

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111122\
 Data File : BM037482.D
 Acq On : 12 Nov 2022 00:19
 Operator : CG/JU
 Sample : N5530-09
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-09

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_M\Methods\8270-BM102822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM037482.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.299	202	206	219	rVB	97943	141437	1.33%	0.253%
2	4.910	305	310	322	rBV	1045479	1419319	13.35%	2.540%
3	5.375	383	389	407	rBV	4280437	6169997	58.05%	11.043%
4	6.987	655	663	684	rBV	3908460	6211234	58.43%	11.116%
5	7.804	795	802	811	rBV	808601	1281102	12.05%	2.293%
6	8.975	993	1001	1021	rBV	2356029	3942196	37.09%	7.055%
7	10.410	1236	1245	1258	rBV2	47479	174607	1.64%	0.312%
8	10.604	1271	1278	1295	rBV	964494	1664427	15.66%	2.979%
9	13.069	1690	1697	1720	rBV	5593939	8540698	80.35%	15.285%
10	14.445	1925	1931	1943	rBV	1300617	1995491	18.77%	3.571%
11	15.939	2179	2185	2203	rBV	4149403	5953613	56.01%	10.655%
12	17.192	2392	2398	2411	rBV	1340725	2070684	19.48%	3.706%
13	18.092	2546	2551	2561	rBV	201374	401347	3.78%	0.718%
14	19.374	2765	2769	2777	rBV2	143539	258805	2.43%	0.463%
15	19.821	2840	2845	2855	rBV	9133711	10629676	100.00%	19.024%
16	20.586	2971	2975	2978	rBV	145730	177073	1.67%	0.317%
17	21.092	3057	3061	3070	rBV2	307591	526299	4.95%	0.942%
18	21.380	3105	3110	3120	rBV	1580935	2208142	20.77%	3.952%
19	23.715	3502	3507	3517	rVB2	1078173	2108463	19.84%	3.774%

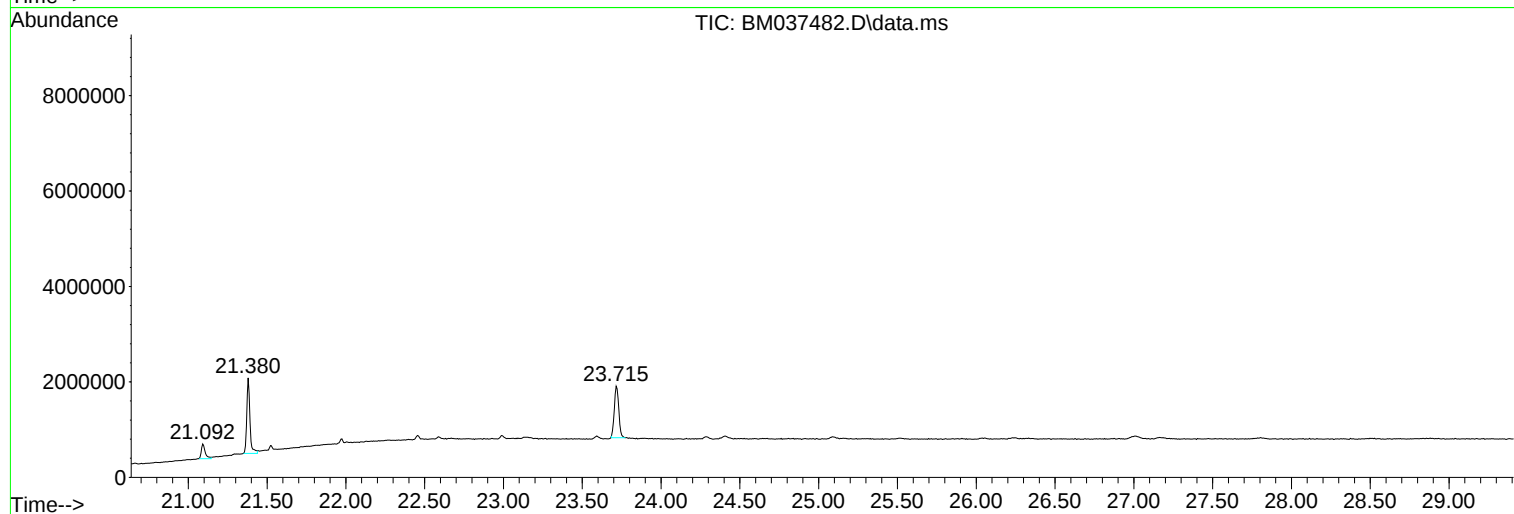
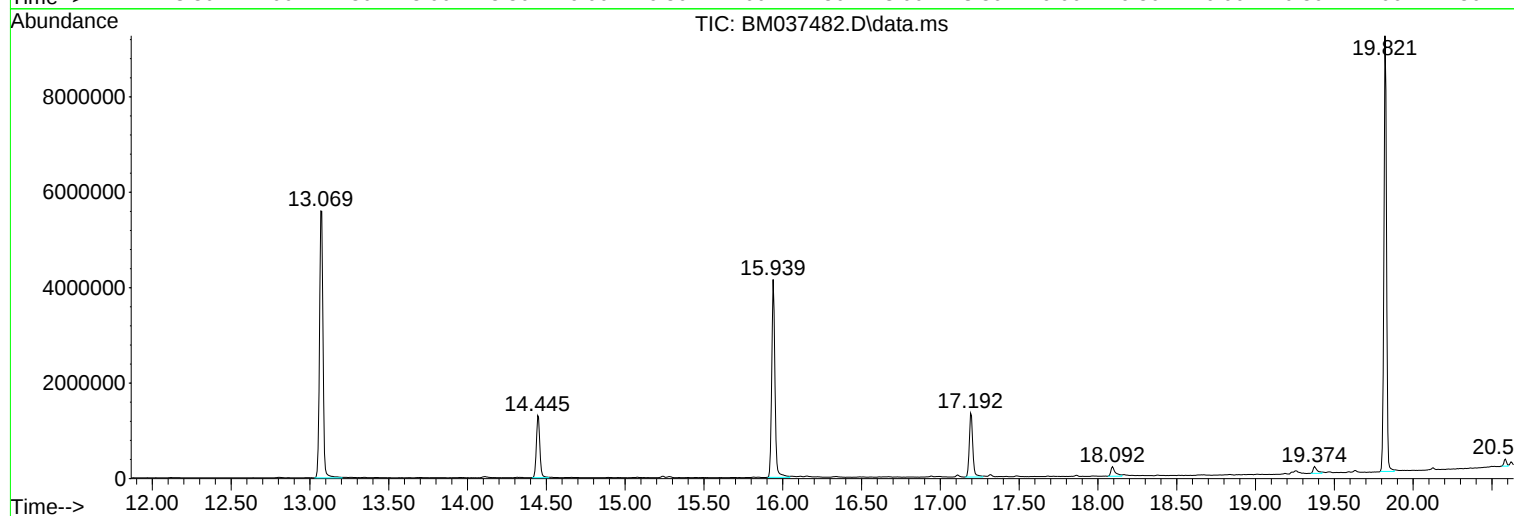
