

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022023\
 Data File : BM038793.D
 Acq On : 20 Feb 2023 18:57
 Operator : CG/JU
 Sample : 01593-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B-26-SB03

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: BM038793.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	294	301	310	rBV	247562	334622	13.90%	2.774%
2	5.434	375	382	392	rBV	728367	1024404	42.54%	8.494%
3	7.057	650	658	670	rBV	680458	1016565	42.22%	8.429%
4	7.875	791	797	804	rVB	185489	273167	11.34%	2.265%
5	9.057	989	998	1009	rBV	406138	638802	26.53%	5.296%
6	10.692	1267	1276	1283	rBV	217646	351408	14.59%	2.914%
7	13.157	1688	1695	1705	rBV	1215058	1689896	70.18%	14.011%
8	14.533	1923	1929	1937	rVB	336531	469823	19.51%	3.895%
9	15.892	2154	2160	2166	rBV	113903	150928	6.27%	1.251%
10	16.027	2177	2183	2193	rBV	966055	1306720	54.27%	10.834%
11	17.280	2390	2396	2402	rBV	375578	501834	20.84%	4.161%
12	18.168	2542	2547	2556	rBV	166576	231116	9.60%	1.916%
13	18.592	2613	2619	2622	rBV	31339	35780	1.49%	0.297%
14	19.445	2760	2764	2772	rBV	73155	106367	4.42%	0.882%
15	19.903	2837	2842	2849	rBV	2178117	2407944	100.00%	19.965%
16	21.162	3052	3056	3063	rBV	134857	180021	7.48%	1.493%
17	21.468	3103	3108	3113	rBV	484140	606110	25.17%	5.025%
18	23.844	3506	3512	3521	rVB2	375435	735475	30.54%	6.098%

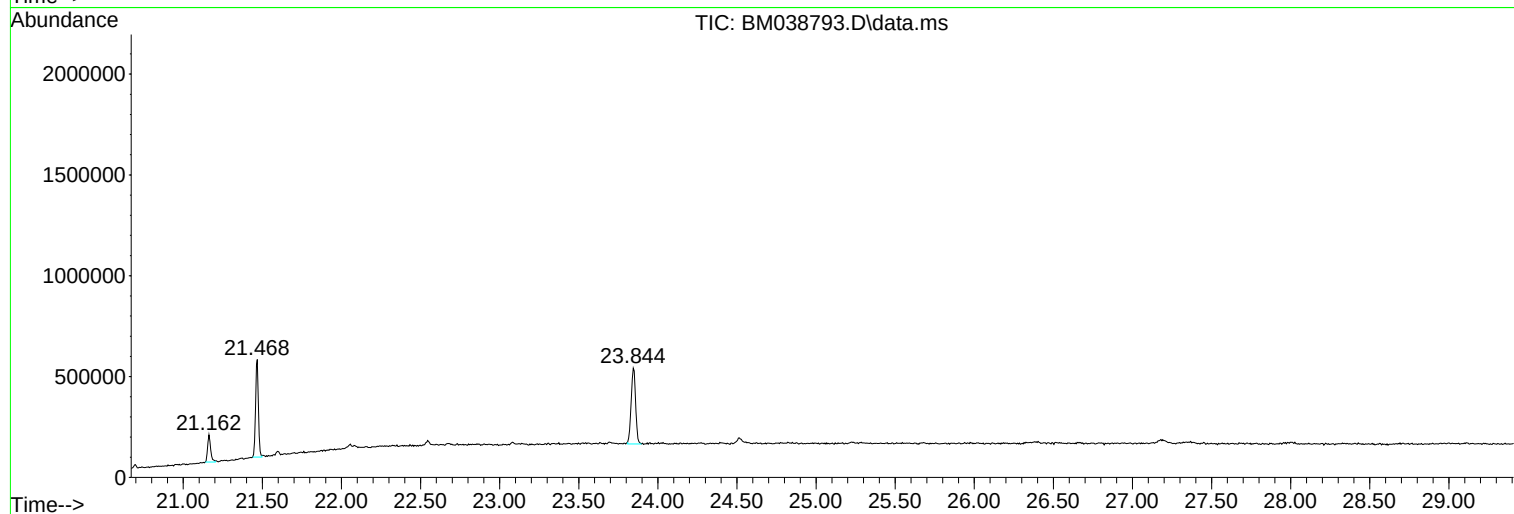
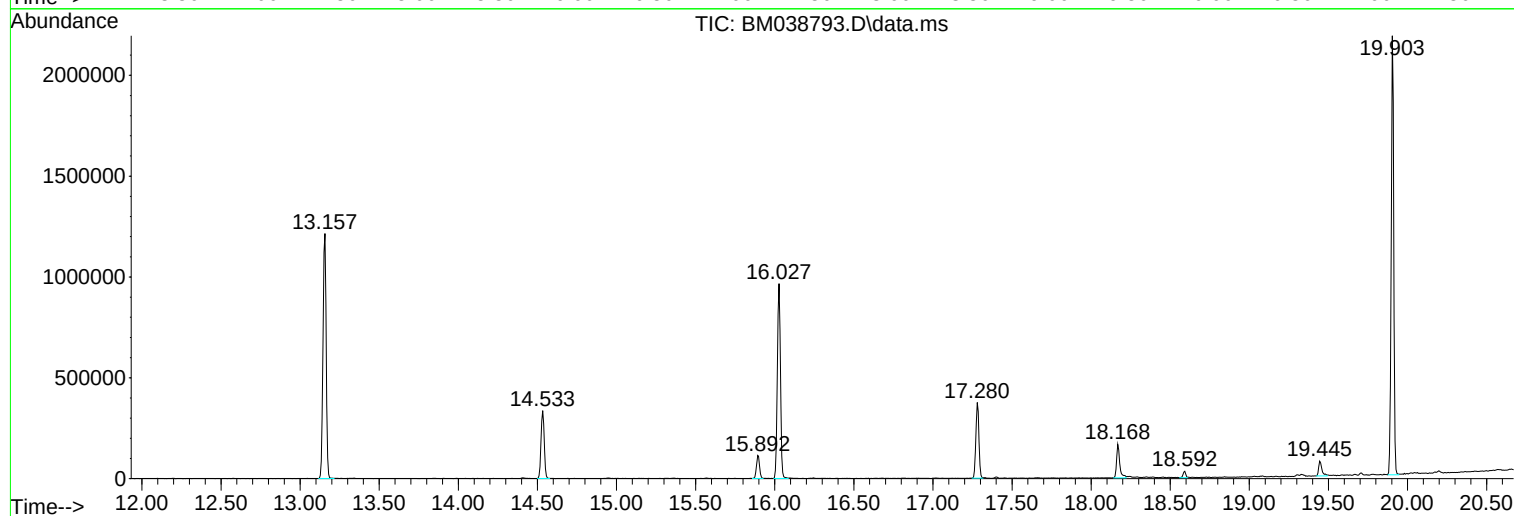
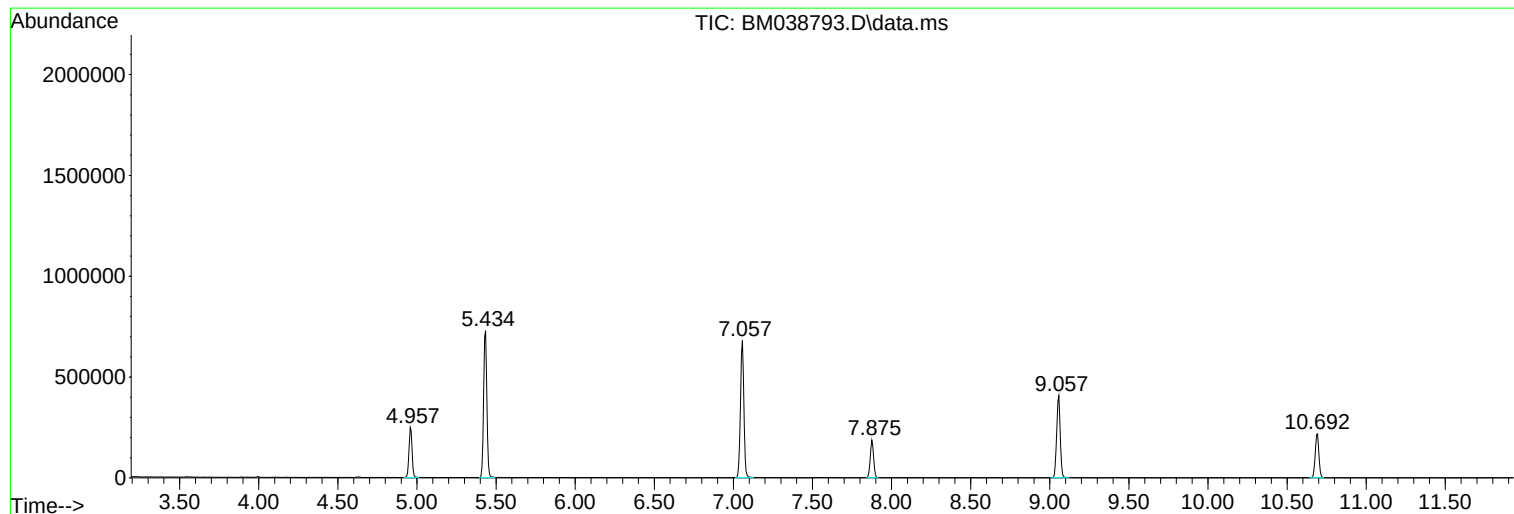
