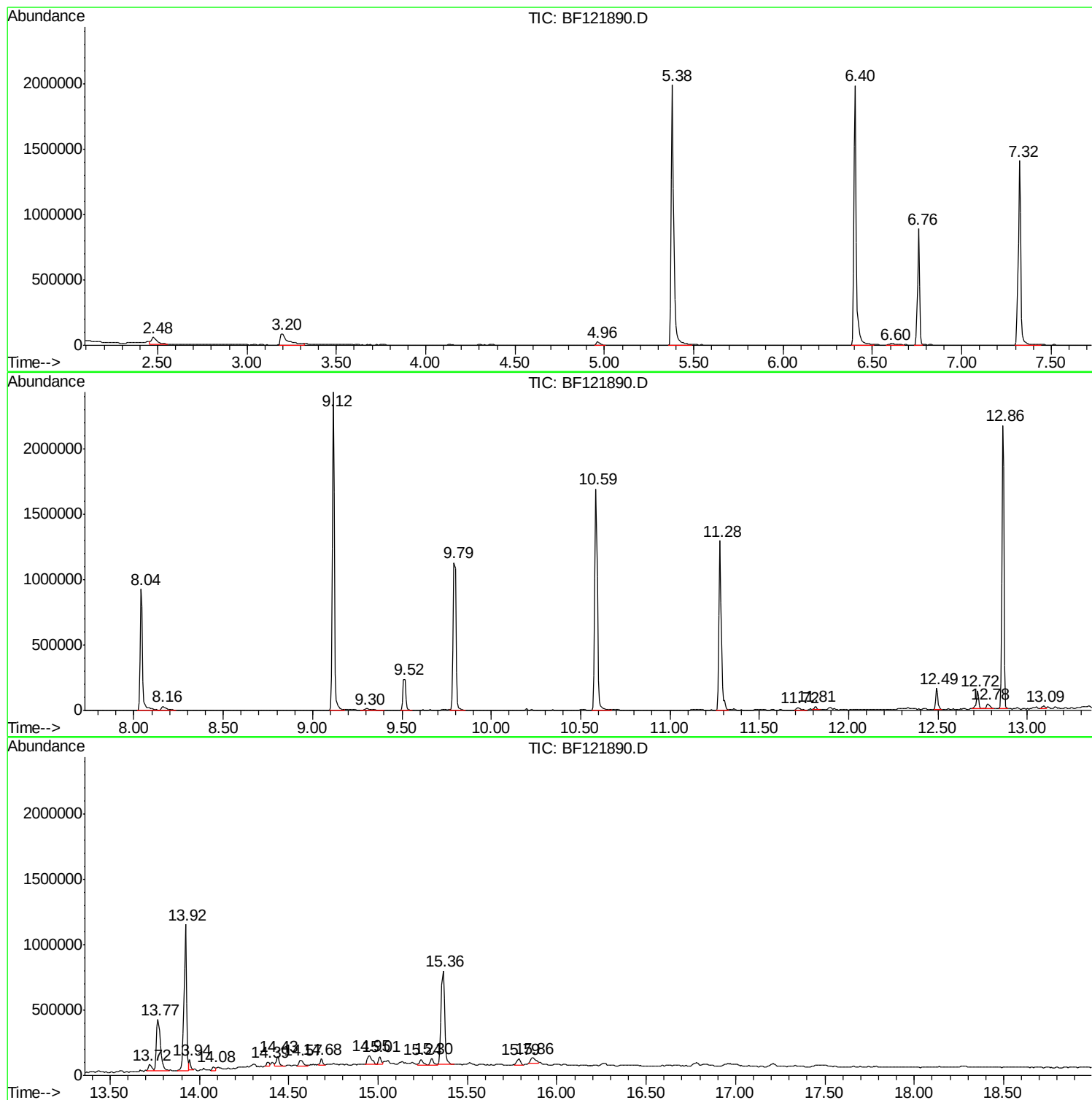
Sum of corrected areas: 19425004

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100820\
Data File : BF121890.D
Acq On : 8 Oct 2020 15:43
Operator : JU/CG
Sample : L4297-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
RO-RBR-200034

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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\BF100820\
Data File : BF121890.D
Acq On : 8 Oct 2020 15:43
Operator : JU/CG
Sample : L4297-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-RBR-200034

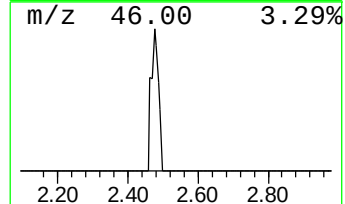
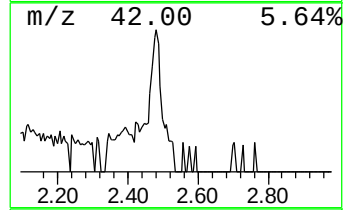
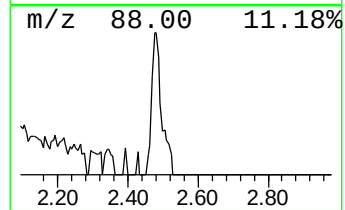
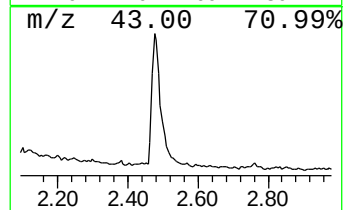
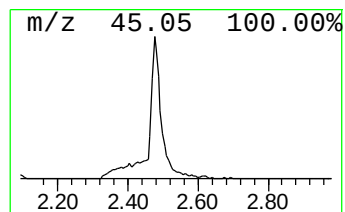
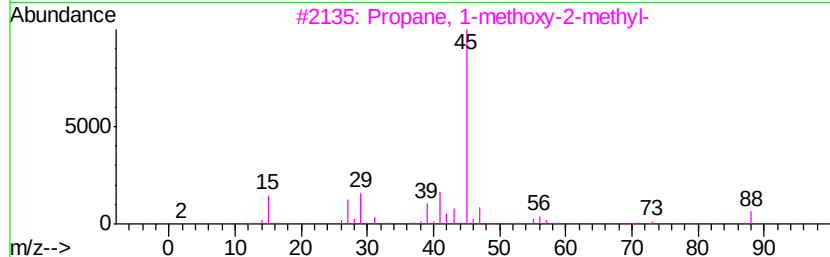