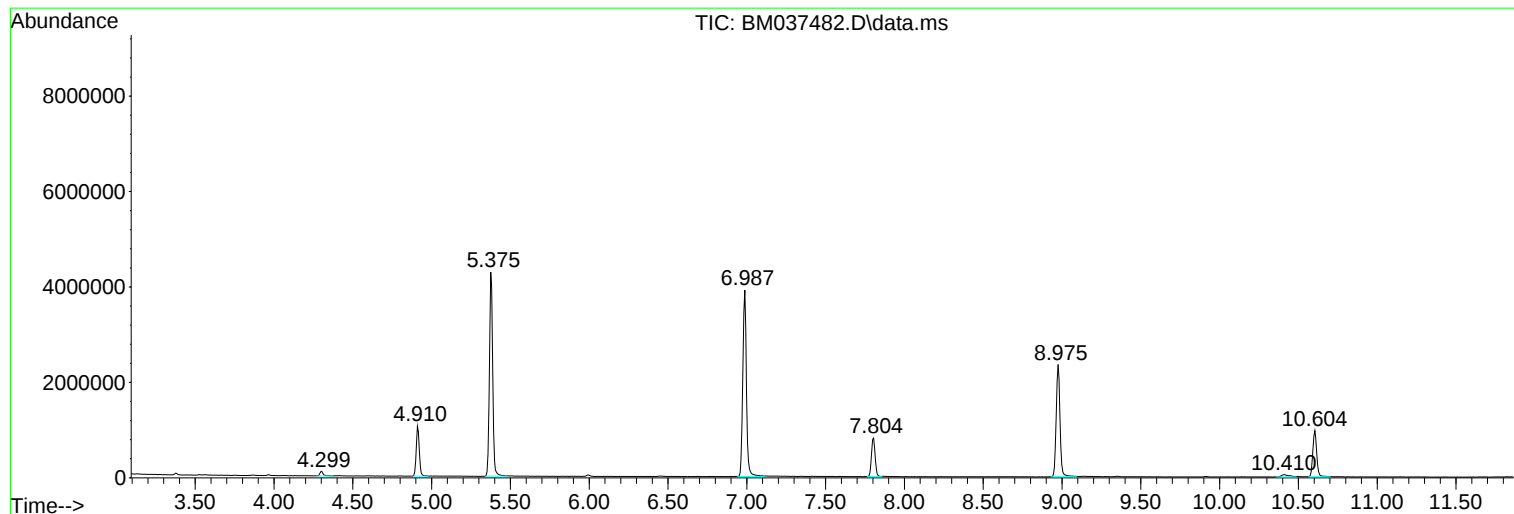
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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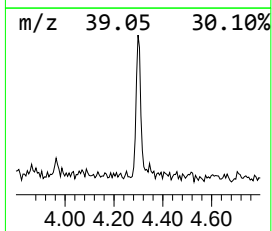
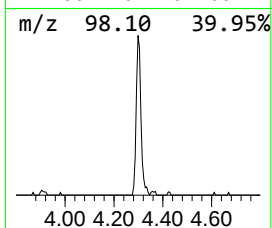
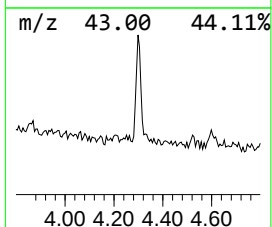
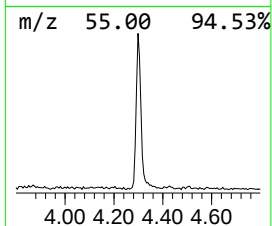
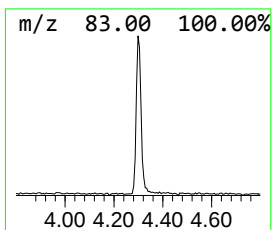
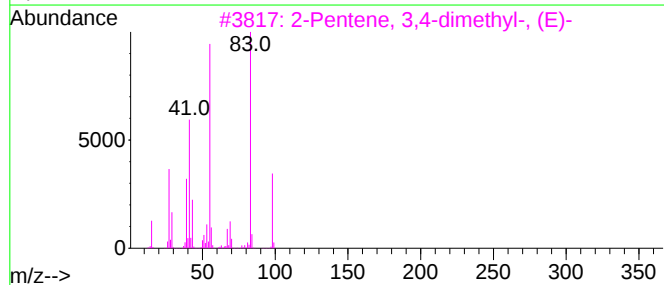
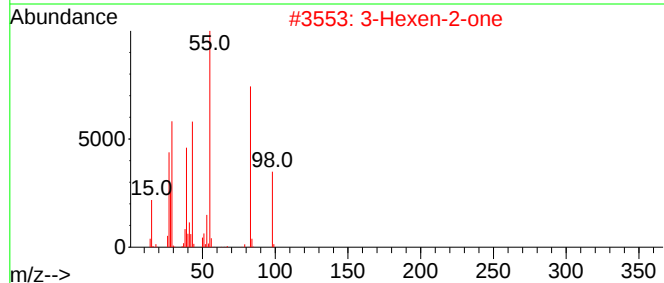
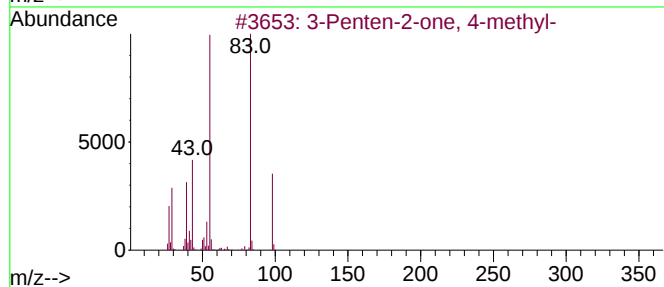
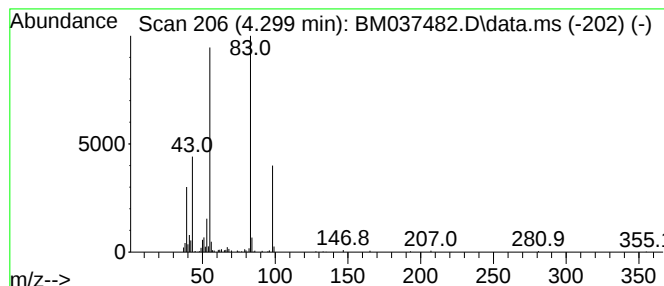
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.299	2.21 ng	141437	1,4-Dichlorobenzene-d4	7.804

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	90
5		2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	90



