

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
 Data File : BF125210.D
 Acq On : 25 Aug 2021 15:20
 Operator : JU/CG
 Sample : M3524-08
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-6D

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: BF125210.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	15	21	28	rVB	1017233	1316473	33.90%	4.374%
2	5.139	511	519	524	rBV	75432	94104	2.42%	0.313%
3	5.534	581	586	589	rBV	3454440	3350441	86.27%	11.131%
4	6.534	751	756	759	rBV	3210053	3388243	87.25%	11.257%
5	6.739	788	791	801	rBV2	37943	59251	1.53%	0.197%
6	6.916	817	821	824	rBV	987392	860853	22.17%	2.860%
7	7.475	911	916	919	rBV	2509174	2234173	57.53%	7.423%
8	8.092	1018	1021	1035	rBV	1298321	1535704	39.54%	5.102%
9	8.198	1035	1039	1042	rVB	1338883	1112753	28.65%	3.697%
10	9.269	1217	1221	1224	rBV	4581276	3883471	100.00%	12.902%
11	9.380	1236	1240	1252	rVB	529689	511655	13.18%	1.700%
12	9.533	1262	1266	1272	rBV	59385	58505	1.51%	0.194%
13	9.951	1333	1337	1340	rBV	1504709	1206938	31.08%	4.010%
14	10.739	1467	1471	1474	rBV	2892376	2432255	62.63%	8.081%
15	11.439	1586	1590	1593	rBV	1246597	1143097	29.43%	3.798%
16	11.821	1652	1655	1659	rVB	204815	167882	4.32%	0.558%
17	11.957	1674	1678	1683	rBV	401671	362974	9.35%	1.206%
18	12.533	1768	1776	1778	rBV	479179	425375	10.95%	1.413%
19	12.615	1787	1790	1793	rVB	220288	159153	4.10%	0.529%
20	12.739	1808	1811	1825	rBV	163165	173411	4.47%	0.576%
