

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM020323\
 Data File : BM038685.D
 Acq On : 03 Feb 2023 18:47
 Operator : CG/JU
 Sample : 01414-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SASP2-123-2(30-40)

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: BM038685.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	322	rBV	269488	356569	13.88%	2.652%
2	5.487	385	391	403	rBV	770724	1102404	42.90%	8.199%
3	7.104	659	666	681	rBV	714749	1098738	42.76%	8.172%
4	7.922	798	805	813	rBV	196402	310705	12.09%	2.311%
5	9.098	997	1005	1017	rBV	424123	669437	26.05%	4.979%
6	10.733	1275	1283	1290	rBV	232251	373939	14.55%	2.781%
7	13.192	1694	1701	1713	rBV	1311960	1855766	72.22%	13.802%
8	14.562	1928	1934	1943	rBV	405923	565918	22.02%	4.209%
9	15.921	2159	2165	2171	rBV	55969	73226	2.85%	0.545%
10	16.051	2182	2187	2199	rBV	1141199	1603533	62.40%	11.926%
11	17.309	2395	2401	2407	rBV	496646	677518	26.37%	5.039%
12	18.192	2545	2551	2561	rBV	222778	346573	13.49%	2.578%
13	19.468	2763	2768	2780	rBV	92876	162593	6.33%	1.209%
14	19.921	2840	2845	2856	rBV	2136831	2569713	100.00%	19.112%
15	21.174	3055	3058	3063	rBV2	89446	106807	4.16%	0.794%
16	21.486	3106	3111	3116	rBV	582113	746091	29.03%	5.549%
17	23.880	3512	3518	3525	rVB2	418119	825905	32.14%	6.143%

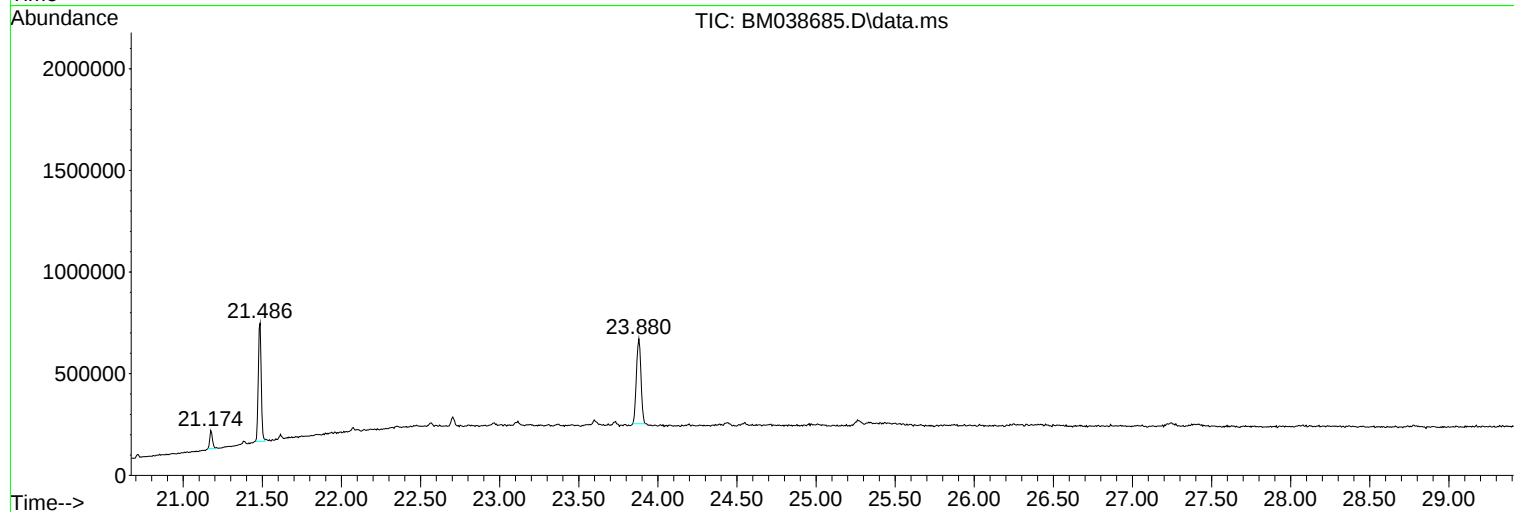
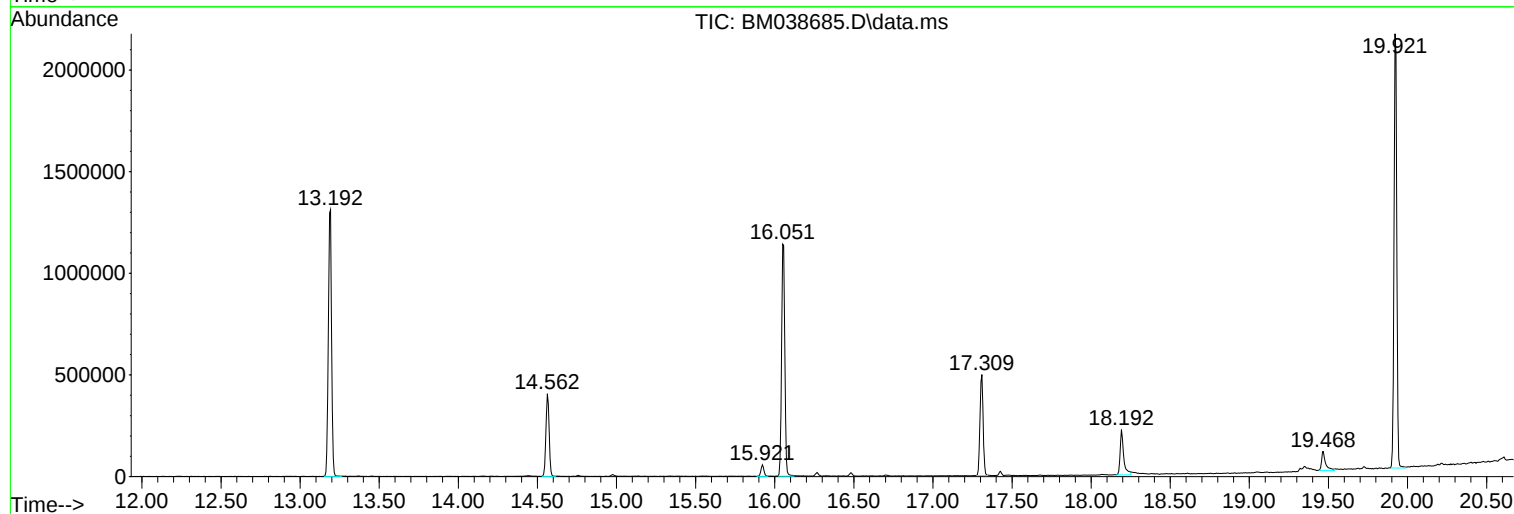
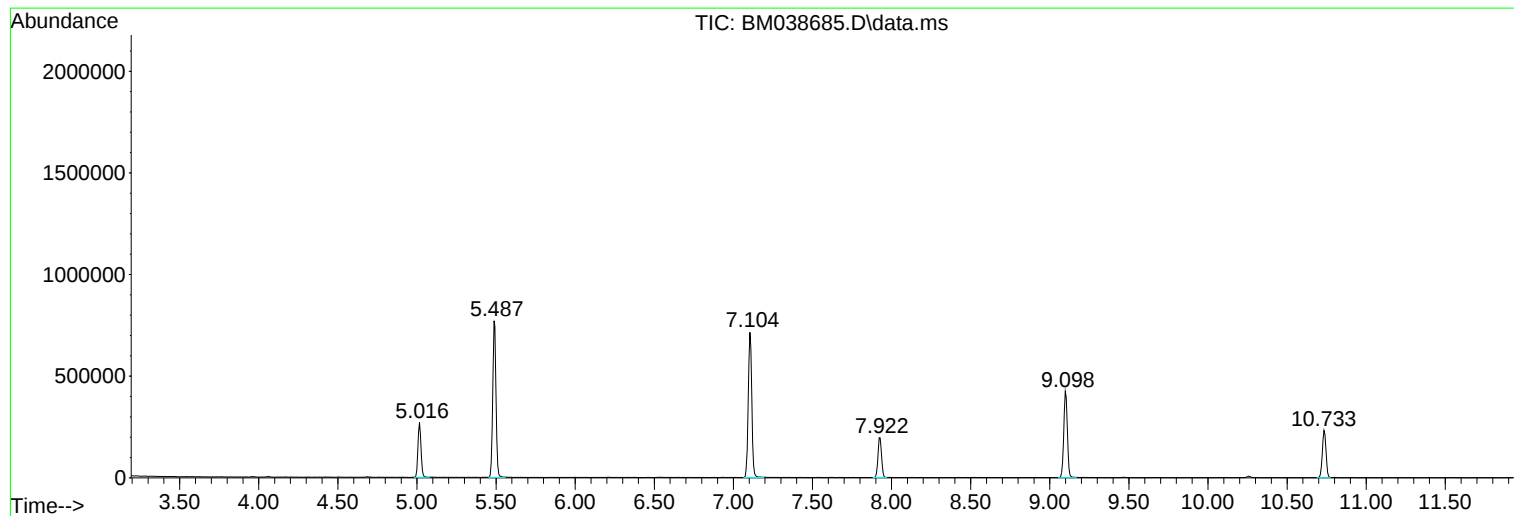
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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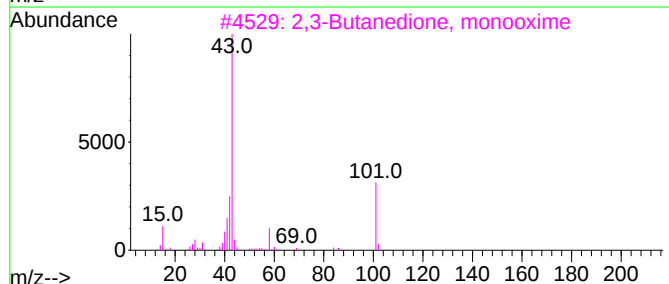
