

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
 Data File : BF125167.D
 Acq On : 23 Aug 2021 21:50
 Operator : JU/CG
 Sample : M3430-07
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-7

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125167.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.211	15	21	27	rVB	1246176	1599210	40.59%	5.164%
2	5.146	516	520	525	rVB	107815	122136	3.10%	0.394%
3	5.534	581	586	590	rBV	3368903	3560894	90.39%	11.499%
4	6.540	751	757	760	rBV	3560159	3551366	90.14%	11.468%
5	6.922	818	822	825	rVB	1124294	963050	24.45%	3.110%
6	7.481	912	917	920	rBV	2568199	2299305	58.36%	7.425%
7	8.098	1019	1022	1036	rBV	904921	837184	21.25%	2.704%
8	8.204	1036	1040	1043	rVV	1520094	1252310	31.79%	4.044%
9	9.281	1218	1223	1226	rBV	4480830	3939644	100.00%	12.722%
10	9.957	1335	1338	1342	rBV	1686475	1405400	35.67%	4.538%
11	10.745	1468	1472	1476	rBV	2811279	2630470	66.77%	8.495%
12	11.445	1587	1591	1594	rBV	1682195	1404400	35.65%	4.535%
13	11.963	1674	1679	1684	rBV2	312855	306599	7.78%	0.990%
14	12.657	1794	1797	1801	rBV	132233	119880	3.04%	0.387%
15	12.751	1810	1813	1817	rBV2	85805	88376	2.24%	0.285%
16	12.886	1831	1836	1841	rBV	119597	133777	3.40%	0.432%
17	13.033	1856	1861	1864	rBV	4075381	3539260	89.84%	11.429%
18	13.951	2010	2017	2031	rBV5	112392	386384	9.81%	1.248%
19	14.086	2035	2040	2043	rBV	1208500	1067543	27.10%	3.447%
20	14.598	2121	2127	2139	rVB3	70645	183979	4.67%	0.594%
21	14.945	2183	2186	2190	rVB2	35416	43942	1.12%	0.142%
22	15.139	2216	2219	2223	rBV	49850	87515	2.22%	0.283%
23	15.216	2229	2232	2237	rVB2	55388	65082	1.65%	0.210%
24	15.298	2244	2246	2257	rVB7	39035	81325	2.06%	0.263%
25	15.516	2279	2283	2288	rBV	46587	57655	1.46%	0.186%
26	15.586	2290	2295	2307	rVB	795289	1079229	27.39%	3.485%
27	16.063	2372	2376	2382	rVB2	65234	94712	2.40%	0.306%
