

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
 Data File : BM038732.D
 Acq On : 14 Feb 2023 16:18
 Operator : CG/JU
 Sample : 01329-06
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 COMP-7-BORING-2-14-21

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: BM038732.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.993	301	307	321	rVB	352203	467224	16.76%	3.220%
2	5.463	380	387	400	rBV	1009728	1408813	50.52%	9.710%
3	7.081	654	662	671	rBV	894664	1362470	48.86%	9.390%
4	7.898	795	801	808	rBV	180635	275901	9.89%	1.902%
5	9.075	994	1001	1011	rBV	530688	846991	30.37%	5.838%
6	10.710	1272	1279	1285	rBV	205223	331892	11.90%	2.287%
7	13.169	1690	1697	1705	rBV	1557081	2155871	77.31%	14.859%
8	14.539	1924	1930	1942	rBV	308746	432483	15.51%	2.981%
9	16.033	2177	2184	2199	rBV	1194621	1623531	58.22%	11.190%
10	17.280	2391	2396	2405	rBV	333489	461400	16.55%	3.180%
11	18.168	2542	2547	2557	rBV	203563	299711	10.75%	2.066%
12	19.445	2759	2764	2771	rBV	89038	126419	4.53%	0.871%
13	19.721	2806	2811	2816	rBV	19142	30041	1.08%	0.207%
14	19.903	2836	2842	2847	rBV	2542964	2788533	100.00%	19.219%
15	21.156	3051	3055	3065	rBV2	108233	162856	5.84%	1.122%
16	21.462	3102	3107	3114	rBV	422687	546487	19.60%	3.766%
17	22.327	3250	3254	3260	rVB	139499	182067	6.53%	1.255%
18	22.674	3309	3313	3319	rVB	224470	296569	10.64%	2.044%
19	23.838	3505	3511	3519	rVB2	367224	709947	25.46%	4.893%

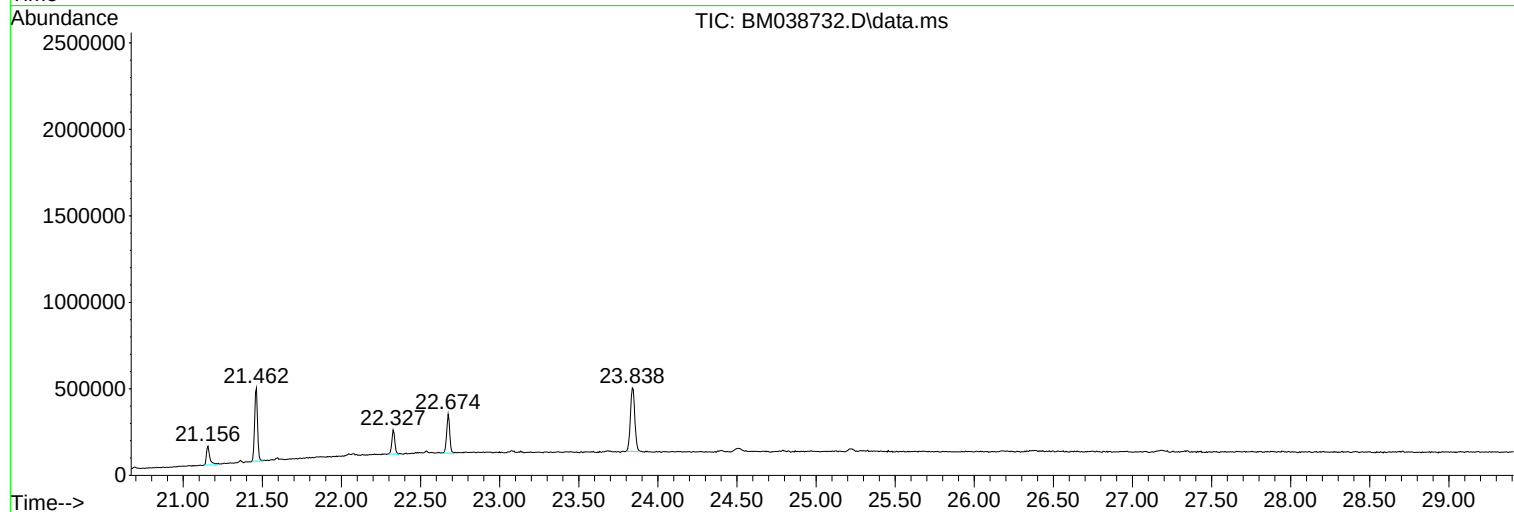
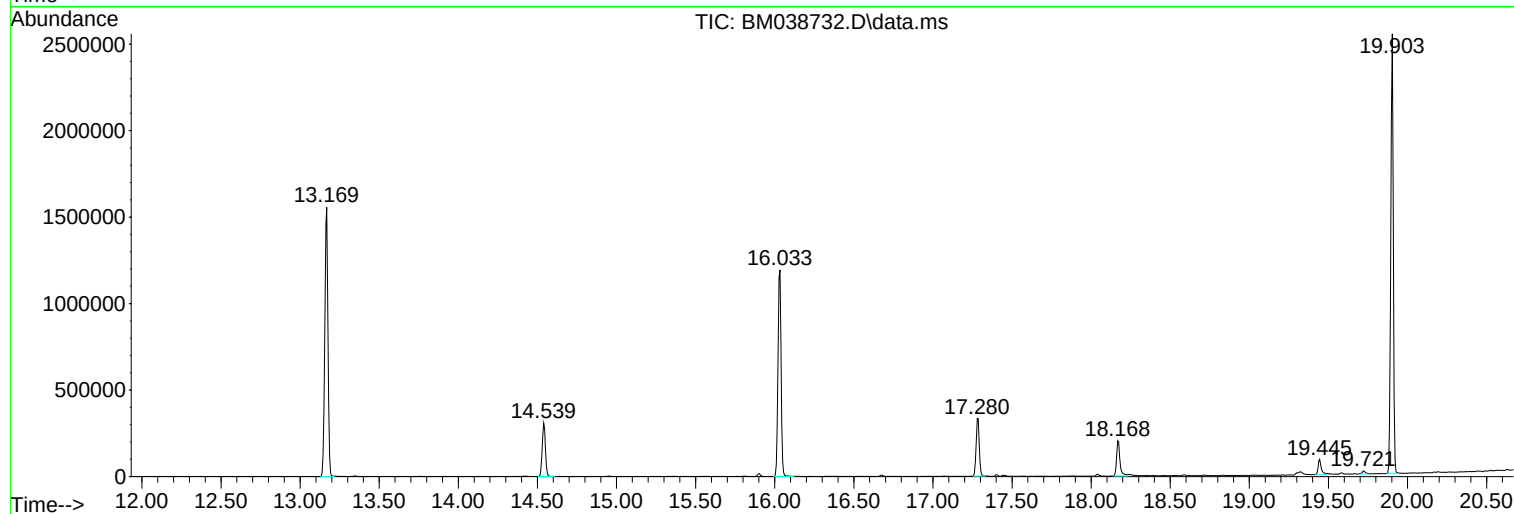
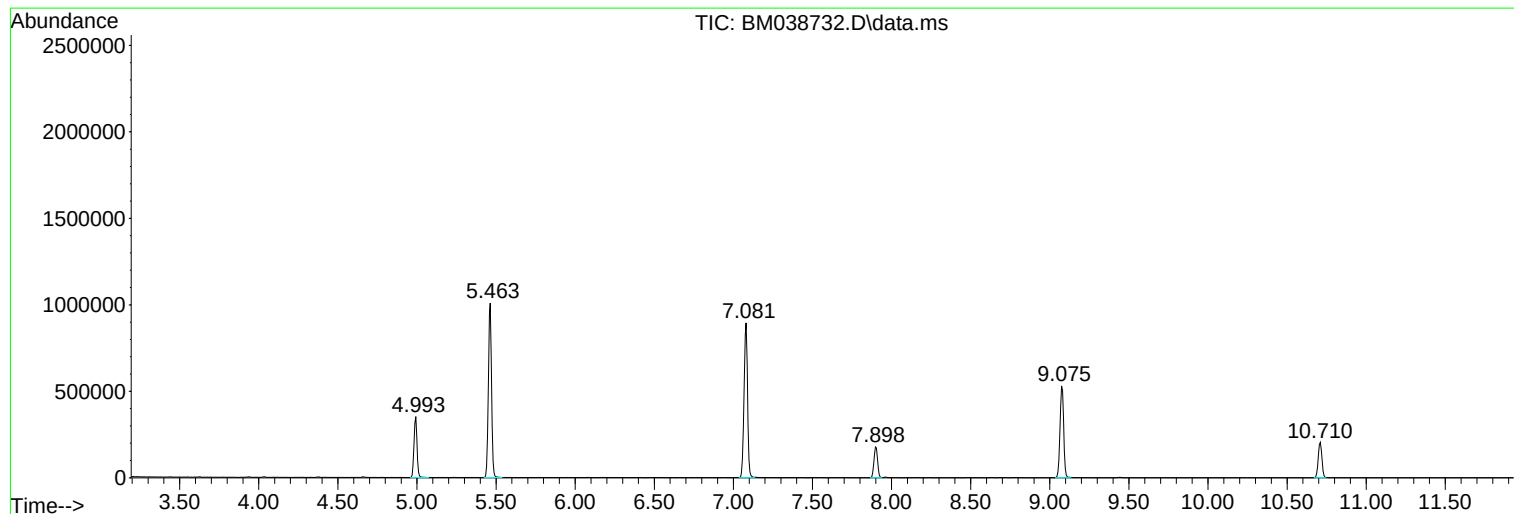
Sum of corrected areas: 14509206

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