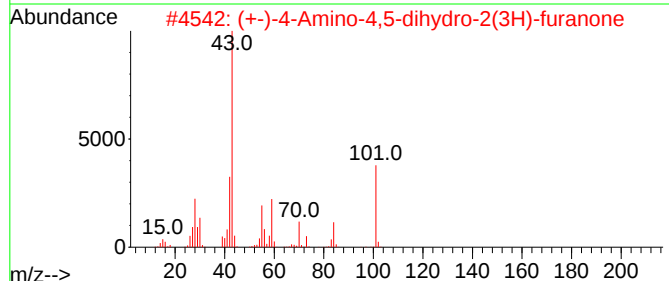
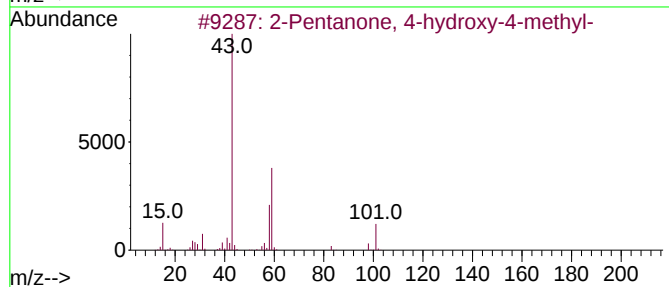
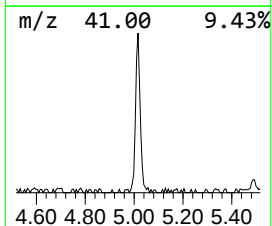
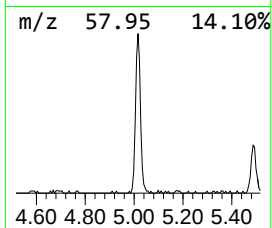
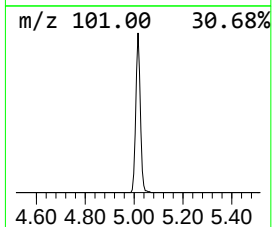
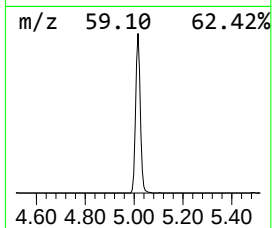
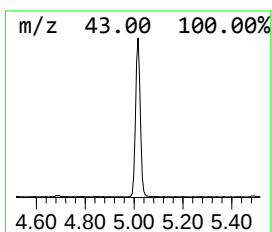
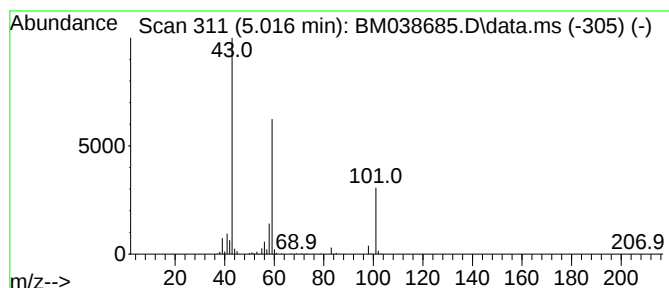
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.016	22.95 ng	356569	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			2,4-Pentanedione, 3-(1-methyleth...	142	C8H14O2	001540-38-1	12
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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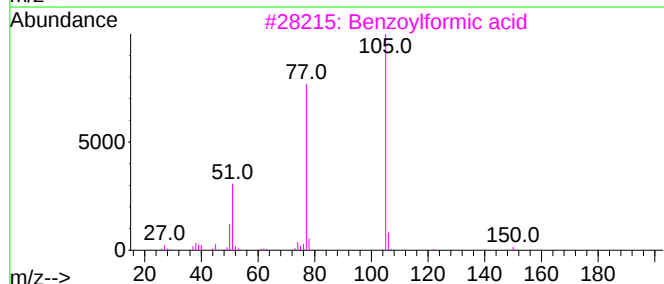
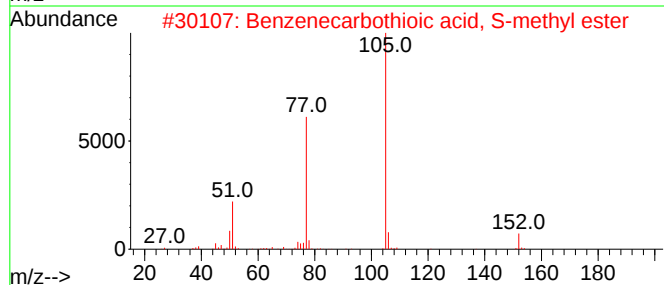
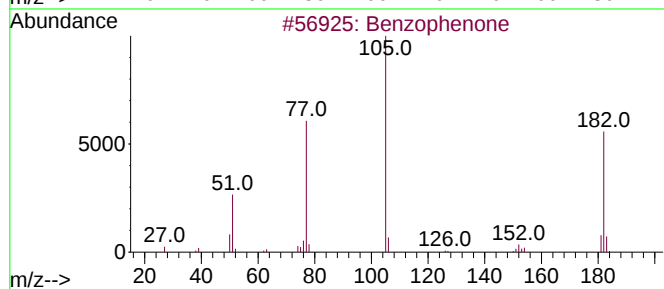