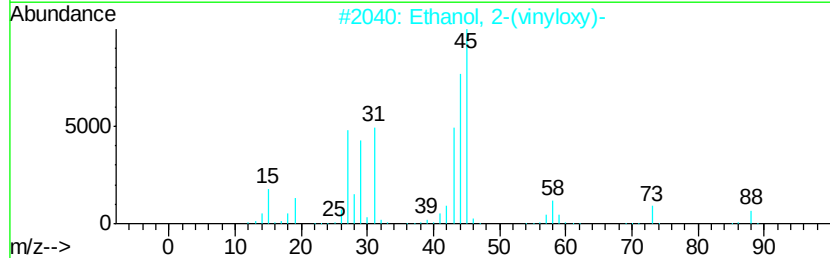
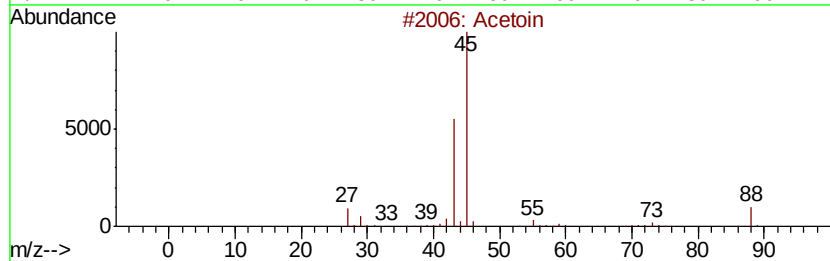
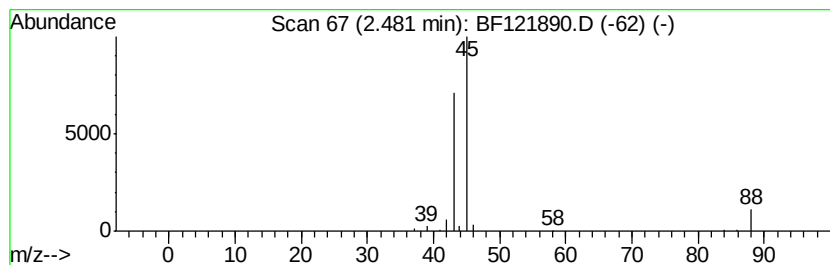
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Acetoin Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.48	3.06 ng	104433	1,4-Dichlorobenzene-d4	6.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetoin	88	C4H8O2	000513-86-0	83
2			Ethanol, 2-(vinlyoxy)-	88	C4H8O2	000764-48-7	9
3			Propane, 1-methoxy-2-methyl-	88	C5H12O	000625-44-5	9
4			2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	9
5			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	7



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100820\
Data File : BF121890.D
Acq On : 8 Oct 2020 15:43
Operator : JU/CG
Sample : L4297-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-RBR-200034