21	13.021	1855	1859	1863	rBV	3902984	3452815	88.91%	11.472%
22	13.910	2007	2010	2013	rBV2	43468	52504	1.35%	0.174%
23	13.945	2013	2016	2018	rVV	103379	96804	2.49%	0.322%
24	13.992	2018	2024	2032	rVV10	55495	192872	4.97%	0.641%
25	14.074	2035	2038	2042	rVB	899474	814768	20.98%	2.707%
26	15.574	2287	2293	2304	rVB2	754720	967356	24.91%	3.214%
27	16.574	2457	2463	2467	rBV5	22883	45161	1.16%	0.150%

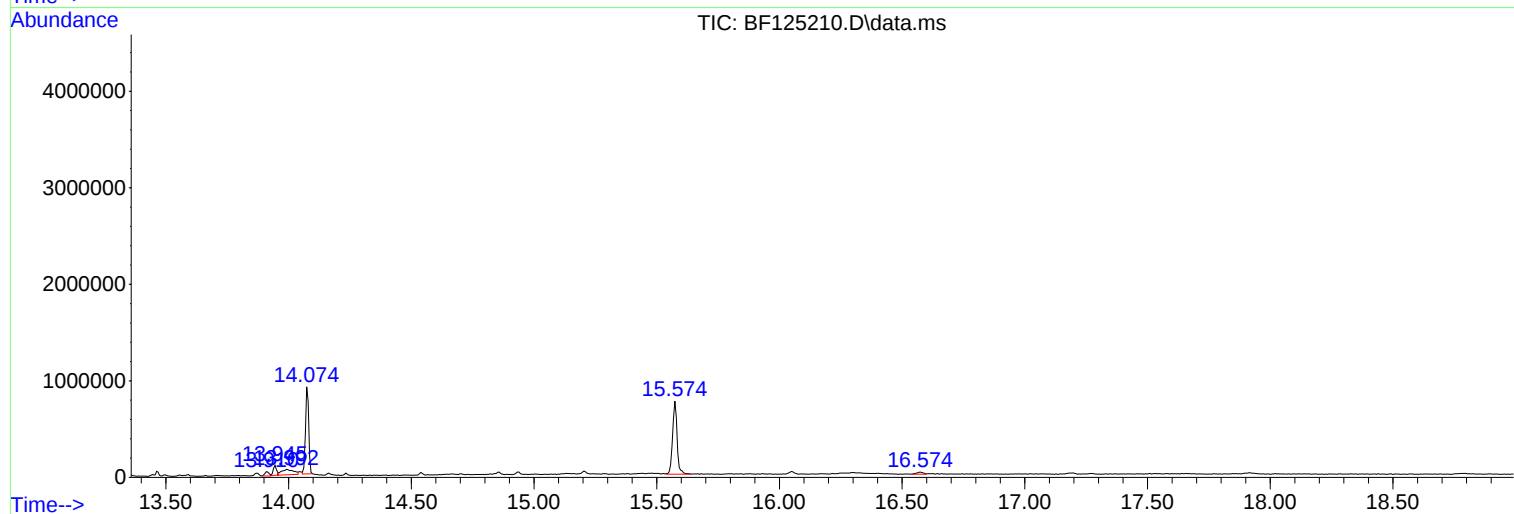
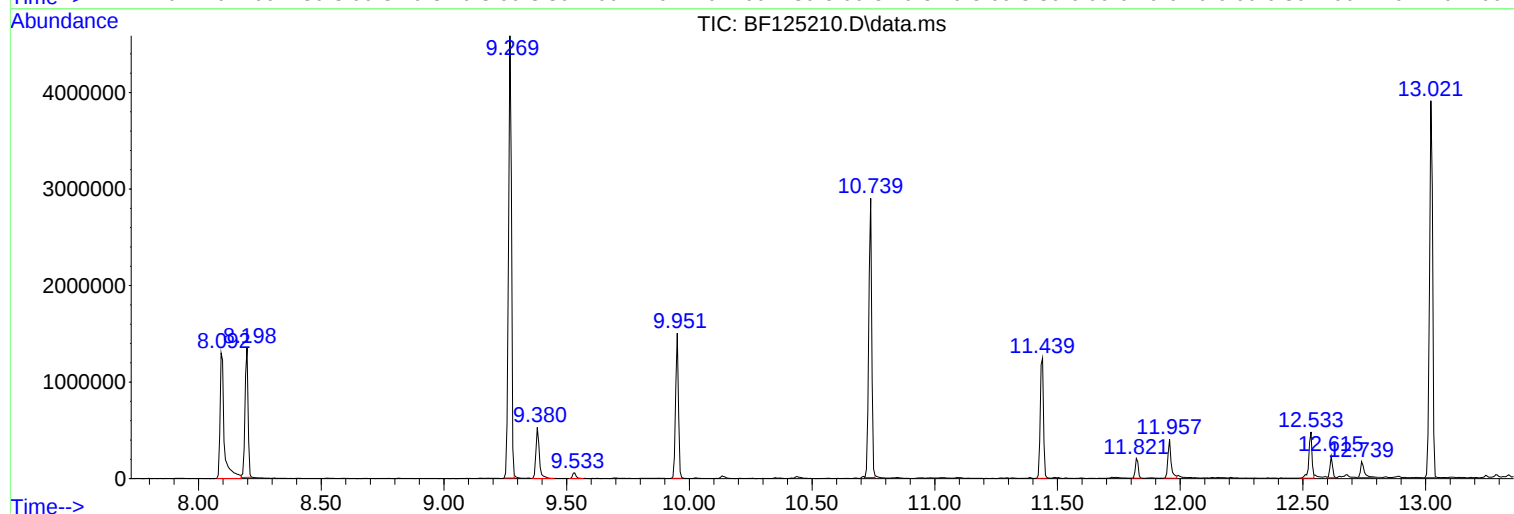
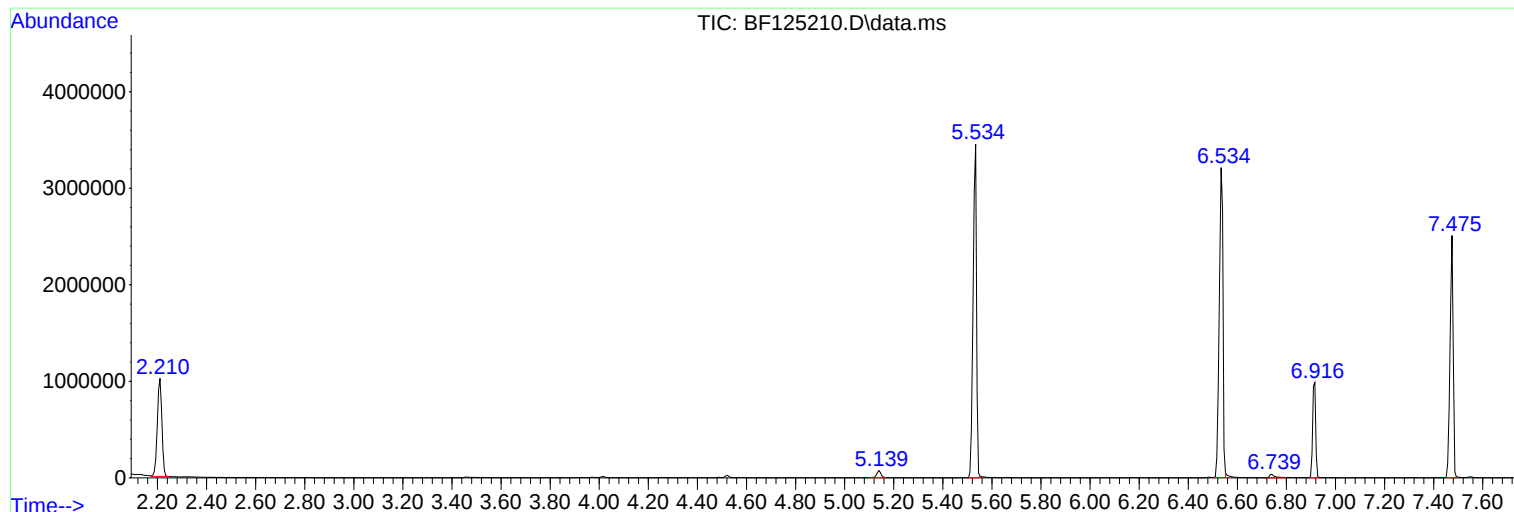
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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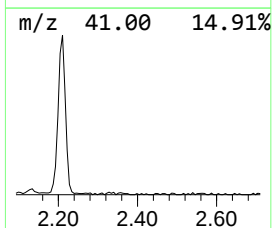
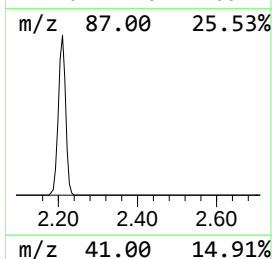
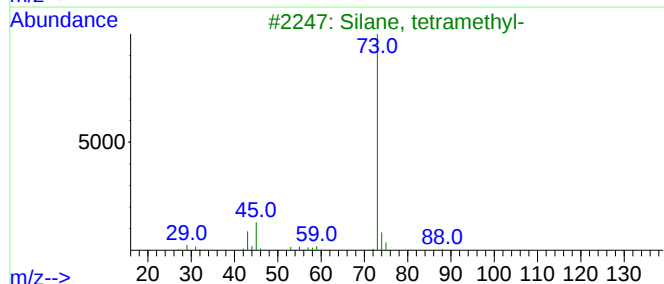
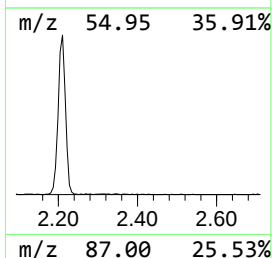
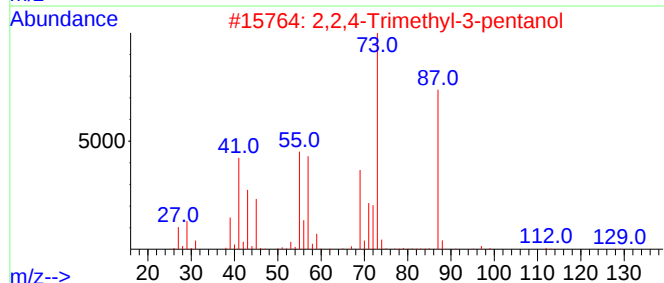
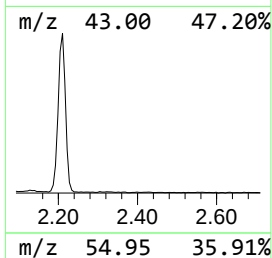
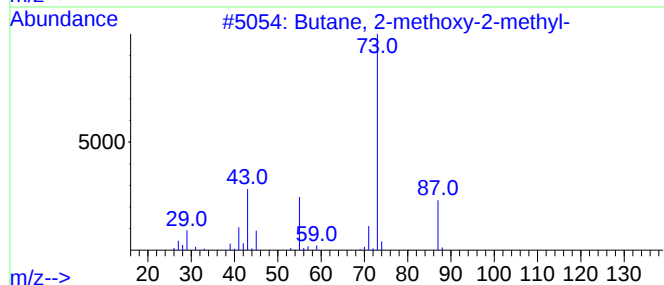
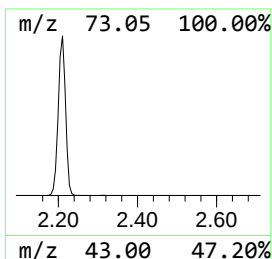
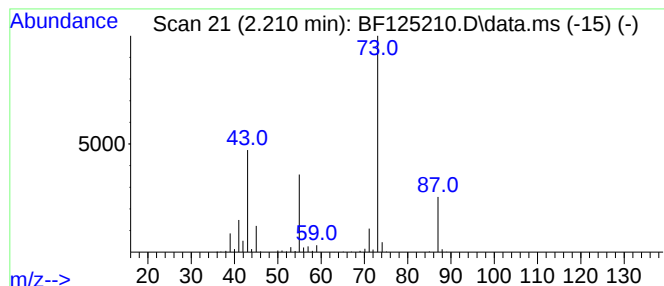
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.210	30.59 ng	1316470	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			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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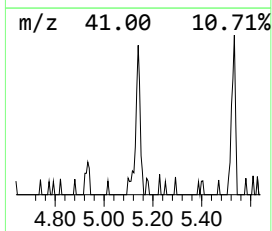
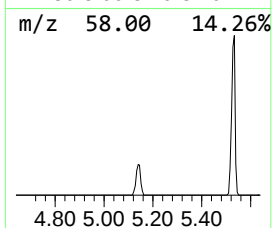
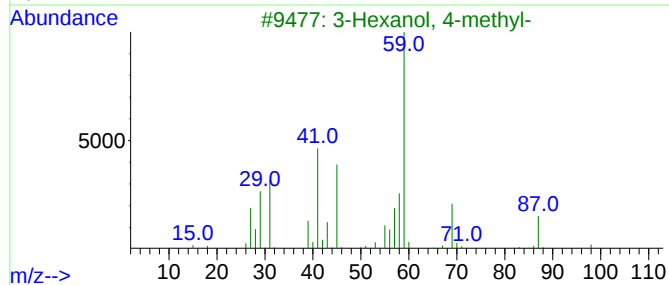
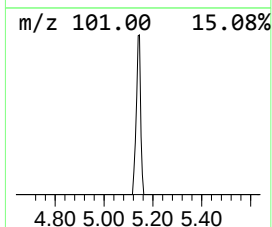
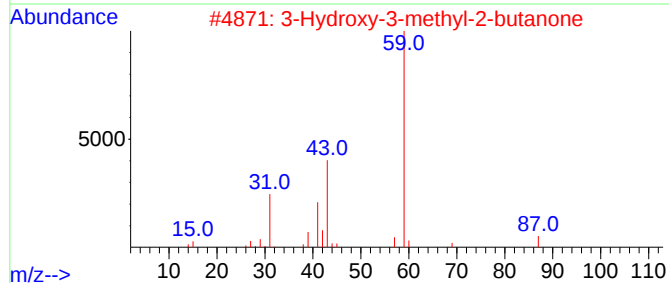
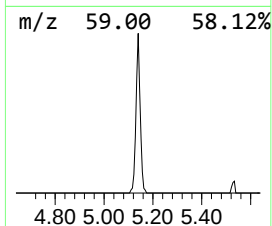
