

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
 Data File : BF125605.D
 Acq On : 23 Sep 2021 22:22
 Operator : JU/CG
 Sample : M3889-04
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUP-UST-04-(13-15)

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-BF092121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125605.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	12	20	26	rVB	1354233	1798837	33.34%	4.374%
2	5.516	577	583	586	rBV	3952395	4185370	77.57%	10.177%
3	6.516	747	753	755	rBV	3661518	4172003	77.32%	10.144%
4	6.892	814	817	821	rVB	1562514	1234296	22.88%	3.001%
5	7.451	907	912	915	rBV	2929346	2729105	50.58%	6.636%
6	8.075	1014	1018	1021	rBV	1625994	1324005	24.54%	3.219%
7	8.175	1031	1035	1038	rBV	2127543	1732356	32.11%	4.212%
8	9.251	1213	1218	1221	rBV	5901374	5172002	95.86%	12.576%
9	9.933	1329	1334	1337	rBV	2250836	2017894	37.40%	4.907%
10	10.716	1463	1467	1482	rVB	3563466	3383688	62.71%	8.228%
11	11.416	1582	1586	1589	rBV	2614177	2105392	39.02%	5.119%
12	11.810	1650	1653	1656	rBV	186206	137343	2.55%	0.334%
13	11.939	1671	1675	1680	rBV	312062	278856	5.17%	0.678%
14	12.516	1767	1773	1777	rBV	109541	96287	1.78%	0.234%
15	12.727	1805	1809	1815	rBV	89737	102363	1.90%	0.249%
16	13.004	1851	1856	1859	rBV	5782592	5395495	100.00%	13.119%
17	13.692	1967	1973	1983	rVB10	23479	74088	1.37%	0.180%
18	13.898	2004	2008	2023	rBV	422701	544069	10.08%	1.323%
19	14.057	2030	2035	2038	rBV	2058847	1955401	36.24%	4.755%
20	14.221	2058	2063	2067	rBV	57258	57154	1.06%	0.139%
21	14.527	2112	2115	2123	rBV3	79682	122518	2.27%	0.298%
22	14.921	2177	2182	2186	rBV	309760	320795	5.95%	0.780%