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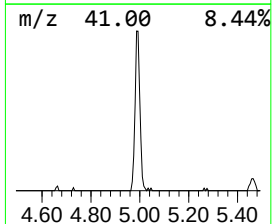
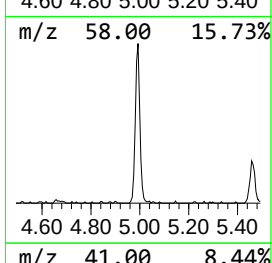
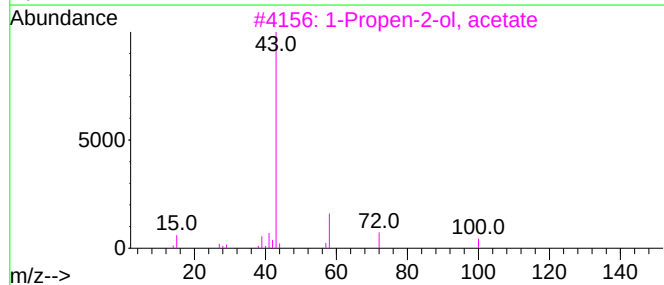
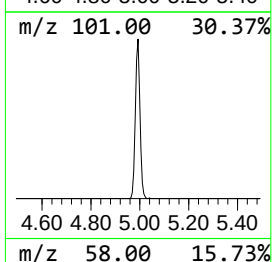
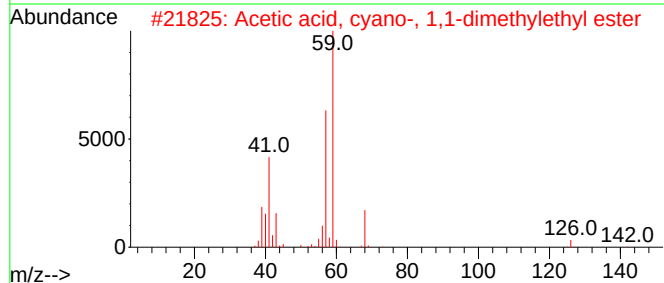
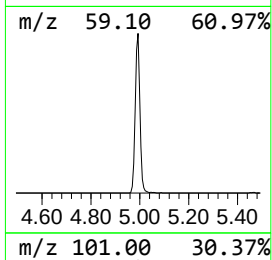
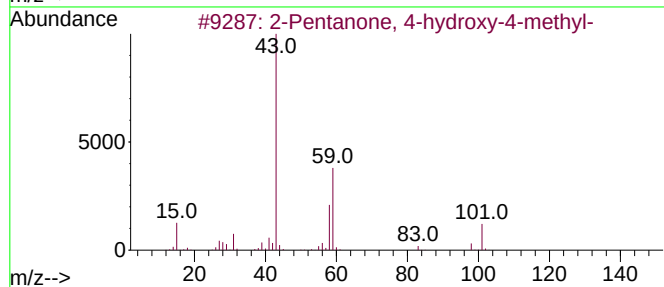
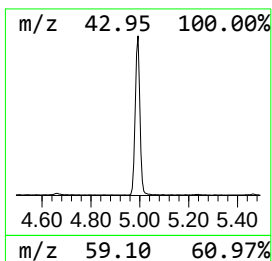
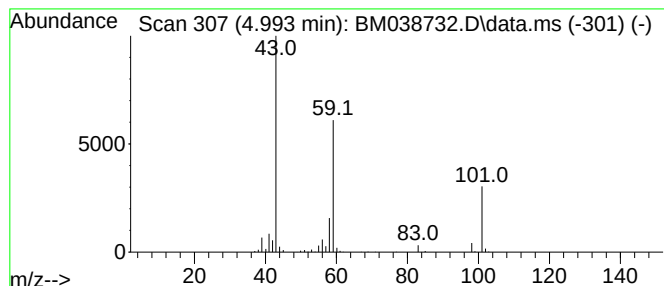
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.993	33.87 ng	467224	1,4-Dichlorobenzene-d4	7.898

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	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Butane	58	C4H10	000106-97-8	9		



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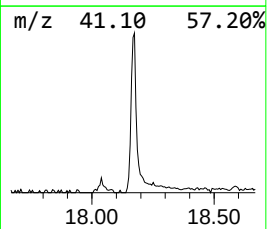
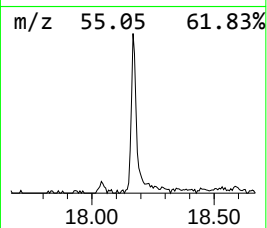