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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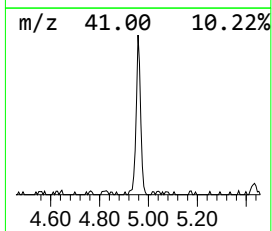
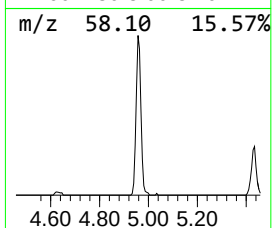
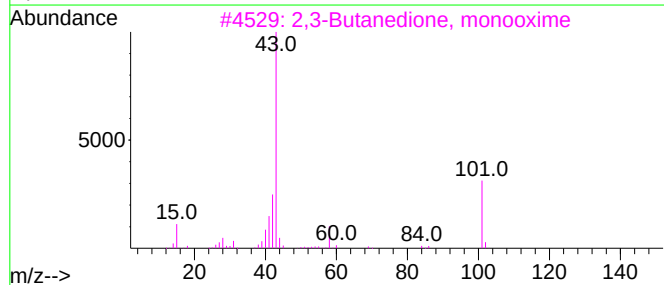
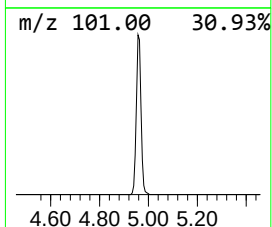
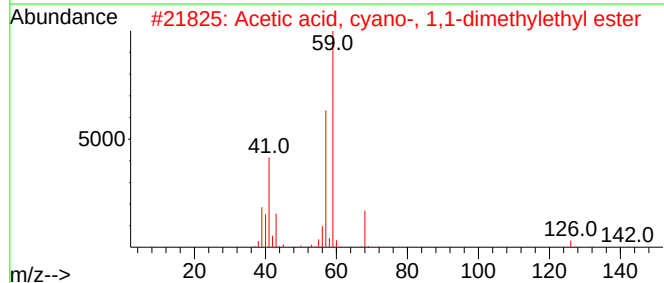
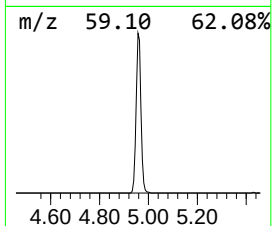
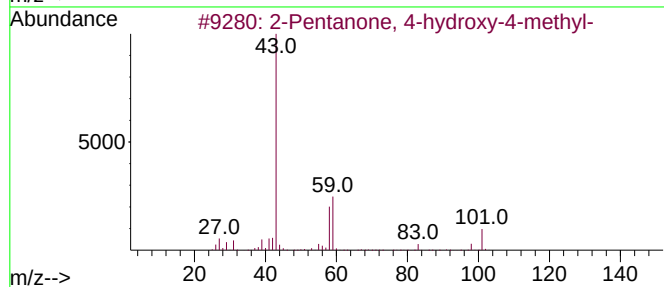
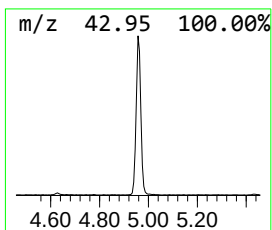
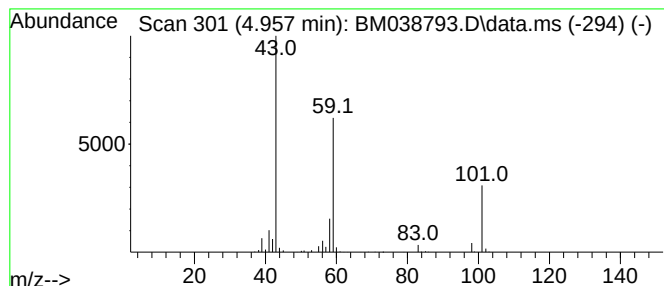
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	24.50 ng	334622	1,4-Dichlorobenzene-d4	7.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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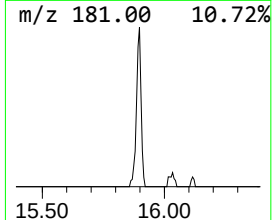
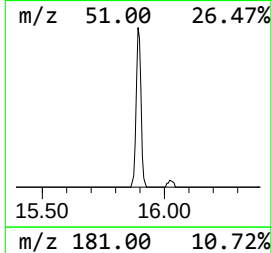