23	15.186	2223	2227	2231	rBV	64114	71202	1.32%	0.173%
24	15.533	2281	2286	2291	rBV	1343658	1737349	32.20%	4.224%
25	15.574	2291	2293	2300	rVB	67516	91169	1.69%	0.222%
26	16.027	2365	2370	2374	rBV	57227	82682	1.53%	0.201%
27	16.080	2374	2379	2387	rVV9	30385	68895	1.28%	0.168%
28	16.545	2453	2458	2466	rVB3	43689	70621	1.31%	0.172%
29	17.162	2556	2563	2568	rBV5	28204	64779	1.20%	0.158%

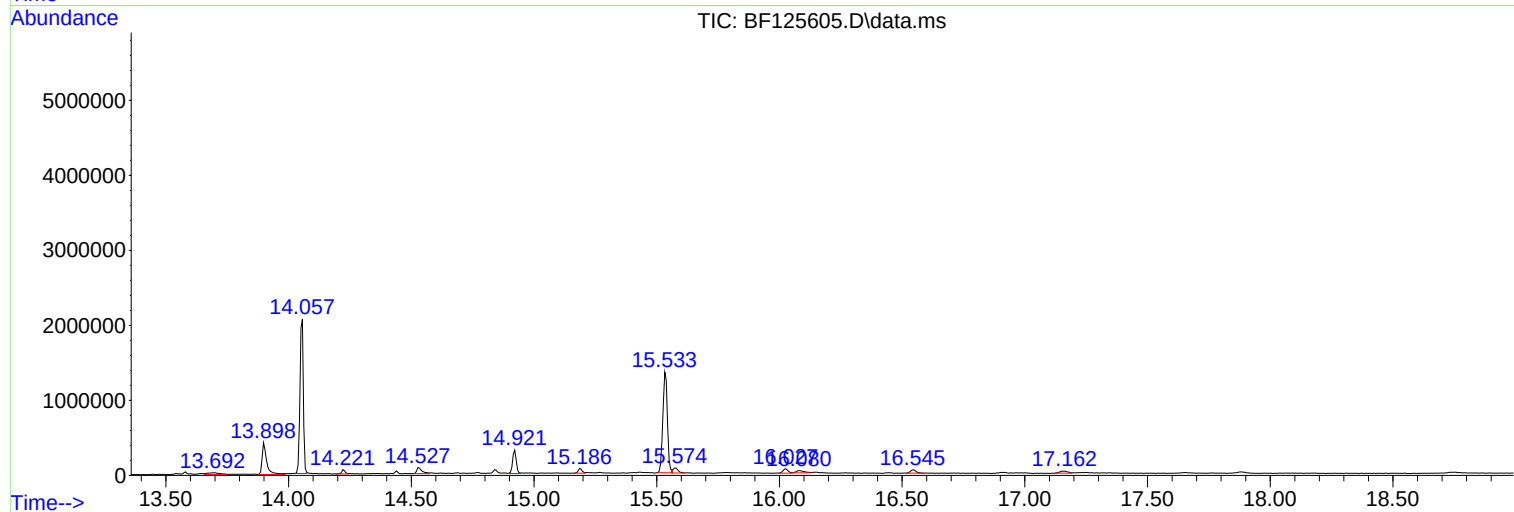
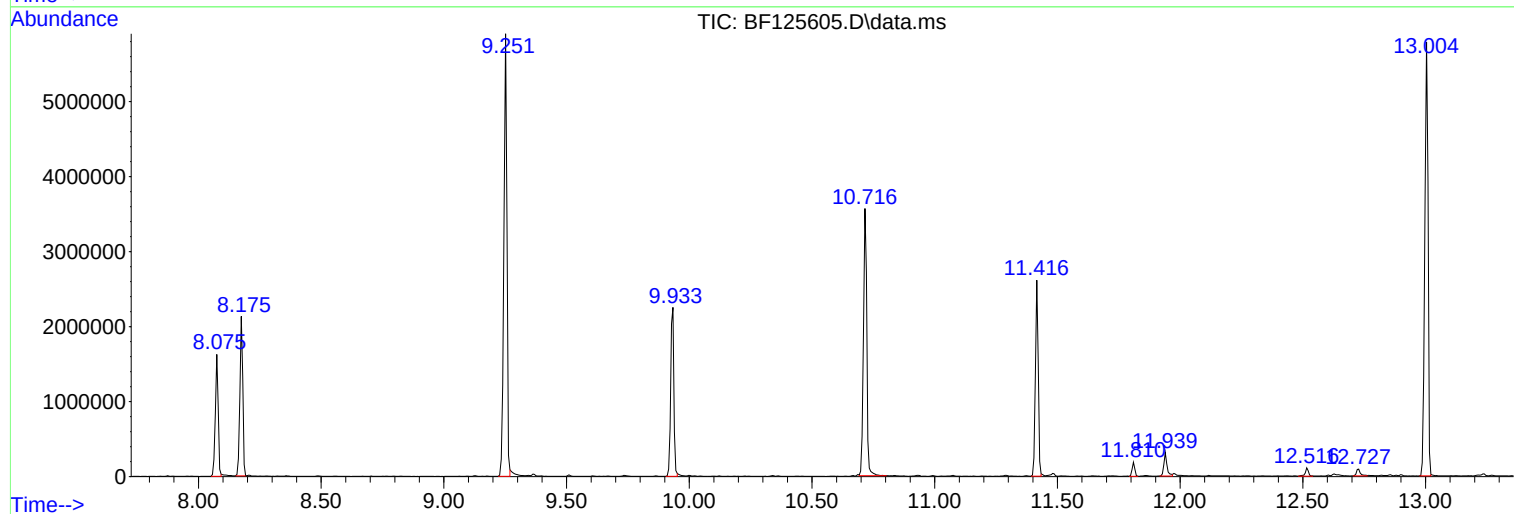
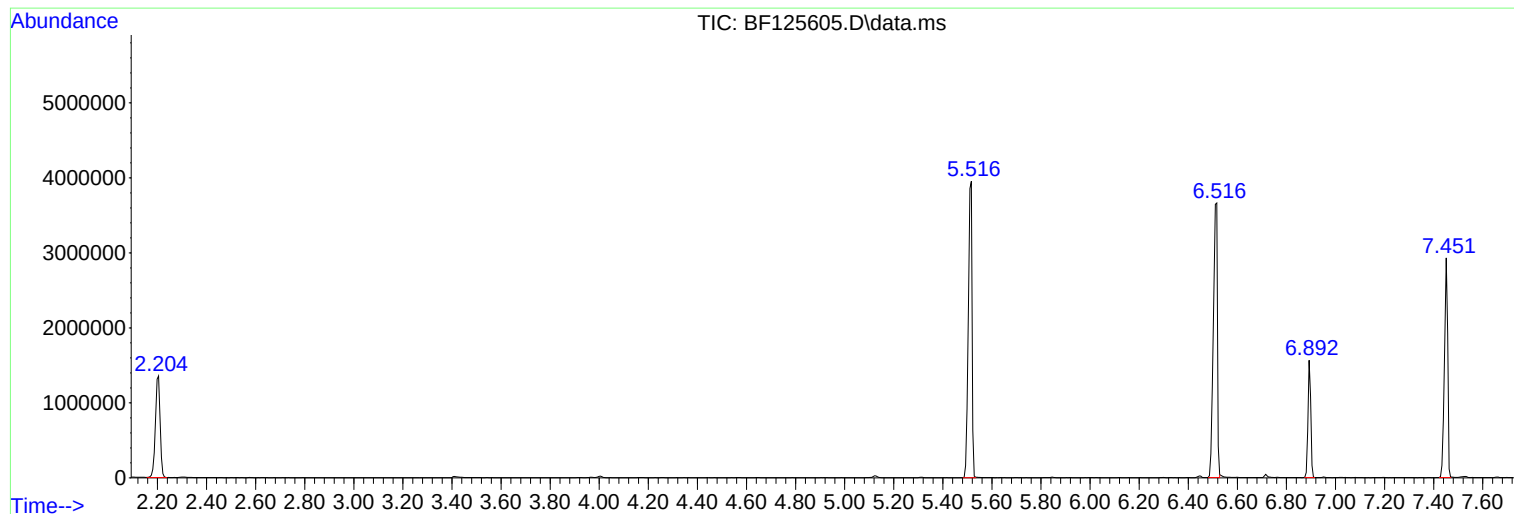
Sum of corrected areas: 41126014

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
Data File : BF125605.D
Acq On : 23 Sep 2021 22:22
Operator : JU/CG
Sample : M3889-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-UST-04-(13-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.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\BF092321\
