

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022322\
 Data File : BM034055.D
 Acq On : 23 Feb 2022 16:38
 Operator : CG/JU
 Sample : N1602-09
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 20220084B-AMENDED-BERKELEY-4B-COMP

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-BM022222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM034055.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.101	312	317	323	rVB	136118	191940	1.55%	0.282%
2	5.566	389	396	407	rBV	3871115	5444759	44.02%	7.988%
3	7.172	660	669	681	rVB	3997641	6378193	51.57%	9.357%
4	8.019	804	813	821	rBV	736131	1155765	9.34%	1.696%
5	9.178	1002	1010	1019	rBV	2482400	4082012	33.01%	5.989%
6	10.607	1247	1253	1262	rBV	236443	374368	3.03%	0.549%
7	10.836	1283	1292	1299	rBV	915099	1520377	12.29%	2.231%
8	13.283	1701	1708	1716	rBV	6706247	9545320	77.18%	14.004%
9	13.995	1822	1829	1833	rBV	117979	177082	1.43%	0.260%
10	14.654	1934	1941	1948	rBV	1342496	1981181	16.02%	2.907%
11	16.130	2186	2192	2200	rBV	4398365	6114794	49.44%	8.971%
12	17.395	2400	2407	2413	rBV	1528182	2257704	18.25%	3.312%
13	18.077	2518	2523	2527	rVB	135868	177489	1.44%	0.260%
14	18.295	2553	2560	2578	rBV	1494245	2616281	21.15%	3.838%
15	19.571	2770	2777	2800	rBV	4020194	6281841	50.79%	9.216%
16	20.012	2846	2852	2857	rBV	9761035	12367822	100.00%	18.145%
17	20.659	2957	2962	2965	rBV	640139	800029	6.47%	1.174%
18	20.695	2965	2968	2974	rVB4	220133	301280	2.44%	0.442%
19	21.277	3063	3067	3072	rBV	815048	1044985	8.45%	1.533%
20	21.565	3111	3116	3121	rBV	1943612	2551796	20.63%	3.744%
21	24.024	3528	3534	3543	rVB2	1397840	2796511	22.61%	4.103%

Sum of corrected areas: 68161529

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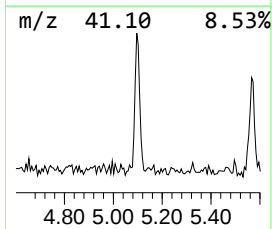
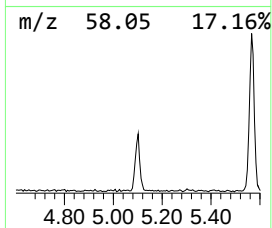
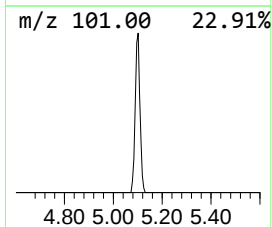
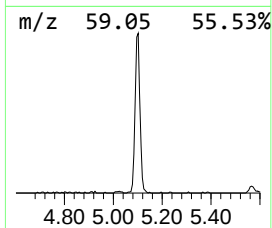
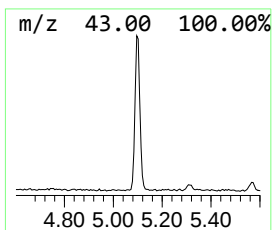
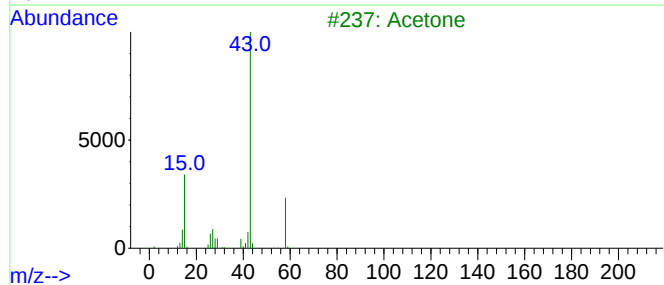
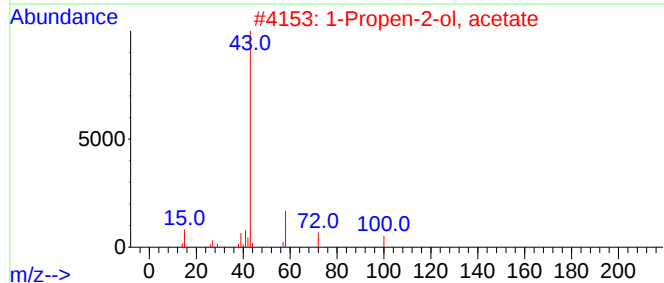
