

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032422\
 Data File : BM034365.D
 Acq On : 24 Mar 2022 16:50
 Operator : CG/JU
 Sample : N1949-11
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 CP-BH2-031422-4-6

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-BM031522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM034365.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.596	58	61	77	rVB	79775	119473	2.07%	0.331%
2	5.490	377	383	394	rBV	2178843	3223519	55.88%	8.939%
3	7.095	649	656	675	rBV	1963196	3310949	57.40%	9.182%
4	7.937	792	799	808	rBV	647964	1008423	17.48%	2.797%
5	9.101	986	997	1007	rBV	1191659	2094371	36.31%	5.808%
6	10.748	1269	1277	1291	rBV	758910	1334646	23.14%	3.701%
7	13.207	1687	1695	1711	rBV	2986953	4525550	78.45%	12.550%
8	13.413	1726	1730	1738	rVB	63870	87127	1.51%	0.242%
9	14.577	1920	1928	1943	rBV	1065701	1630357	28.26%	4.521%
10	16.060	2174	2180	2198	rBV	2031010	3226881	55.94%	8.949%
11	17.318	2387	2394	2403	rBV	1119148	1690453	29.31%	4.688%
12	17.706	2455	2460	2471	rBV5	42132	92771	1.61%	0.257%
13	17.995	2505	2509	2514	rVB	68865	89679	1.55%	0.249%
14	18.089	2521	2525	2533	rBV6	40206	85029	1.47%	0.236%
15	18.218	2542	2547	2556	rBV	510972	827682	14.35%	2.295%
16	19.077	2688	2693	2700	rBV	199173	317917	5.51%	0.882%
17	19.159	2703	2707	2712	rVB3	163451	210896	3.66%	0.585%
18	19.295	2727	2730	2736	rBV	86553	105717	1.83%	0.293%
19	19.389	2739	2746	2751	rVV	190959	320793	5.56%	0.890%
20	19.489	2759	2763	2774	rBV2	133491	259073	4.49%	0.718%
21	19.842	2820	2823	2827	rBV	49785	62105	1.08%	0.172%
22	19.936	2834	2839	2850	rBV	4700723	5768466	100.00%	15.997%
23	21.200	3051	3054	3065	rBV	566165	811982	14.08%	2.252%
24	21.406	3086	3089	3094	rVB	176849	193729	3.36%	0.537%
25	21.489	3099	3103	3118	rVV	1133860	1774601	30.76%	4.921%
26	22.753	3314	3318	3328	rVB	676692	1006011	17.44%	2.790%
27	23.906	3509	3514	3522	rVB2	903422	1881733	32.62%	5.218%