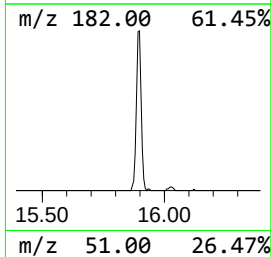
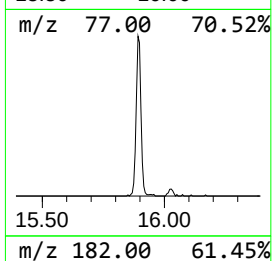
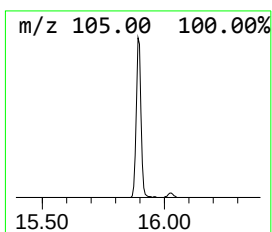
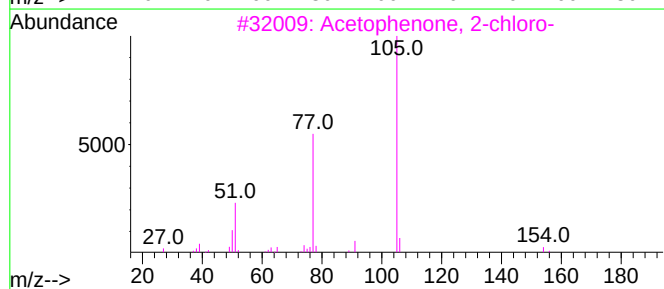
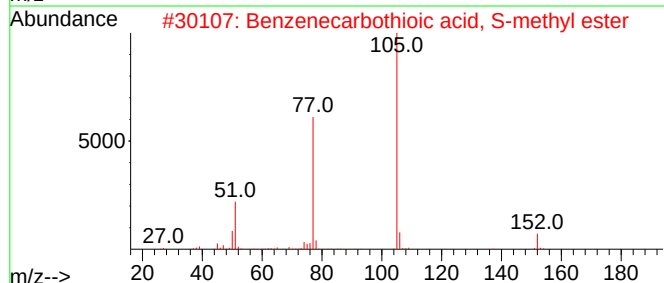
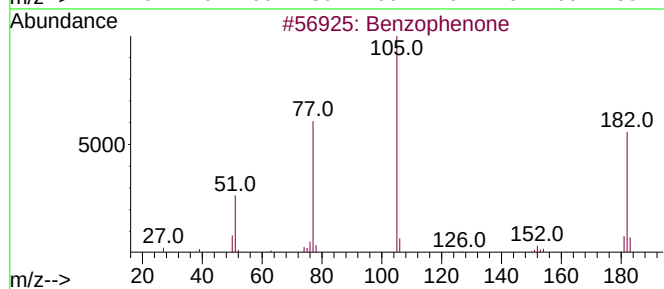
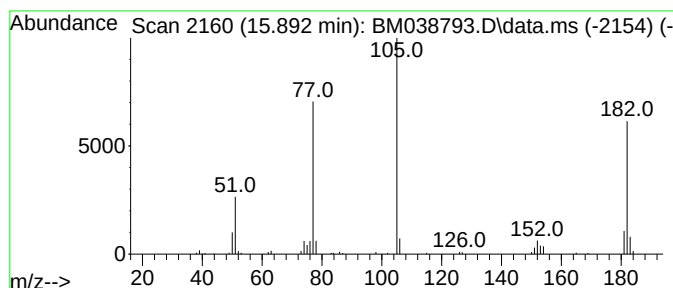
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.892	6.42 ng	150928	Acenaphthene-d10	14.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4			Benzoylformic acid	150	C8H6O3	000611-73-4	43
5			Ethyl 2-benzoyl-4-cyanobutanoate	245	C14H15NO3	1000486-83-9	38



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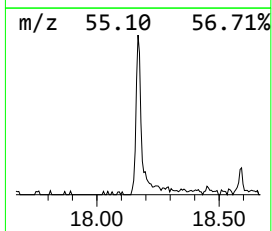
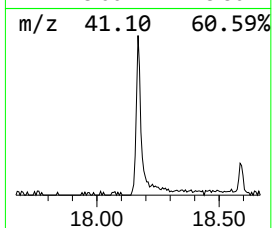
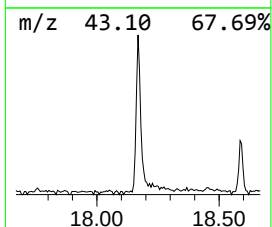
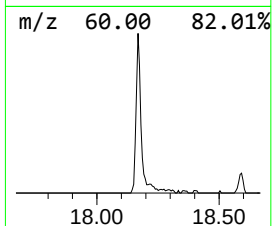