28	17.215	2567	2572	2580	rVB3	28889	65705	1.67%	0.212%

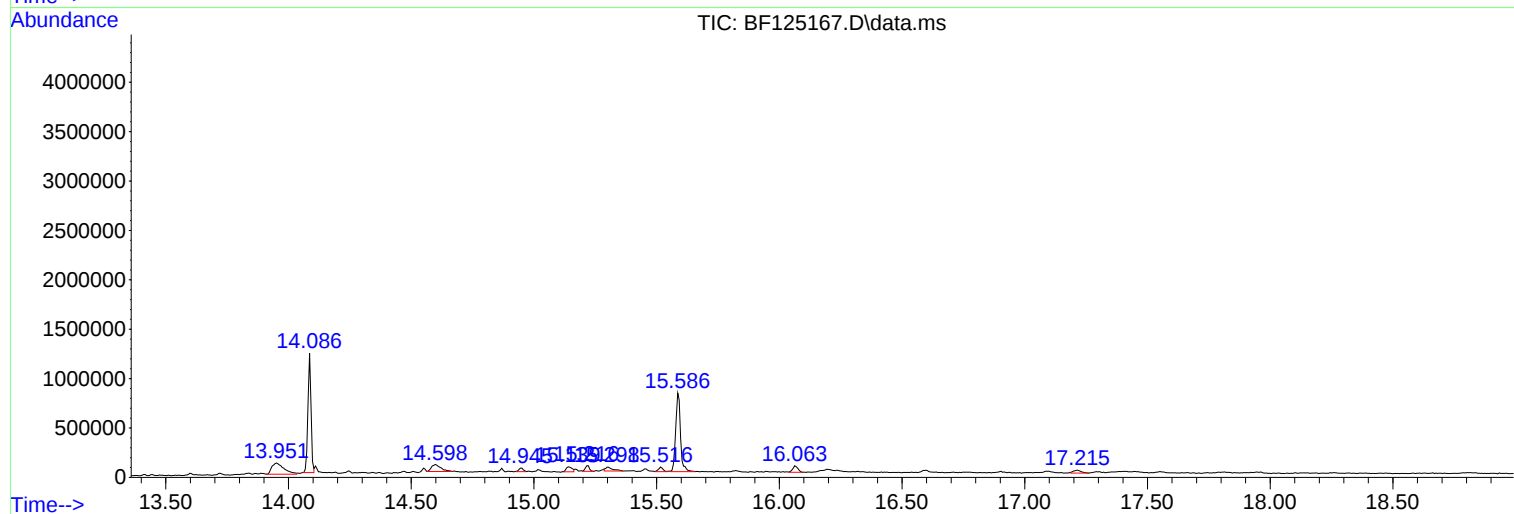
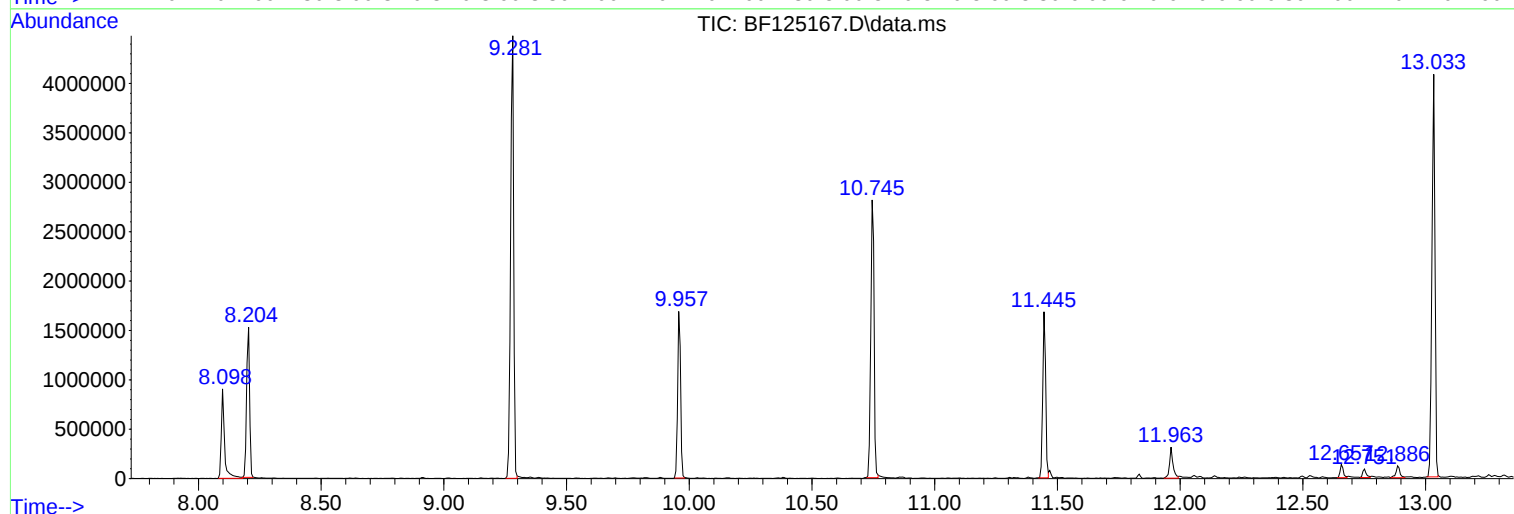
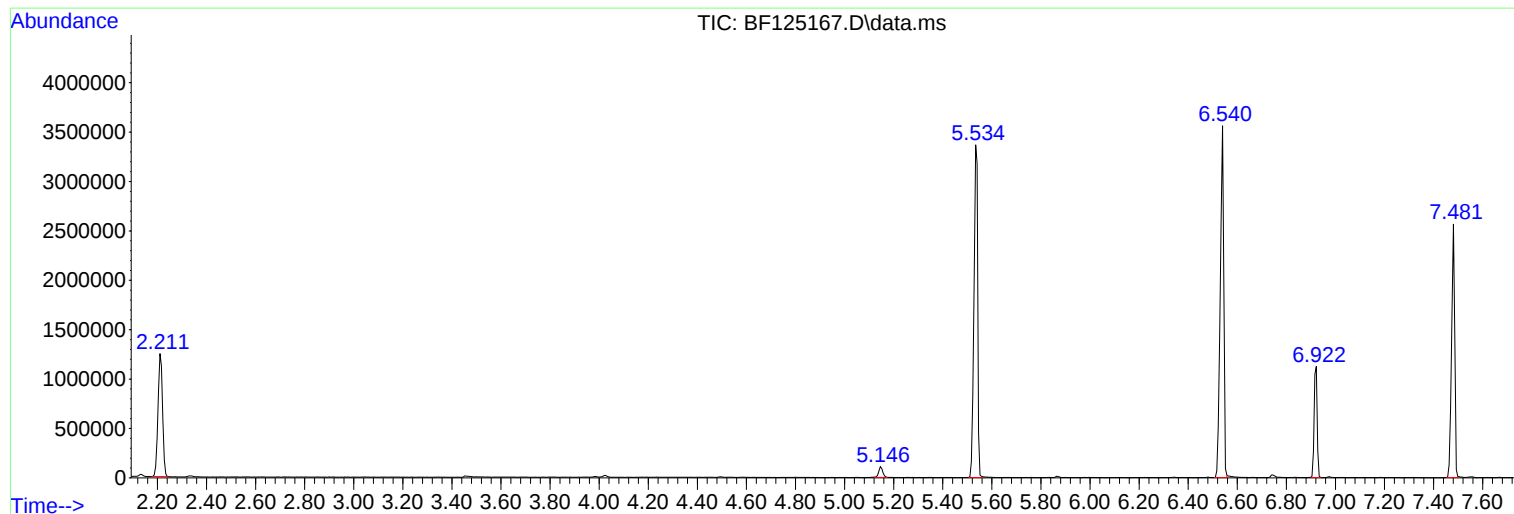
Sum of corrected areas: 30966332

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125167.D
Acq On : 23 Aug 2021 21:50
Operator : JU/CG
Sample : M3430-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125167.D
Acq On : 23 Aug 2021 21:50
Operator : JU/CG
Sample : M3430-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PE-7

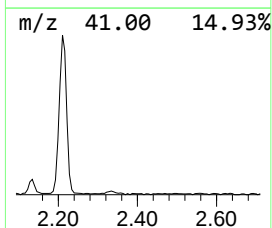
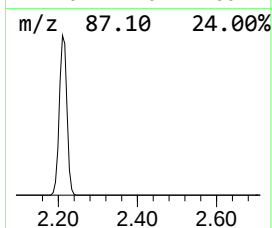
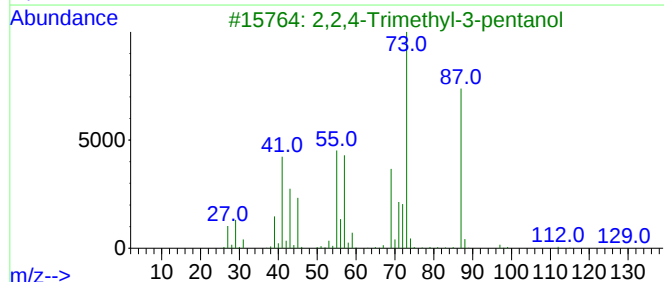
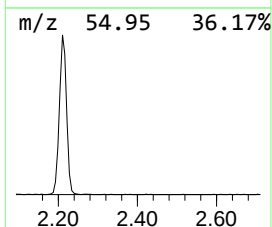
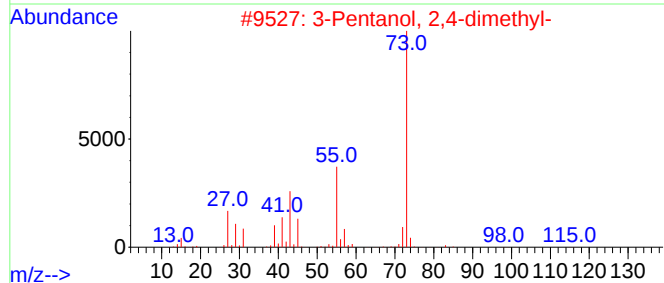
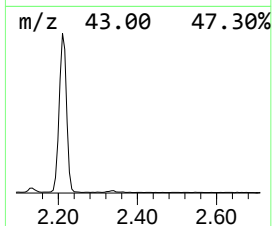
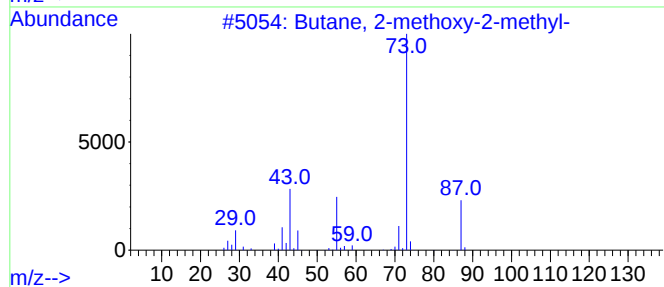
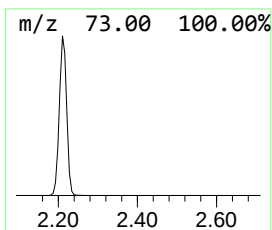
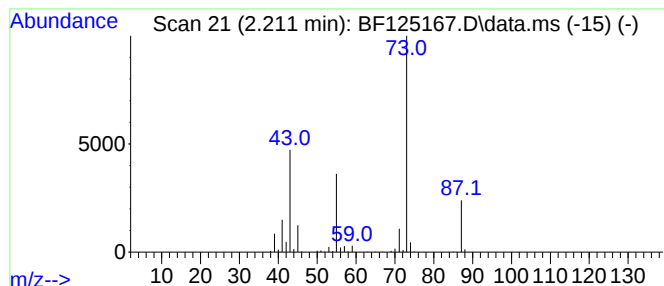
