

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
 Data File : BM041312.D
 Acq On : 07 Aug 2023 14:58
 Operator : MA/JU
 Sample : 03903-13
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-03W

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-BM072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041312.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.363	361	370	380	rBV	1422265	2094791	6.60%	2.043%
2	6.969	637	643	659	rVB	848136	1409276	4.44%	1.374%
3	7.786	775	782	789	rBV	534575	836549	2.63%	0.816%
4	8.969	975	983	999	rBV	2002892	3205212	10.09%	3.126%
5	10.392	1217	1225	1238	rBV	3851912	6643485	20.92%	6.479%
6	10.592	1253	1259	1272	rVB	738156	1280718	4.03%	1.249%
7	13.074	1673	1681	1692	rBV	5514469	7835091	24.67%	7.641%
8	14.457	1909	1916	1924	rBV	1201092	1807033	5.69%	1.762%
9	15.515	2090	2096	2103	rBV	991438	1475801	4.65%	1.439%
10	15.957	2165	2171	2186	rBV	4858639	6879843	21.66%	6.709%
11	16.727	2298	2302	2309	rBV	281095	366486	1.15%	0.357%
12	17.215	2380	2385	2391	rBV	1589158	2087993	6.58%	2.036%
13	18.121	2534	2539	2549	rBV	1215756	1710150	5.39%	1.668%
14	18.921	2661	2675	2701	rBV	12180134	31756045	100.00%	30.968%
15	19.403	2753	2757	2765	rBV	722319	954176	3.00%	0.931%
16	19.856	2829	2834	2839	rBV	8722505	10440572	32.88%	10.182%
17	21.127	3046	3050	3059	rVB	360601	449231	1.41%	0.438%
18	21.421	3095	3100	3105	rBV	1628814	1951325	6.14%	1.903%
19	22.603	3294	3301	3317	rVB	12008518	17685441	55.69%	17.247%
20	23.791	3498	3503	3514	rVB	882456	1674880	5.27%	1.633%