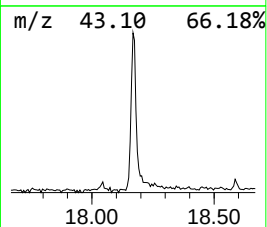
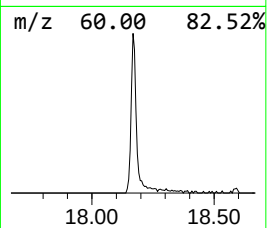
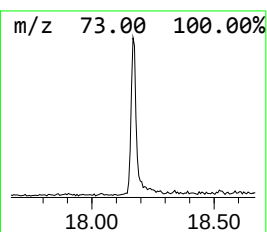
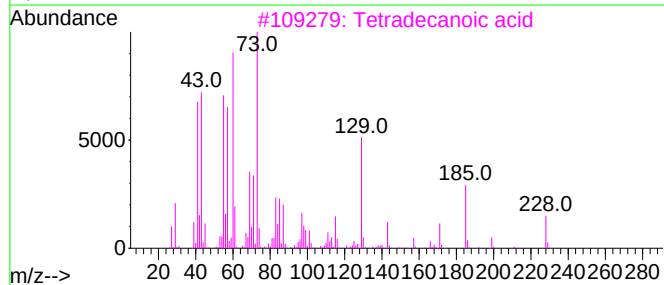
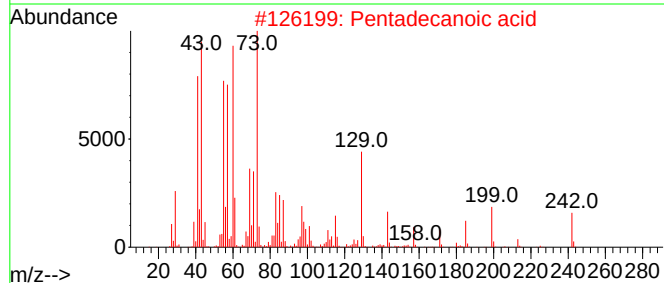
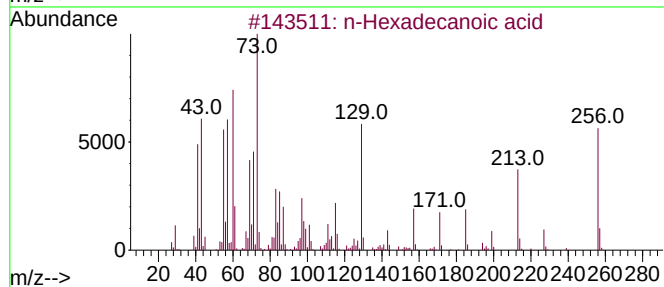
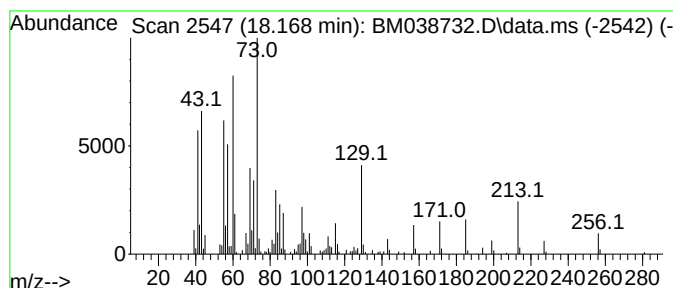
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.168	12.99 ng	299711	Phenanthrene-d10	17.280

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	70
4			n-Decanoic acid	172	C10H20O2	000334-48-5	53
5			Tridecanoic acid	214	C13H26O2	000638-53-9	52



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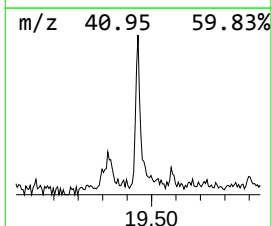
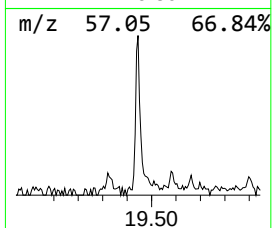
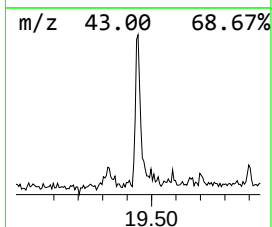
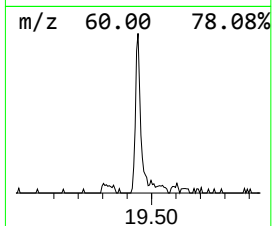
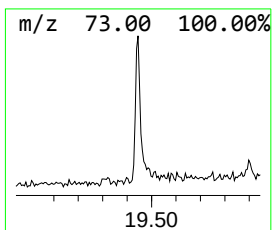
