

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM020223\
 Data File : BM038673.D
 Acq On : 02 Feb 2023 21:10
 Operator : CG/JU
 Sample : 01348-05
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MID2-H5(32-34)

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-BM020123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM038673.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	305	311	319	rBV	343660	471198	18.17%	3.076%
2	5.493	386	392	406	rBV	1055407	1432638	55.24%	9.354%
3	7.110	660	667	680	rBV	904389	1363801	52.58%	8.904%
4	7.928	798	806	814	rBV	307288	446110	17.20%	2.913%
5	9.104	999	1006	1018	rBV	547111	842992	32.50%	5.504%
6	10.739	1277	1284	1292	rBV	318698	516328	19.91%	3.371%
7	13.192	1694	1701	1712	rBV	1812056	2452547	94.56%	16.012%
8	14.569	1927	1935	1942	rBV	502231	704355	27.16%	4.599%
9	16.057	2182	2188	2199	rBV	1204827	1559536	60.13%	10.182%
10	17.310	2393	2401	2408	rBV	539960	720499	27.78%	4.704%
11	18.192	2547	2551	2560	rBV	126787	190824	7.36%	1.246%
12	19.468	2763	2768	2775	rBV2	72885	107238	4.13%	0.700%
13	19.927	2840	2846	2852	rBV	2307564	2593639	100.00%	16.934%
14	20.609	2957	2962	2967	rBV	159216	187754	7.24%	1.226%
15	21.180	3055	3059	3069	rBV2	146156	203063	7.83%	1.326%
16	21.486	3107	3111	3117	rBV	523435	650556	25.08%	4.247%
17	22.709	3316	3319	3324	rVB	78769	98621	3.80%	0.644%
18	23.886	3513	3519	3527	rVB2	417591	774870	29.88%	5.059%

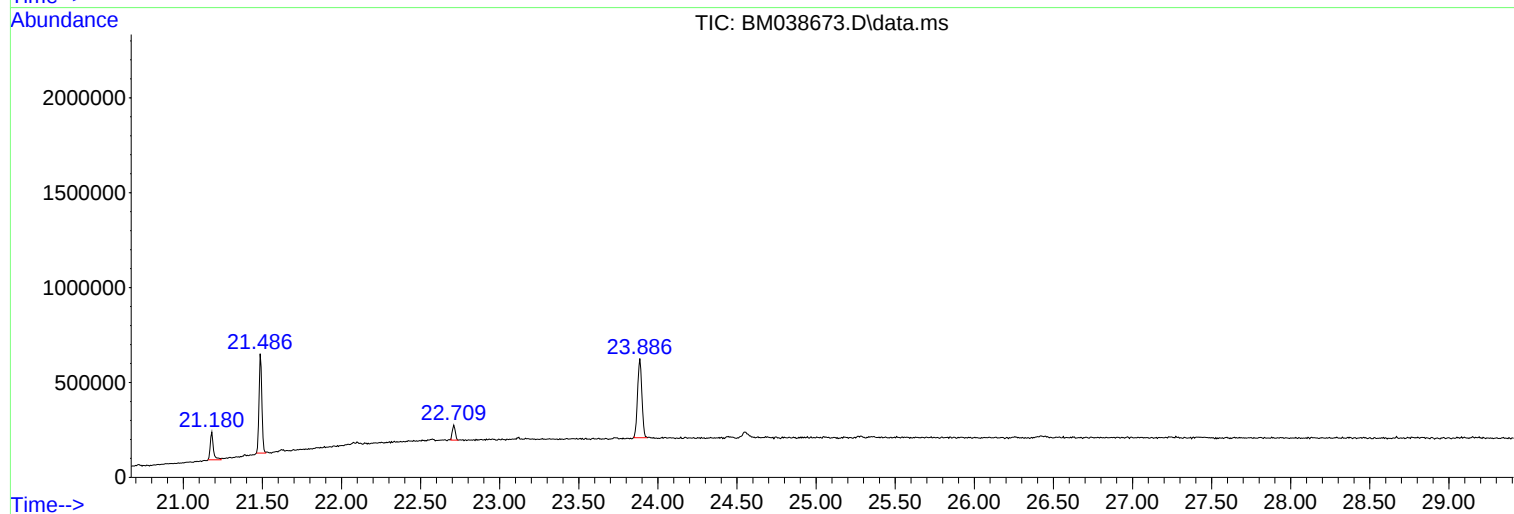
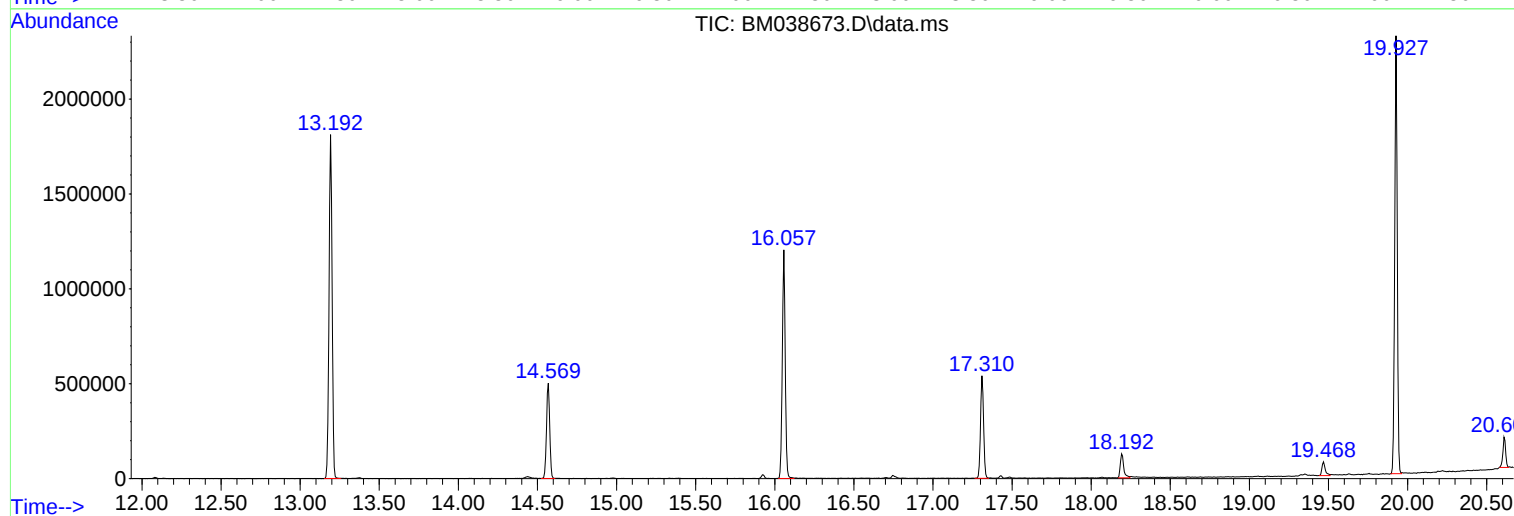
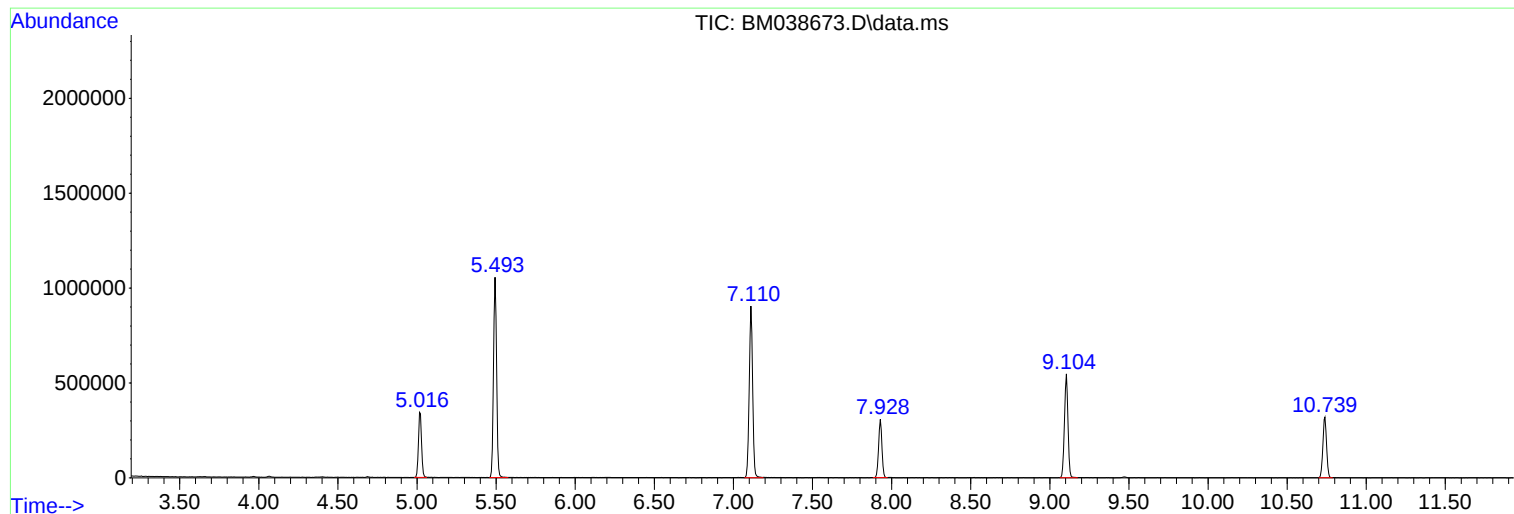
Sum of corrected areas: 15316569

