

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
 Data File : BF125112.D
 Acq On : 19 Aug 2021 13:55
 Operator : JU/CG
 Sample : M3443-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 210812088-02

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: BF125112.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	16	22	28	rBV	2403600	3223242	62.55%	12.735%
2	5.128	513	517	521	rBV	519910	494163	9.59%	1.953%
3	6.916	818	821	825	rVB	1144064	957211	18.58%	3.782%
4	7.481	912	917	920	rBV	3226521	3209975	62.29%	12.683%
5	8.098	1018	1022	1035	rBV	500235	493962	9.59%	1.952%
6	8.198	1035	1039	1043	rVB	1471580	1270183	24.65%	5.019%
7	9.280	1217	1223	1226	rBV	4928552	5153024	100.00%	20.360%
8	9.957	1334	1338	1341	rBV	1765013	1398458	27.14%	5.525%
9	11.445	1587	1591	1594	rBV	1639844	1456607	28.27%	5.755%
10	11.957	1674	1678	1684	rBV	166553	186727	3.62%	0.738%
11	12.745	1808	1812	1823	rBV	60967	82645	1.60%	0.327%
12	13.033	1856	1861	1864	rBV	5338029	5130718	99.57%	20.272%
13	13.933	2008	2014	2032	rBV6	32419	126977	2.46%	0.502%
14	14.080	2032	2039	2043	rBV	1248693	1146674	22.25%	4.531%
15	14.945	2183	2186	2193	rBV	76047	78458	1.52%	0.310%
16	15.580	2288	2294	2298	rBV	714009	900158	17.47%	3.557%

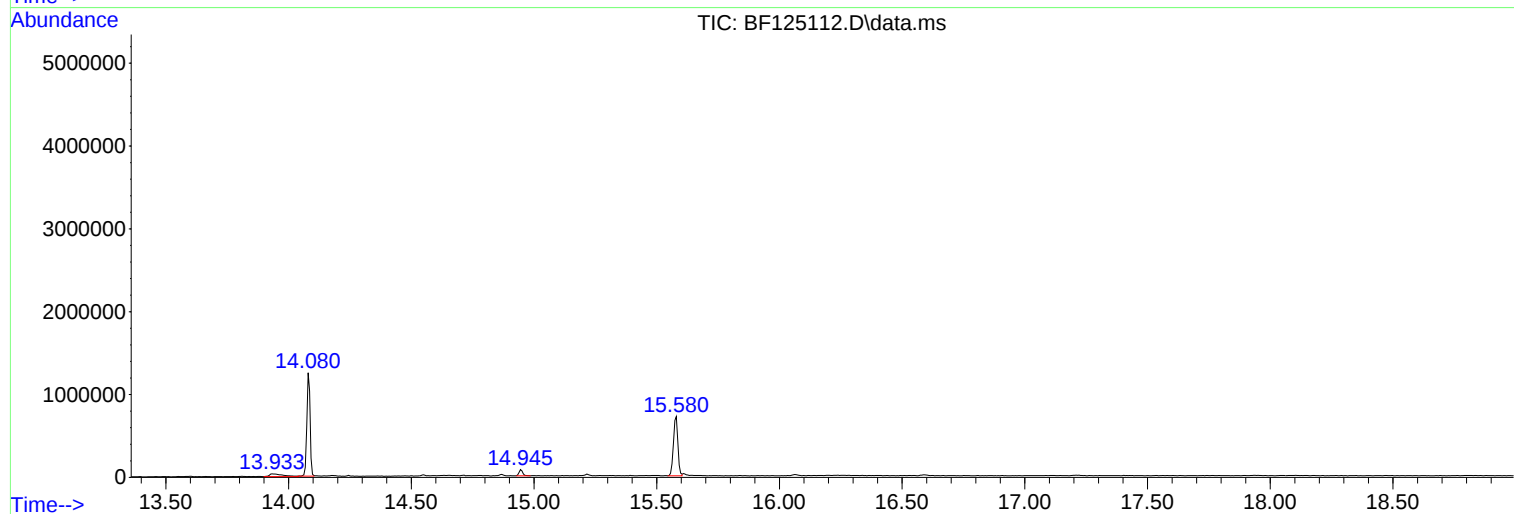
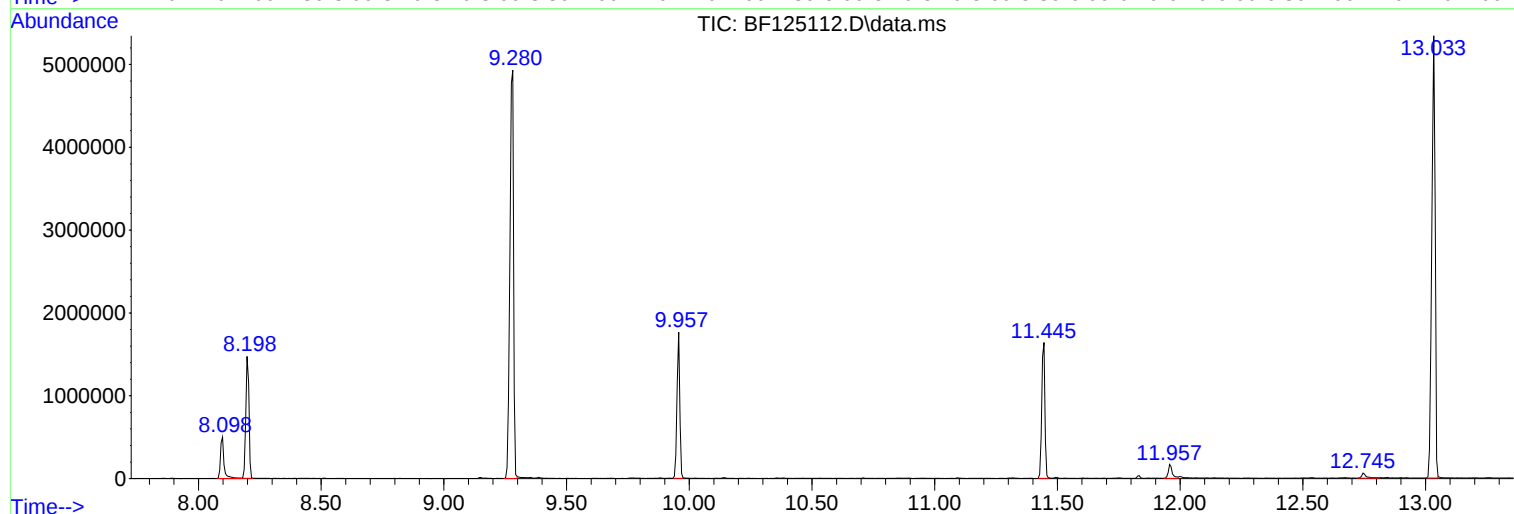
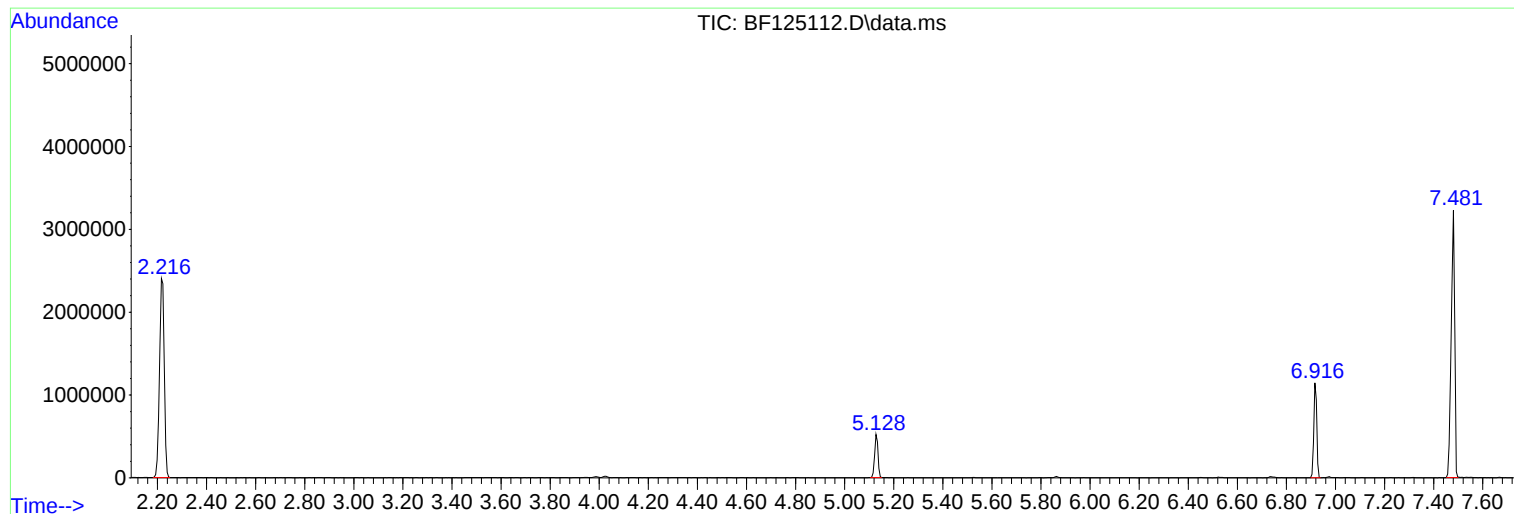
Sum of corrected areas: 25309182

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125112.D
Acq On : 19 Aug 2021 13:55
Operator : JU/CG
Sample : M3443-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
210812088-02

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\BF081921\
Data File : BF125112.D