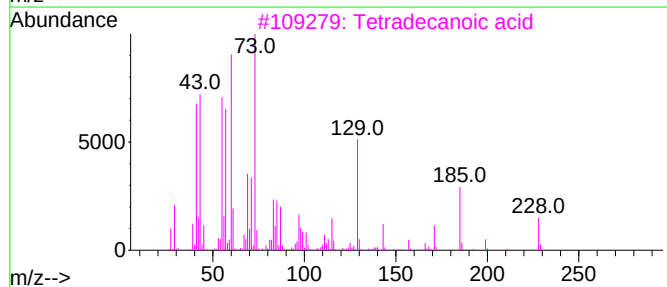
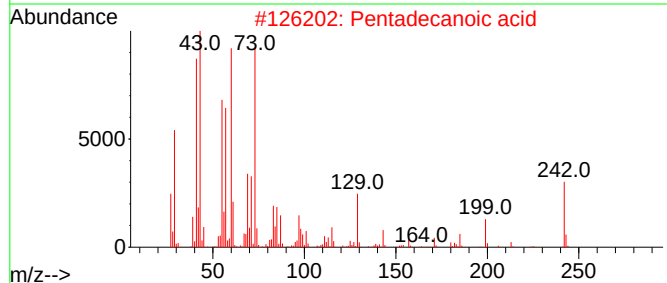
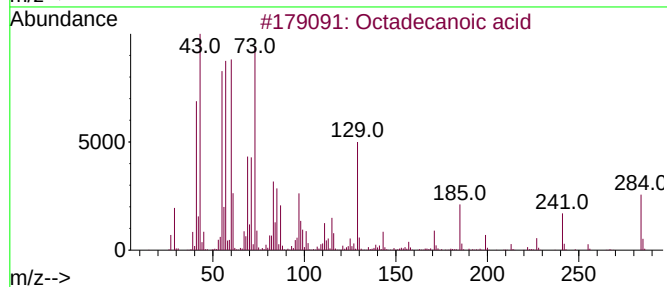
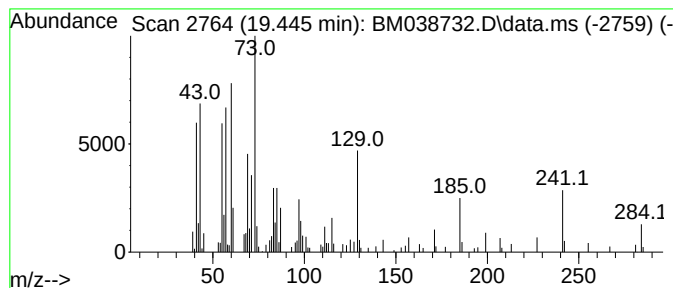
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Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	4.63 ng	126419	Chrysene-d12	21.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



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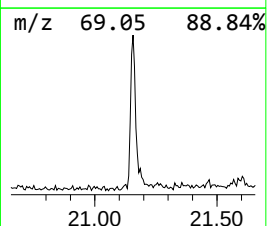
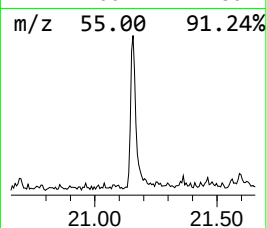
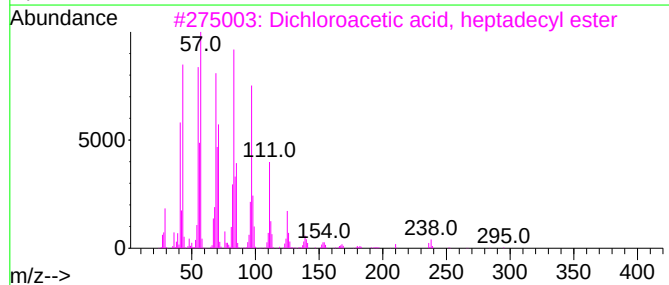
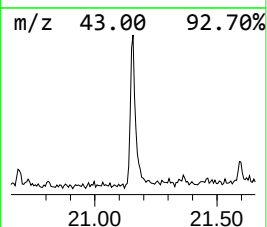
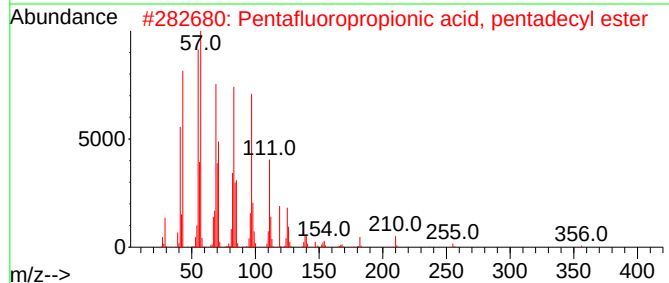
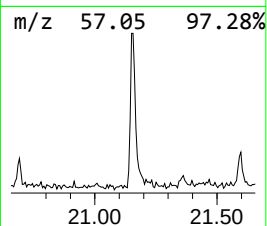
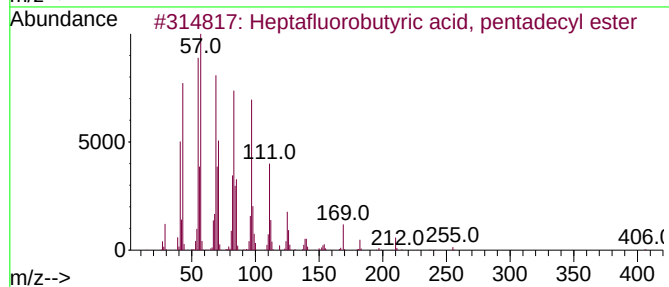
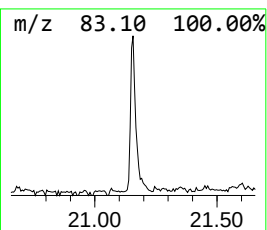
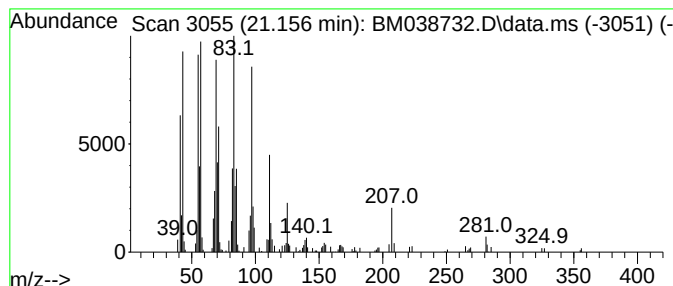