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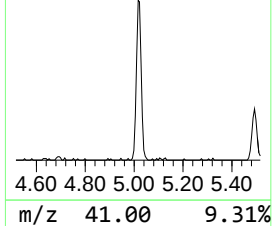
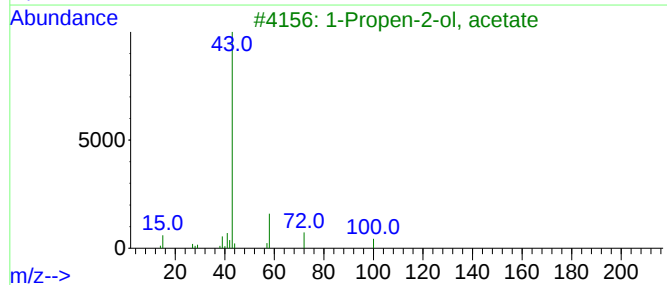
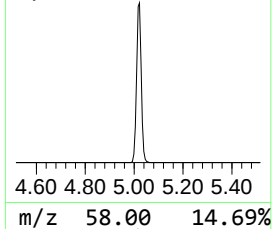
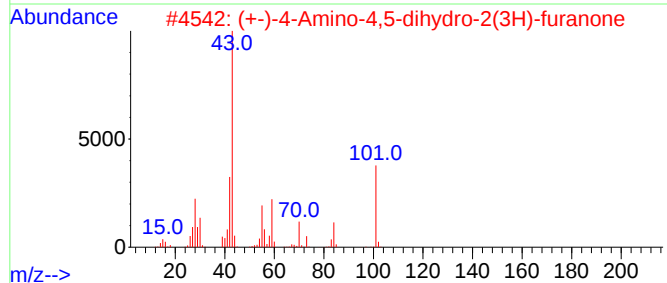
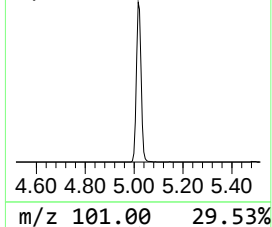
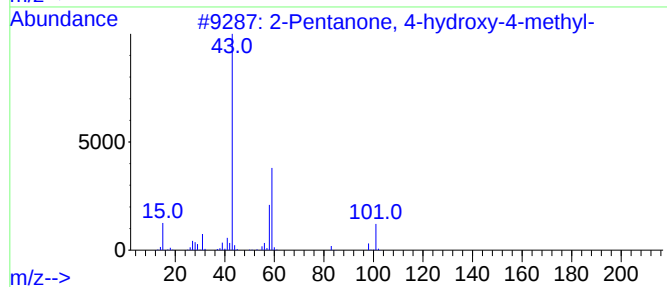
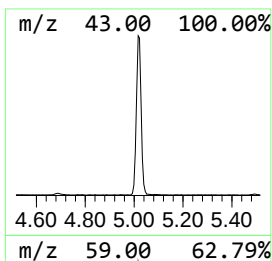
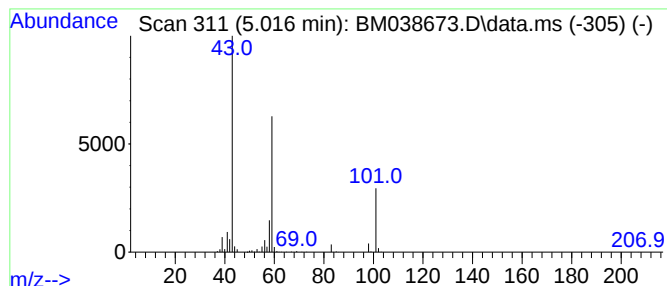
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	21.12 ng	471198	1,4-Dichlorobenzene-d4	7.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	38		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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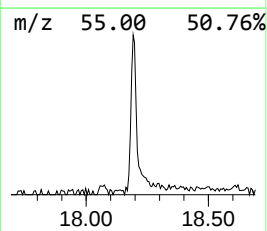
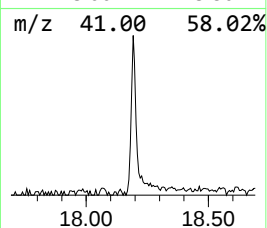
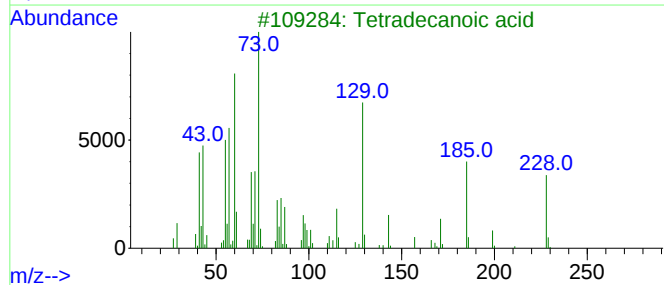
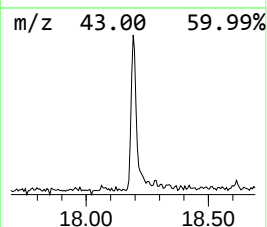
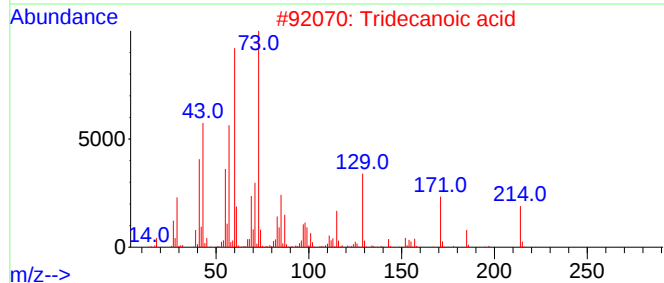