Sum of corrected areas: 36059933

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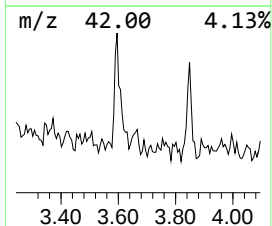
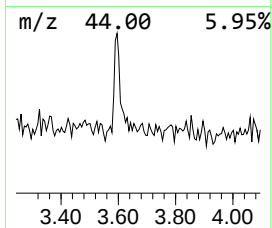
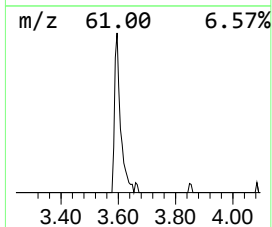
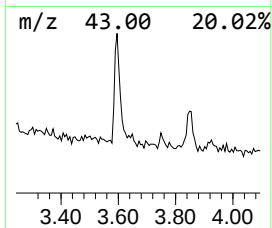
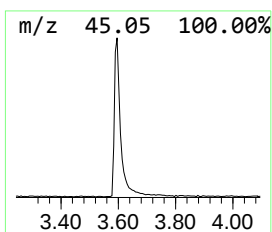
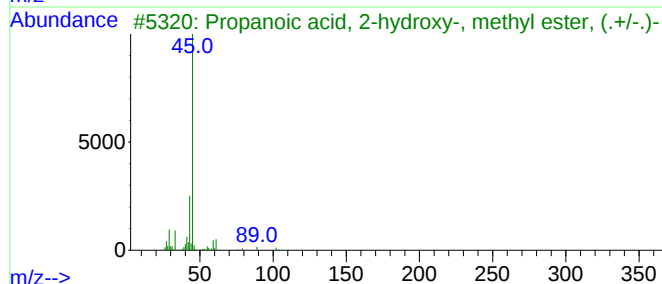
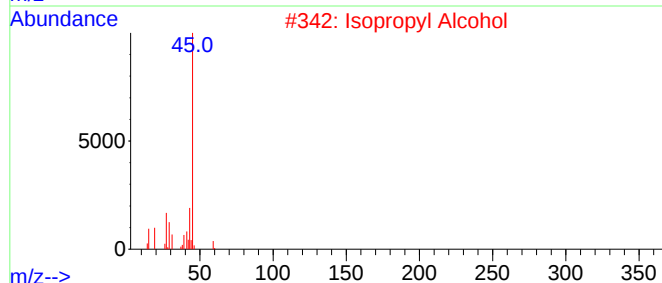
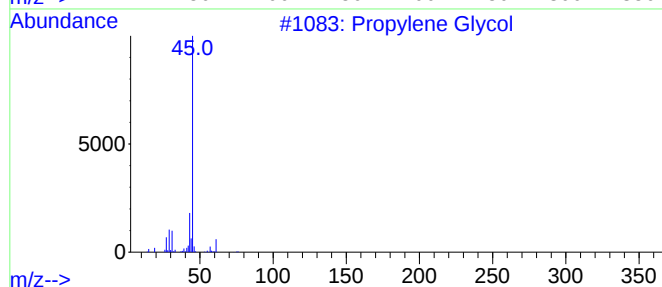
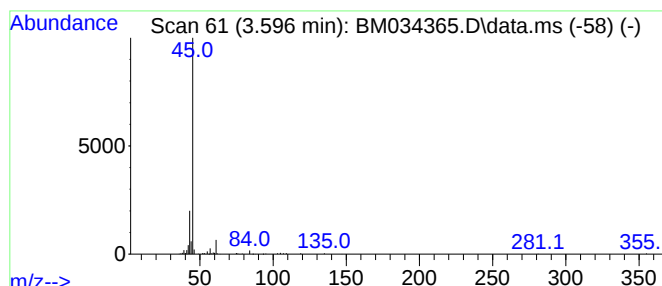
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.596	2.37 ng	119473	1,4-Dichlorobenzene-d4	7.936

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	72
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	40
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
4			2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	9
5			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9



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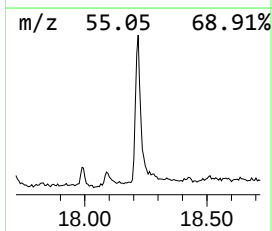
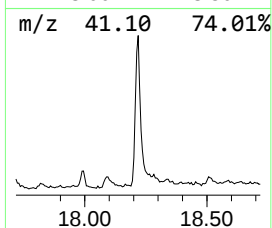
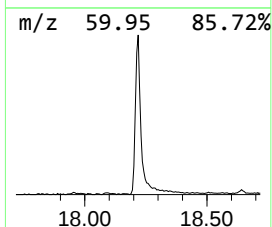
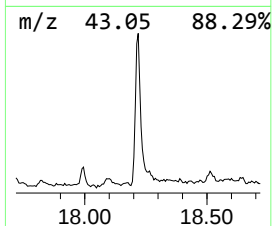
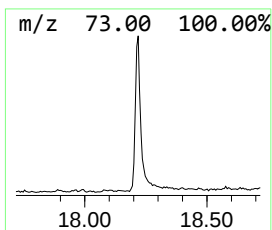
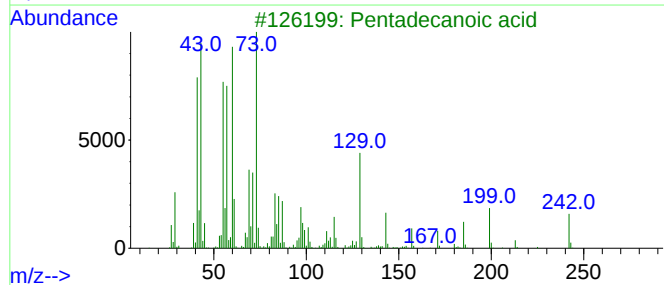
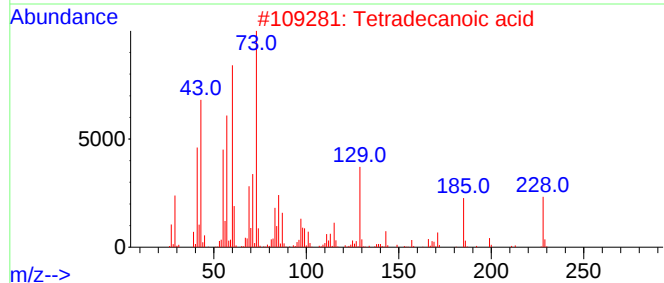
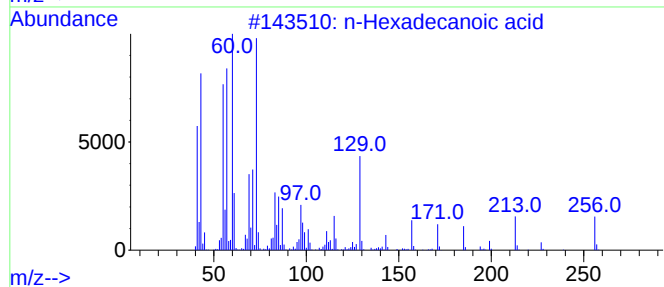
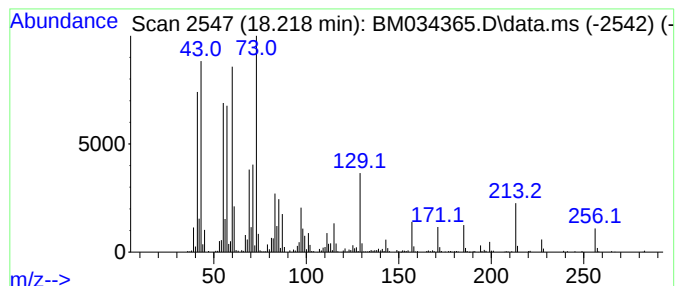
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.218	9.79 ng	827682	Phenanthrene-d10	17.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	68
5			Nonanoic acid	158	C9H18O2	000112-05-0	45