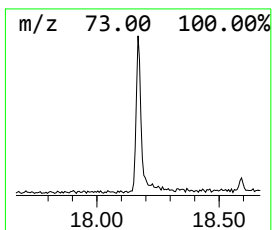
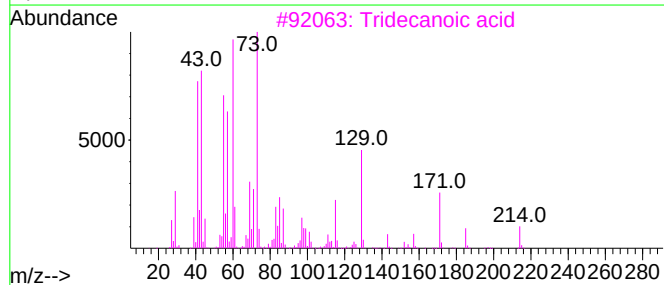
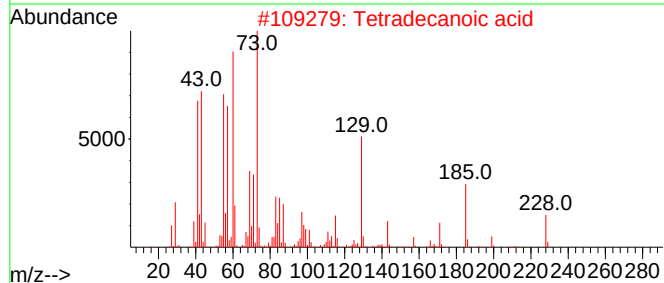
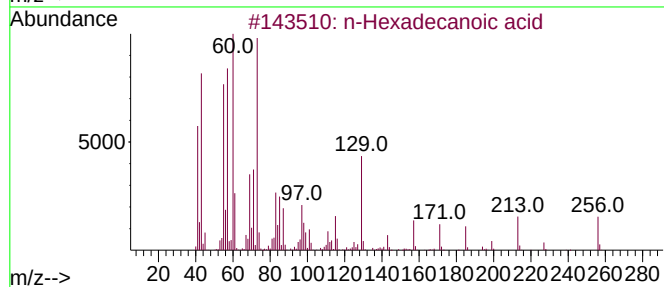
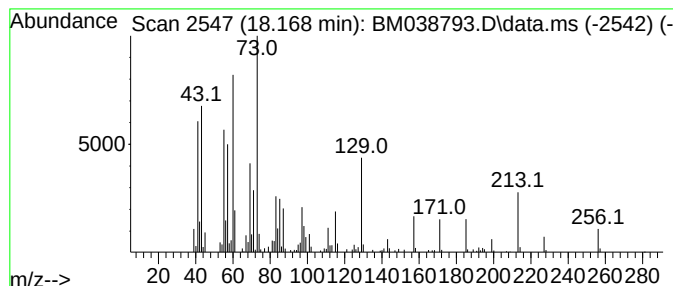
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.168	9.21 ng	231116	Phenanthrene-d10	17.280

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	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5			Undecanoic acid	186	C11H22O2	000112-37-8	50



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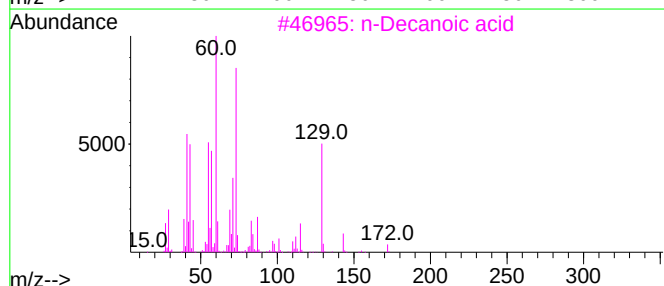
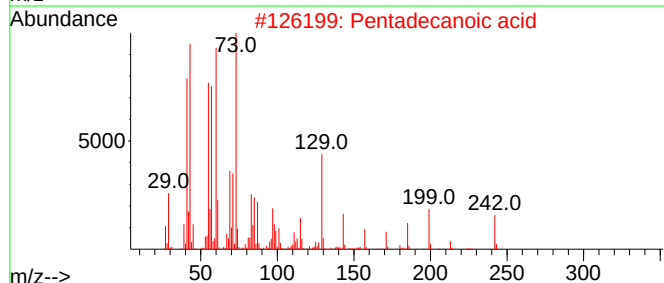
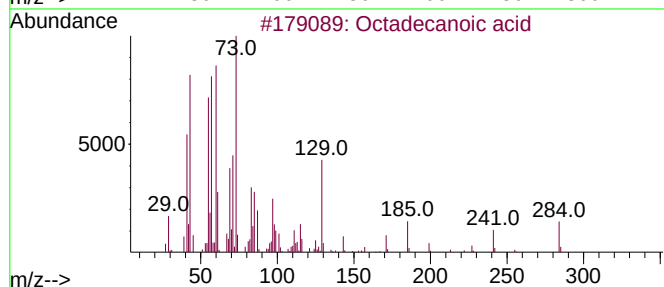
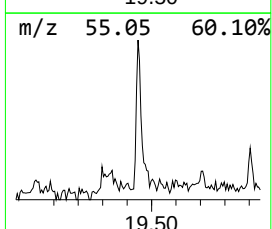
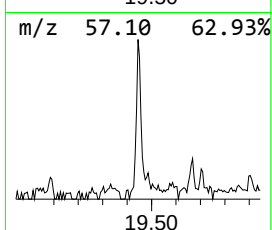