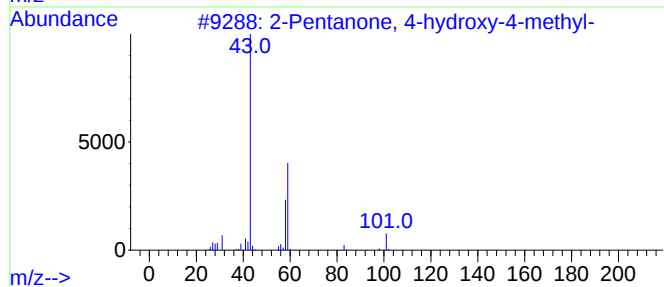
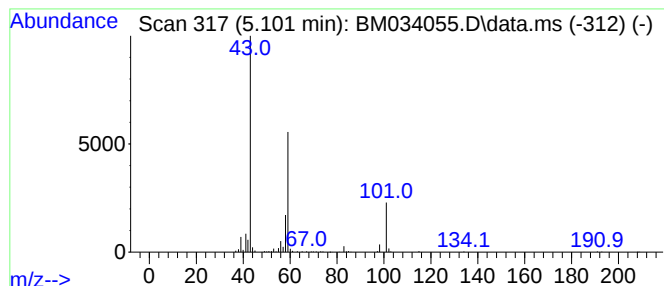
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.101	3.32 ng	191940	1,4-Dichlorobenzene-d4	8.019

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3			Acetone	58	C3H6O	000067-64-1	10
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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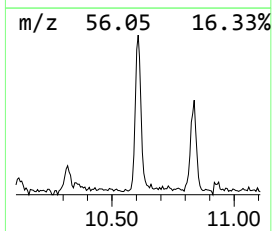
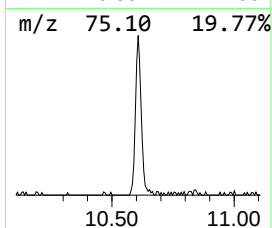
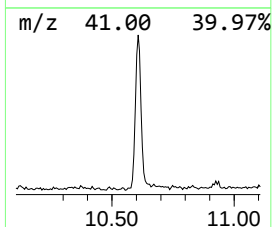
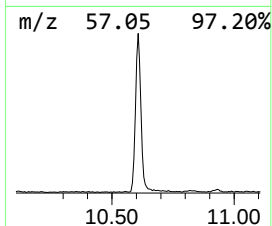
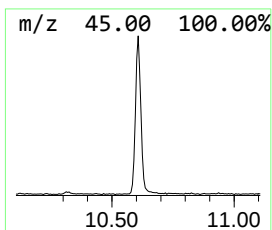
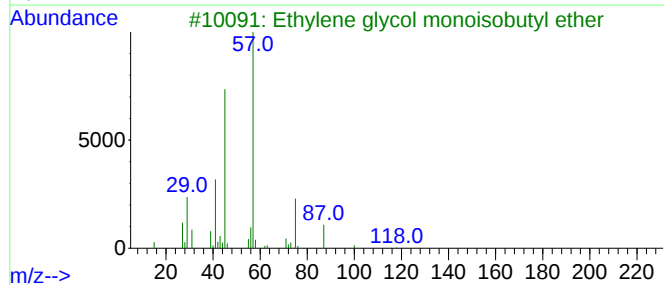
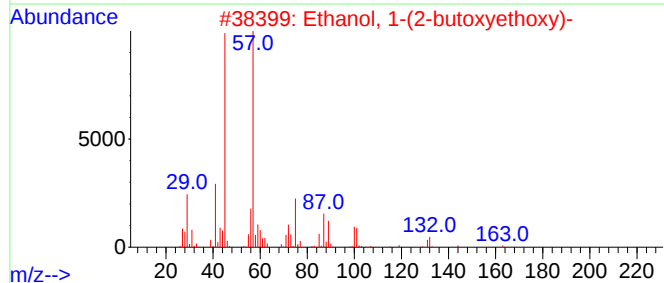
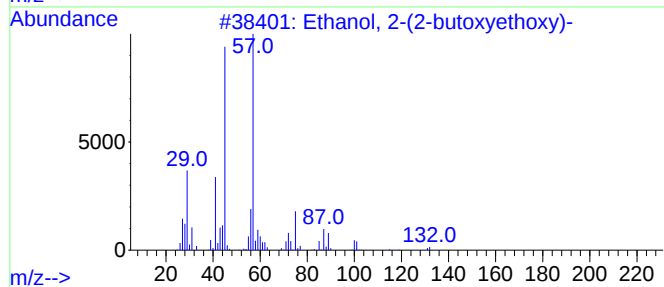
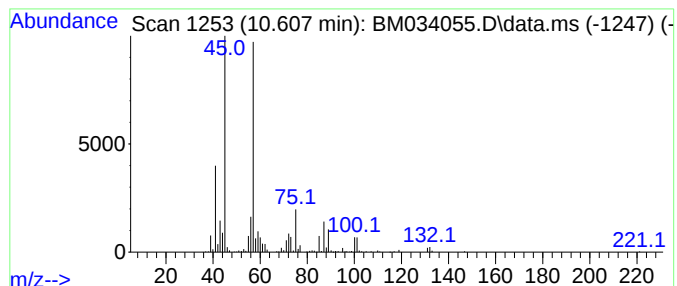
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.607	4.92 ng	374368	Naphthalene-d8	10.836

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	59
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Methyl-2,3,5-tri-O-methyl-4-thio...	222	C9H18O4S	051306-30-0	53