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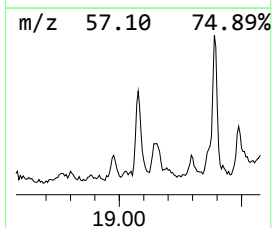
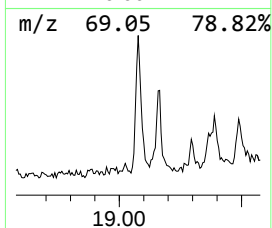
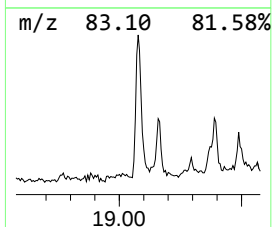
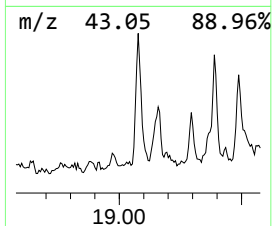
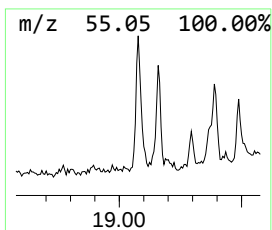
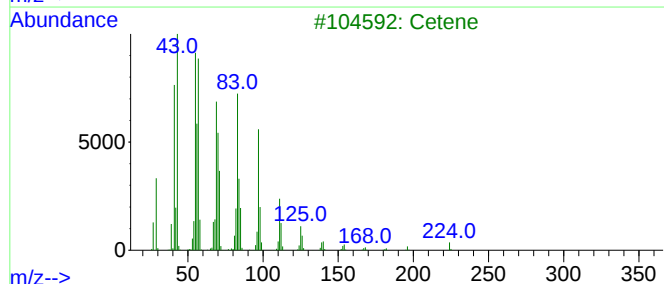
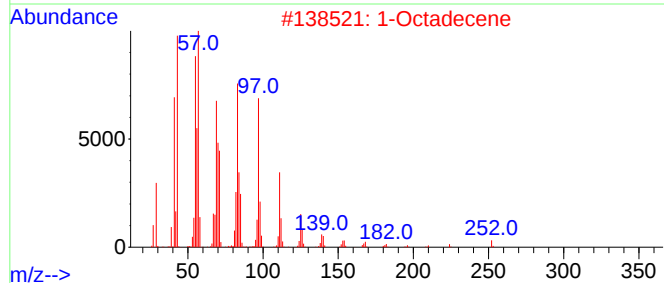
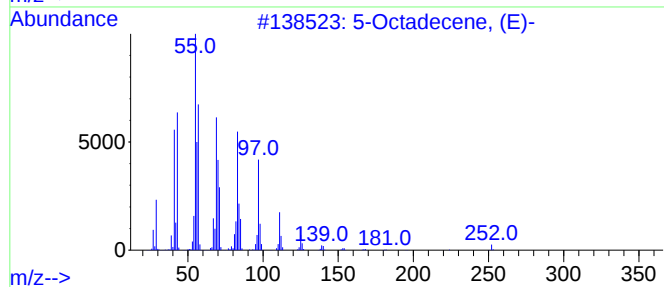
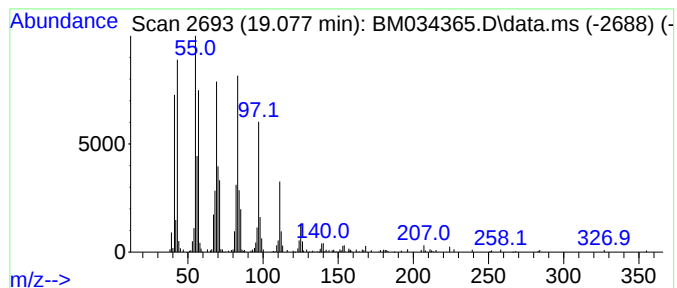
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 5-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.077	3.76 ng	317917	Phenanthrene-d10	17.318