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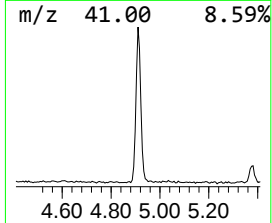
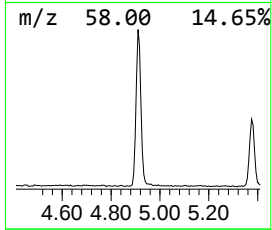
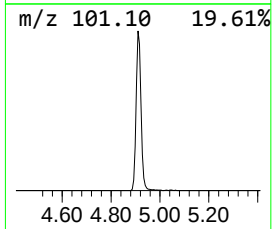
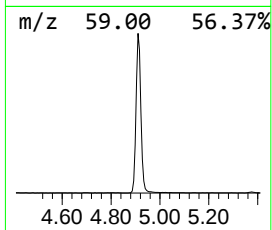
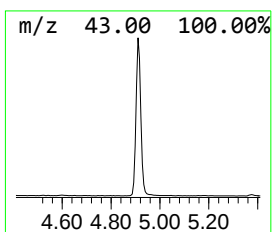
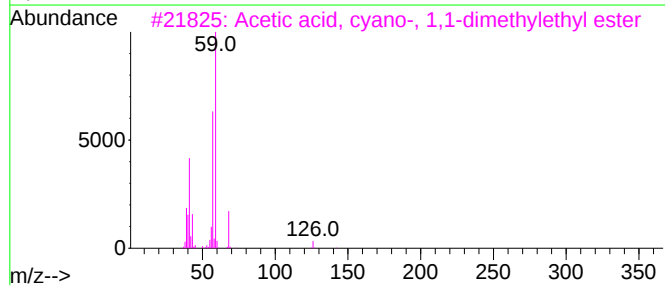
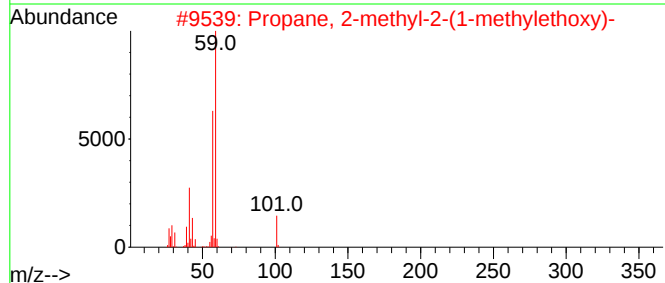
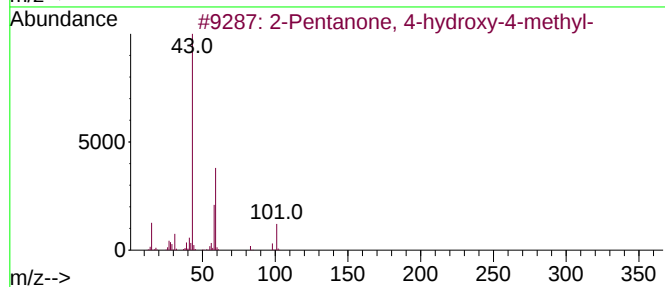
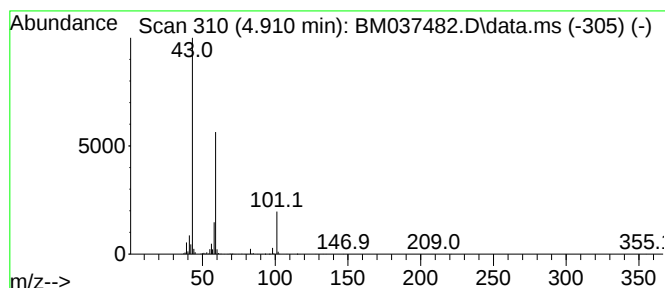
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.910	22.16 ng	1419320	1,4-Dichlorobenzene-d4	7.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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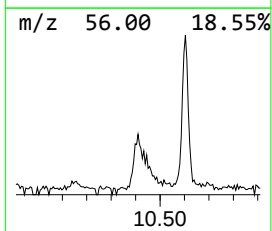
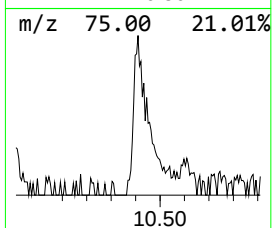
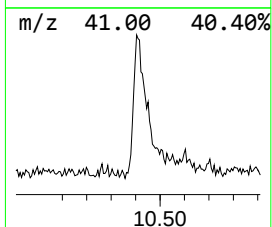
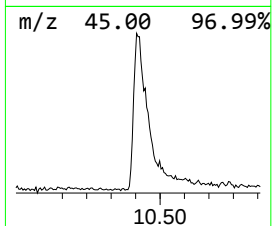