Data File : BF125605.D
Acq On : 23 Sep 2021 22:22
Operator : JU/CG
Sample : M3889-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-UST-04-(13-15)

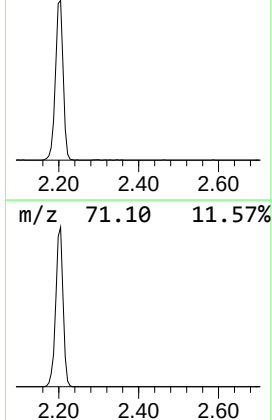
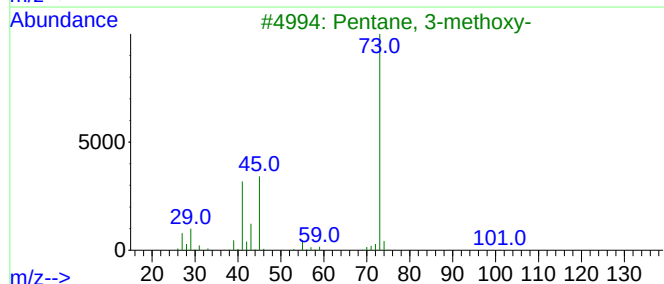
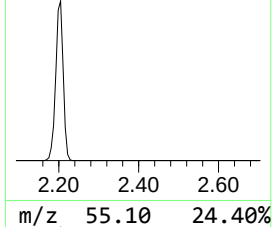
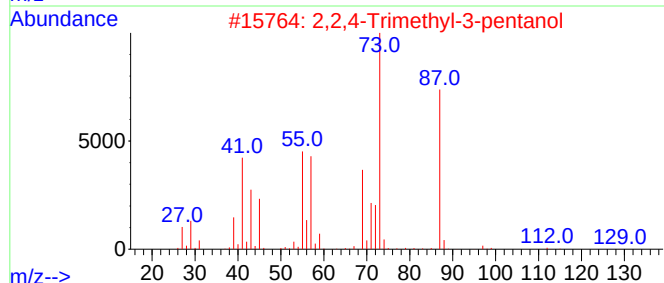
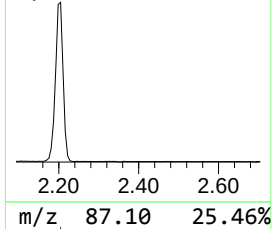
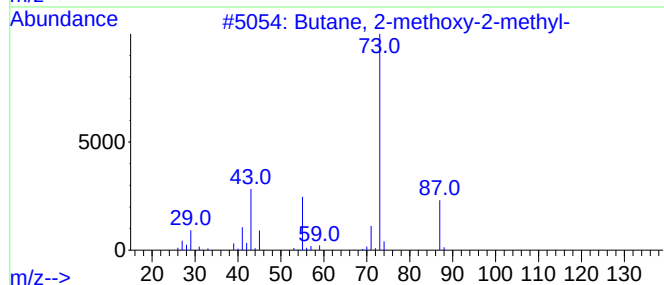
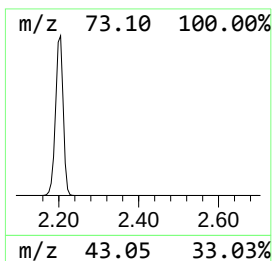
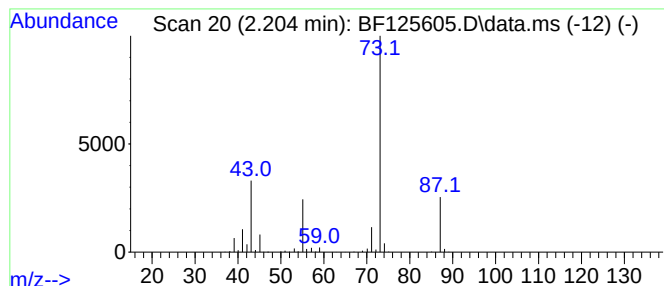
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.204	29.15 ng	1798840	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
Data File : BF125605.D
Acq On : 23 Sep 2021 22:22
Operator : JU/CG
Sample : M3889-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-UST-04-(13-15)