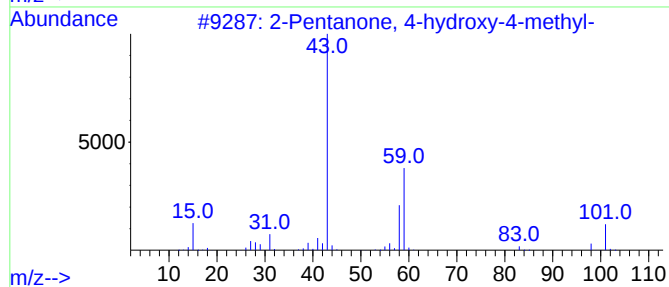
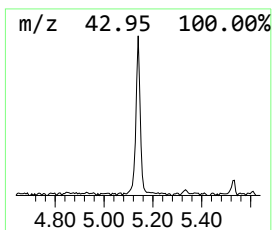
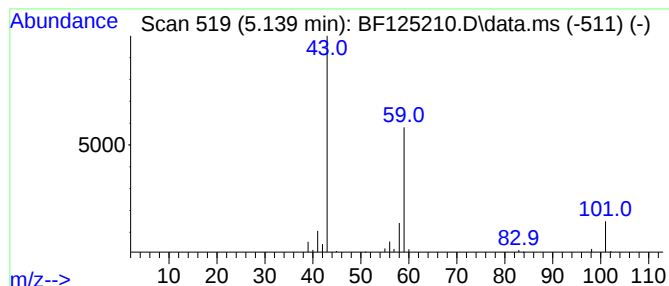
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.139	2.19 ng	94104	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	64		
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	38		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	3-Pentanol	88	C5H12O	000584-02-1	28		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		



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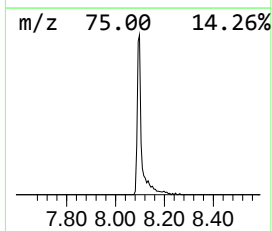
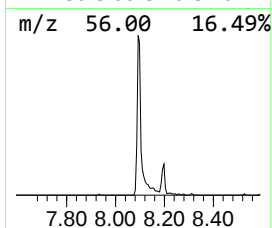
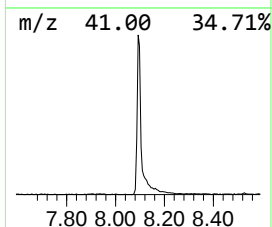
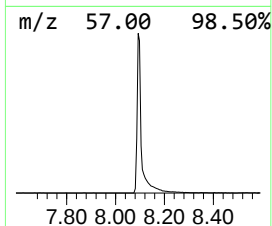
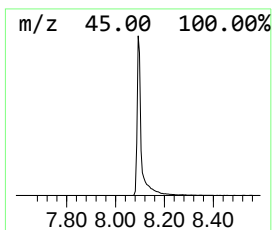
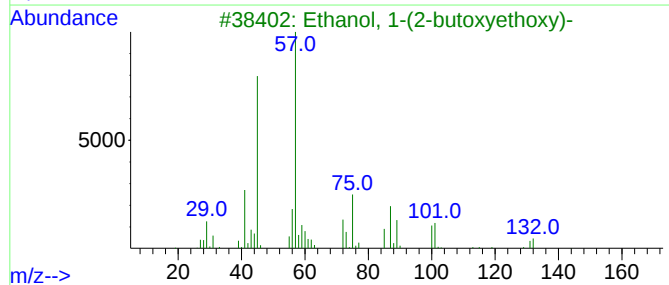
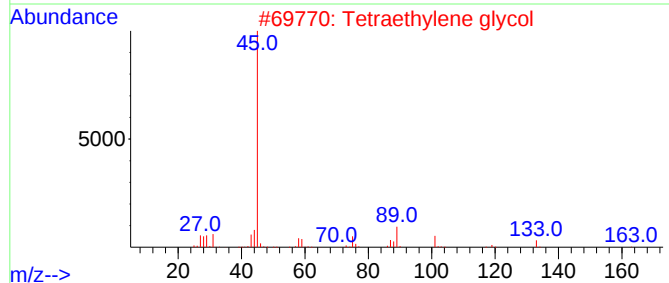
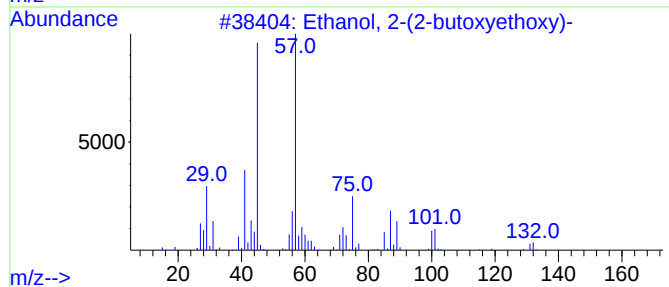
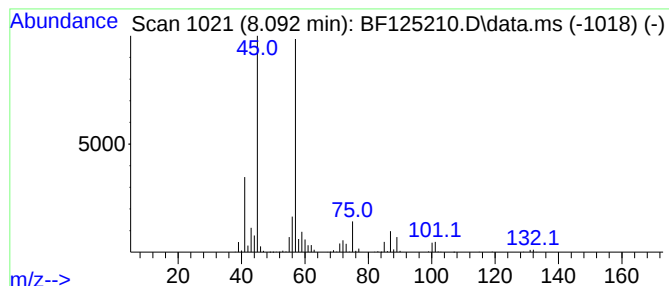
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	27.60 ng	1535700	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2			Tetraethylene glycol	194	C8H18O5	000112-60-7	53
3			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	47



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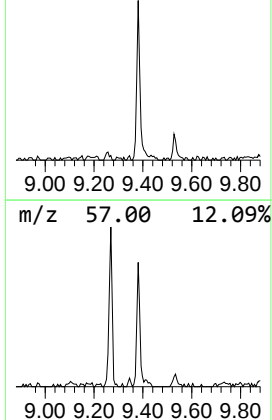
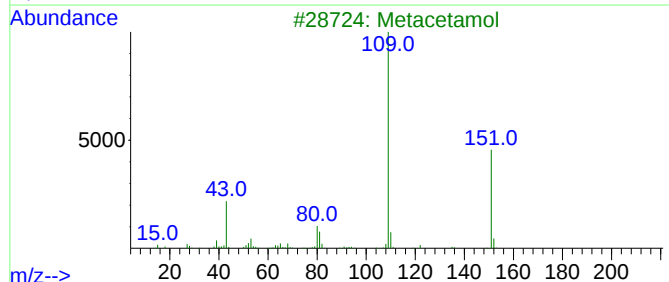
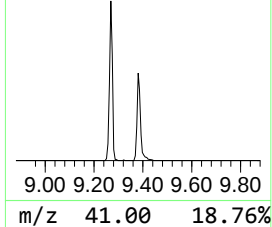
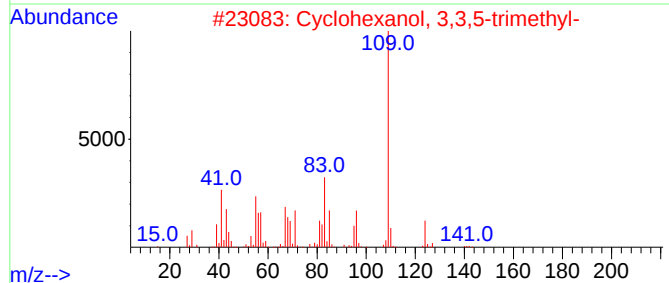
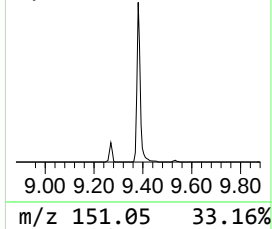
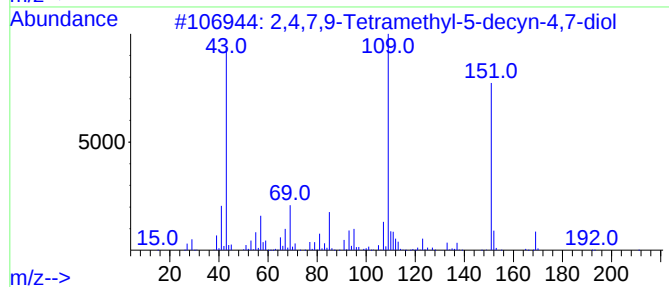