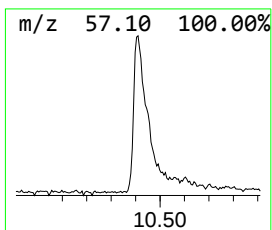
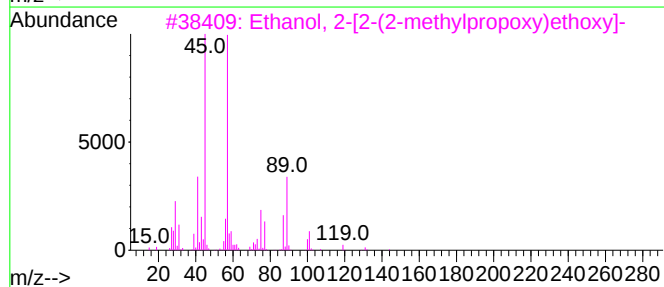
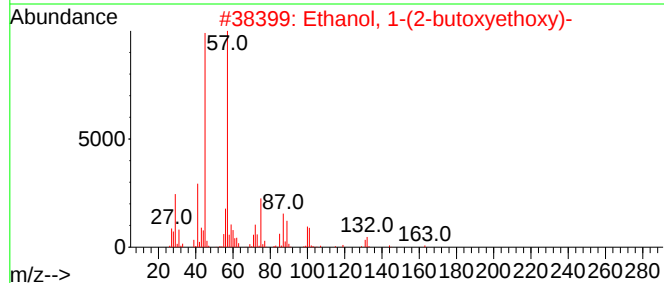
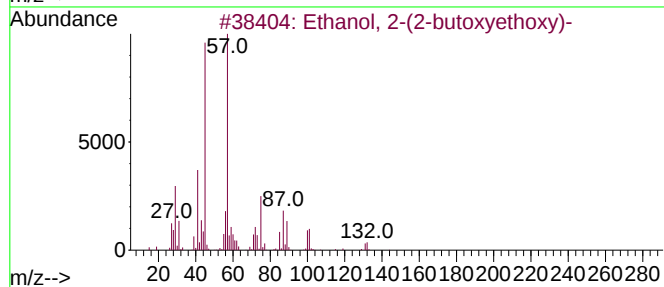
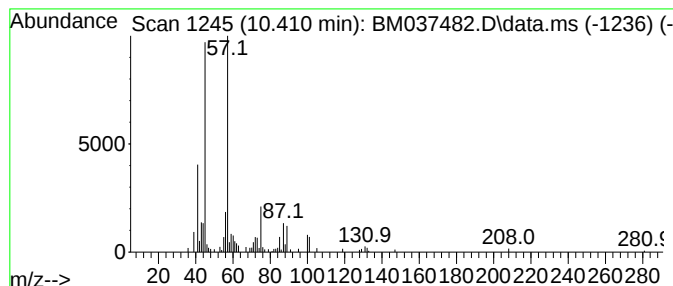
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.410	2.10 ng	174607	Naphthalene-d8	10.604	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	86
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
5	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	59



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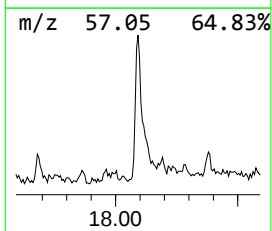
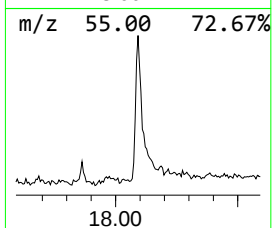
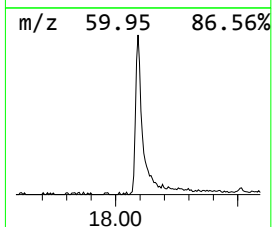
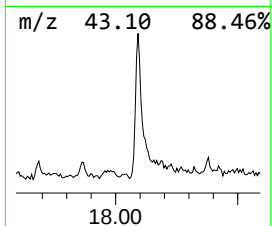
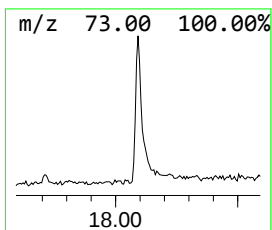
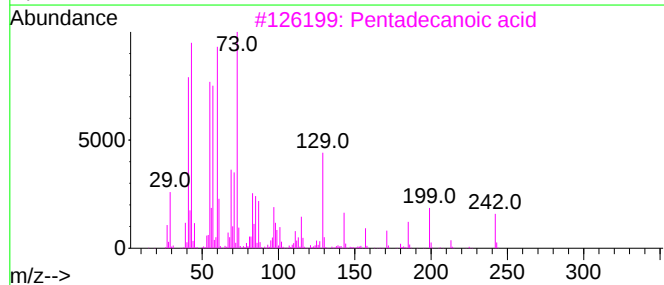