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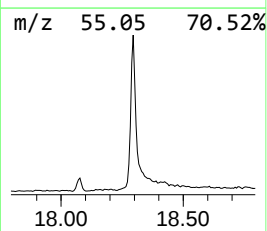
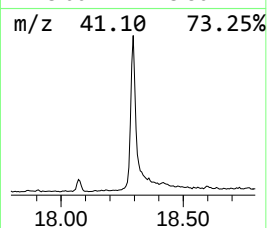
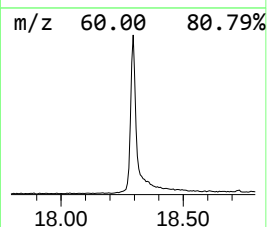
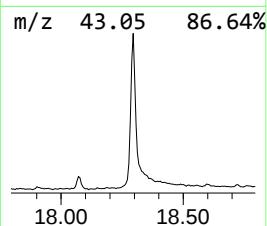
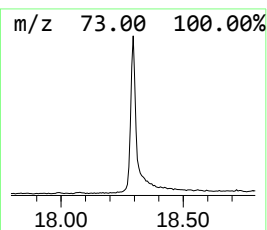
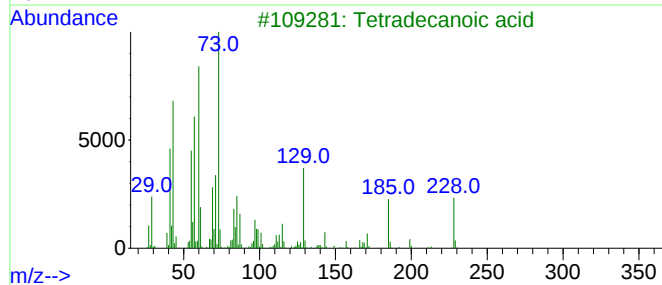
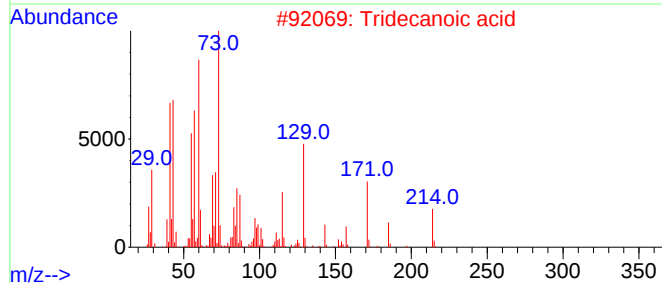
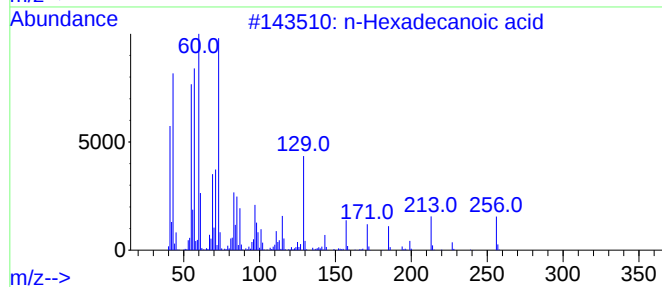
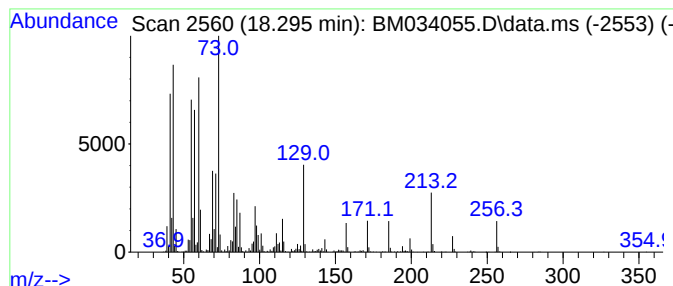
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.295	23.18 ng	2616280	Phenanthrene-d10	17.395

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			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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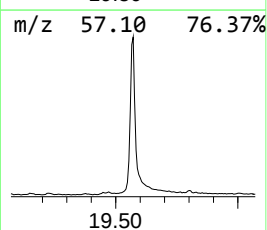
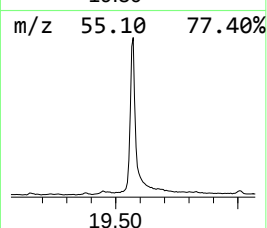
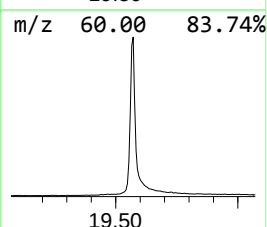
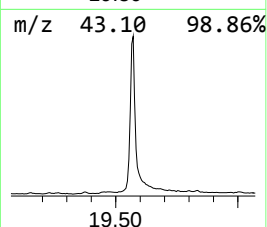
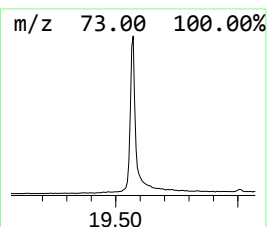
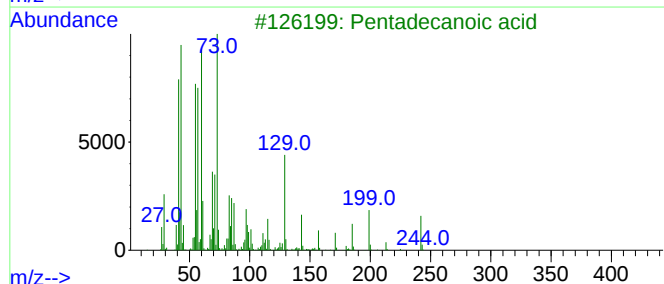
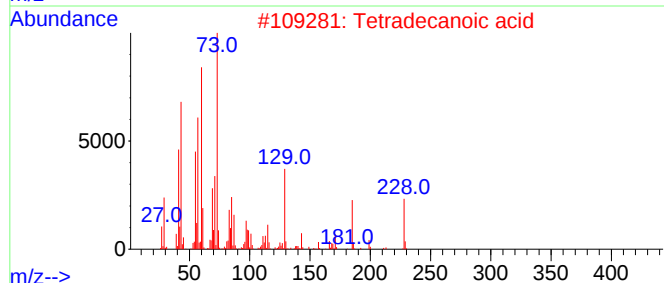
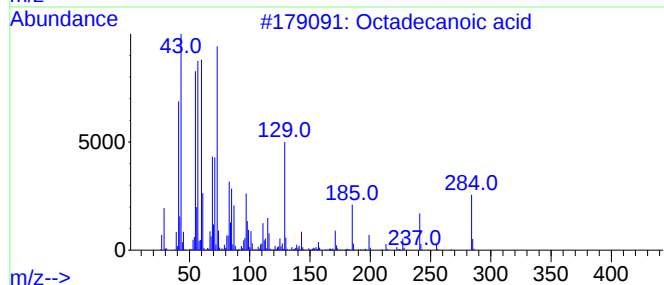