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Octadecene, (E)-	252	C18H36	007206-21-5	99
2		1-Octadecene	252	C18H36	000112-88-9	97
3		Cetene	224	C16H32	000629-73-2	95
4		n-Heptadecanol-1	256	C17H36O	001454-85-9	95
5		9-Eicosene, (E)-	280	C20H40	074685-29-3	94



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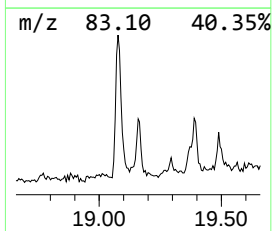
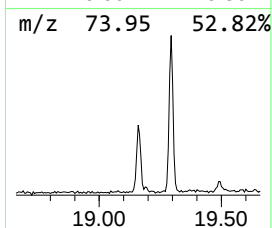
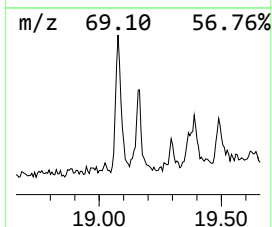
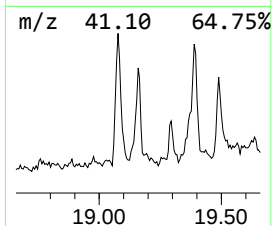
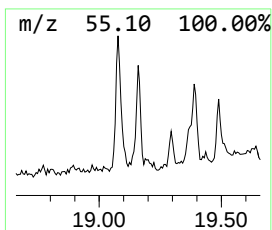
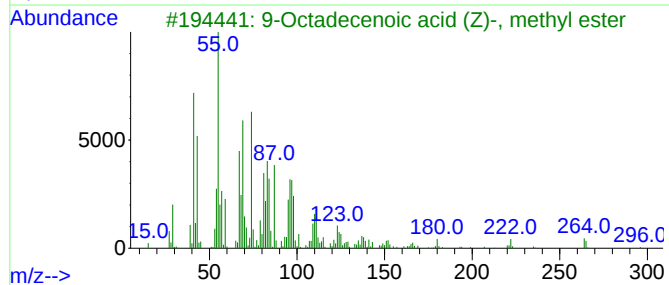
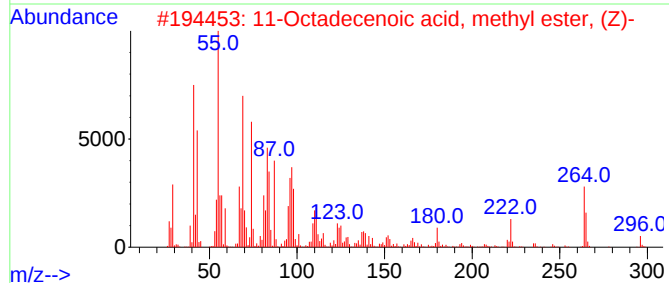
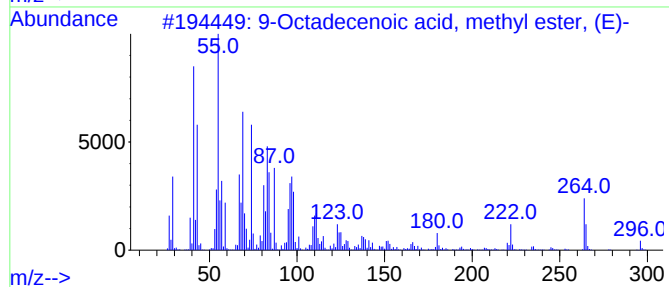
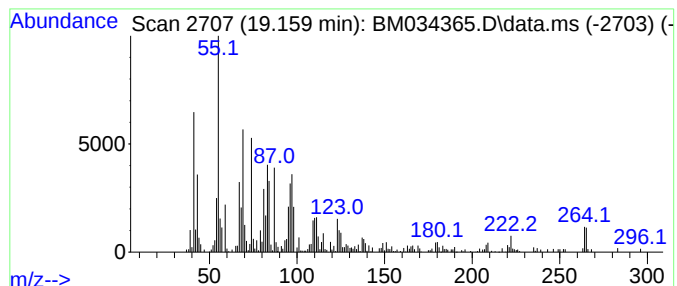
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenoic acid, methyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.159	2.50 ng	210896	Phenanthrene-d10	17.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
2			11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
3			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
4			11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
5			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	97