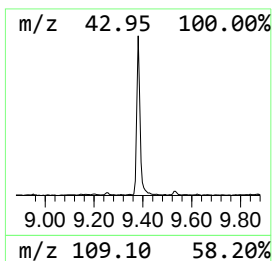
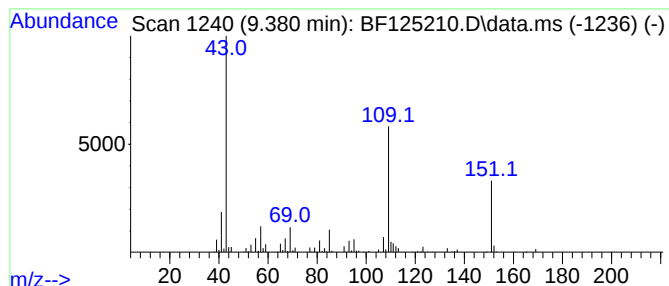
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.380	8.48 ng	511655	Acenaphthene-d10	9.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	86		
2	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	50		
3	Metacetamol	151	C8H9NO2	000621-42-1	46		
4	Acetaminophen	151	C8H9NO2	000103-90-2	43		
5	Glutaric acid, (2-methylcyclohex...	324	C19H32O4	1000405-50-3	37		



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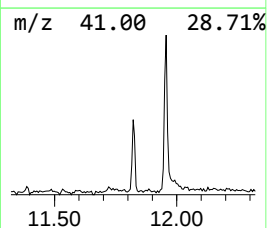
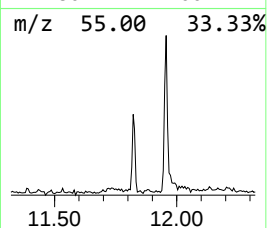
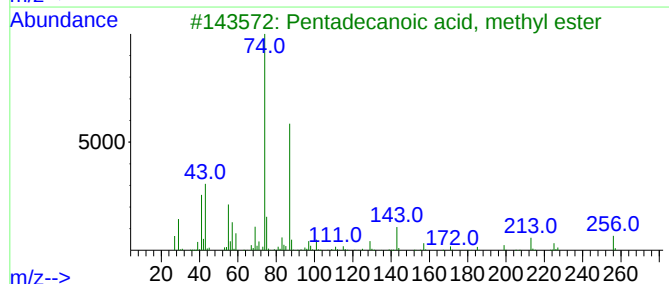
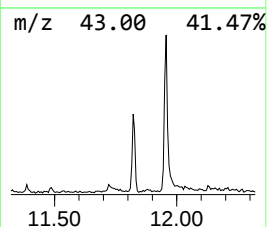
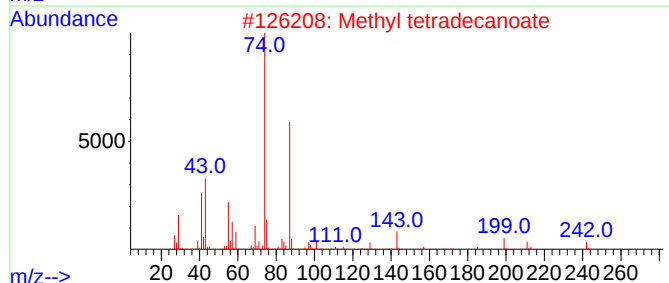
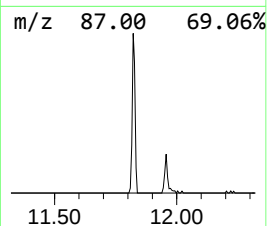
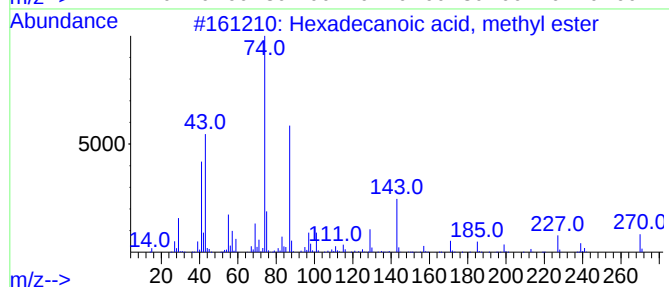
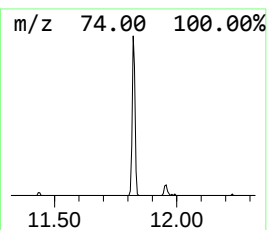
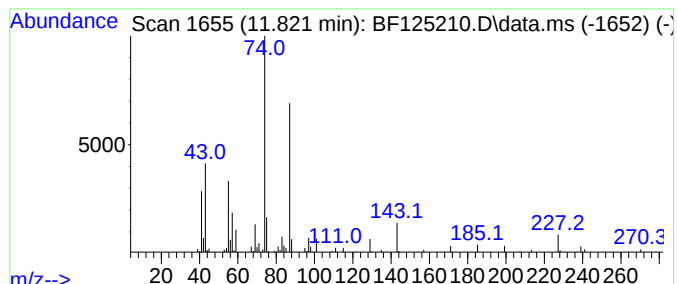
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Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.821	2.94 ng	167882	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	94
2			Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	90
5			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87



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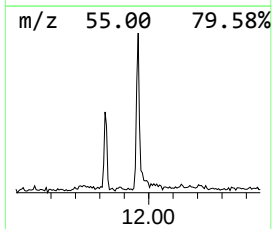
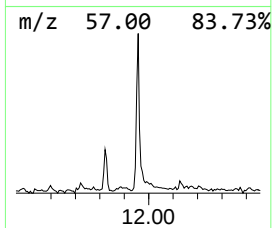
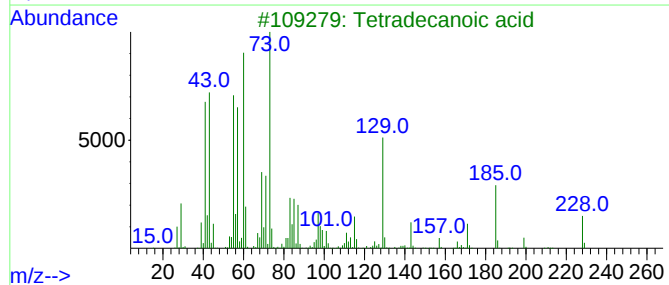
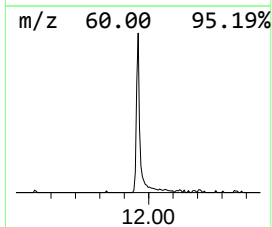
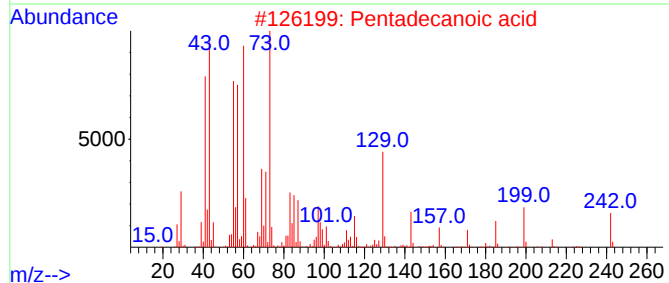