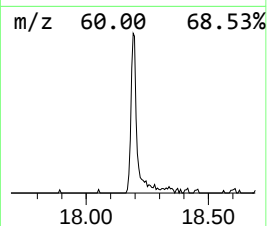
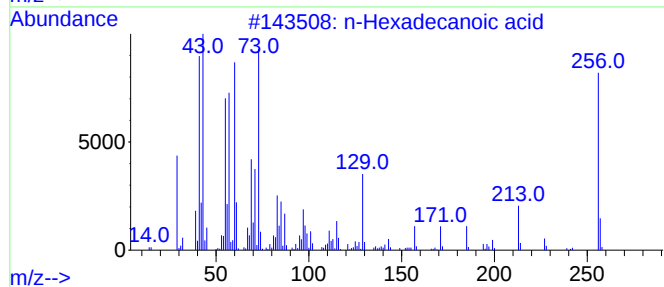
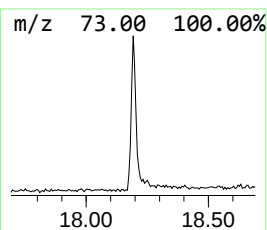
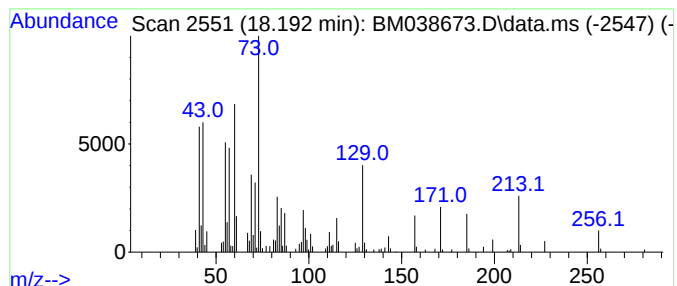
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	5.30 ng	190824	Phenanthrene-d10	17.310

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	76
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	46



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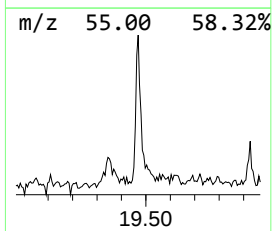
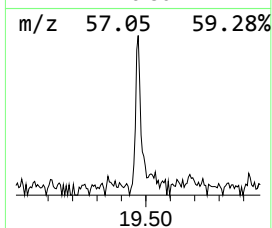
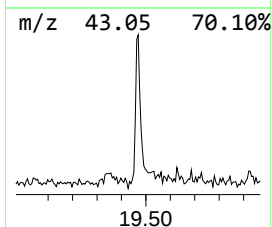
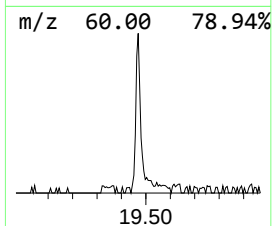
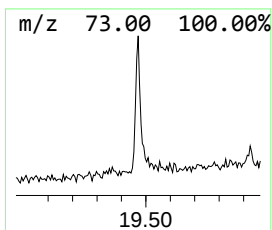
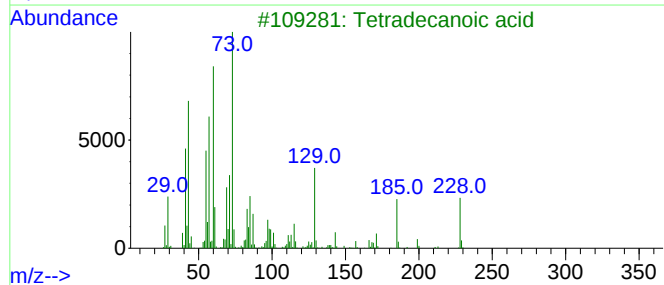
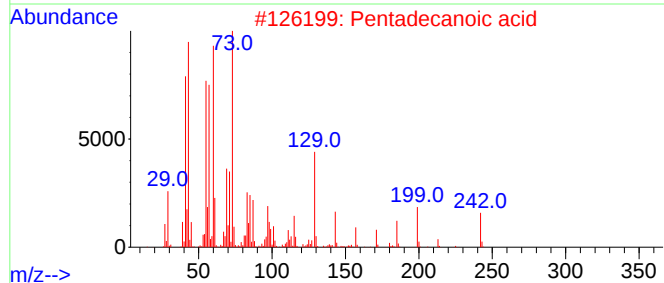
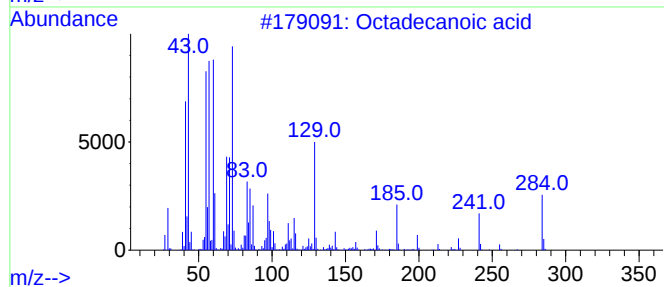
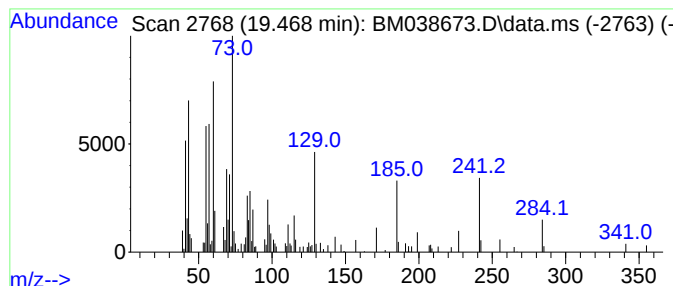