Acq On : 19 Aug 2021 13:55
Operator : JU/CG
Sample : M3443-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
210812088-02

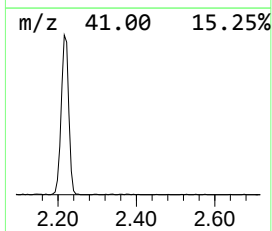
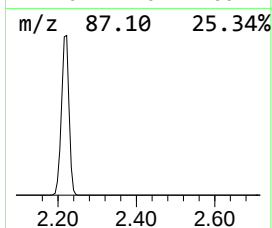
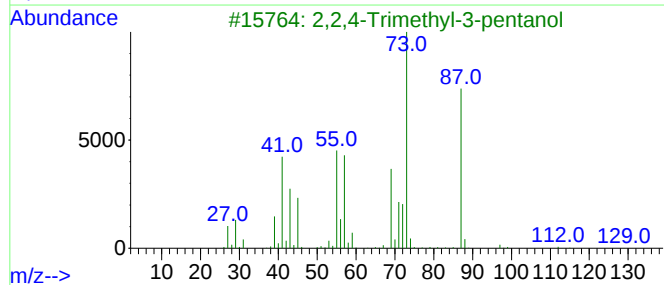
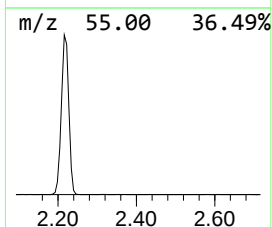
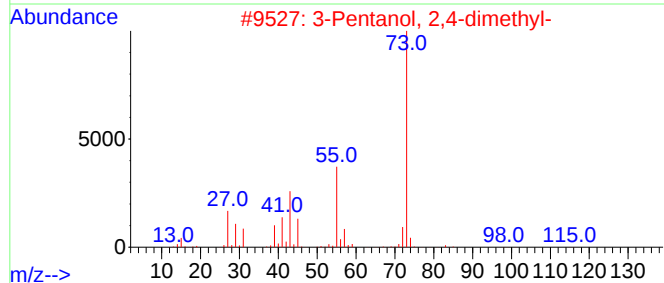
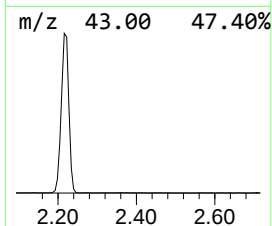
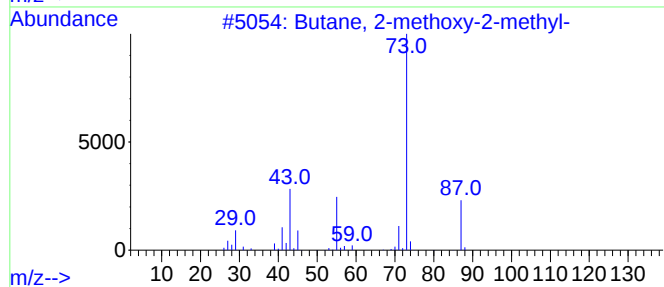
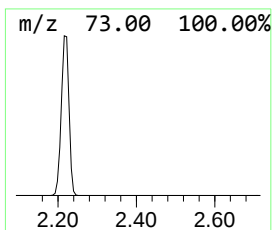
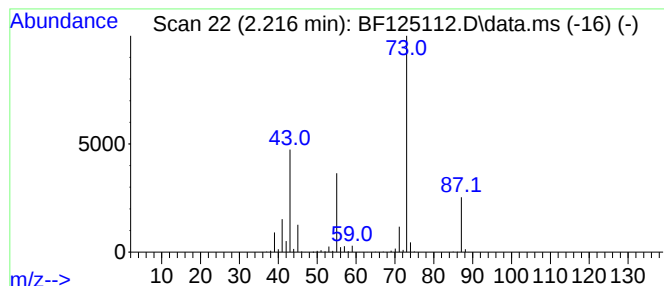
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.216	67.35 ng	3223240	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125112.D
Acq On : 19 Aug 2021 13:55
Operator : JU/CG
Sample : M3443-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

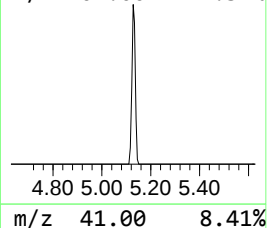