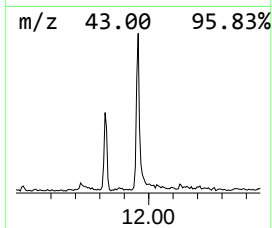
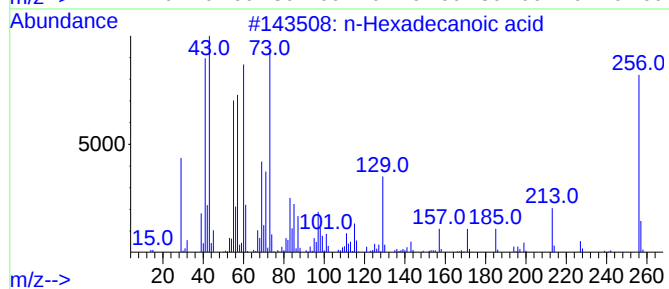
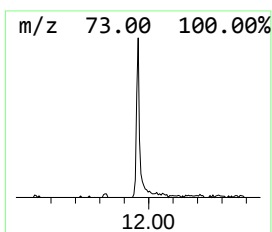
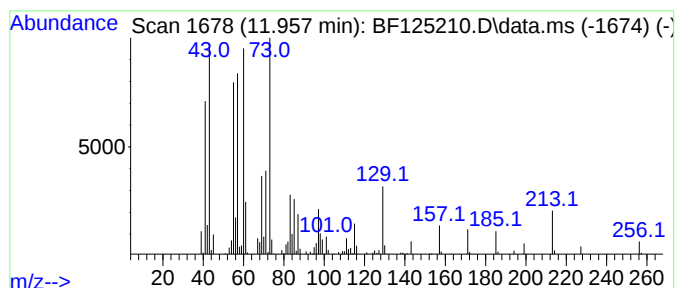
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	6.35 ng	362974	Phenanthrene-d10	11.439

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	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		Tridecanoic acid	214	C13H26O2	000638-53-9	83
5		Nonanoic acid	158	C9H18O2	000112-05-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125210.D
Acq On : 25 Aug 2021 15:20
Operator : JU/CG
Sample : M3524-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-6D

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

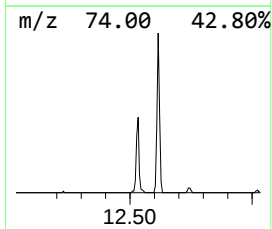
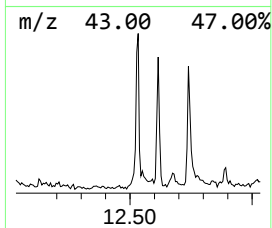
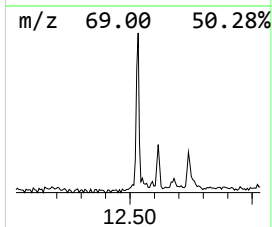
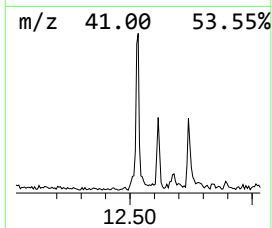
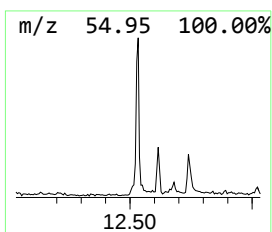
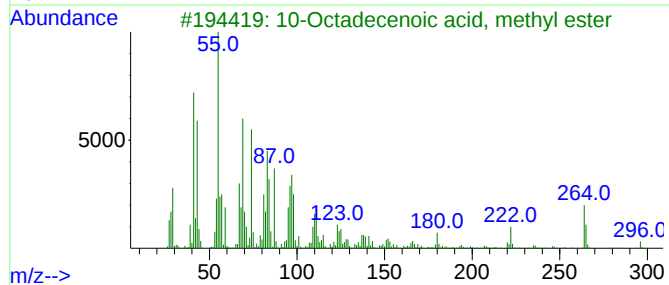
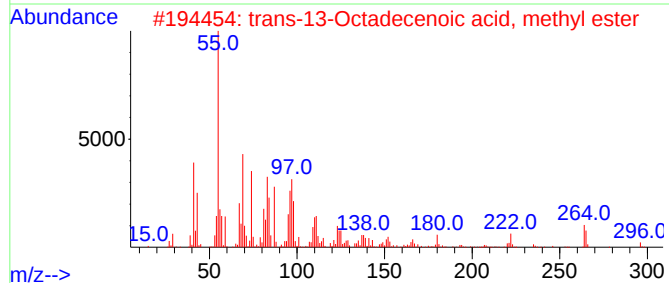
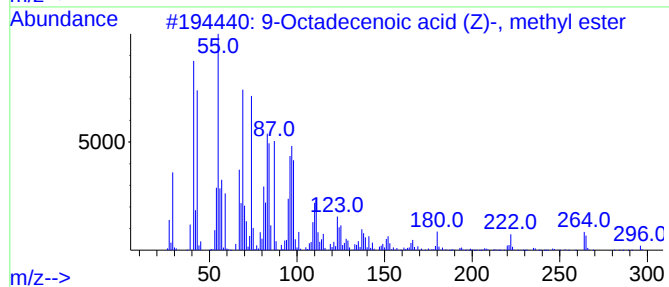
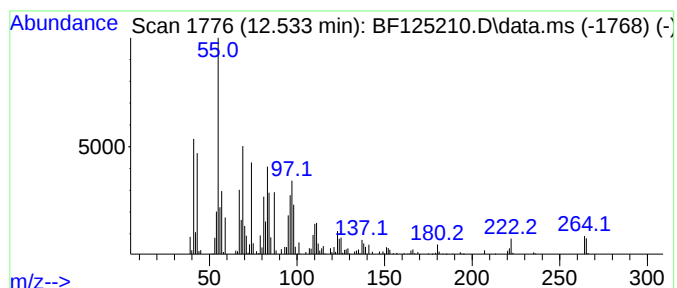
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 9-Octadecenoic acid (Z)-, m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.533	7.44 ng	425375	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	95
3			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
4			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
5			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125210.D