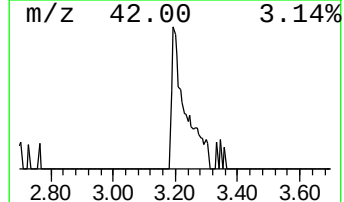
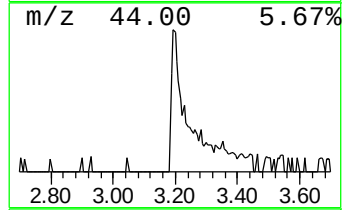
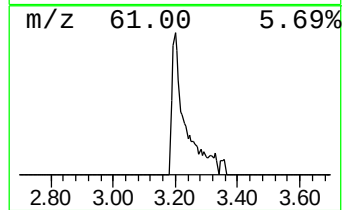
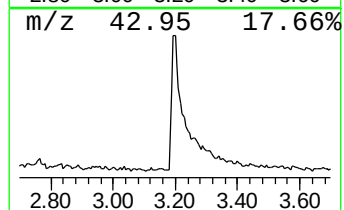
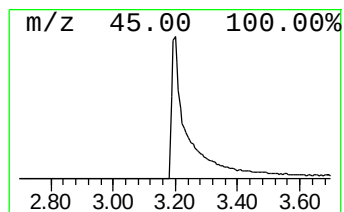
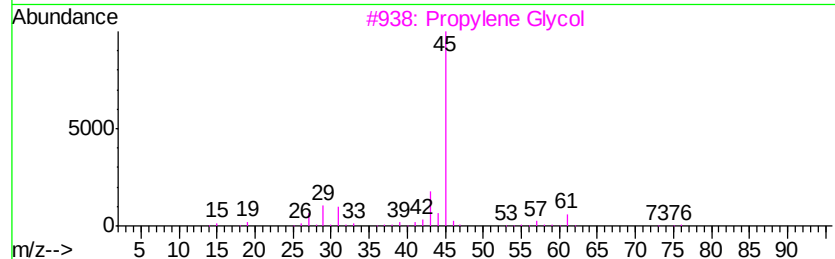
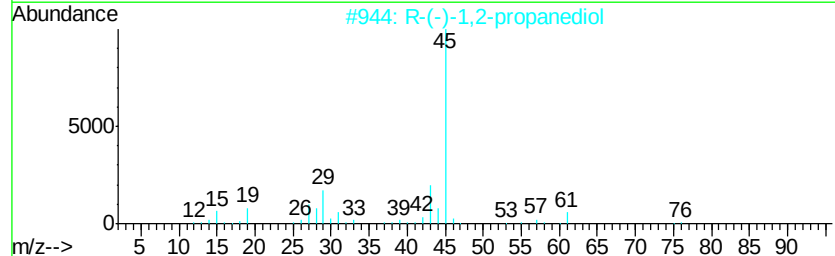
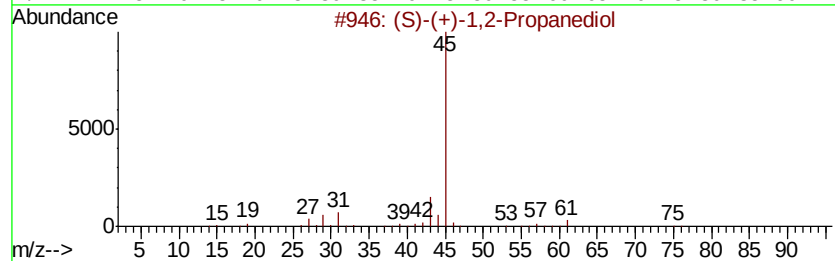
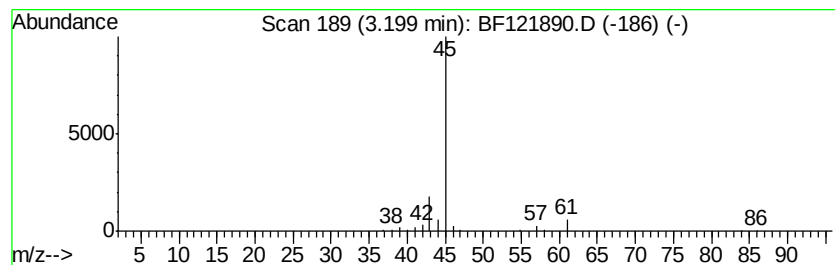
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	7.18 ng	245592	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3		Propylene Glycol	76	C3H8O2	000057-55-6	43
4		2-Butanol	74	C4H10O	000078-92-2	9
5		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100820\
Data File : BF121890.D
Acq On : 8 Oct 2020 15:43
Operator : JU/CG
Sample : L4297-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