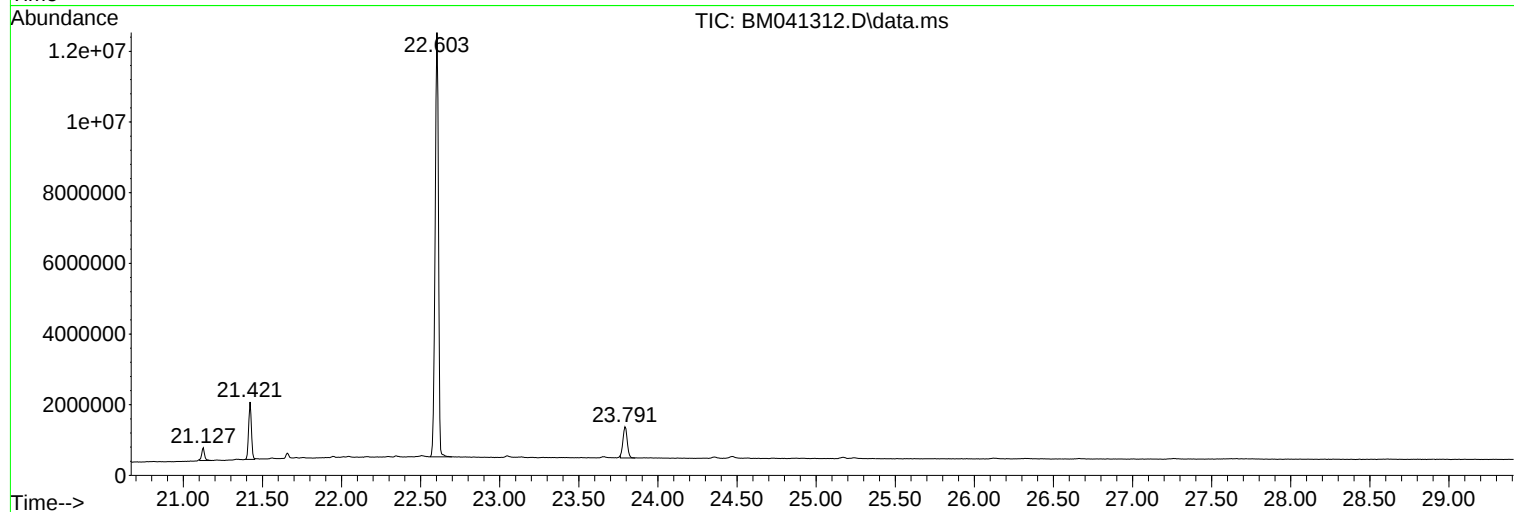
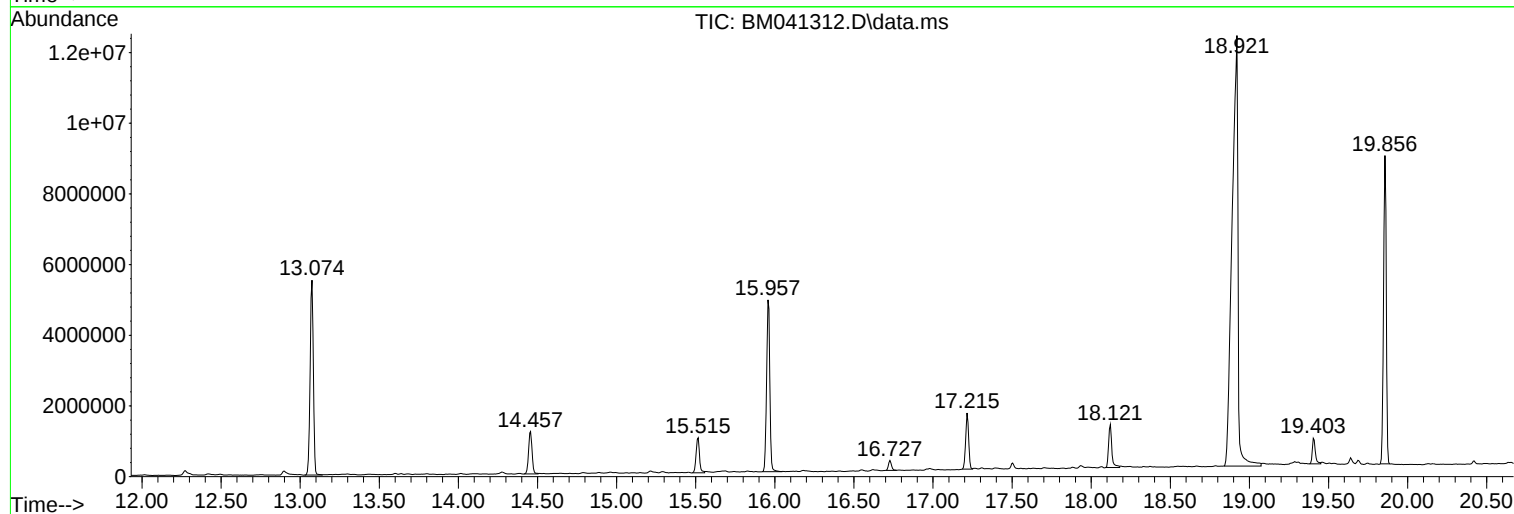
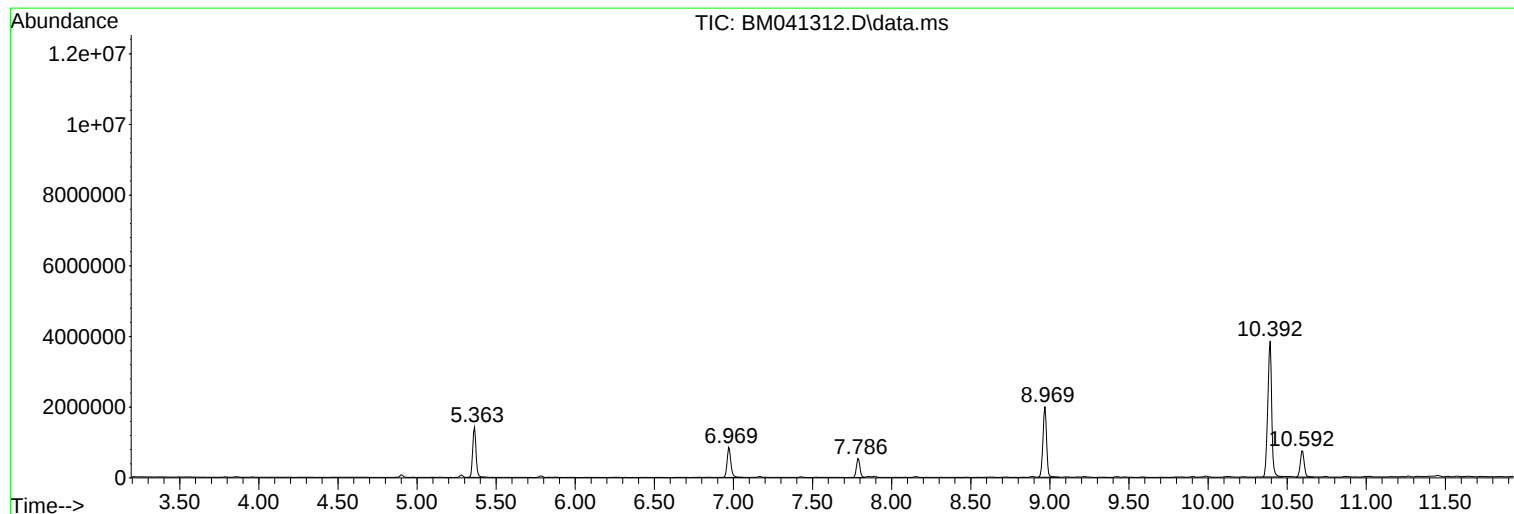
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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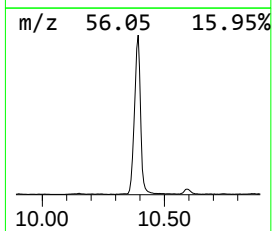
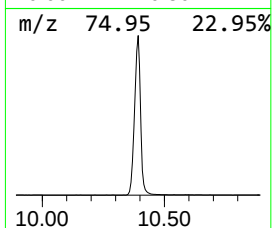
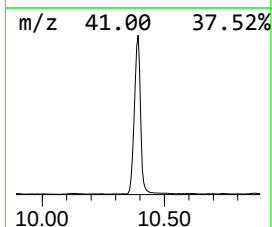
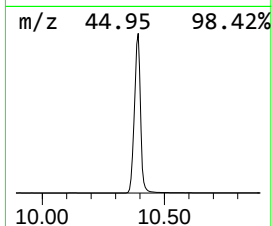
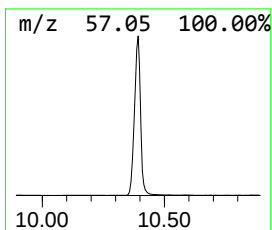
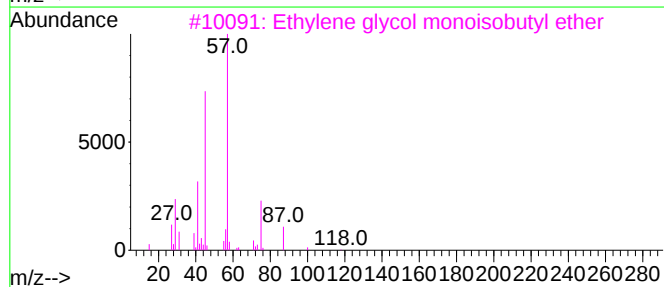
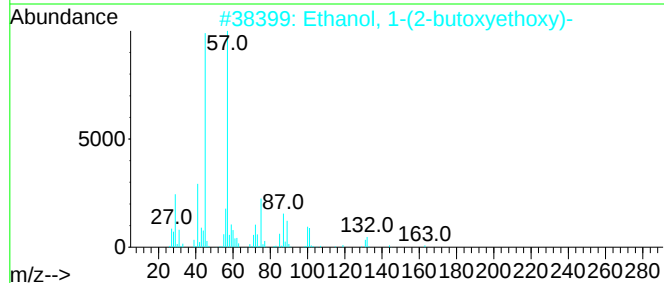
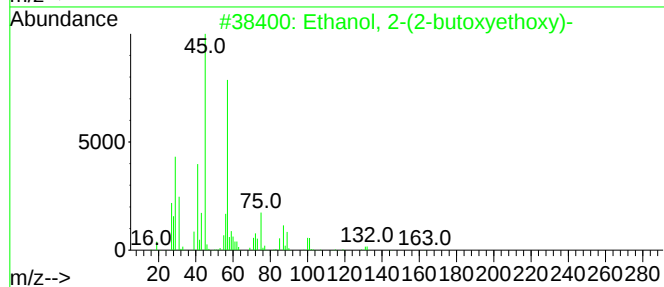
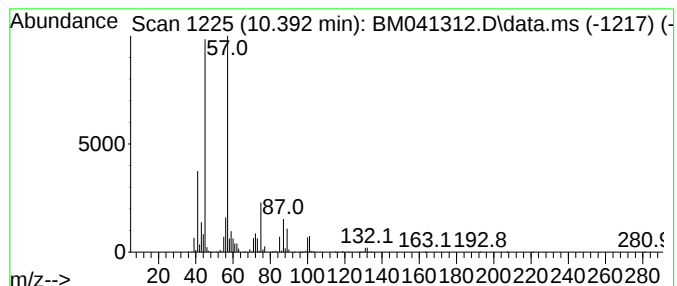
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.392	103.75 ng	6643490	Naphthalene-d8	10.592