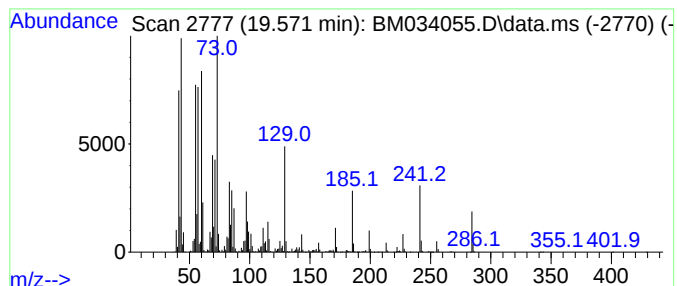
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.571	49.23 ng	6281840	Chrysene-d12	21.565

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
5			Tridecanoic acid	214	C13H26O2	000638-53-9	68



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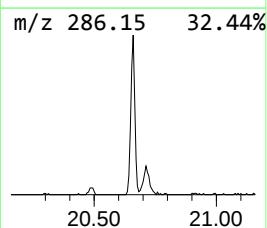
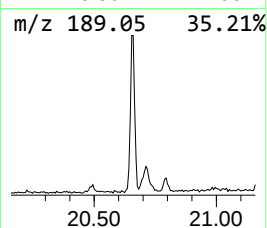
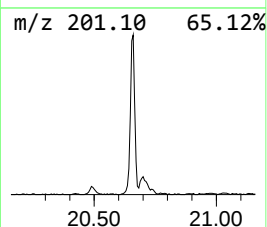
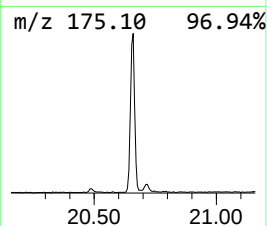
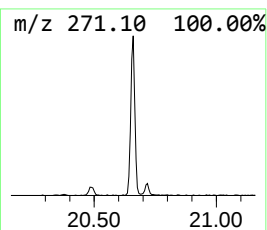
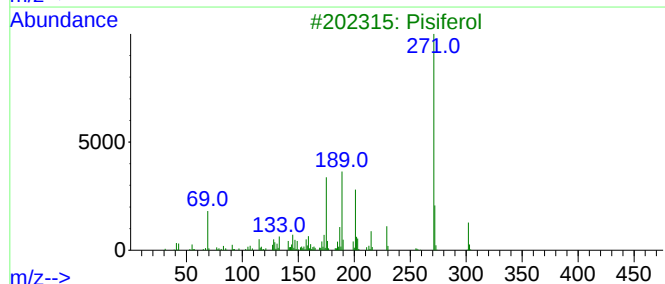
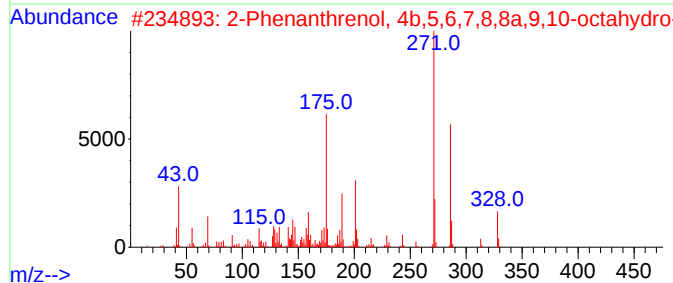
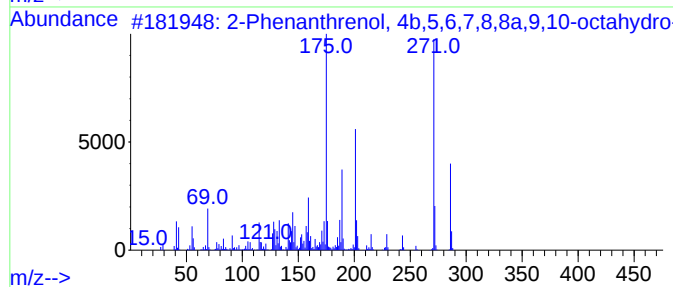
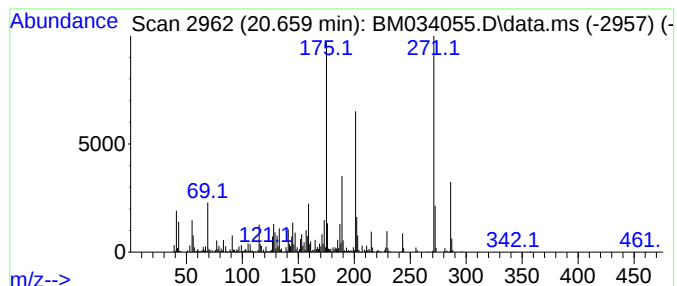
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Peak Number 5 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.659	6.27 ng	800029	Chrysene-d12	21.565

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	99
2		2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	90
3		Pisiferol	302	C20H30O2	024035-36-7	49