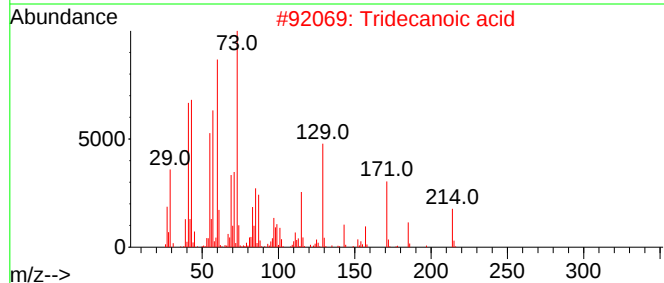
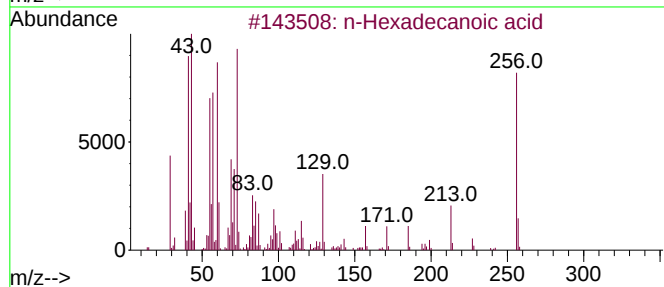
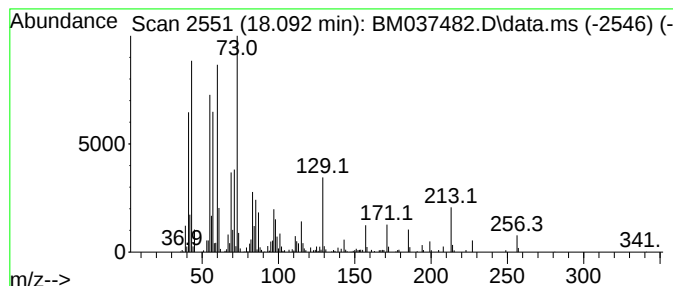
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	3.88 ng	401347	Phenanthrene-d10	17.192

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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Dodecanoic acid	200	C12H24O2	000143-07-7	52



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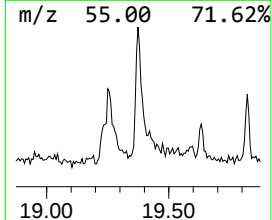
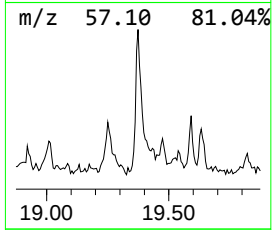
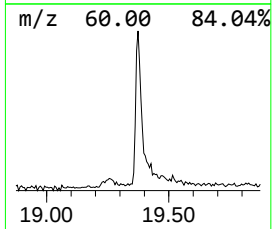
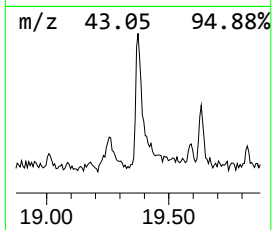
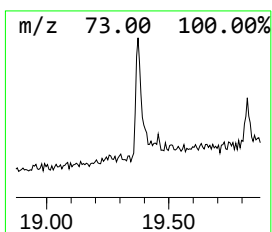
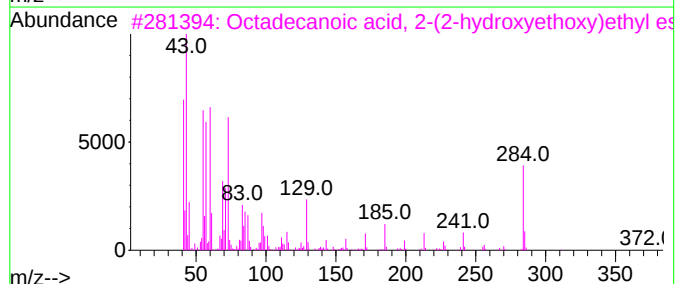
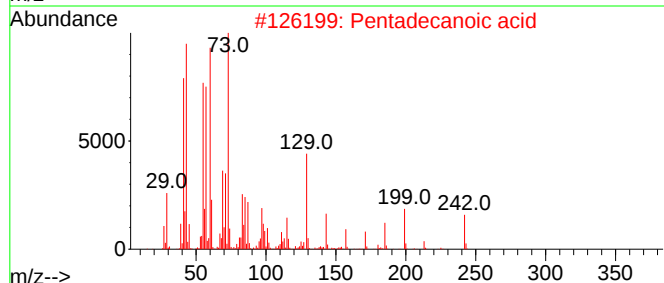
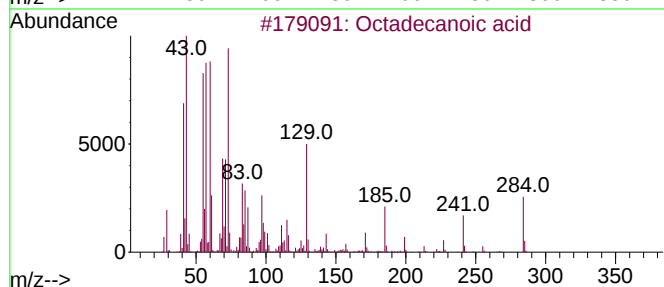
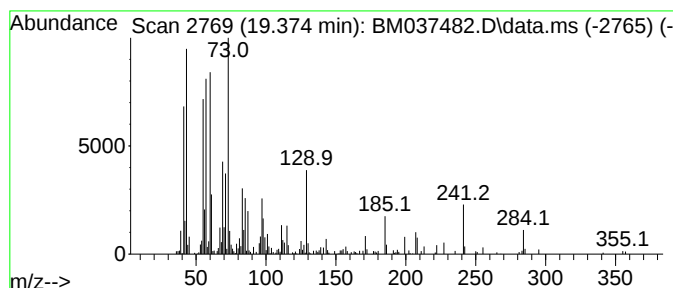