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	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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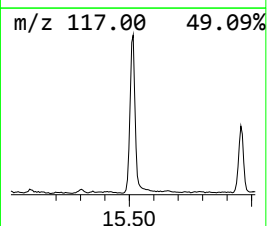
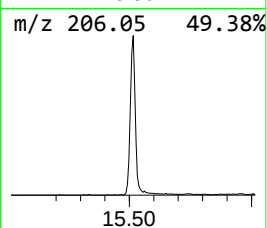
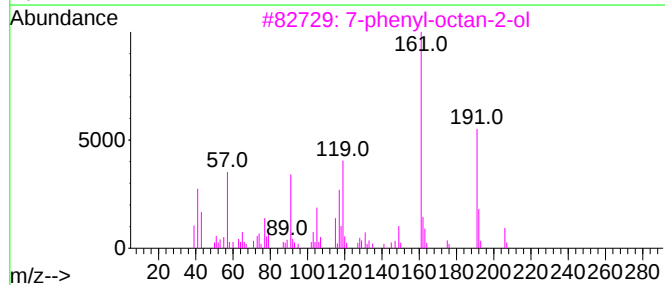
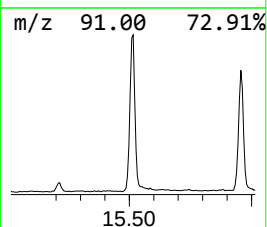
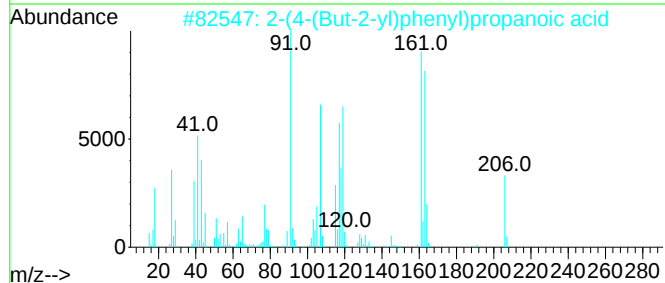
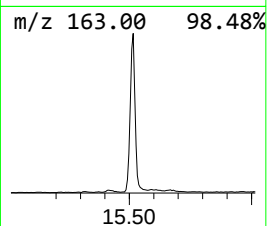
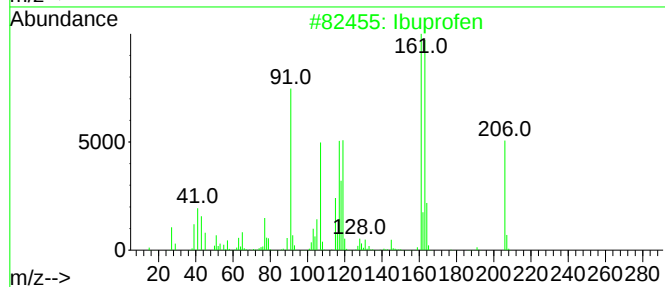
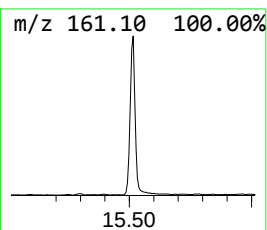
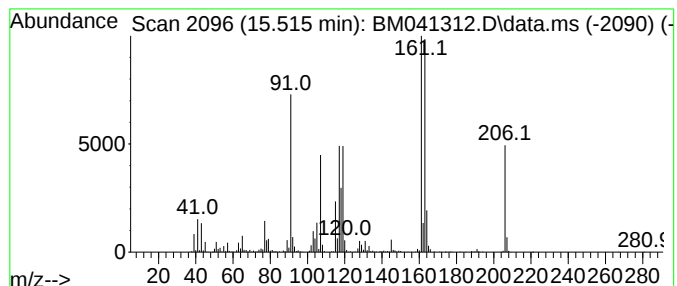
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Peak Number 2 Ibuprofen Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.515	16.33 ng	1475800	Acenaphthene-d10	14.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ibuprofen	206	C13H18O2	015687-27-1	99
2			2-(4-(But-2-yl)phenyl)propanoic ...	206	C13H18O2	064451-76-9	98
3			7-phenyl-octan-2-ol	206	C14H22O	1000383-47-6	27
4			1,2,3,5-Tetramethylbenzene, 2-ox...	163	C10H13NO	1010127-21-8	22
5			Silane, triethoxy-2-propenyl-	204	C9H20O3Si	002550-04-1	22