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Peak Number 4 Heptafluorobutyric acid, pe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.156	5.96 ng	162856	Chrysene-d12	21.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
5			1-Heneicosyl formate	340	C22H44O2	077899-03-7	93



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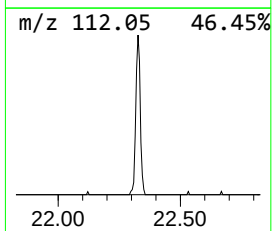
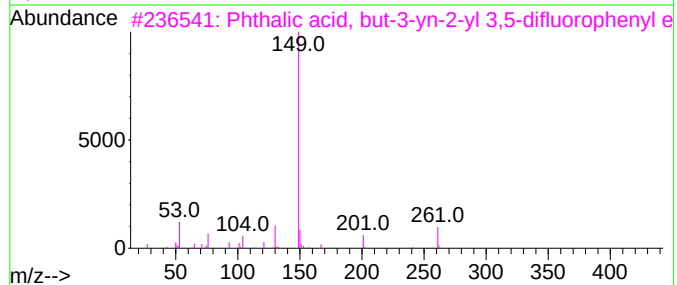
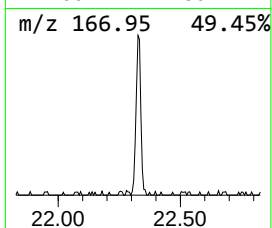
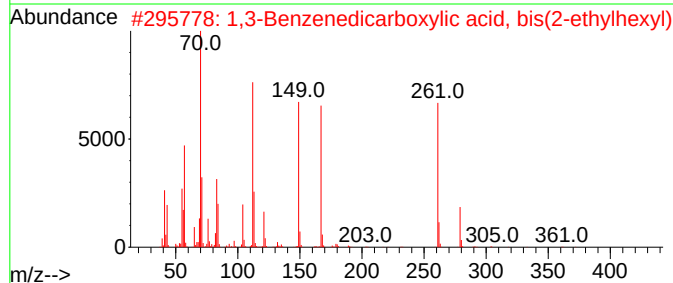
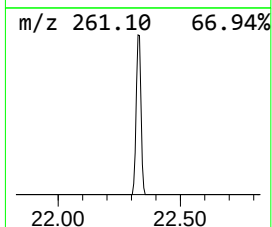
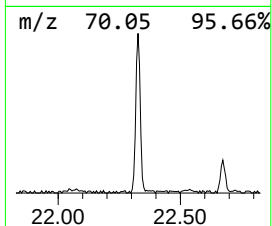
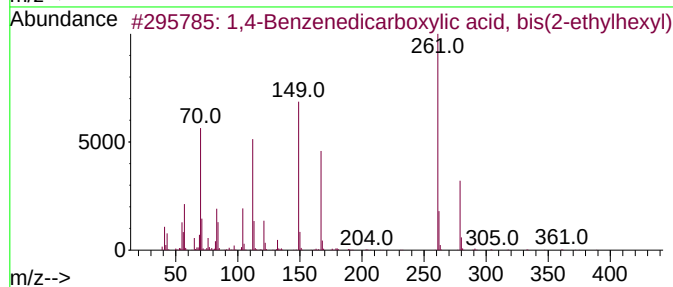
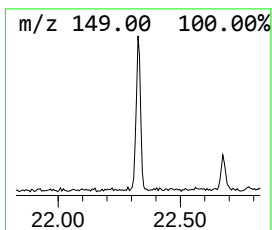
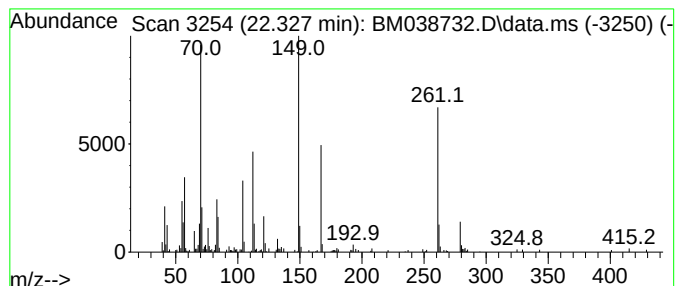
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Peak Number 5 1,4-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.327	6.66 ng	182067	Chrysene-d12		21.462	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...		