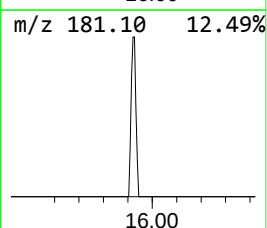
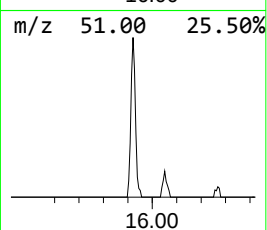
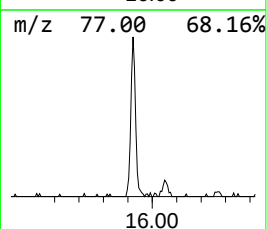
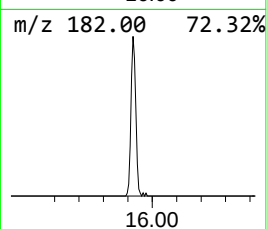
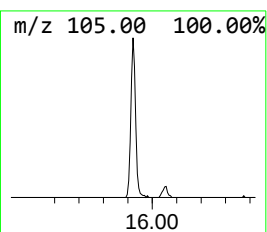
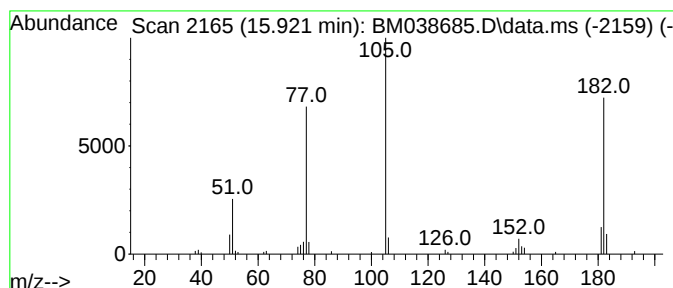
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	2.59 ng	73226	Acenaphthene-d10	14.563

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	53
3			Benzoylformic acid	150	C8H6O3	000611-73-4	46
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	46
5			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	43



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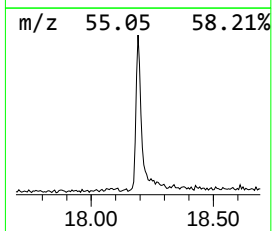
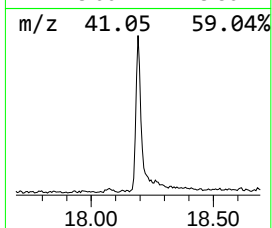
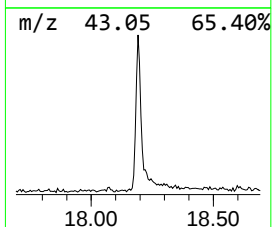
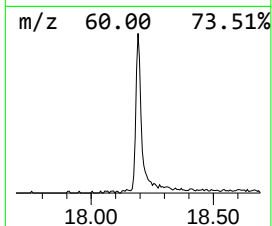