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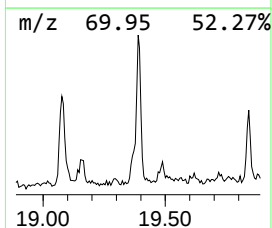
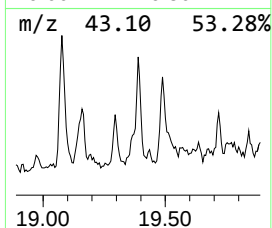
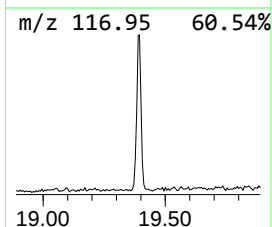
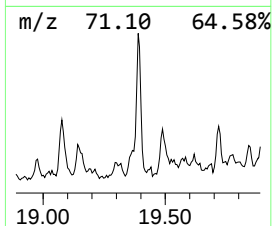
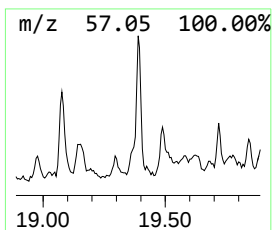
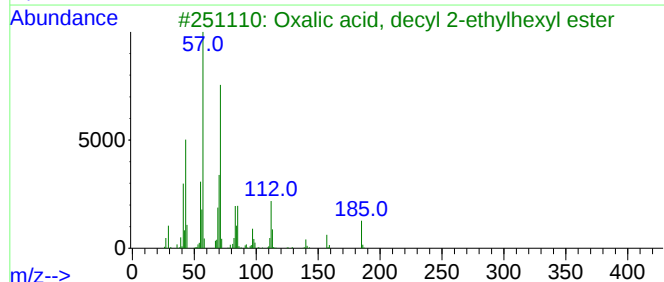
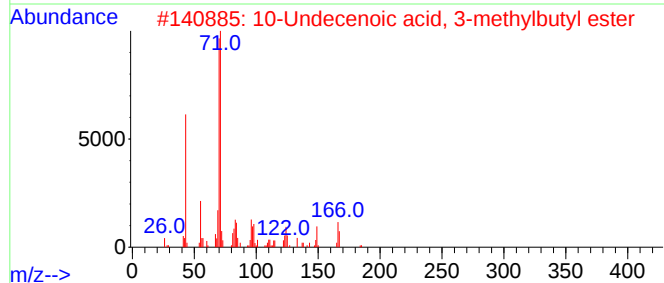
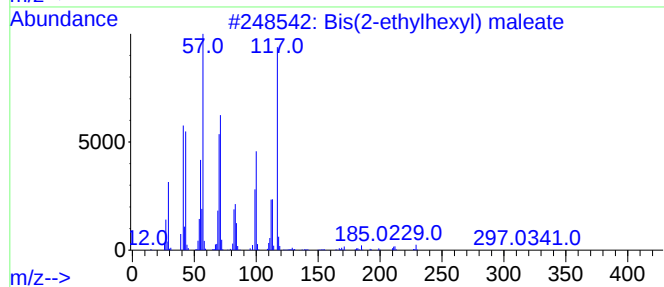
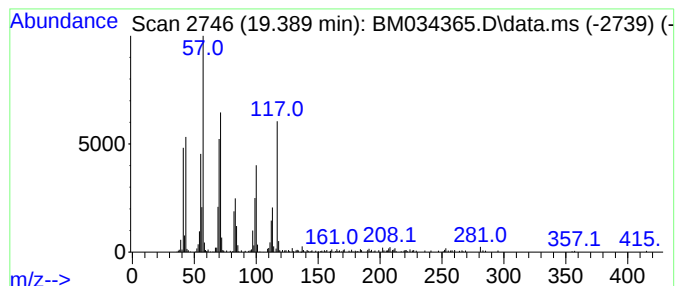
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Peak Number 5 Bis(2-ethylhexyl) maleate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.389	3.80 ng	320793	Phenanthrene-d10	17.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	87
2			10-Undecenoic acid, 3-methylbuty...	254	C16H30O2	010214-27-4	27
3			Oxalic acid, decyl 2-ethylhexyl ...	342	C20H38O4	1000309-39-3	27
4			Heptane, 3-(bromomethyl)-	192	C8H17Br	018908-66-2	22
5			2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	959012-82-9	22