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Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.468	3.30 ng	107238	Chrysene-d12	21.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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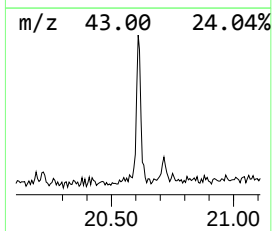
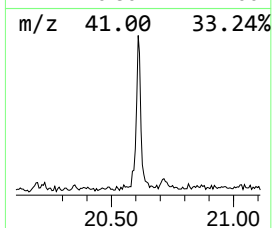
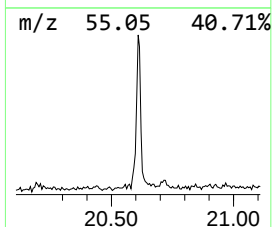
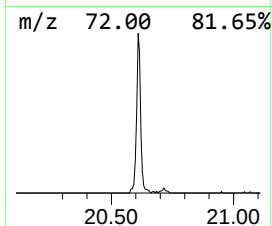
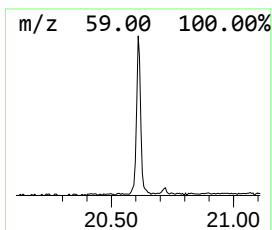
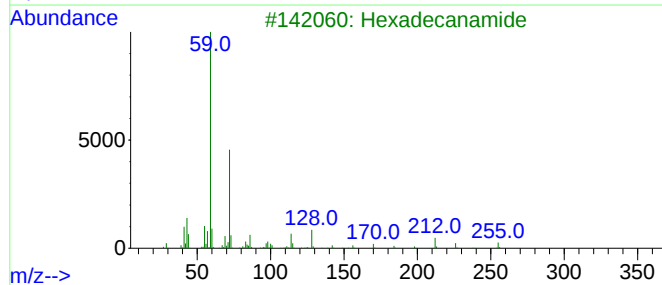
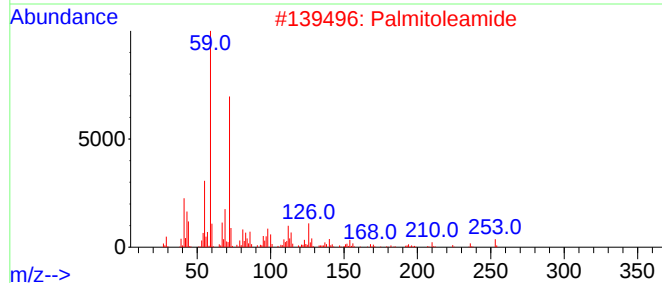
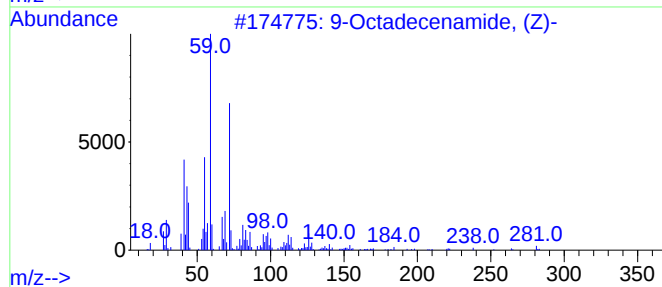
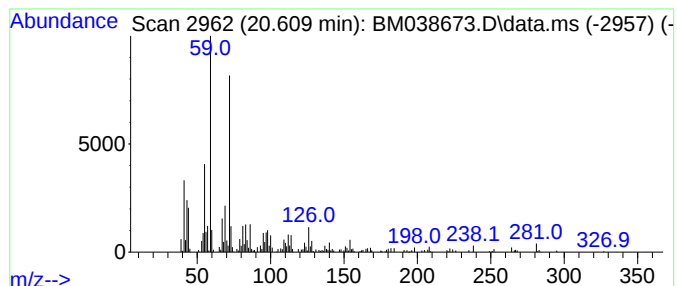
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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.609	5.77 ng	187754	Chrysene-d12	21.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2			Palmitoleamide	253	C16H31NO	106010-22-4	58