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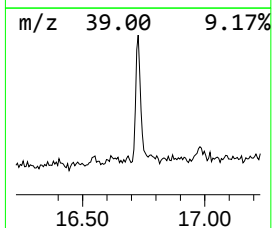
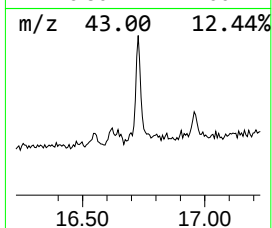
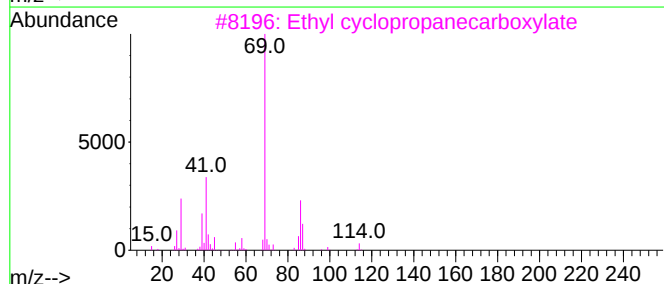
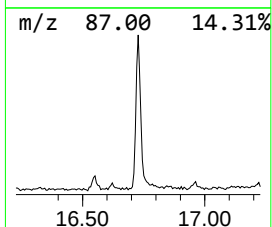
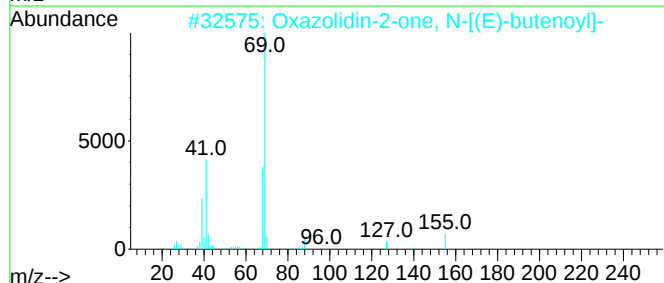
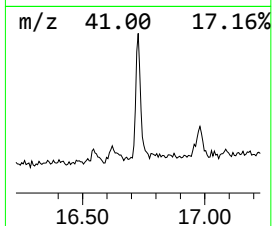
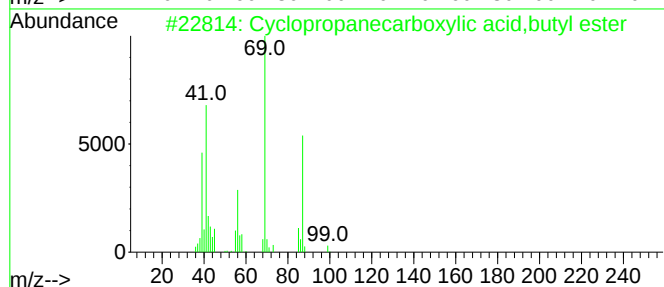
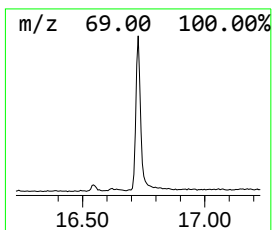
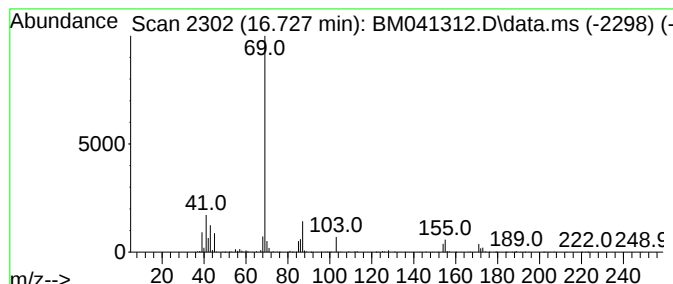
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Peak Number 3 Cyclopropanecarboxylic acid... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.727	3.51 ng	366486	Phenanthrene-d10	17.215

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanecarboxylic acid, buty...	142	C8H14O2	054947-39-6	59
2			Oxazolidin-2-one, N-[(E)-butenyl]-	155	C7H9NO3	1010156-45-5	50
3			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	38
4			(E)-2-Methylbut-2-en-1-yl methac...	154	C9H14O2	088142-95-4	38
5			Cyclopropanecarboxylic acid, isop...	128	C7H12O2	006887-83-8	36