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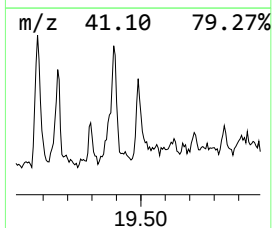
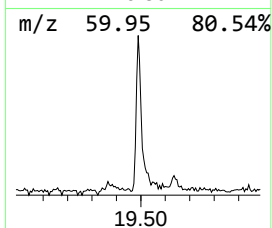
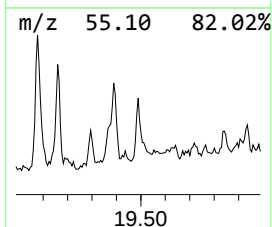
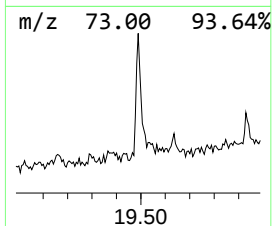
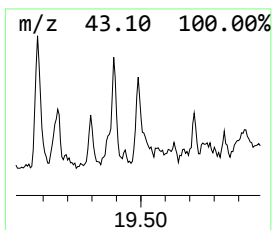
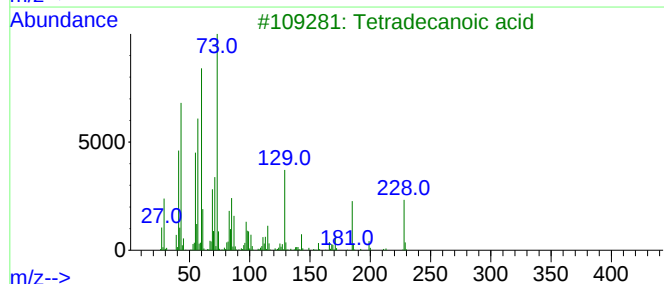
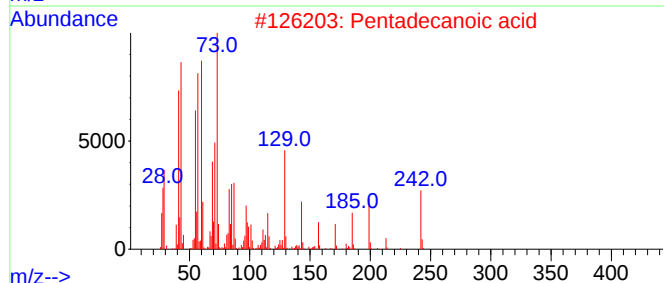
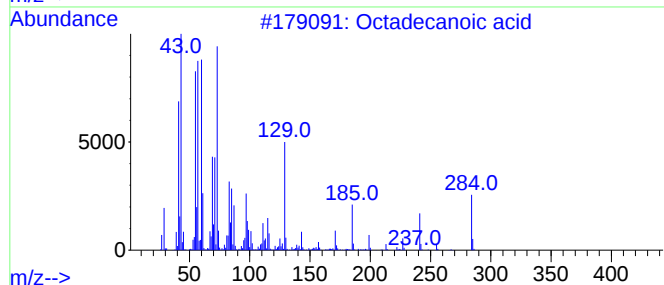
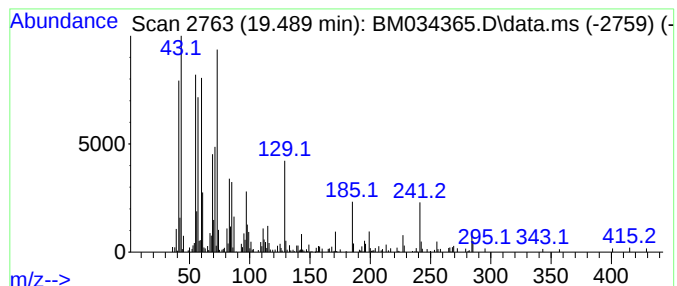
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.489	2.92 ng	259073	Chrysene-d12	21.494

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5			Methyl 6-O-[1-methylpropyl]-.bet...	250	C11H22O6	1010126-15-7	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032422\
Data File : BM034365.D
Acq On : 24 Mar 2022 16:50
Operator : CG/JU
Sample : N1949-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CP-BH2-031422-4-6