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.211	33.21 ng	1599210	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125167.D
Acq On : 23 Aug 2021 21:50
Operator : JU/CG
Sample : M3430-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-7

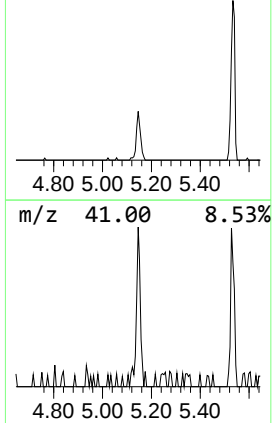
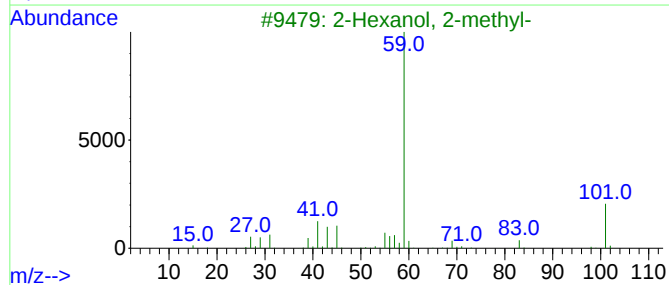
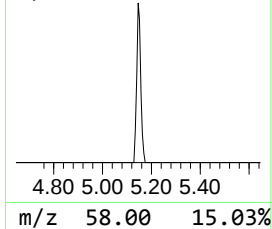
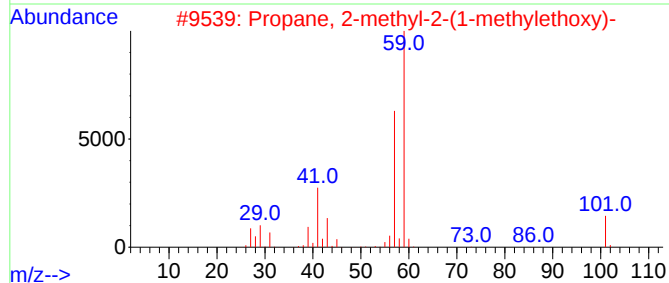
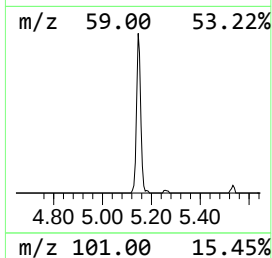
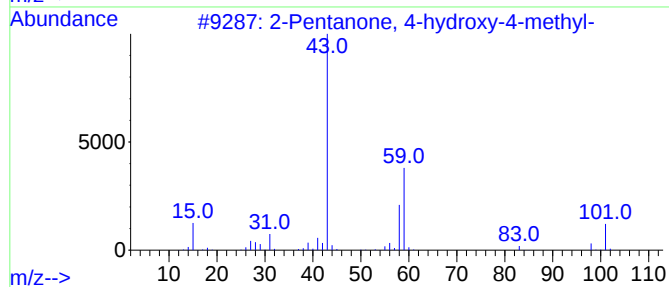
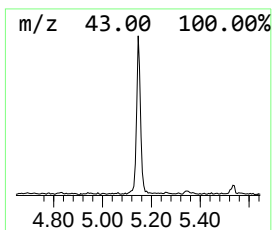
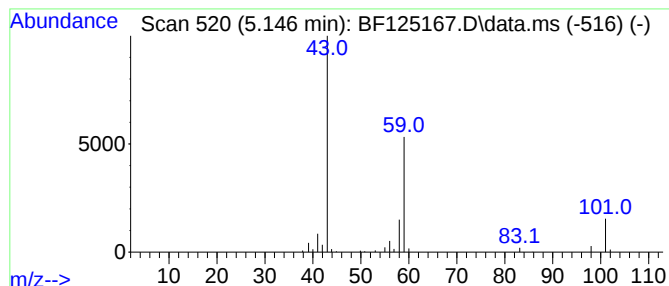
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.146	2.54 ng	122136	1,4-Dichlorobenzene-d4	6.922

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125167.D
Acq On : 23 Aug 2021 21:50
Operator : JU/CG
Sample : M3430-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-7

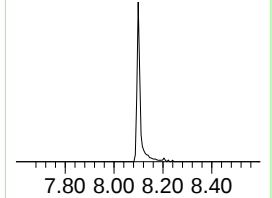
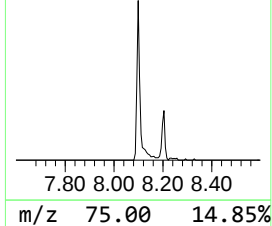