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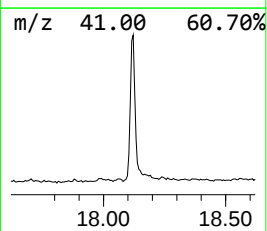
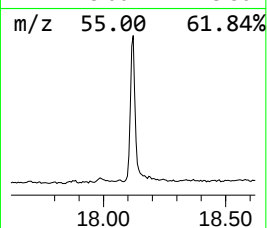
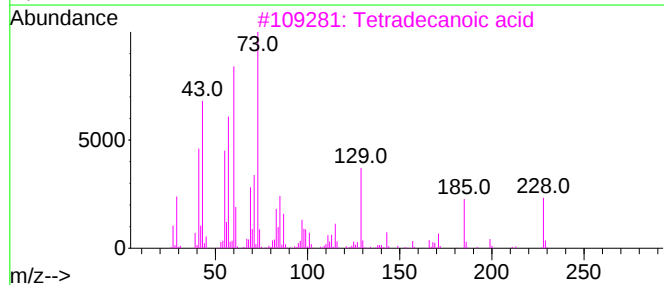
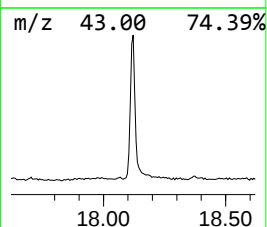
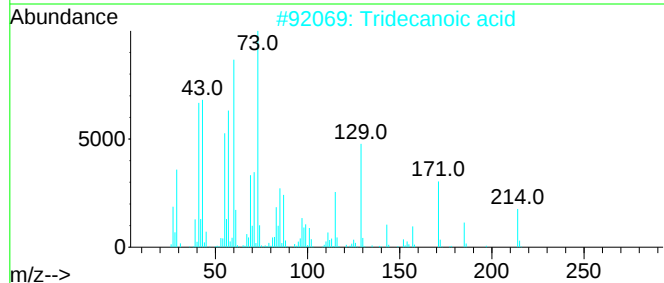
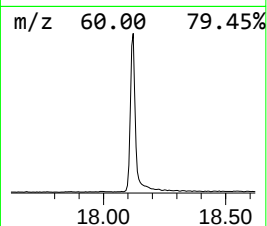
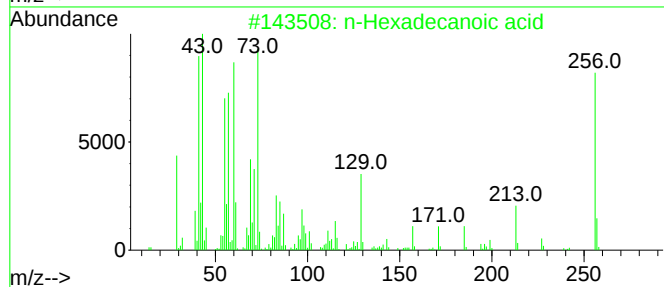
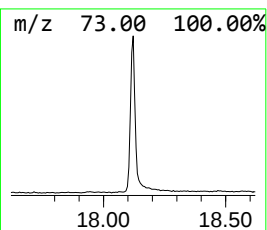
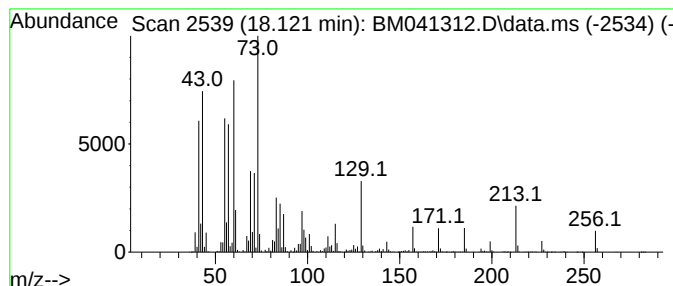
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.121	16.38 ng	1710150	Phenanthrene-d10	17.215	
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	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47