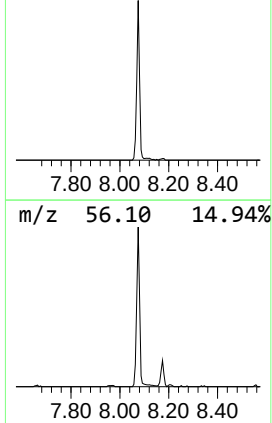
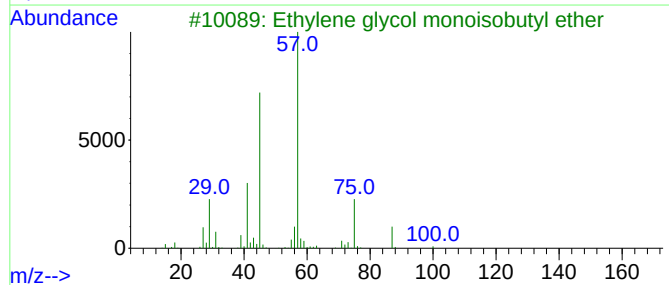
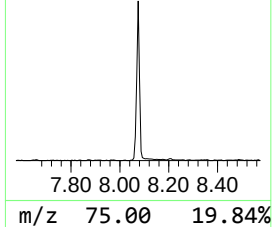
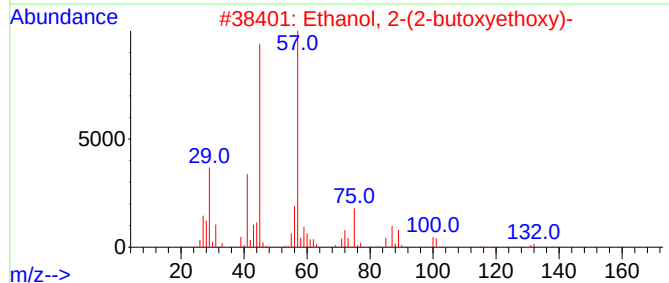
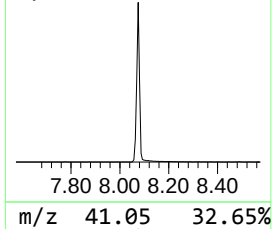
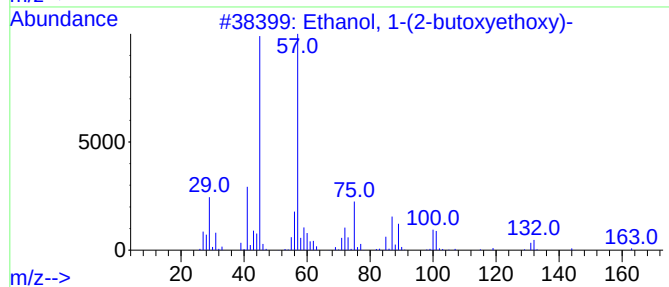
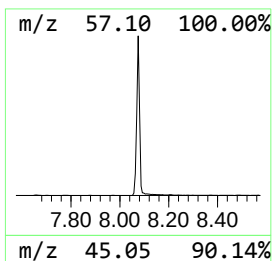
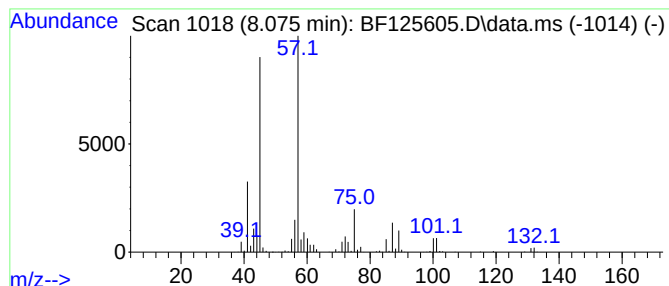
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.075	15.29 ng	1324010	Naphthalene-d8	8.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
Data File : BF125605.D
Acq On : 23 Sep 2021 22:22
Operator : JU/CG
Sample : M3889-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-UST-04-(13-15)

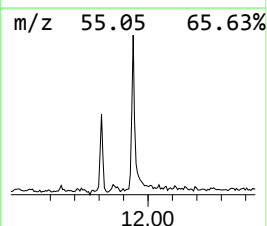
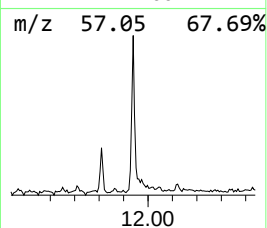
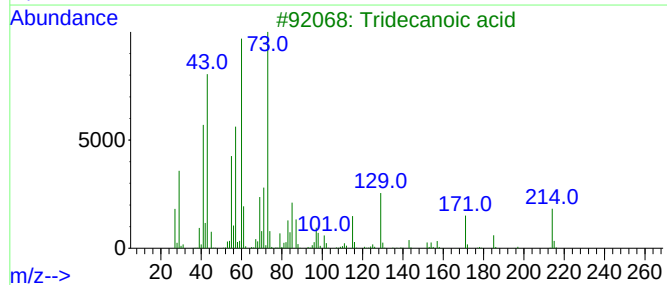
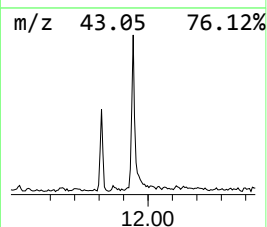