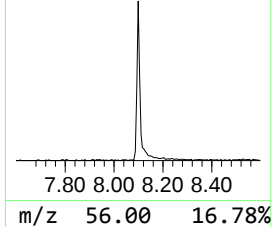
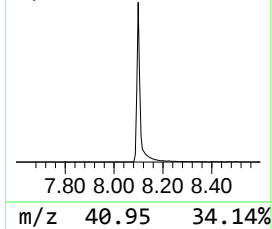
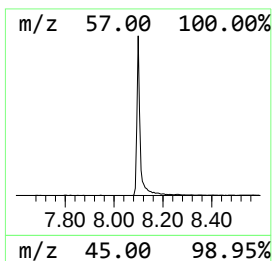
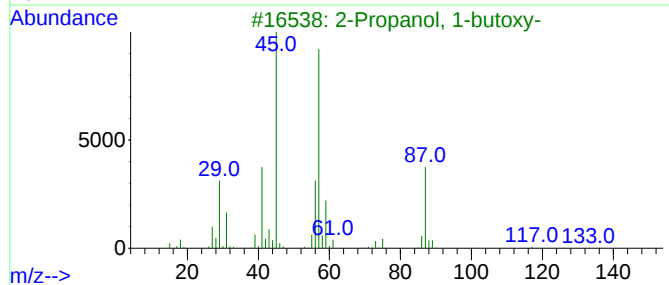
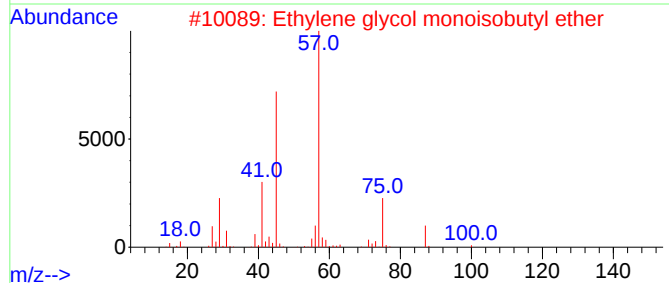
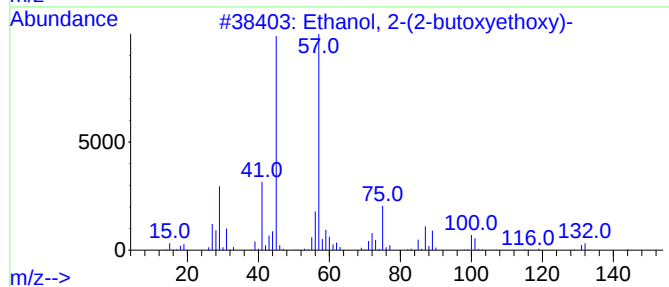
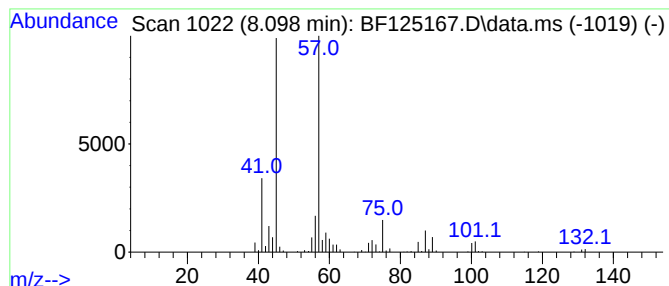
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	13.37 ng	837184	Naphthalene-d8	8.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3			2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	59
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125167.D
Acq On : 23 Aug 2021 21:50
Operator : JU/CG
Sample : M3430-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-7

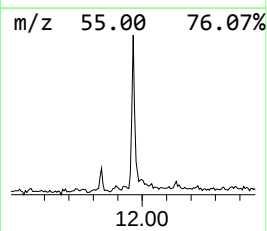
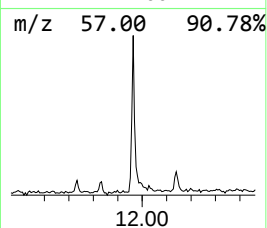
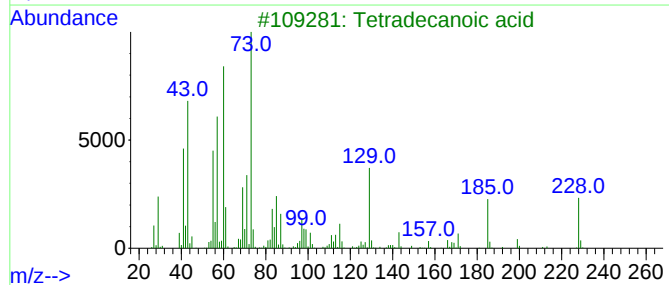
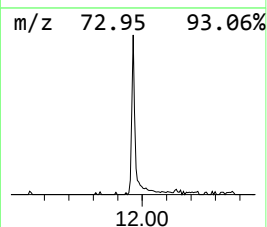
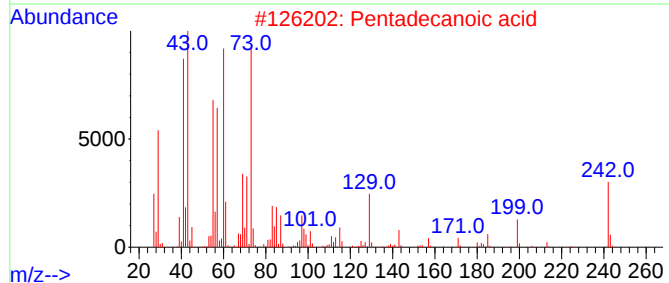
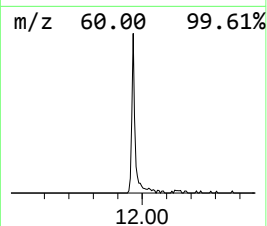