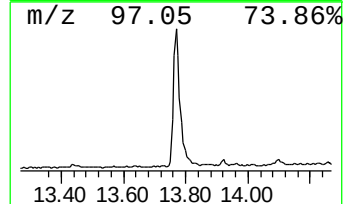
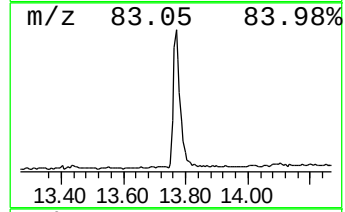
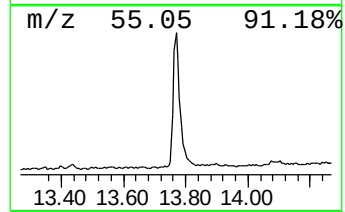
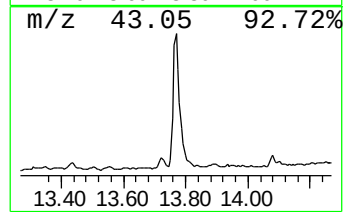
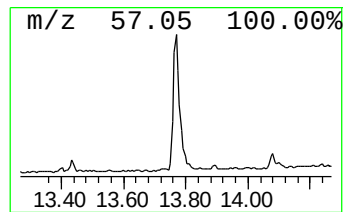
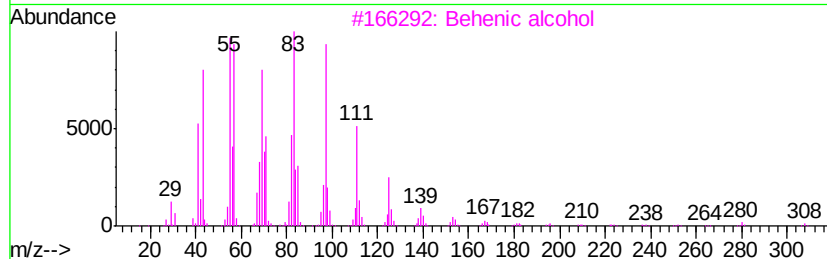
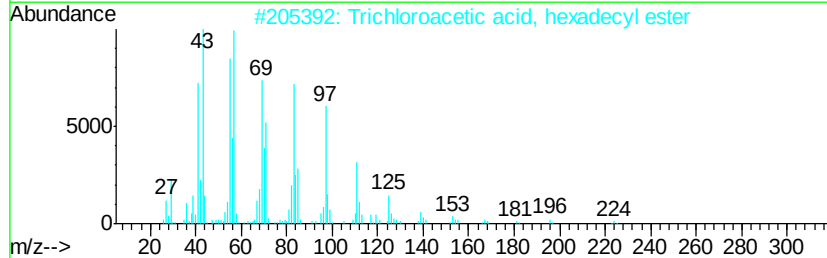
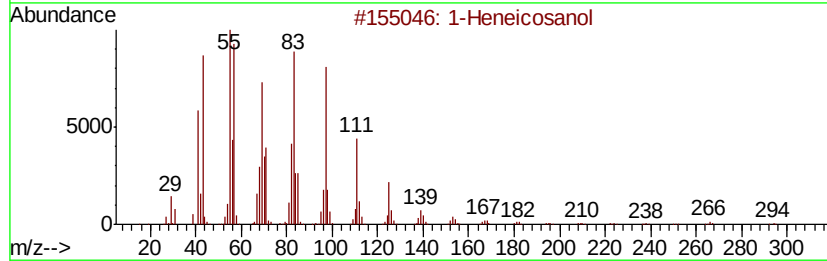
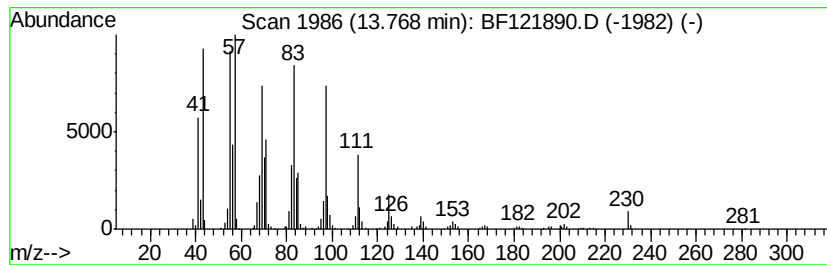
Instrument :
BNA_F
ClientSampleId :
RO-RBR-200034

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	10.91 ng	574442	Chrysene-d12	13.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosanol	312 C21H44O	015594-90-8	95
2	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	94
3	Behenic alcohol	326 C22H46O	000661-19-8	93
4	n-Tetracosanol-1	354 C24H50O	000506-51-4	93