3			Hexadecanamide	255	C16H33NO	000629-54-9	53
4			Octanamide	143	C8H17NO	000629-01-6	47
5			1,1,3-Trimethyl-1-silacyclobutane	114	C6H14Si	002295-13-8	35



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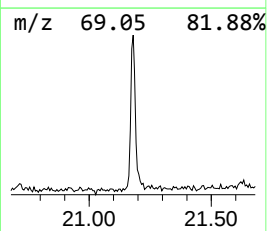
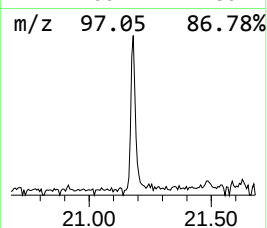
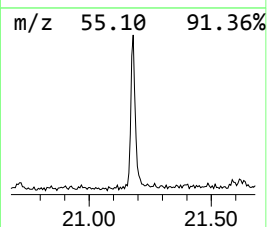
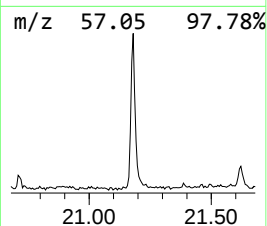
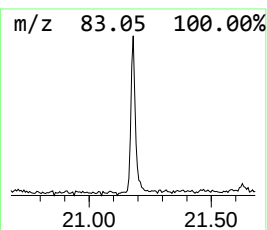
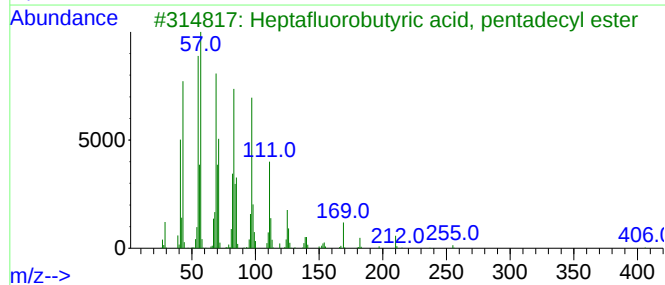
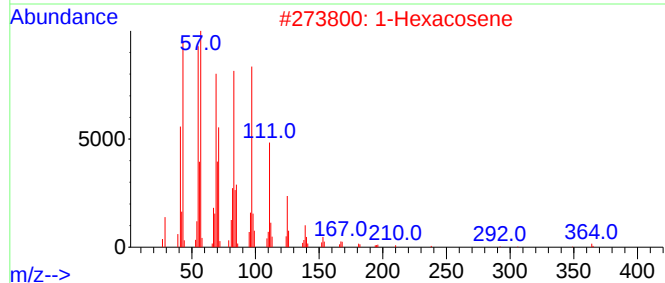
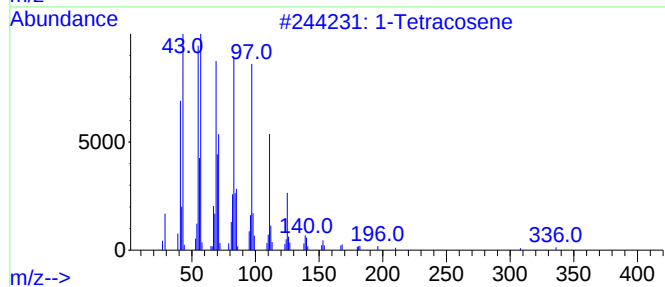
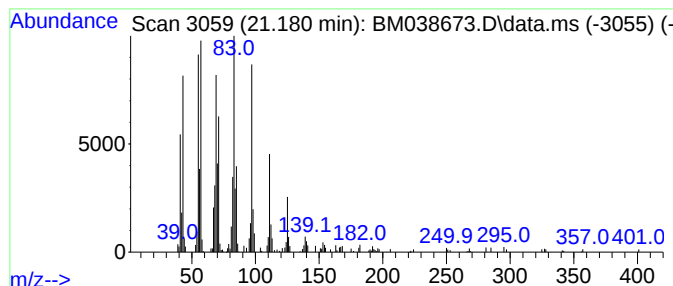
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Peak Number 5 1-Tetracosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.180	6.24 ng	203063	Chrysene-d12	21.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetracosene	336	C24H48	010192-32-2	95