4		13-Isopropylpodocarpene-12-ol-20-al	300	C20H28O2	024035-37-8	49
5		(4Br,8As)-(+)-4B,5,6,7,8,8A,9,10...	346	C22H34O3	1000426-72-2	46



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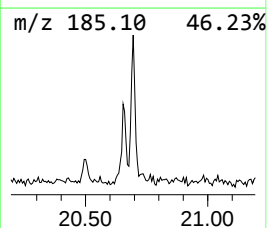
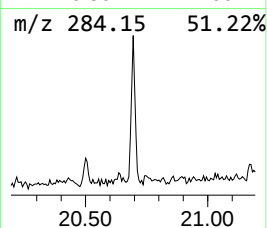
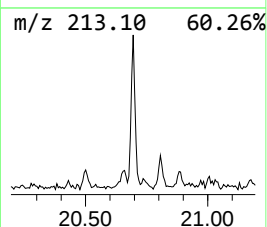
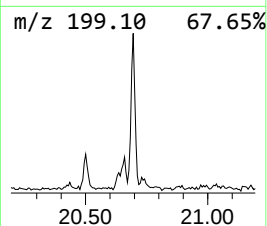
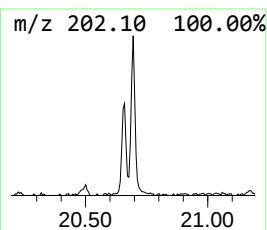
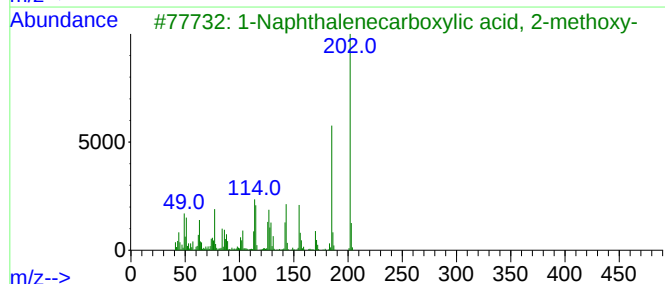
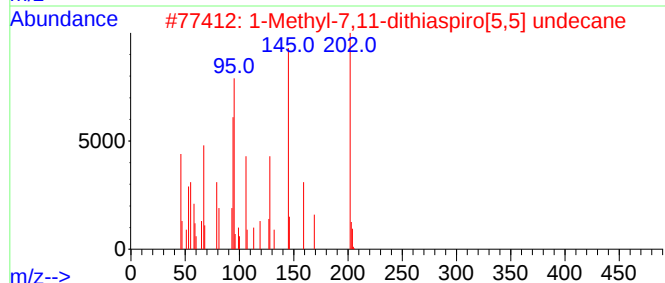
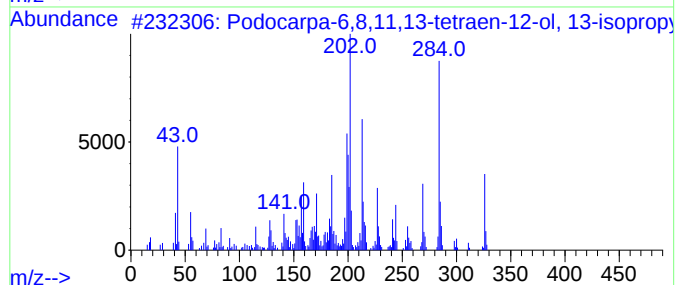
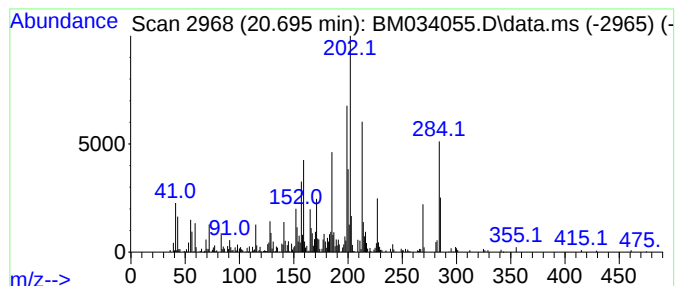
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20220084B-AMENDED-BERKELEY-4B-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Podocarpa-6,8,11,13-tetraen... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
20.695	2.36 ng	301280	Chrysene-d12		21.565	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Podocarpa-6,8,11,13-tetraen-12-o...		326	C22H30O2	022160-86-7	83
2	1-Methyl-7,11-dithiaspiro[5,5] u...		202	C10H18S2	107678-22-8	25