5	Trifluoroacetoxy hexadecane	338 C18H33F3O2	006222-03-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100820\
Data File : BF121890.D
Acq On : 8 Oct 2020 15:43
Operator : JU/CG
Sample : L4297-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-RBR-200034

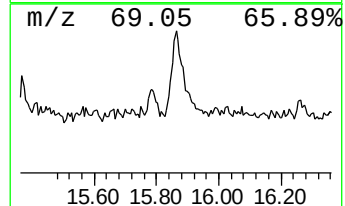
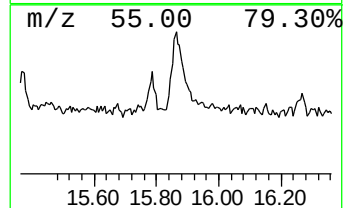
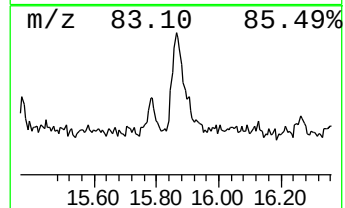
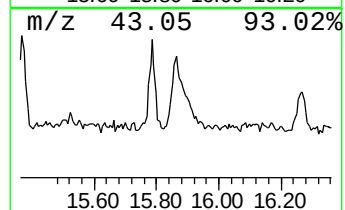
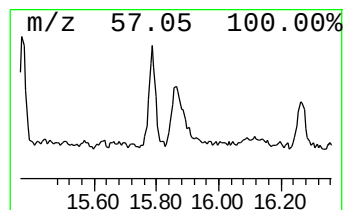
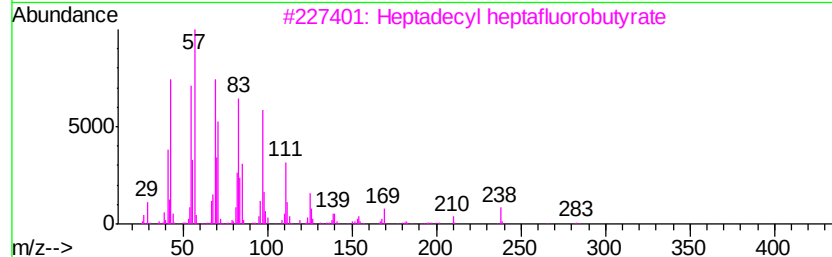
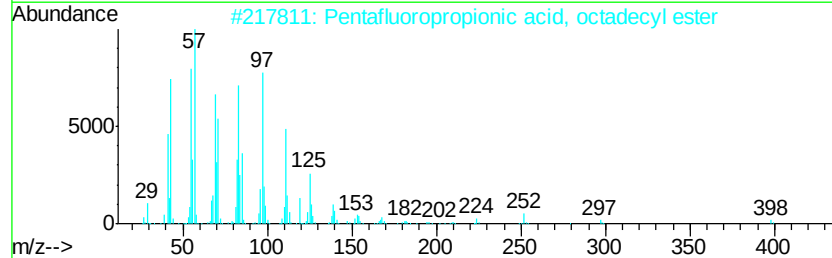
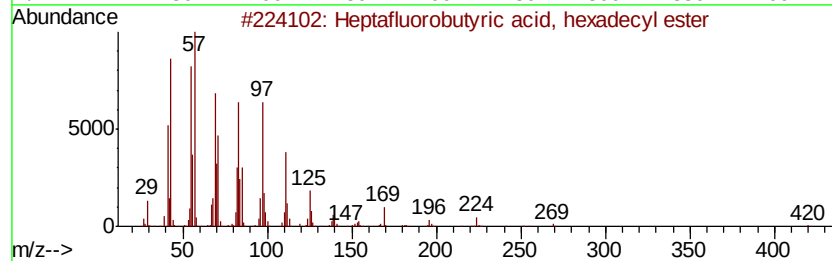
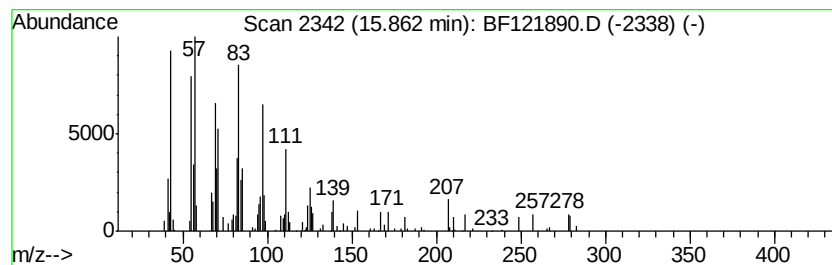
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptafluorobutyric acid, he... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	2.08 ng	97210	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
2		Pentafluoropropionic acid, octadec...	416	C21H37F5O2	959261-25-7	91
3		Heptadecyl heptafluorobutyrat	452	C21H35F7O2	959085-66-6	91
4		Pentafluoropropionic acid, hexadec...	388	C19H33F5O2	006222-07-7	91
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100820\
Data File : BF121890.D
Acq On : 8 Oct 2020 15:43
Operator : JU/CG
Sample : L4297-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-RBR-200034

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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
Acetoin	2.48	3.1	ng	104433	1	6.76	683642	20.0
(S)-(+)-1,2-Propa...	3.20	7.2	ng	245592	1	6.76	683642	20.0
1-Heneicosanol	13.77	10.9	ng	574442	5	13.92	1052990	20.0
Heptafluorobutyri...	15.86	2.1	ng	97210	6	15.36	933443	20.0