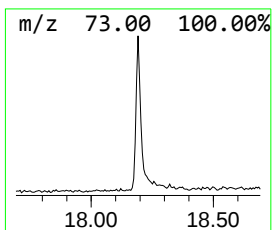
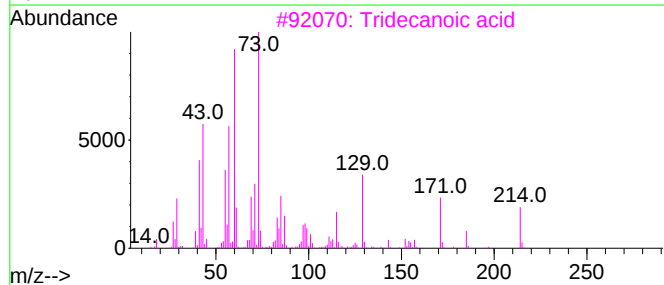
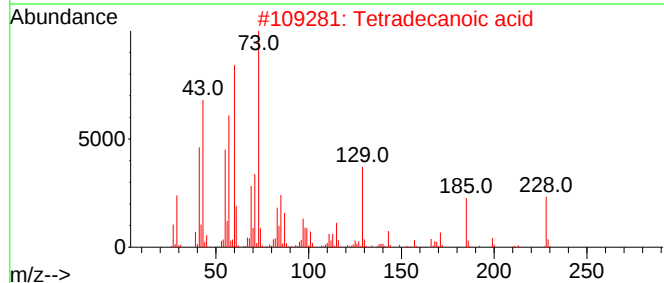
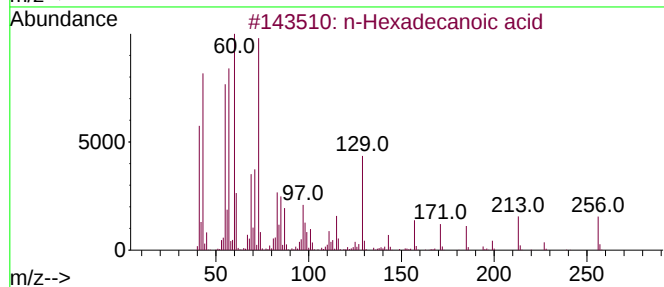
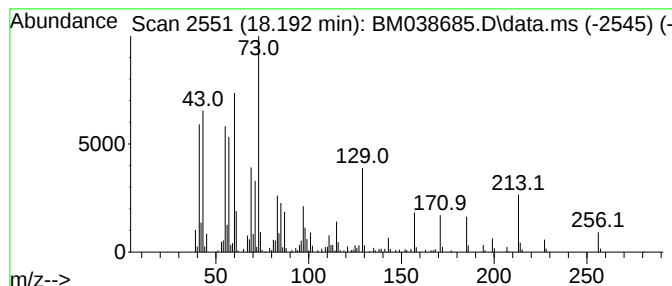
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	10.23 ng	346573	Phenanthrene-d10	17.309

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3			Tridecanoic acid	214	C13H26O2	000638-53-9	68
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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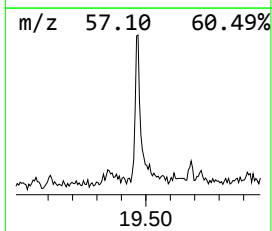
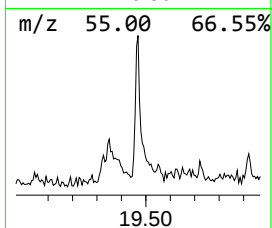
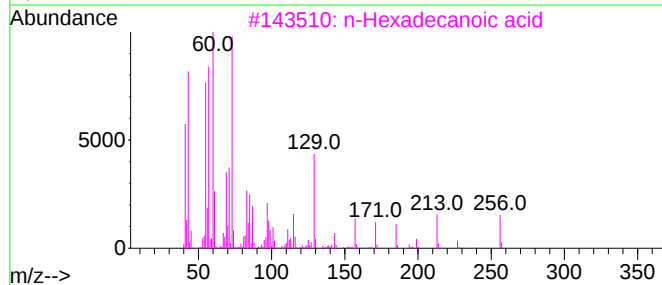
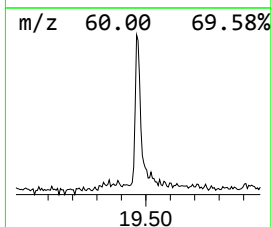
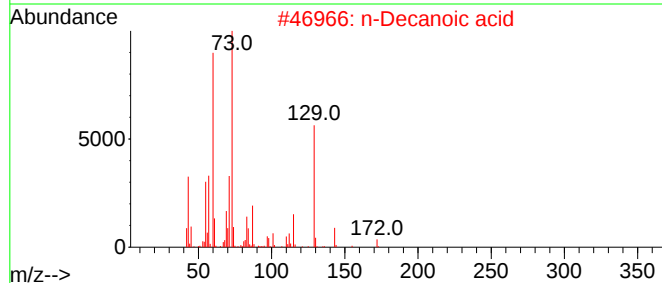
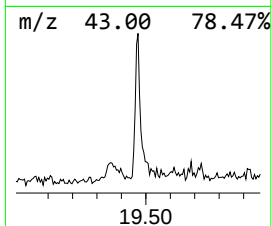
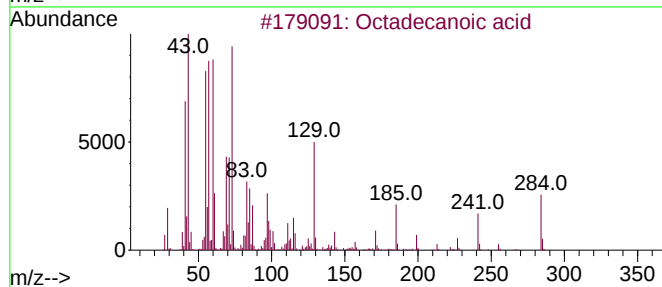