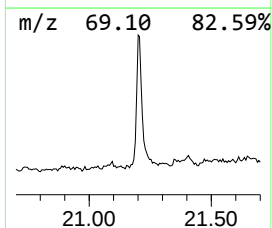
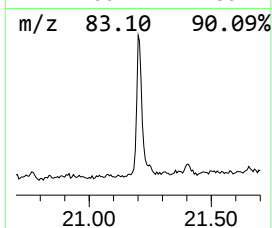
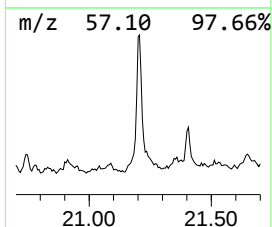
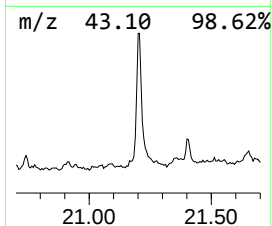
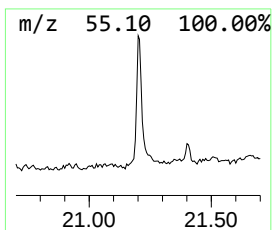
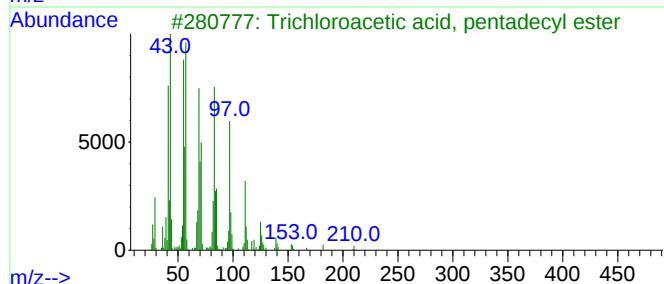
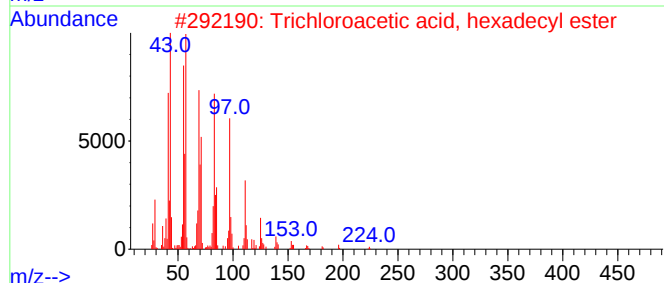
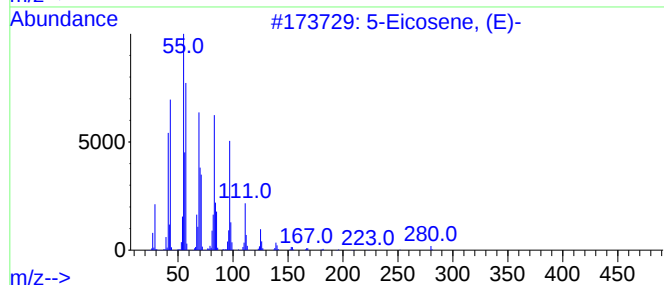
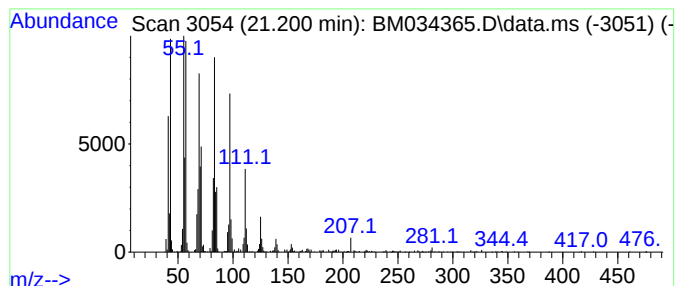
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.200	9.15 ng	811982	Chrysene-d12	21.494

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4			1-Hexacosene	364	C26H52	018835-33-1	94
5			Cyclotetracosane	336	C24H48	000297-03-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032422\
Data File : BM034365.D
Acq On : 24 Mar 2022 16:50
Operator : CG/JU
Sample : N1949-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CP-BH2-031422-4-6