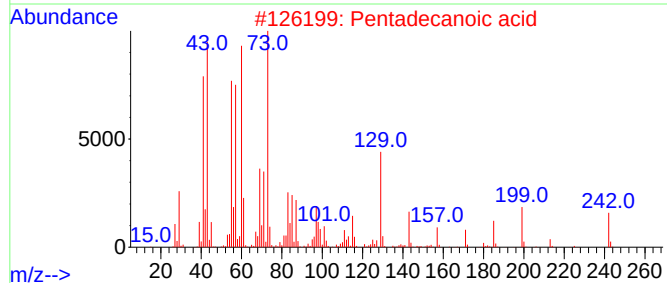
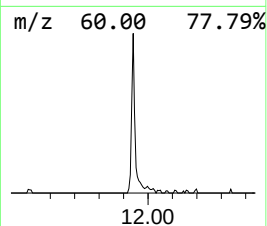
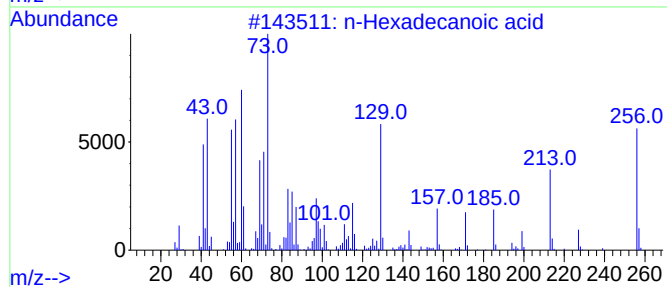
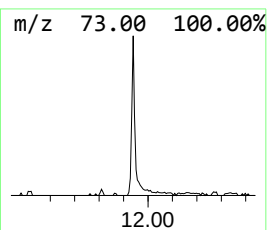
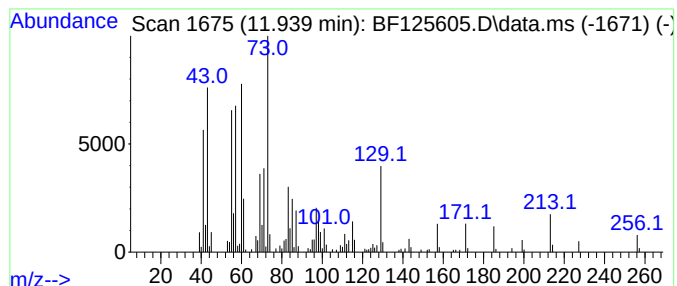
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	2.65 ng	278856	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	87
4			n-Decanoic acid	172	C10H20O2	000334-48-5	68
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
Data File : BF125605.D
Acq On : 23 Sep 2021 22:22
Operator : JU/CG
Sample : M3889-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-UST-04-(13-15)

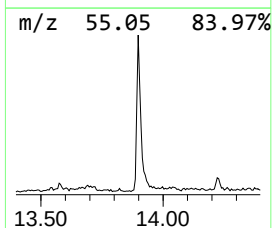
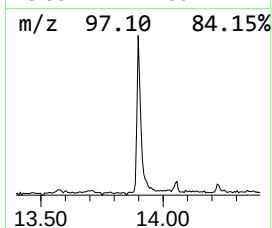
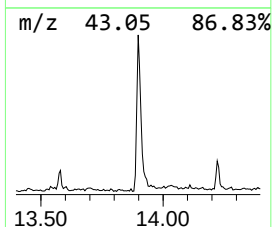
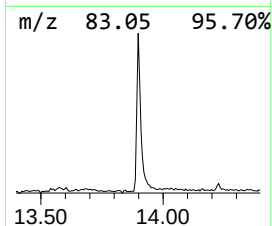
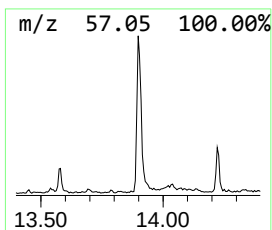
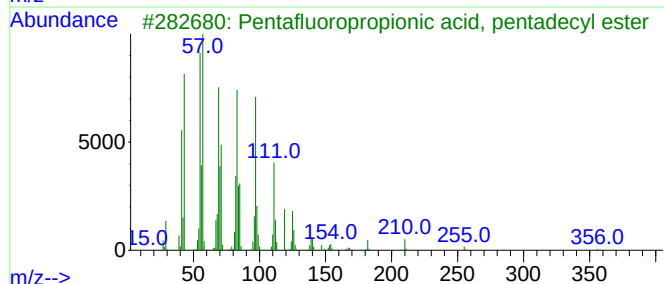