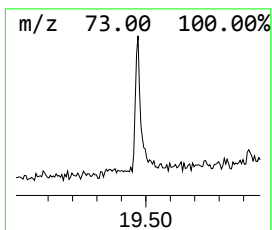
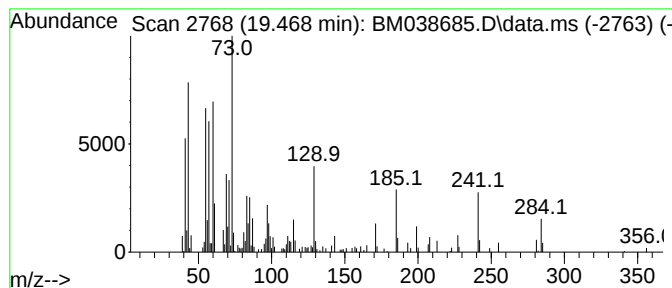
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.468	4.36 ng	162593	Chrysene-d12	21.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Decanoic acid	172	C10H20O2	000334-48-5	95
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	55
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	50



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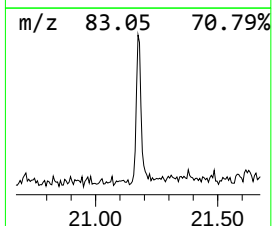
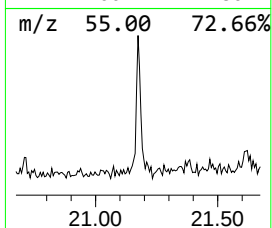
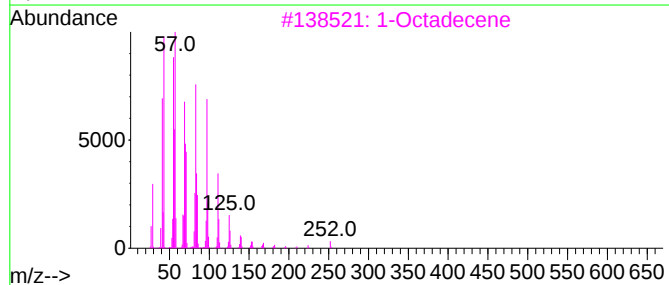
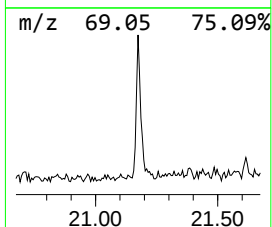
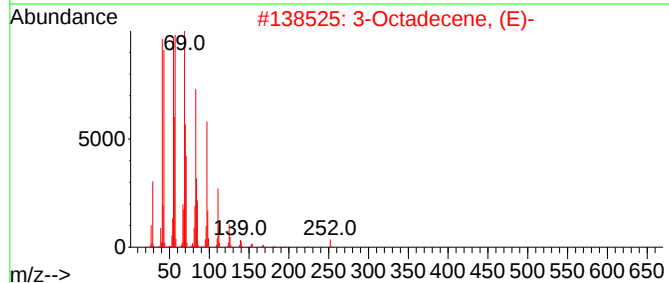
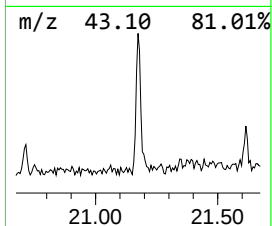
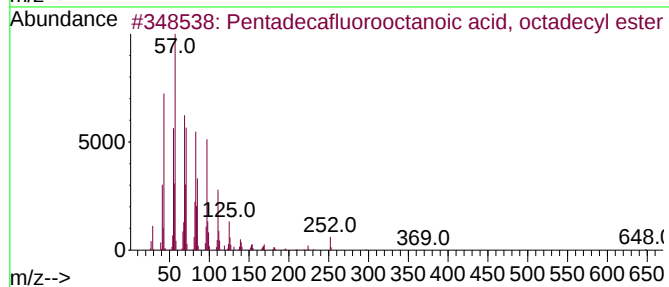
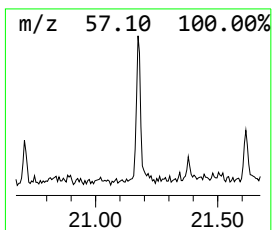