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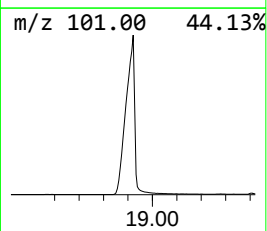
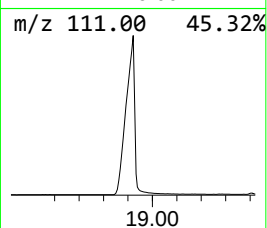
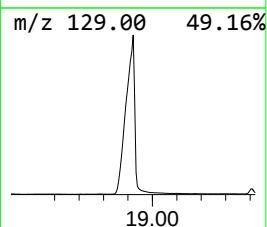
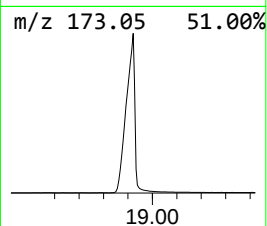
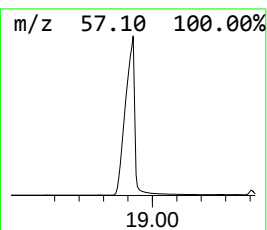
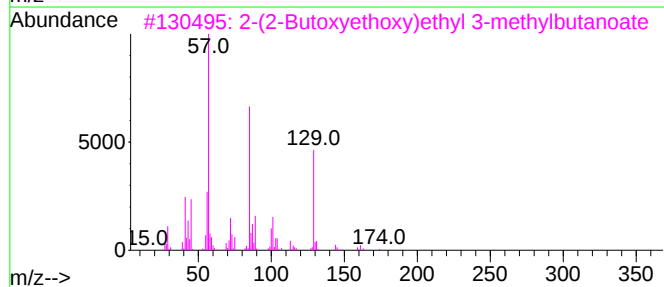
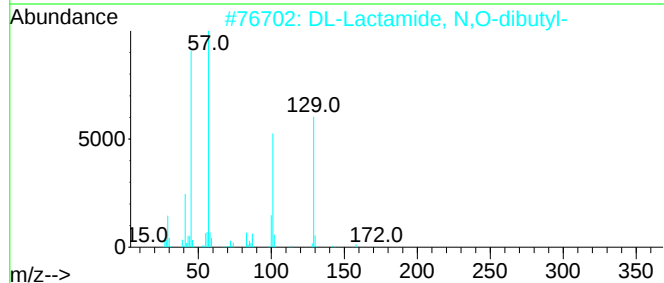
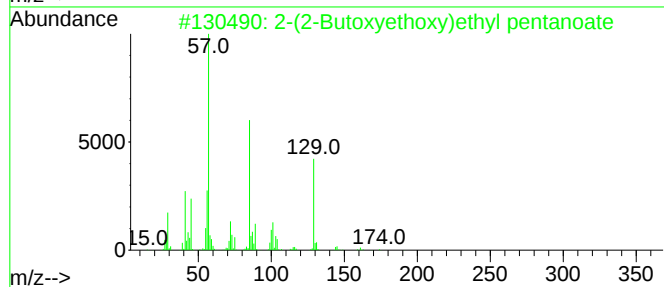
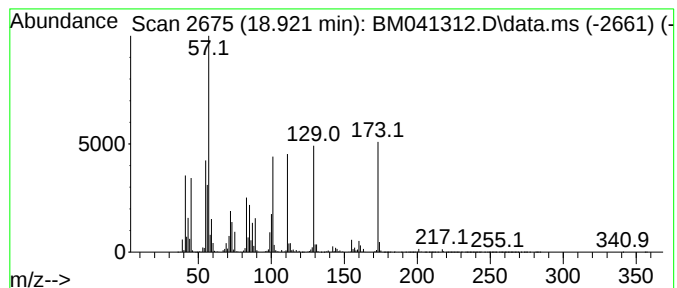
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown18.921 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.921	304.18 ng	31756000	Phenanthrene-d10	17.215

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Butoxyethoxy)ethyl pentanoate	246	C13H26O4	1000367-00-4	22		
2	DL-Lactamide, N,O-dibutyl-	201	C11H23NO2	1000452-56-2	16		
3	2-(2-Butoxyethoxy)ethyl 3-methyl...	246	C13H26O4	1000367-04-5	14		
4	Germane, trimethyl(1-methyl-2-bu...	188	C8H18Ge	006727-43-1	12		
5	8-Methylnonanoic acid, 2-butyl e...	228	C14H28O2	1000452-00-3	12		



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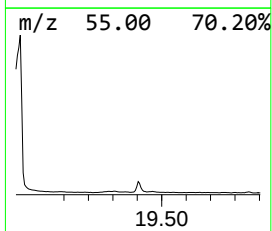
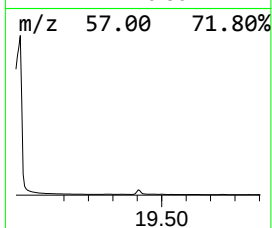
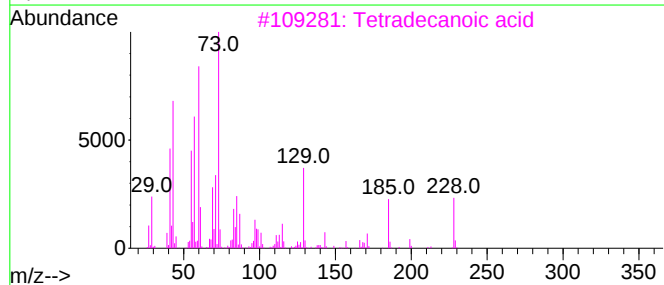
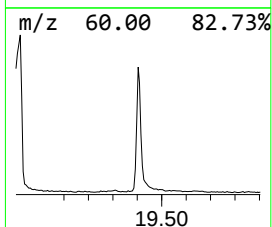
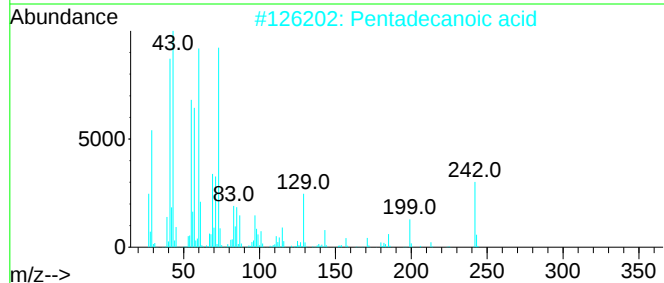
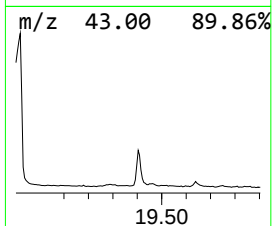
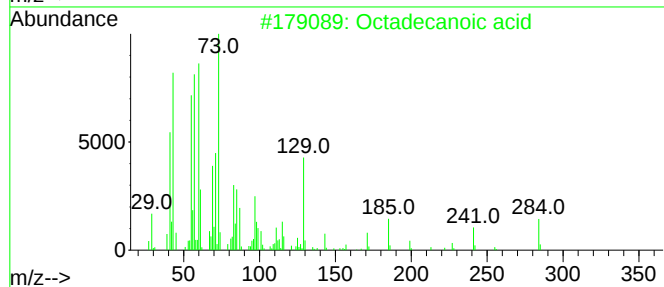
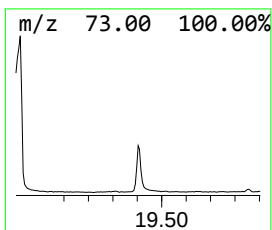
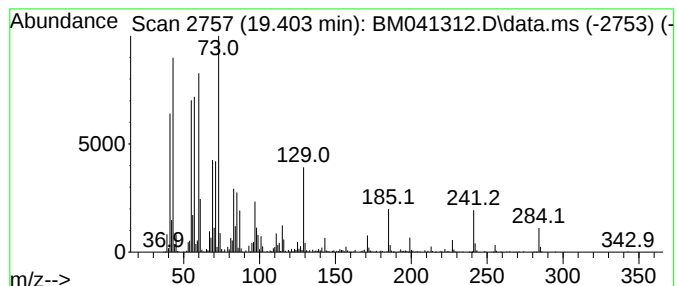
Instrument :
BNA_M
ClientSampleId :
MW-03W