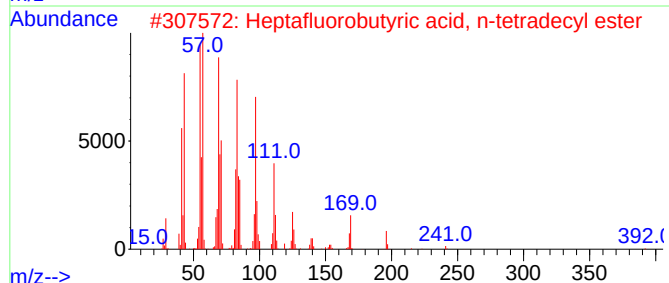
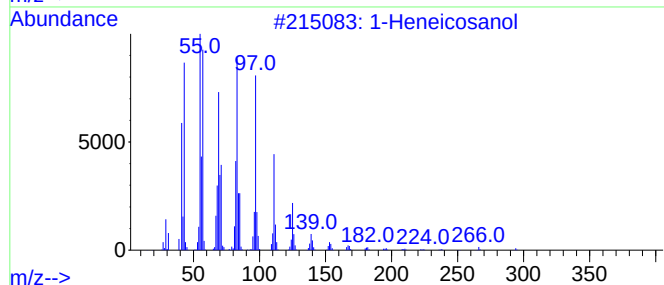
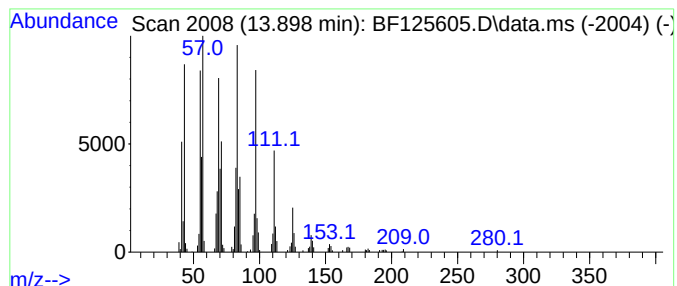
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	5.56 ng	544069	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4			1-Hexacosene	364	C26H52	018835-33-1	94
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
Data File : BF125605.D
Acq On : 23 Sep 2021 22:22
Operator : JU/CG
Sample : M3889-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-UST-04-(13-15)

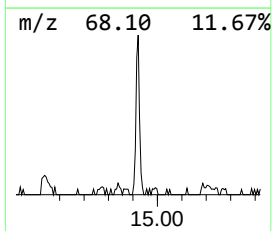
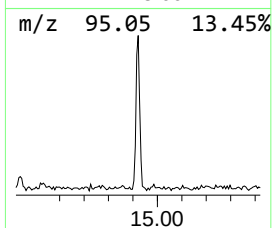
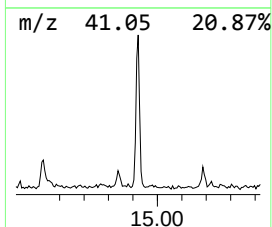
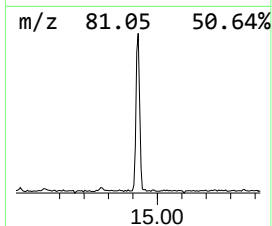
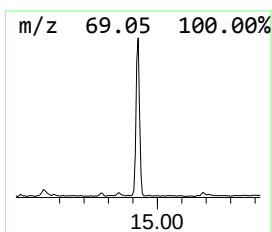
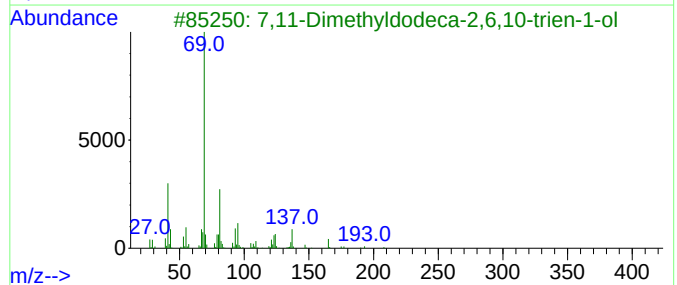
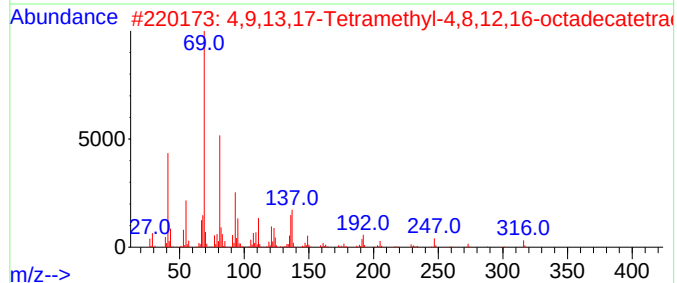
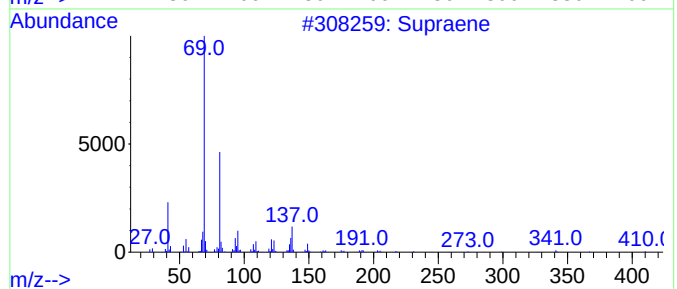