Acq On : 25 Aug 2021 15:20
Operator : JU/CG
Sample : M3524-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-6D

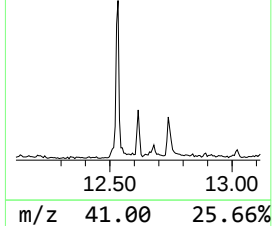
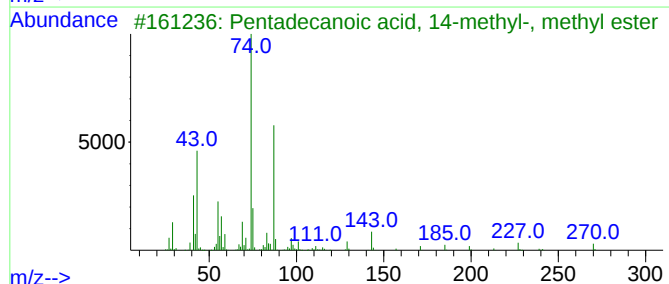
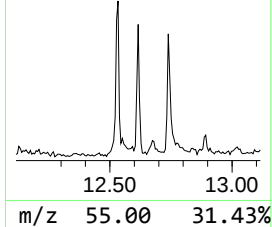
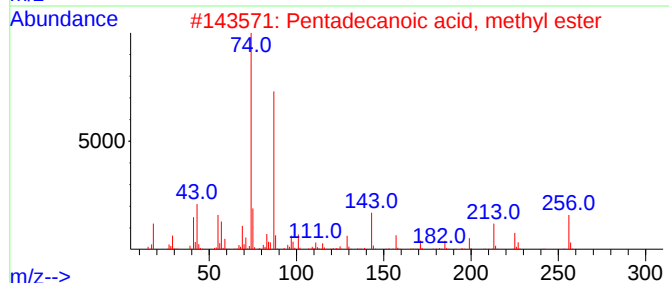
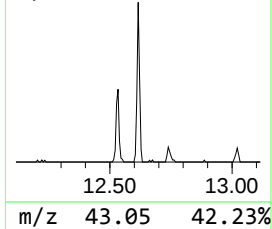
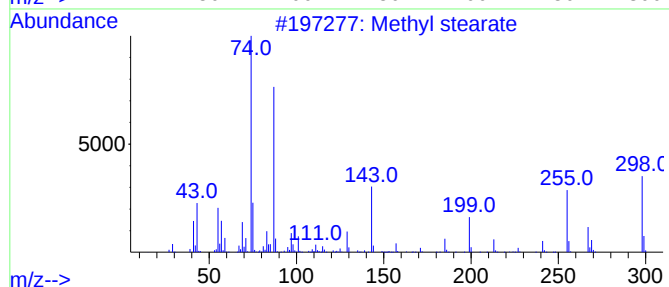
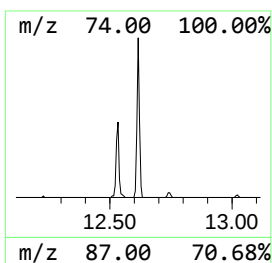
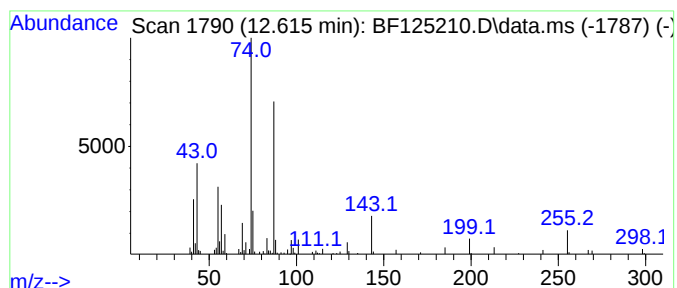
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Methyl stearate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	2.78 ng	159153	Phenanthrene-d10	11.439

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methyl stearate	298	C19H38O2	000112-61-8	91
2		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
3		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
4		Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	87
5		Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125210.D
Acq On : 25 Aug 2021 15:20
Operator : JU/CG
Sample : M3524-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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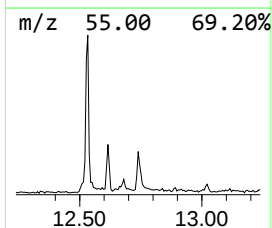
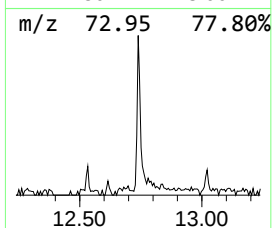
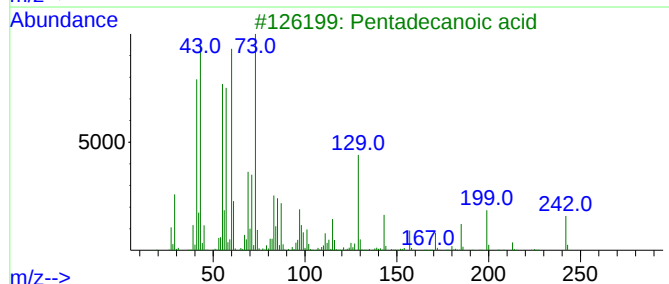
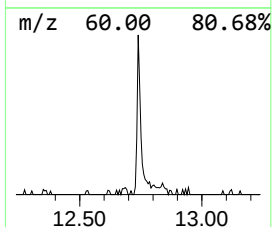
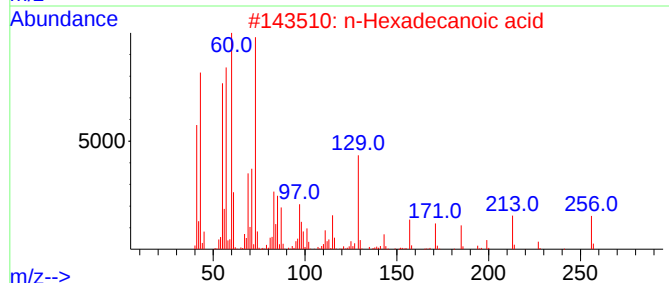
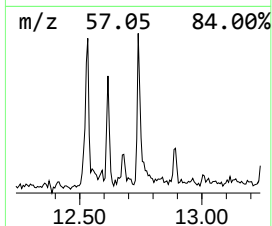
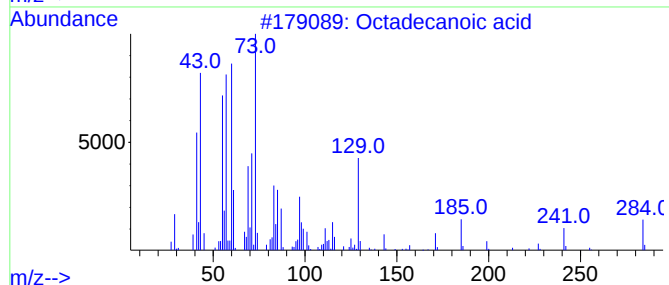
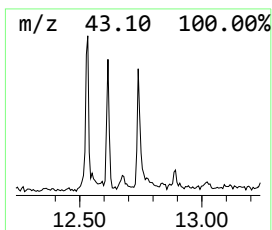