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.403	9.78 ng	954176	Chrysene-d12	21.421	
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	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Tridecanoic acid	214	C13H26O2	000638-53-9	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
Data File : BM041312.D
Acq On : 07 Aug 2023 14:58
Operator : MA/JU
Sample : 03903-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

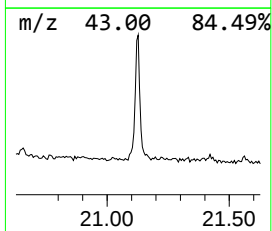
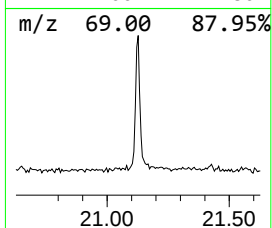
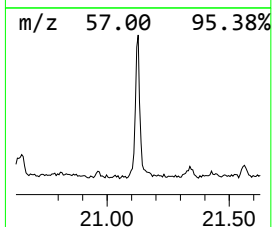
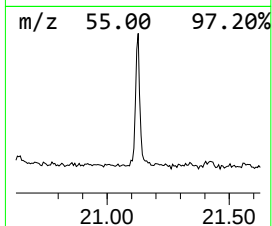
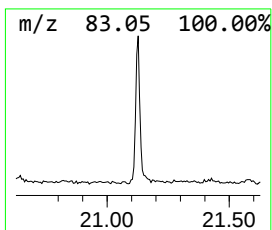
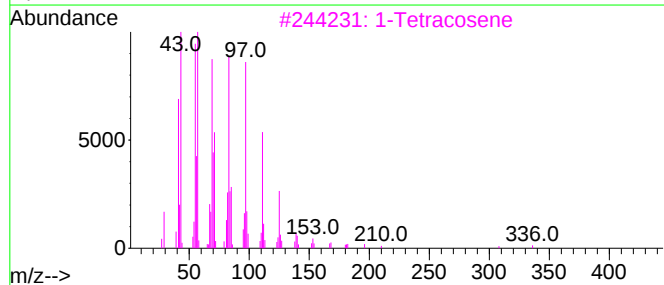
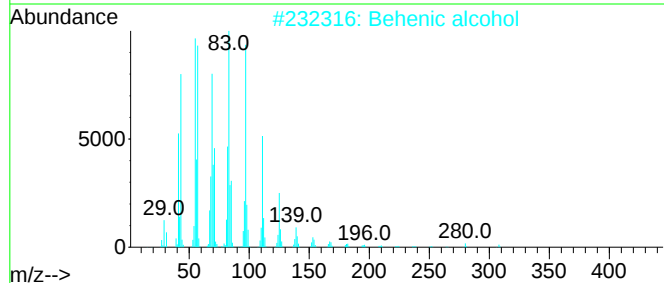
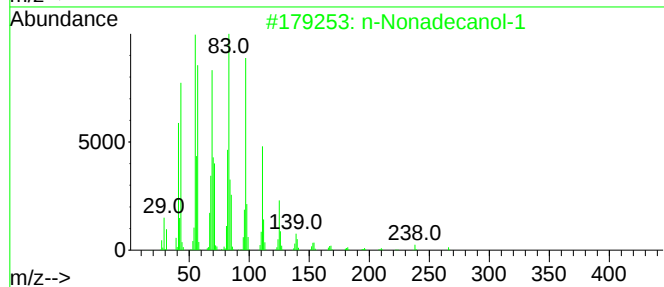
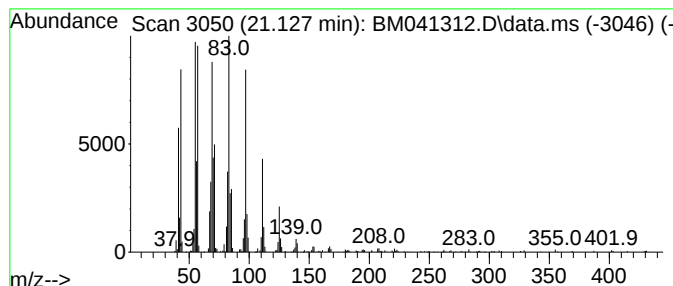
Instrument :
BNA_M
ClientSampleId :
MW-03W