3	1-Naphthalenecarboxylic acid, 2-...		202	C12H10O3	000947-62-6	20
4	3-Trifluoromethylbenzylamine, N-...		329	C19H30F3N	1000310-29-2	18
5	5-Hydroxy-3-methyl-1-phenylpyraz...		202	C11H10N2O2	060484-29-9	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022322\
Data File : BM034055.D
Acq On : 23 Feb 2022 16:38
Operator : CG/JU
Sample : N1602-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20220084B-AMENDED-BERKELEY-4B-COMP

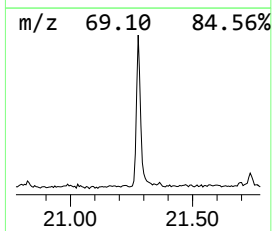
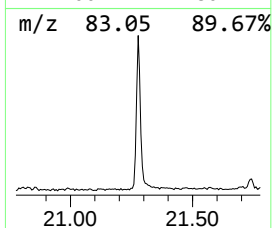
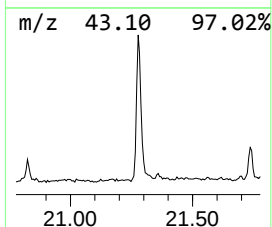
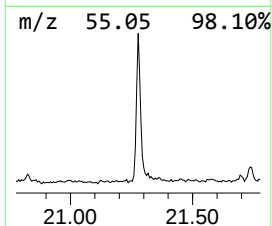
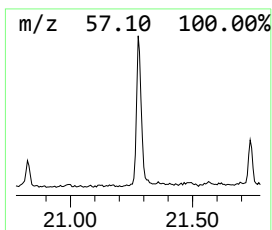
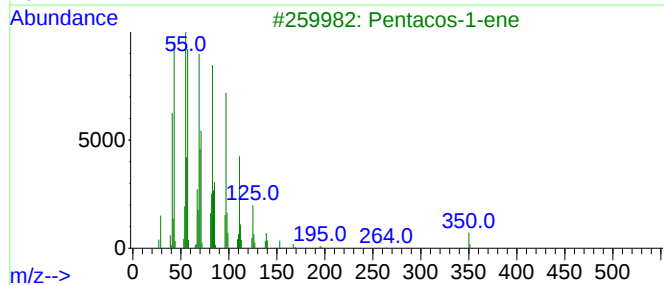
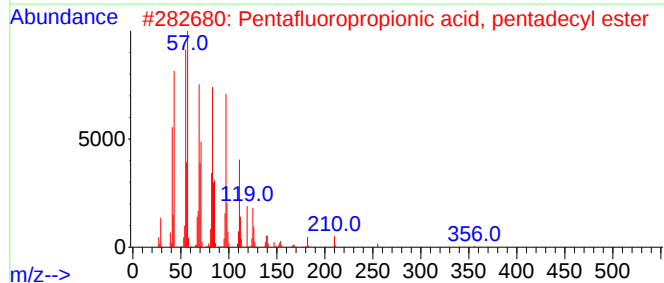
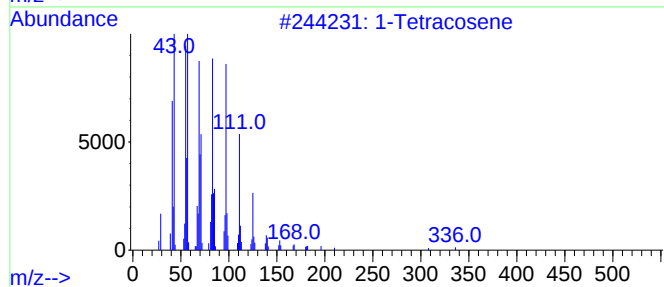
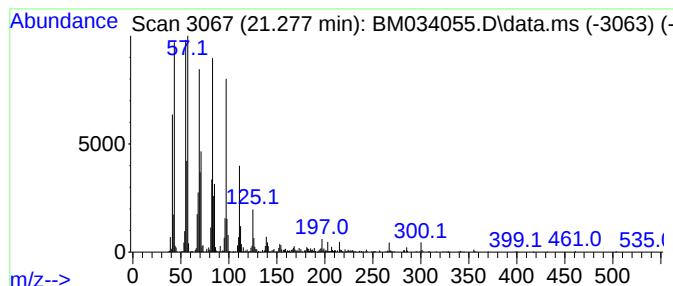
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Tetracosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.277	8.19 ng	1044990	Chrysene-d12	21.565

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetracosene	336	C24H48	010192-32-2	95
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3			Pentacos-1-ene	350	C25H50	016980-85-1	94
4			Behenic alcohol	326	C22H46O	000661-19-8	94
5			1-Heneicosanol	312	C21H44O	015594-90-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022322\
Data File : BM034055.D
Acq On : 23 Feb 2022 16:38
Operator : CG/JU
Sample : N1602-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20220084B-AMENDED-BERKELEY-4B-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022222.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
2-Pentanone, 4-...	5.101	3.3	ng	191940	1	8.019	1155770	20.0
Ethanol, 2-(2-b...	10.607	4.9	ng	374368	2	10.836	1520380	20.0
n-Hexadecanoic ...	18.295	23.2	ng	2616280	4	17.395	2257700	20.0
Octadecanoic acid	19.571	49.2	ng	6281840	5	21.565	2551800	20.0
2-Phenanthrenol...	20.659	6.3	ng	800029	5	21.565	2551800	20.0
Podocarpa-6,8,1...	20.695	2.4	ng	301280	5	21.565	2551800	20.0
1-Tetracosene	21.277	8.2	ng	1044990	5	21.565	2551800	20.0