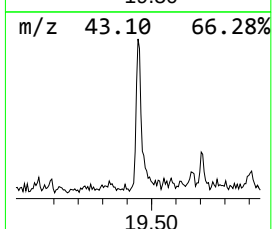
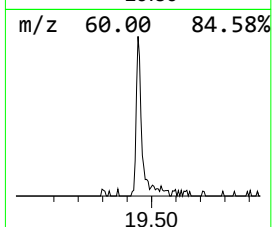
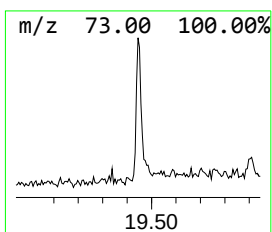
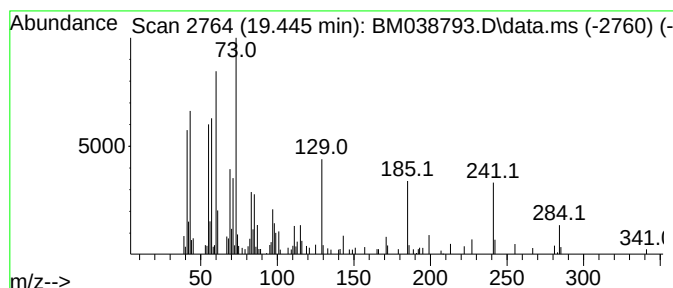
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	3.51 ng	106367	Chrysene-d12	21.468

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	90
3			n-Decanoic acid	172	C10H20O2	000334-48-5	78
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Tridecanoic acid	214	C13H26O2	000638-53-9	68



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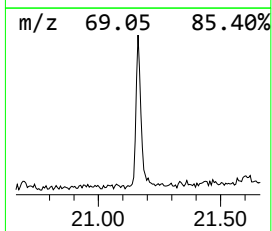
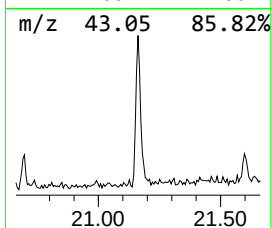
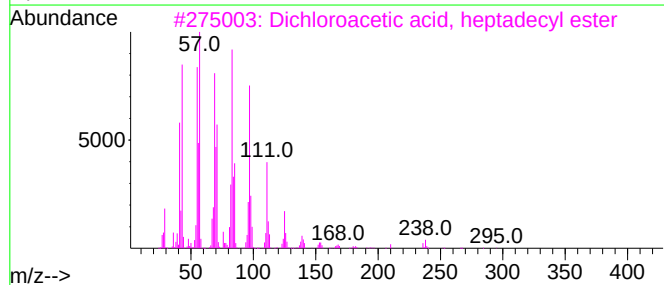
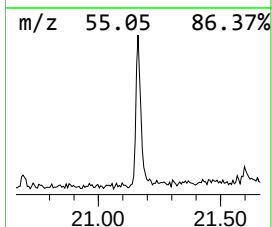
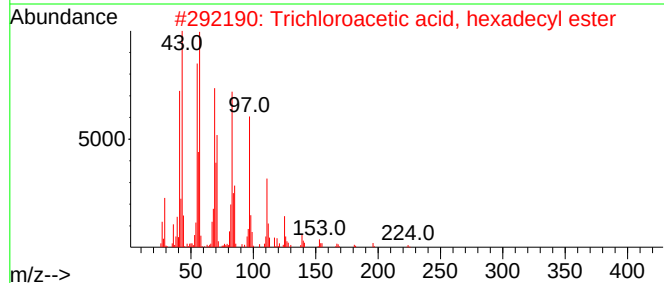
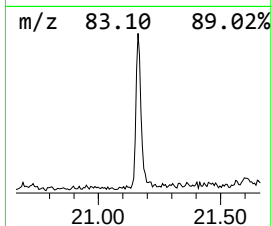