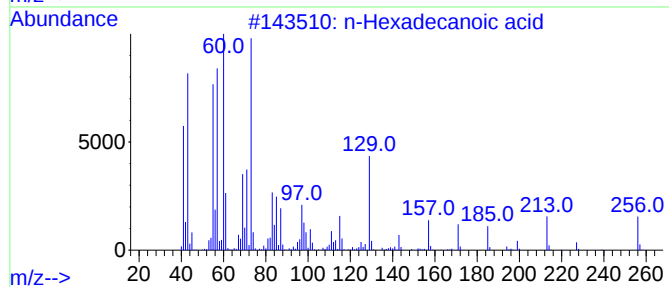
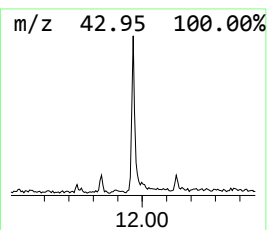
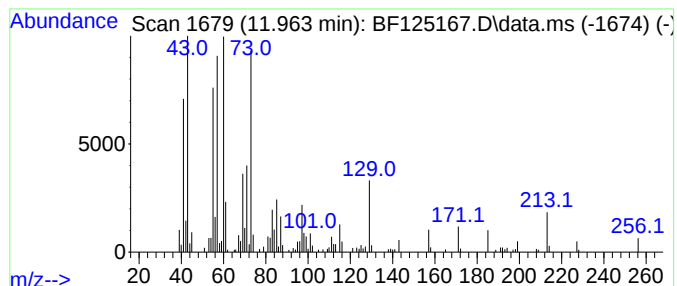
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.963	4.37 ng	306599	Phenanthrene-d10	11.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	70
5			Nonanoic acid	158	C9H18O2	000112-05-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125167.D
Acq On : 23 Aug 2021 21:50
Operator : JU/CG
Sample : M3430-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-7

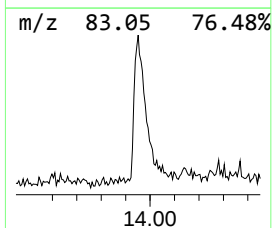
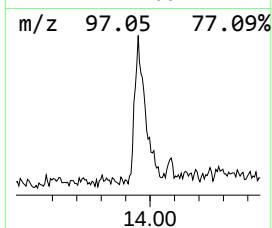
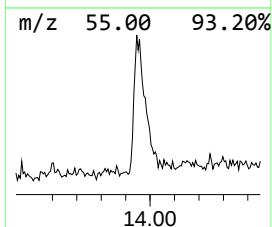
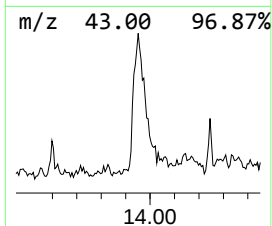
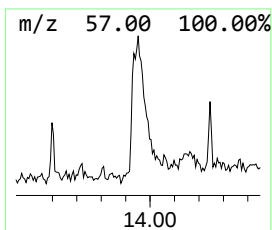
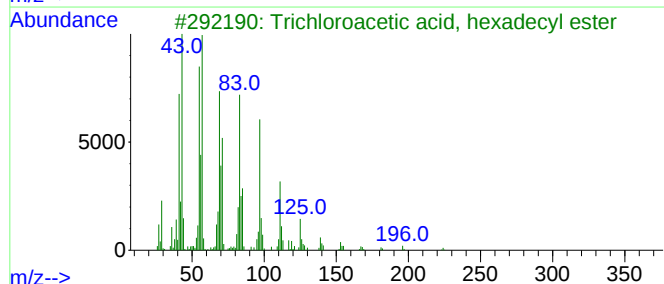
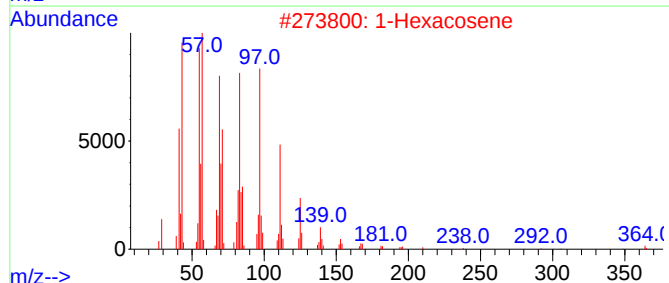
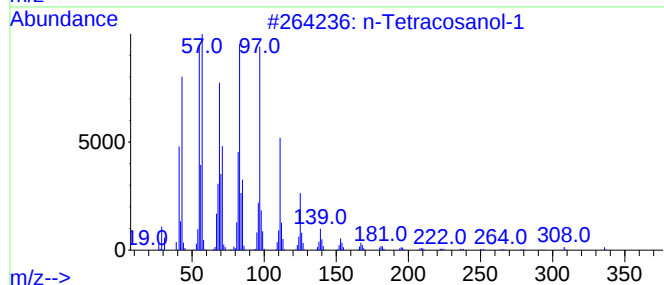
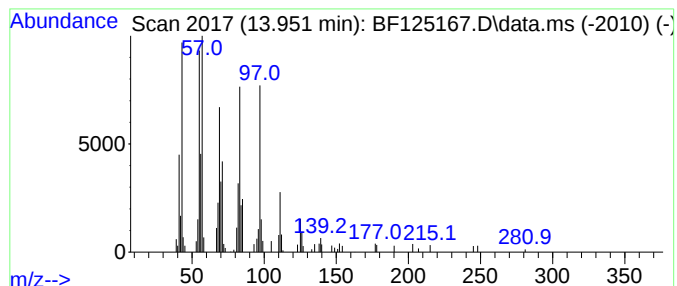