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Nonadecanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.127	4.60 ng	449231	Chrysene-d12		21.421	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1		284	C19H40O	001454-84-8	94
2	Behenic alcohol		326	C22H46O	000661-19-8	94
3	1-Tetracosene		336	C24H48	010192-32-2	94
4	1-Hexacosene		364	C26H52	018835-33-1	94
5	1-Heneicosanol		312	C21H44O	015594-90-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
Data File : BM041312.D
Acq On : 07 Aug 2023 14:58
Operator : MA/JU
Sample : 03903-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-03W

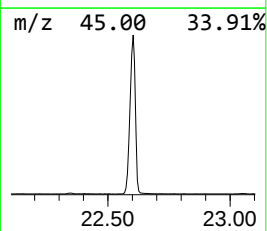
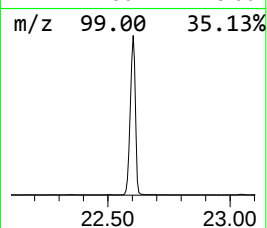
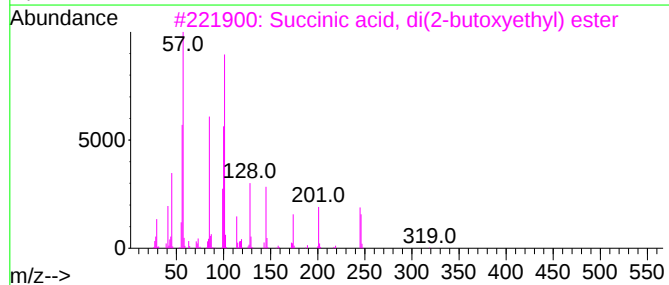
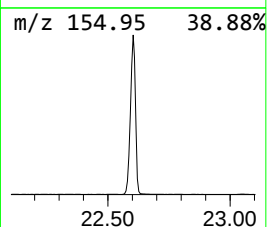
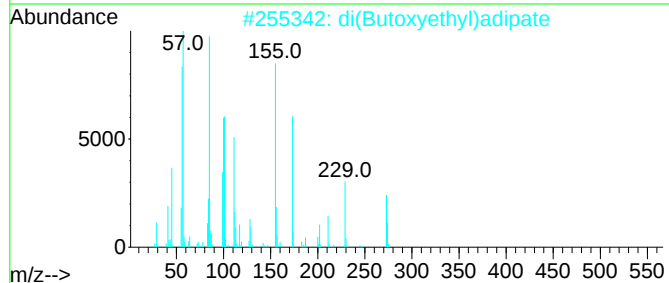
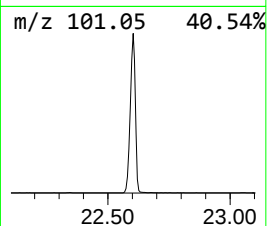
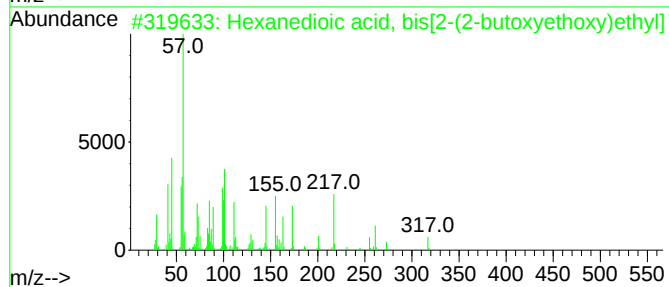
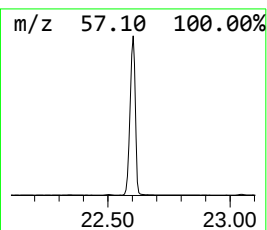
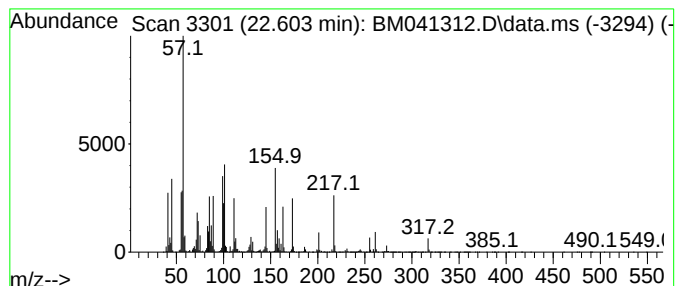
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexanedioic acid, bis[2-(2-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.603	181.27 ng	17685400	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, bis[2-(2-butox...	434	C22H42O8	000141-17-3	93
2			di(Butoxyethyl)adipate	346	C18H34O6	000141-18-4	23
3			Succinic acid, di(2-butoxyethyl)...	318	C16H30O6	1010325-84-7	12
4			H2N(CH2)7NH2	130	C7H18N2	000646-19-5	10
5			1-Decanamine	157	C10H23N	002016-57-1	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
Data File : BM041312.D
Acq On : 07 Aug 2023 14:58
Operator : MA/JU
Sample : 03903-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-03W

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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
Ethanol, 2-(2-b...	10.392	103.8	ng	6643490	2	10.592	1280720	20.0
Ibuprofen	15.515	16.3	ng	1475800	3	14.457	1807030	20.0
Cyclopropanecar...	16.727	3.5	ng	366486	4	17.215	2087990	20.0
n-Hexadecanoic ...	18.121	16.4	ng	1710150	4	17.215	2087990	20.0
unknown18.921	18.921	304.2	ng	31756000	4	17.215	2087990	20.0
Octadecanoic acid	19.403	9.8	ng	954176	5	21.421	1951330	20.0
n-Nonadecanol-1	21.127	4.6	ng	449231	5	21.421	1951330	20.0
Hexanedioic aci...	22.603	181.3	ng	17685400	5	21.421	1951330	20.0