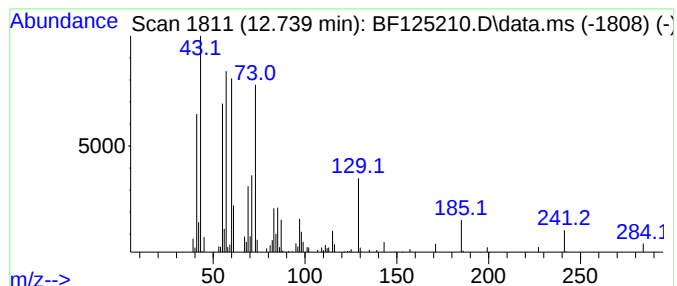
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	3.03 ng	173411	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	91
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125210.D
Acq On : 25 Aug 2021 15:20
Operator : JU/CG
Sample : M3524-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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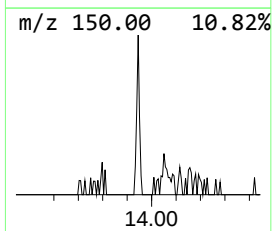
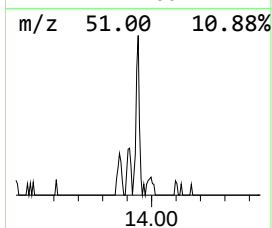
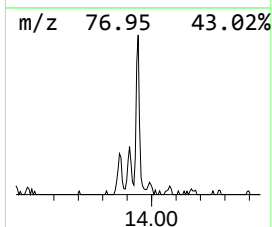
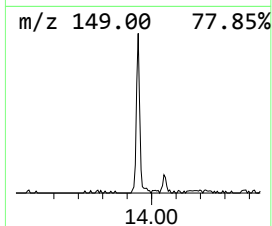
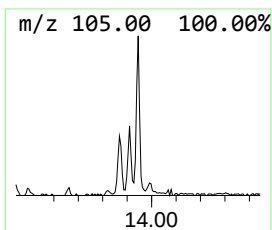
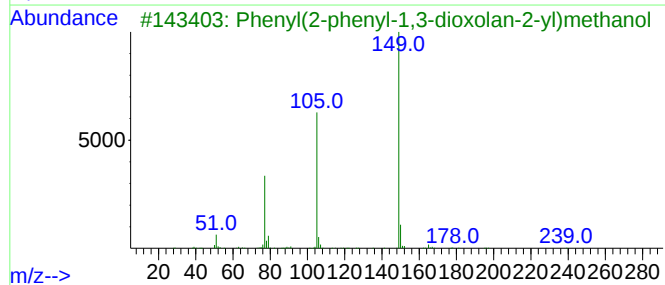
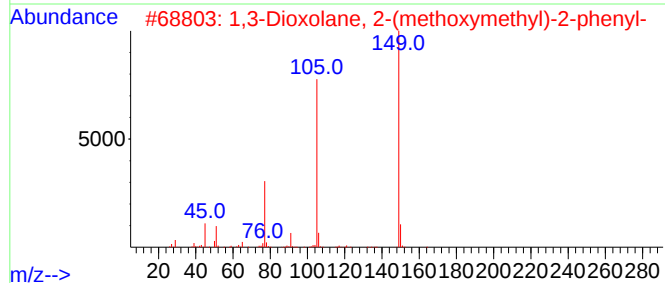
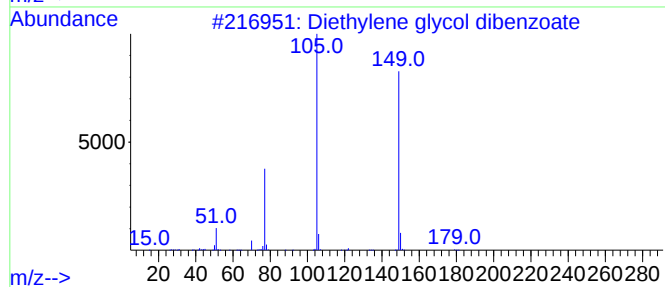
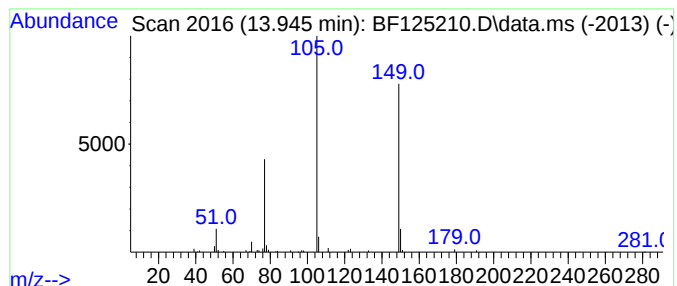
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Diethylene glycol dibenzoate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	2.38 ng	96804	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	83
2			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83
3			Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	78
4			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	72
5			Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125210.D
Acq On : 25 Aug 2021 15:20
Operator : JU/CG
Sample : M3524-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-6D

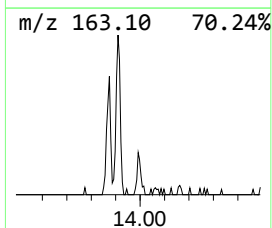
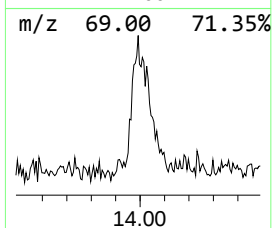
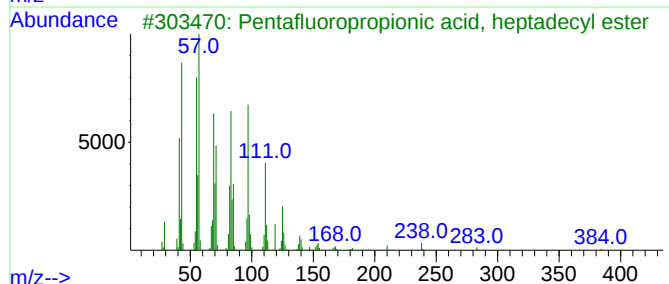