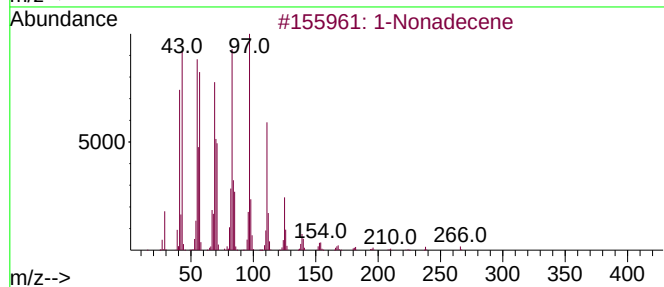
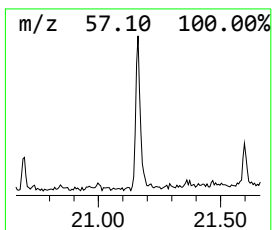
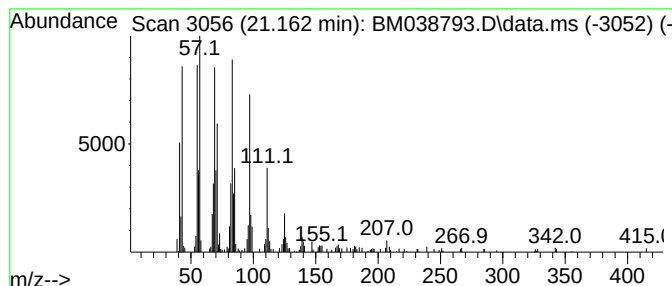
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.162	5.94 ng	180021	Chrysene-d12	21.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonadecene	266	C19H38	018435-45-5	98
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



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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-...	4.957	24.5	ng	334622	1	7.875	273167	20.0
Benzophenone	15.892	6.4	ng	150928	3	14.533	469823	20.0
n-Hexadecanoic ...	18.168	9.2	ng	231116	4	17.280	501834	20.0
Octadecanoic acid	19.445	3.5	ng	106367	5	21.468	606110	20.0
1-Nonadecene	21.162	5.9	ng	180021	5	21.468	606110	20.0