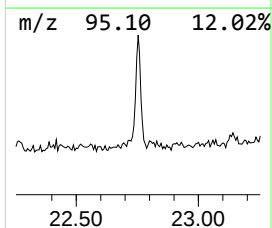
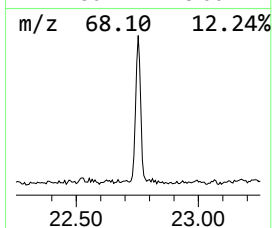
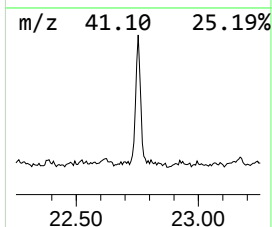
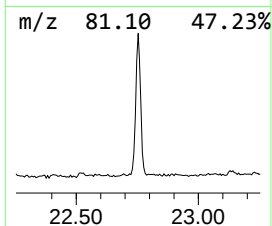
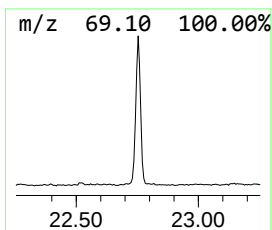
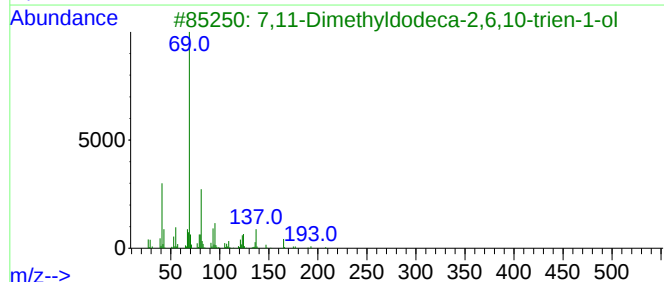
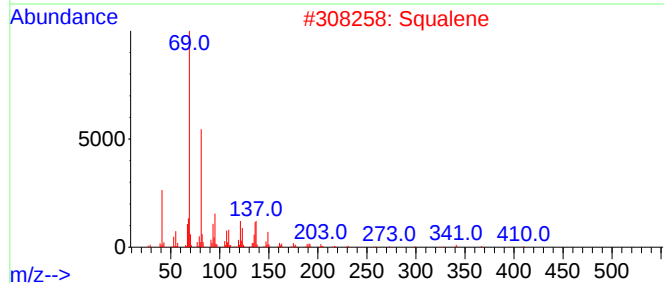
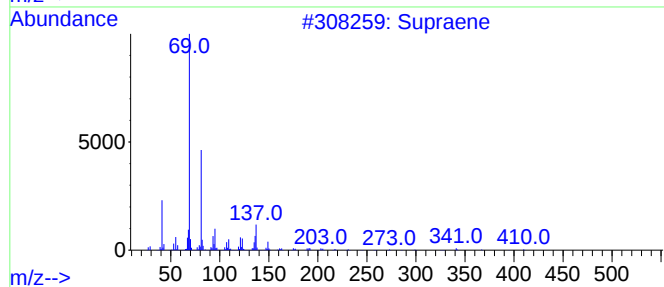
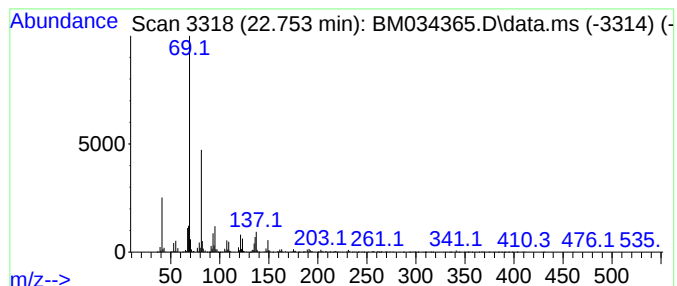
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.753	10.69 ng	1006010	Perylene-d12	23.906

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	89
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	83
4			4,8,12-Tetradecatrilene, 5,9,13-...	248	C17H28O	066408-55-7	72
5			2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032422\
Data File : BM034365.D
Acq On : 24 Mar 2022 16:50
Operator : CG/JU
Sample : N1949-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CP-BH2-031422-4-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.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
Propylene Glycol	3.596	2.4	ng	119473	1	7.936	1008420	20.0
n-Hexadecanoic ...	18.218	9.8	ng	827682	4	17.318	1690450	20.0
5-Octadecene, (E)-	19.077	3.8	ng	317917	4	17.318	1690450	20.0
9-Octadecenoic ...	19.159	2.5	ng	210896	4	17.318	1690450	20.0
Bis(2-ethylhexy...	19.389	3.8	ng	320793	4	17.318	1690450	20.0
Octadecanoic acid	19.489	2.9	ng	259073	5	21.494	1774600	20.0
5-Eicosene, (E)-	21.200	9.2	ng	811982	5	21.494	1774600	20.0
Supraene	22.753	10.7	ng	1006010	6	23.906	1881730	20.0