390	C24H38O4	006422-86-2	50
2	1,3-Benzenedicarboxylic acid, bi...		390	C24H38O4	000137-89-3	49
3	Phthalic acid, but-3-yn-2-yl 3,5...		330	C18H12F2O4	1000315-75-6	27
4	Bis(2-ethylhexyl) phthalate		390	C24H38O4	000117-81-7	27
5	Phthalic acid, 6-ethyloct-3-yl 2...		418	C26H42O4	1000315-53-8	27



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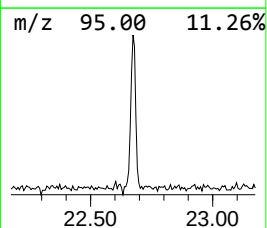
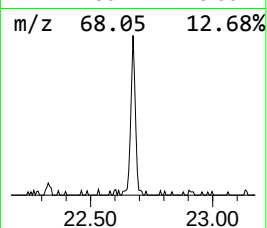
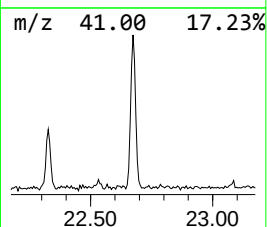
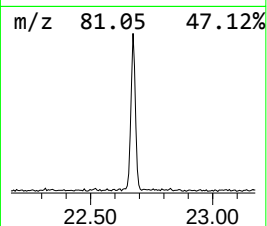
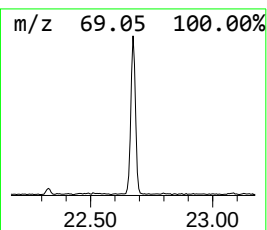
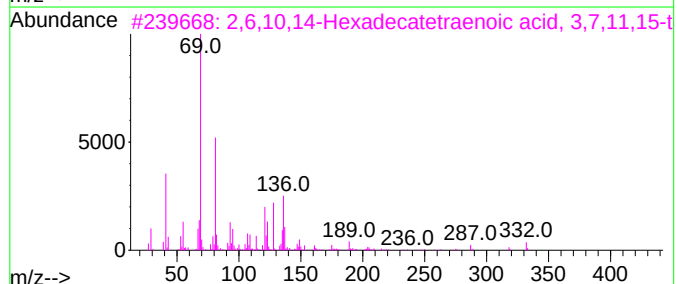
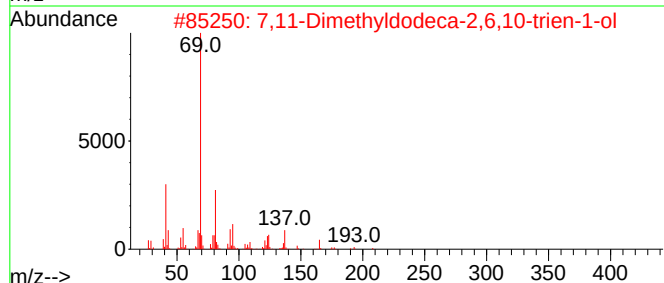
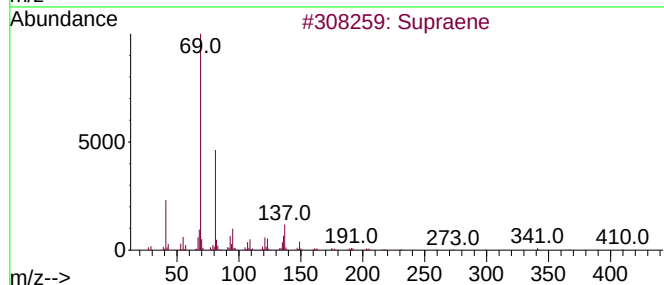
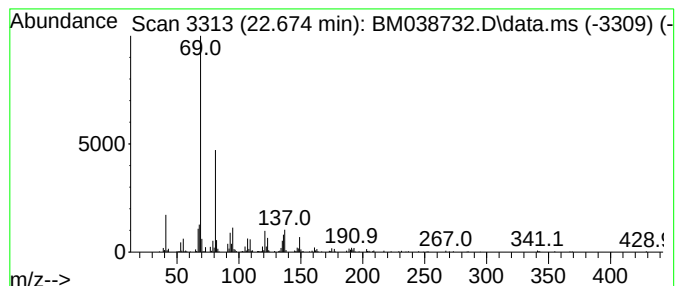
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.674	8.35 ng	296569	Perylene-d12	23.844

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
3			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5			2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038732.D
Acq On : 14 Feb 2023 16:18
Operator : CG/JU
Sample : 01329-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-7-BORING-2-14-21

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-...	4.993	33.9	ng	467224	1	7.898	275901	20.0
n-Hexadecanoic ...	18.168	13.0	ng	299711	4	17.280	461400	20.0
Octadecanoic acid	19.445	4.6	ng	126419	5	21.462	546487	20.0
Heptafluorobuty...	21.156	6.0	ng	162856	5	21.462	546487	20.0
1,4-Benzenedica...	22.327	6.7	ng	182067	5	21.462	546487	20.0
Supraene	22.674	8.3	ng	296569	6	23.844	709947	20.0