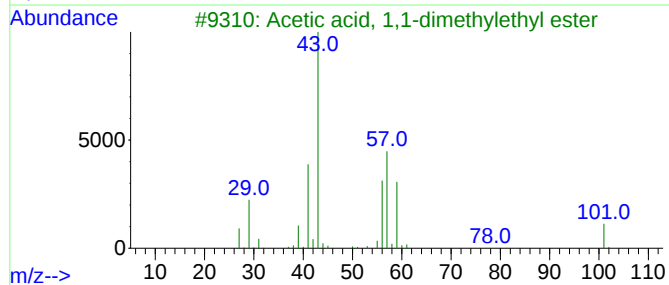
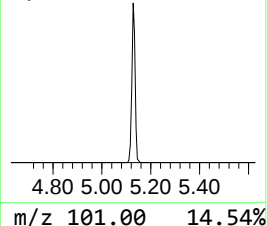
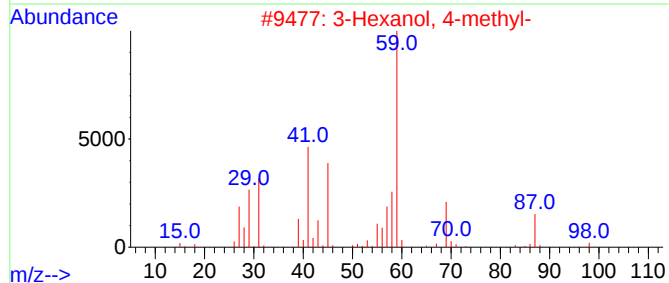
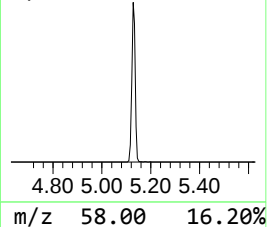
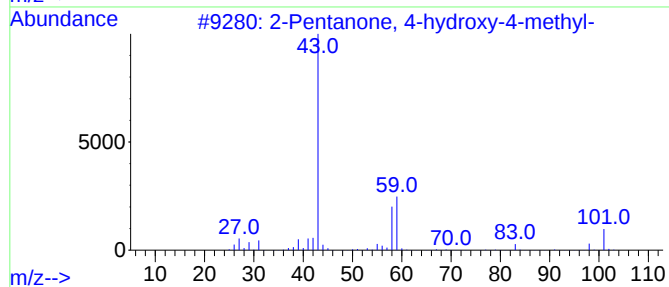
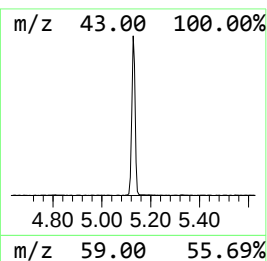
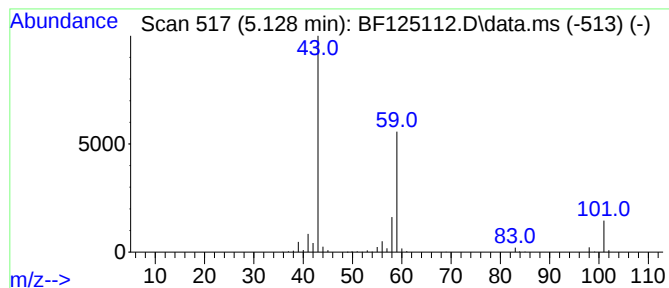
Instrument :
BNA_F
ClientSampleId :
210812088-02

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 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.128	10.33 ng	494163	1,4-Dichlorobenzene-d4	6.916	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	32
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125112.D
Acq On : 19 Aug 2021 13:55
Operator : JU/CG
Sample : M3443-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
210812088-02

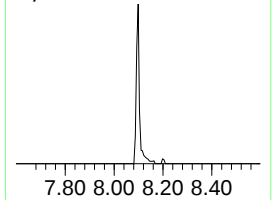
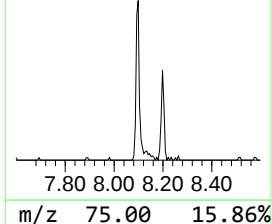