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.951	7.24 ng	386384	Chrysene-d12	14.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2			1-Hexacosene	364	C26H52	018835-33-1	90
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
4			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
5			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125167.D
Acq On : 23 Aug 2021 21:50
Operator : JU/CG
Sample : M3430-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-7

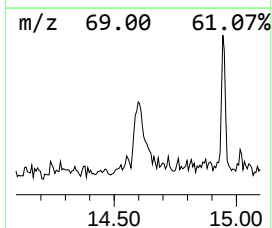
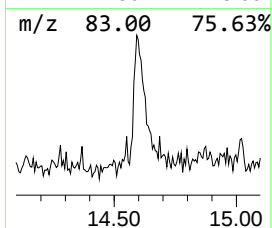
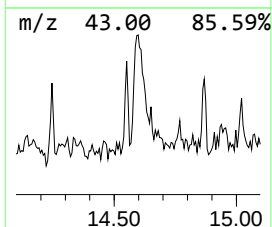
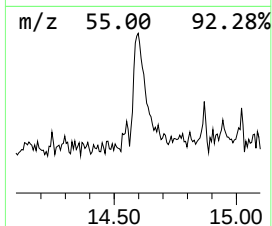
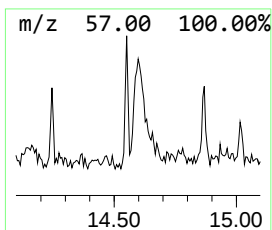
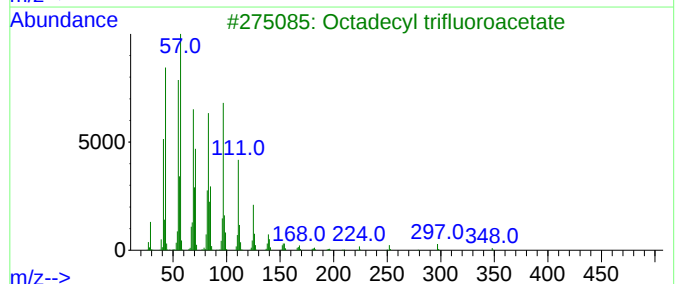
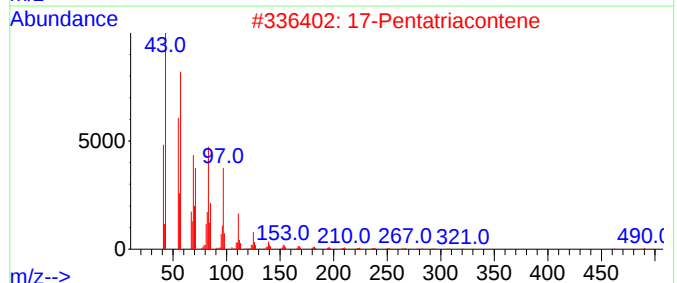
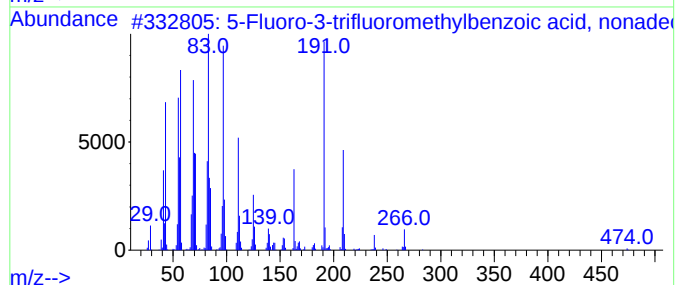
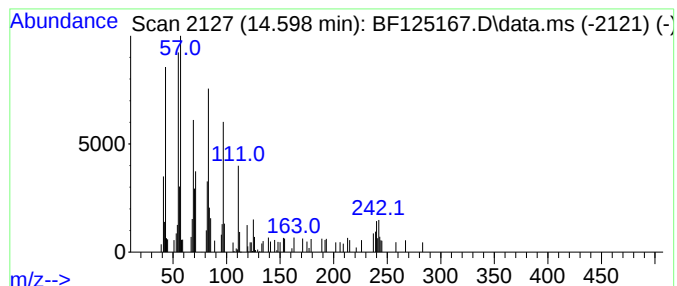
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 5-Fluoro-3-trifluoromethylb... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.598	3.45 ng	183979	Chrysene-d12	14.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Fluoro-3-trifluoromethylbenzoi...	474	C27H42F4O2	1000338-91-1	81
2			17-Pentatriacontene	491	C35H70	006971-40-0	74
3			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	74
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	74
5			1-Tricosene	322	C23H46	018835-32-0	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125167.D
Acq On : 23 Aug 2021 21:50
Operator : JU/CG
Sample : M3430-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.211	33.2	ng	1599210	1	6.922	963050	20.0
2-Pentanone, 4-...	5.146	2.5	ng	122136	1	6.922	963050	20.0
Ethanol, 2-(2-b...	8.098	13.4	ng	837184	2	8.204	1252310	20.0
n-Hexadecanoic ...	11.963	4.4	ng	306599	4	11.445	1404400	20.0
n-Tetracosanol-1	13.951	7.2	ng	386384	5	14.086	1067540	20.0
5-Fluoro-3-trif...	14.598	3.5	ng	183979	5	14.086	1067540	20.0