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.374	2.34 ng	258805	Chrysene-d12	21.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	68



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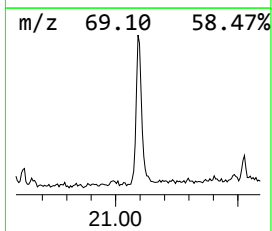
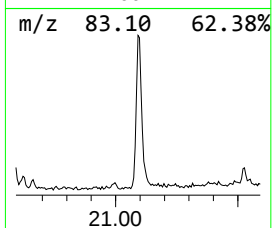
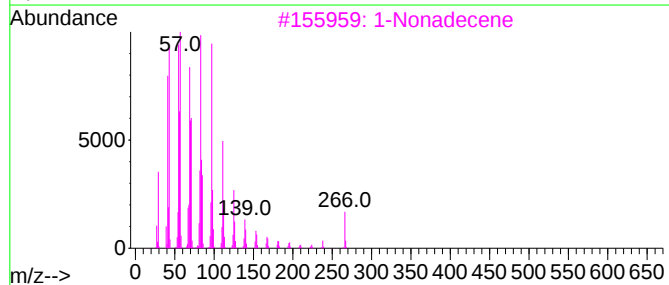
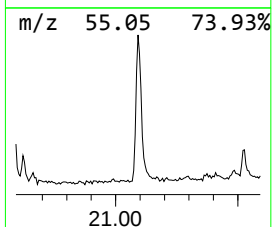
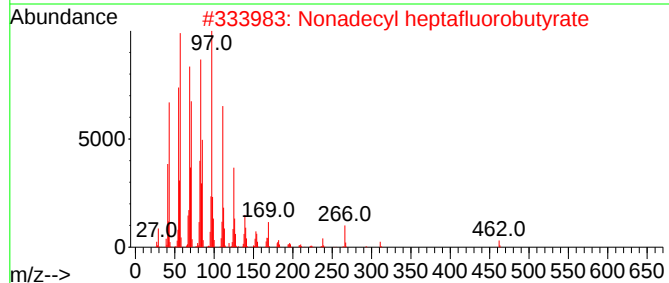
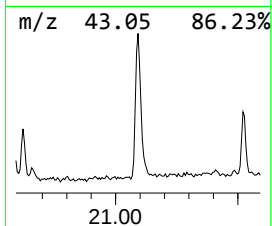
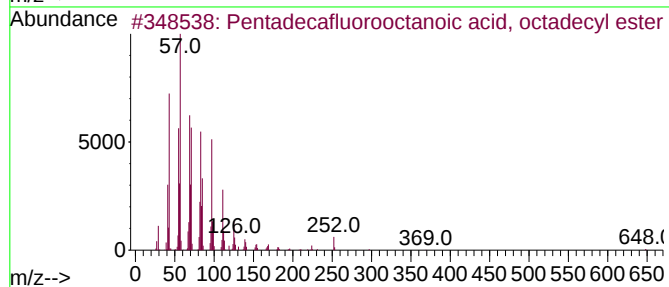
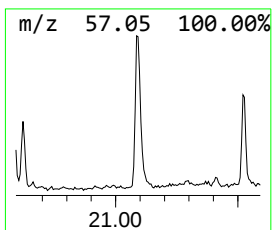
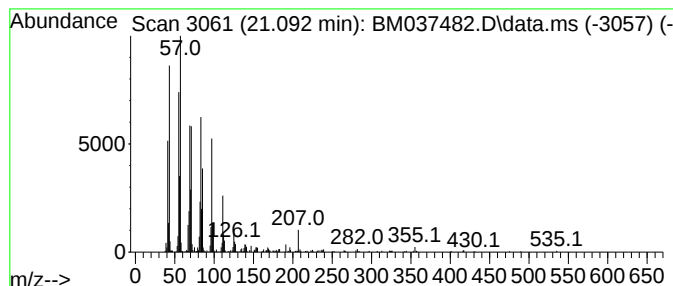
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	4.77 ng	526299	Chrysene-d12	21.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2			Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	91
3			1-Nonadecene	266	C19H38	018435-45-5	89
4			1-Hexacosene	364	C26H52	018835-33-1	89
5			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111122\
Data File : BM037482.D
Acq On : 12 Nov 2022 00:19
Operator : CG/JU
Sample : N5530-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-09

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.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
3-Penten-2-one,...	4.299	2.2	ng	141437	1	7.804	1281100	20.0
2-Pentanone, 4-...	4.910	22.2	ng	1419320	1	7.804	1281100	20.0
Ethanol, 2-(2-b...	10.410	2.1	ng	174607	2	10.604	1664430	20.0
n-Hexadecanoic ...	18.092	3.9	ng	401347	4	17.192	2070680	20.0
Octadecanoic acid	19.374	2.3	ng	258805	5	21.380	2208140	20.0
Pentadecafluoro...	21.092	4.8	ng	526299	5	21.380	2208140	20.0