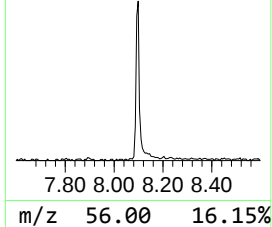
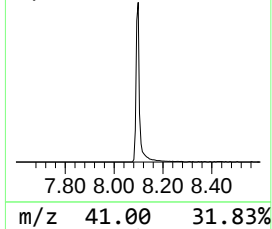
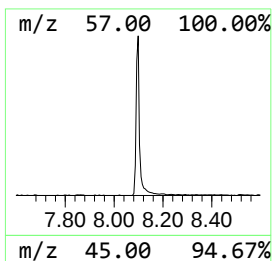
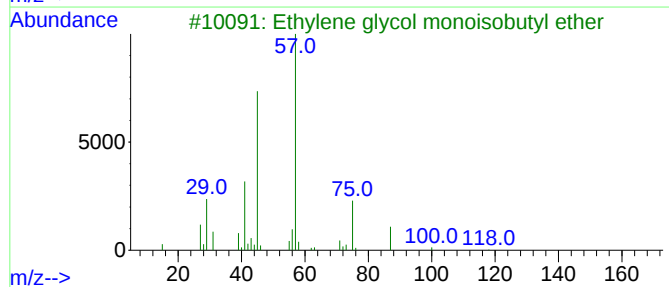
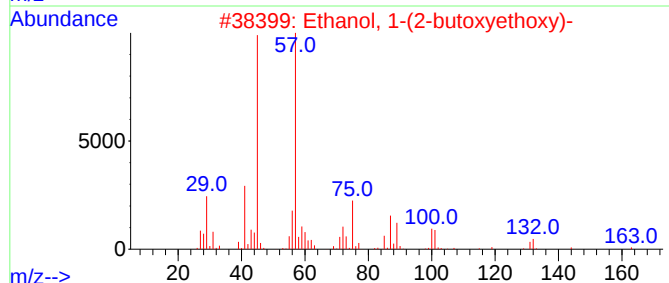
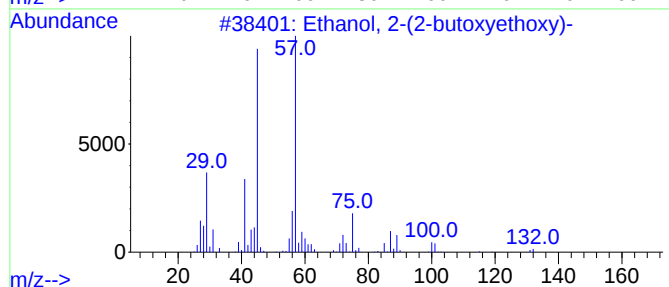
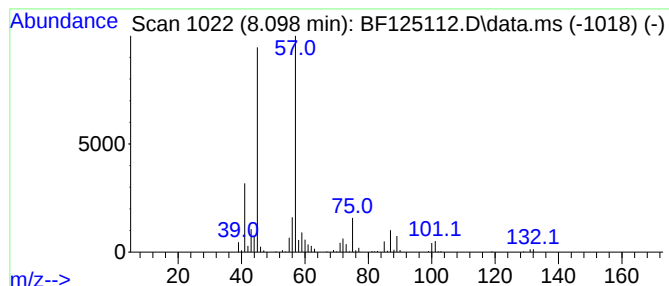
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	7.78 ng	493962	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125112.D
Acq On : 19 Aug 2021 13:55
Operator : JU/CG
Sample : M3443-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
210812088-02

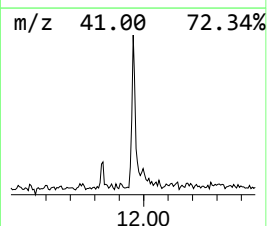
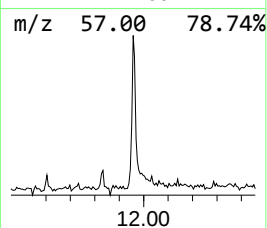
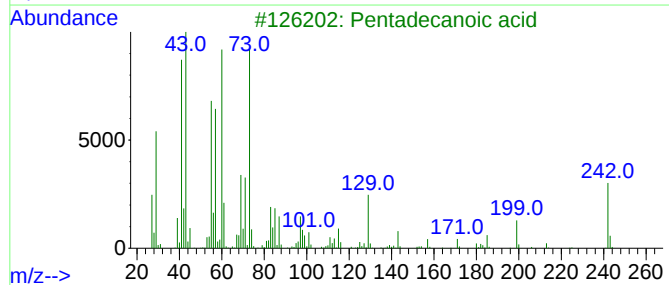
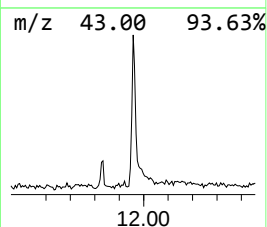
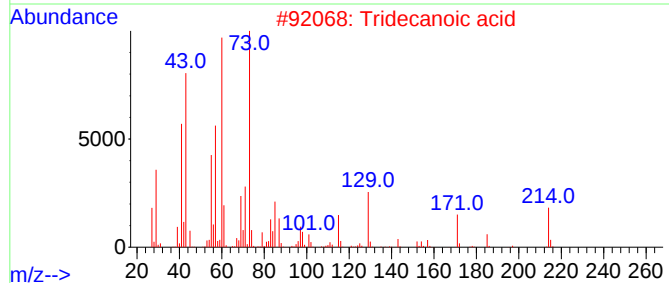
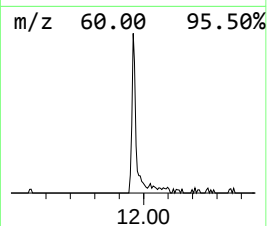
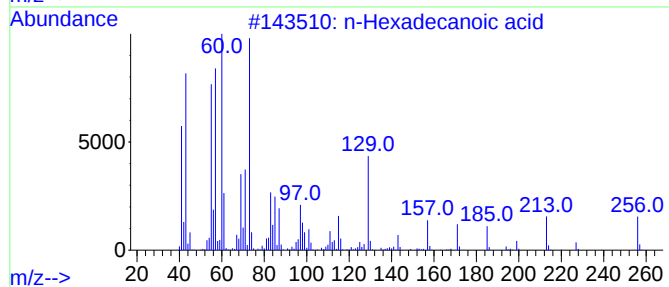