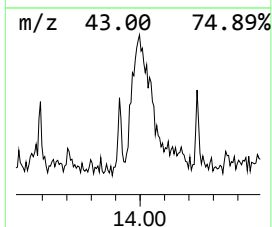
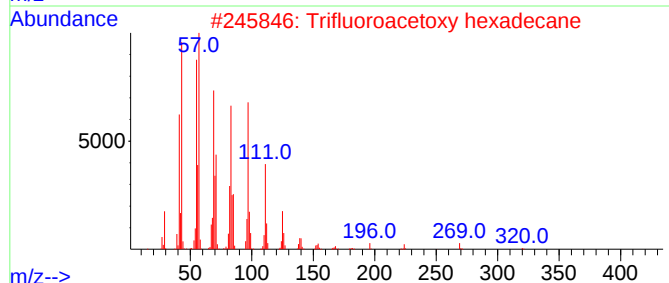
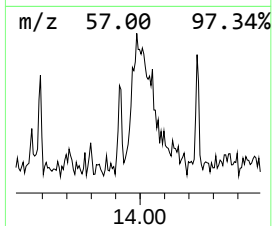
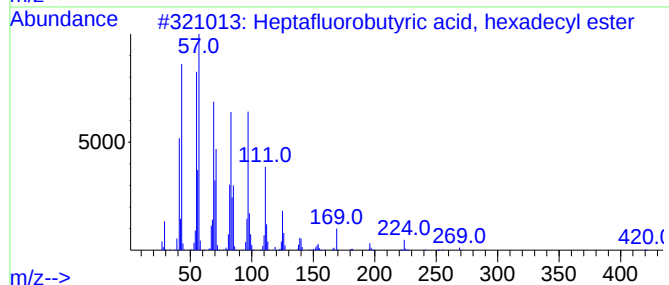
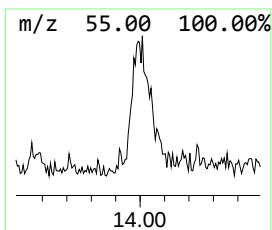
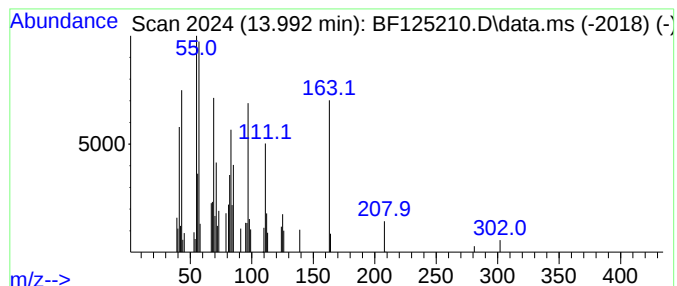
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptafluorobutyric acid, he... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.992	4.73 ng	192872	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	64
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	64
3			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	64
4			1-Hexacosene	364	C26H52	018835-33-1	64
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125210.D
Acq On : 25 Aug 2021 15:20
Operator : JU/CG
Sample : M3524-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-6D

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-...	5.139	2.2	ng	94104	1	6.916	860853	20.0
Ethanol, 2-(2-b...	8.092	27.6	ng	1535700	2	8.198	1112750	20.0
2,4,7,9-Tetrame...	9.380	8.5	ng	511655	3	9.951	1206940	20.0
Hexadecanoic ac...	11.821	2.9	ng	167882	4	11.439	1143100	20.0
n-Hexadecanoic ...	11.957	6.3	ng	362974	4	11.439	1143100	20.0
9-Octadecenoic ...	12.533	7.4	ng	425375	4	11.439	1143100	20.0
Methyl stearate	12.616	2.8	ng	159153	4	11.439	1143100	20.0
Octadecanoic acid	12.739	3.0	ng	173411	4	11.439	1143100	20.0
Diethylene glyc...	13.945	2.4	ng	96804	5	14.074	814768	20.0
Heptafluorobuty...	13.992	4.7	ng	192872	5	14.074	814768	20.0