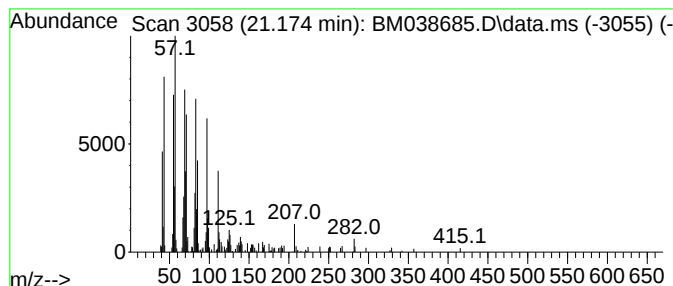
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.174	2.86 ng	106807	Chrysene-d12	21.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			3-Octadecene, (E)-	252	C18H36	007206-19-1	91
3			1-Octadecene	252	C18H36	000112-88-9	83
4			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	83
5			1-Hexacosene	364	C26H52	018835-33-1	83



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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	22.9	ng	356569	1	7.922	310705	20.0
Benzophenone	15.921	2.6	ng	73226	3	14.563	565918	20.0
n-Hexadecanoic ...	18.192	10.2	ng	346573	4	17.309	677518	20.0
Octadecanoic acid	19.468	4.4	ng	162593	5	21.486	746091	20.0
Pentadecafluoro...	21.174	2.9	ng	106807	5	21.486	746091	20.0