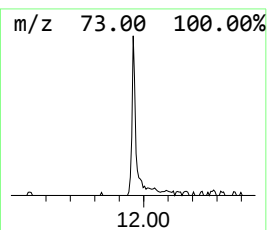
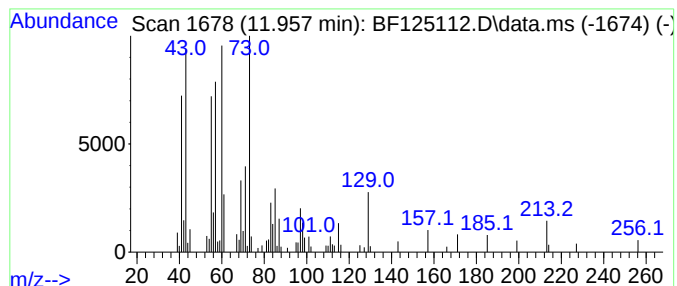
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.957	2.56 ng	186727	Phenanthrene-d10	11.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125112.D
Acq On : 19 Aug 2021 13:55
Operator : JU/CG
Sample : M3443-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
210812088-02

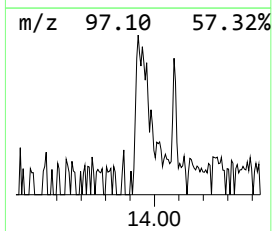
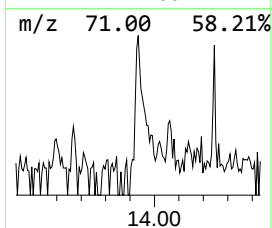
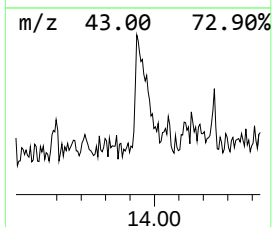
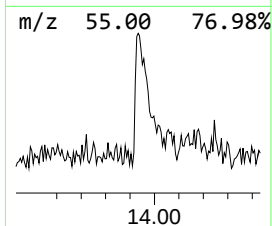
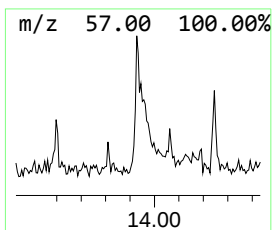
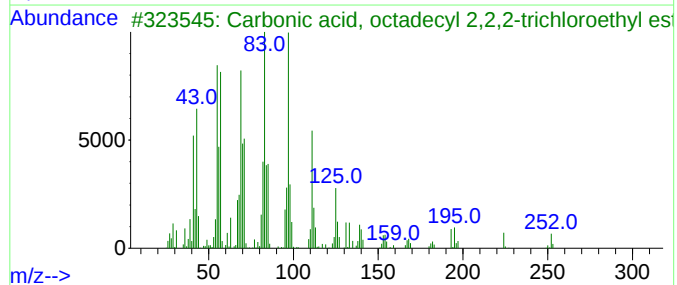
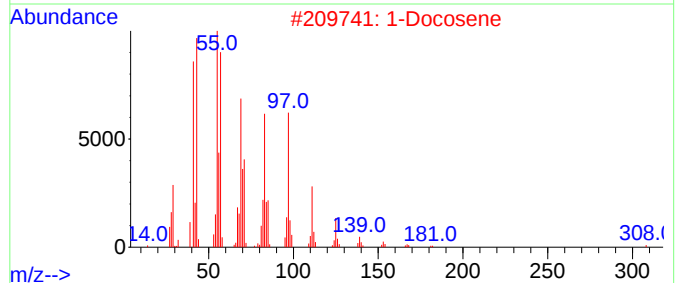
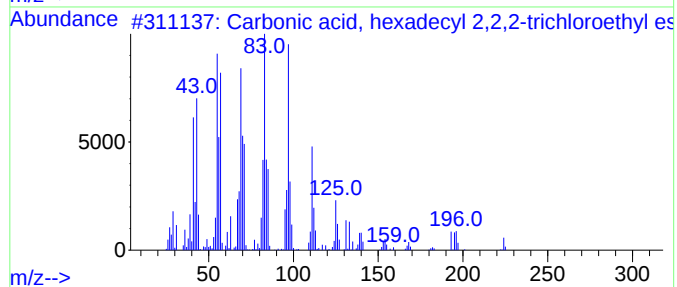
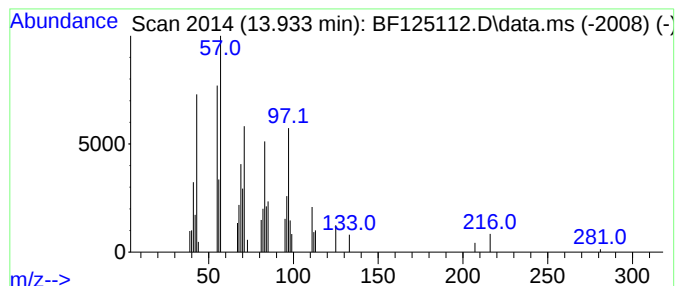
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Carbonic acid, hexadecyl 2,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	2.21 ng	126977	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	81
2			1-Docosene	308	C22H44	001599-67-3	81
3			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	74
4			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	68
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125112.D
Acq On : 19 Aug 2021 13:55
Operator : JU/CG
Sample : M3443-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
210812088-02

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...	2.216	67.3	ng	3223240	1	6.916	957211	20.0
2-Pentanone, 4-...	5.128	10.3	ng	494163	1	6.916	957211	20.0
Ethanol, 2-(2-b...	8.098	7.8	ng	493962	2	8.198	1270180	20.0
n-Hexadecanoic ...	11.957	2.6	ng	186727	4	11.445	1456610	20.0
Carbonic acid, ...	13.933	2.2	ng	126977	5	14.080	1146670	20.0