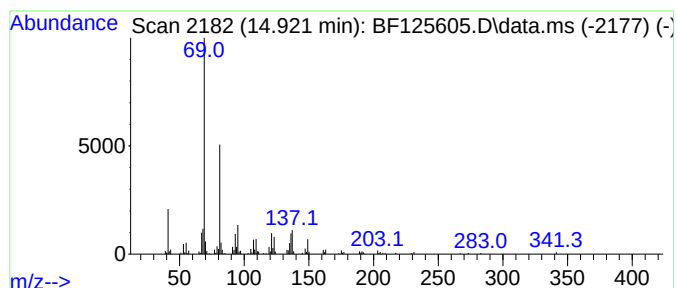
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.921	3.69 ng	320795	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4			Squalene	410	C30H50	000111-02-4	50
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
Data File : BF125605.D
Acq On : 23 Sep 2021 22:22
Operator : JU/CG
Sample : M3889-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-UST-04-(13-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.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...	2.204	29.1	ng	1798840	1	6.892	1234300	20.0
Ethanol, 1-(2-b...	8.075	15.3	ng	1324010	2	8.175	1732360	20.0
n-Hexadecanoic ...	11.939	2.6	ng	278856	4	11.416	2105390	20.0
1-Heneicosanol	13.898	5.6	ng	544069	5	14.057	1955400	20.0
Supraene	14.921	3.7	ng	320795	6	15.533	1737350	20.0