2			1-Hexacosene	364	C26H52	018835-33-1	94
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



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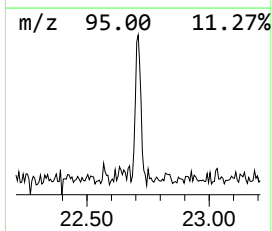
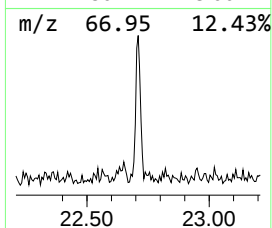
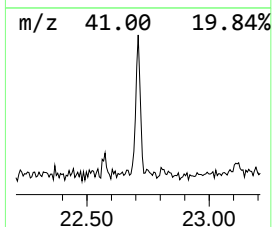
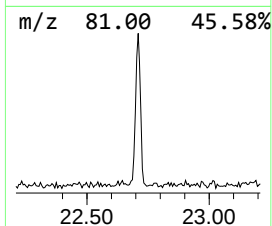
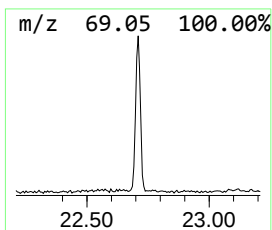
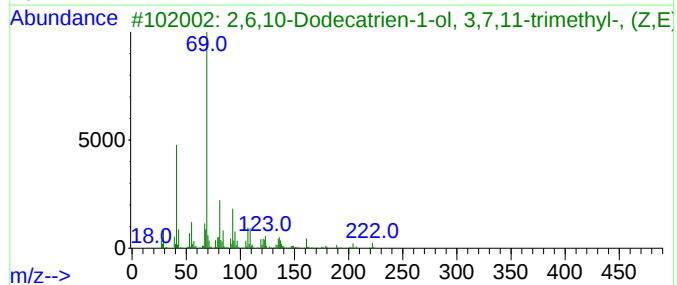
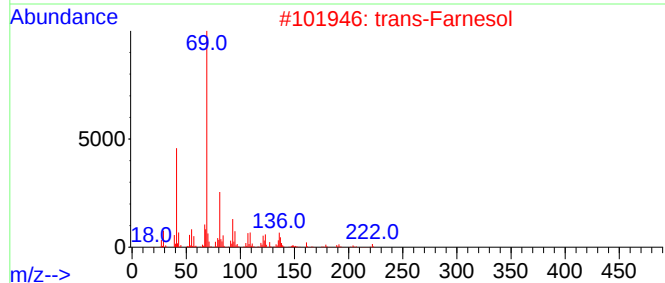
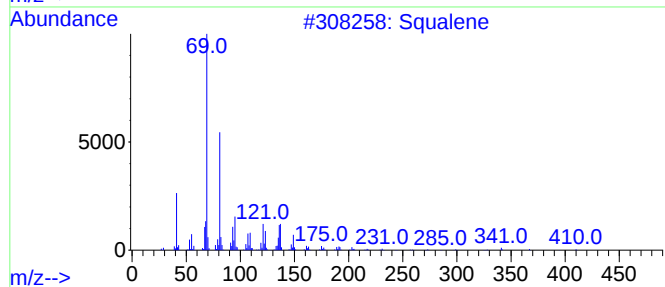
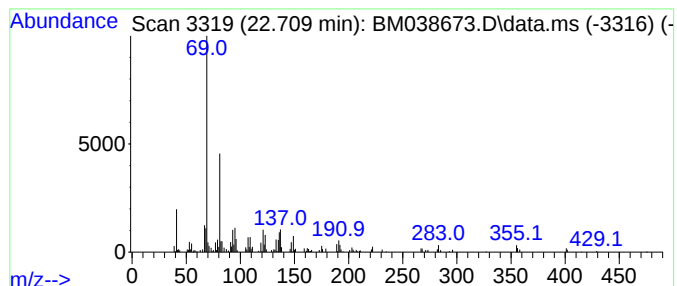
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.709	2.55 ng	98621	Perylene-d12	23.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	87
2			trans-Farnesol	222	C15H26O	000106-28-5	87
3			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	003790-71-4	76
4			Supraene	410	C30H50	007683-64-9	72
5			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM020223\
Data File : BM038673.D
Acq On : 02 Feb 2023 21:10
Operator : CG/JU
Sample : 01348-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MID2-H5(32-34)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.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-...	5.016	21.1	ng	471198	1	7.928	446110	20.0
n-Hexadecanoic ...	18.192	5.3	ng	190824	4	17.310	720499	20.0
Octadecanoic acid	19.468	3.3	ng	107238	5	21.486	650556	20.0
9-Octadecenamid...	20.609	5.8	ng	187754	5	21.486	650556	20.0
1-Tetracosene	21.180	6.2	ng	203063	5	21.486	650556	20.0
Squalene	22.709	2.5	ng	98621	6	23.886	774870	20.0