

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060921\
 Data File : BM030355.D
 Acq On : 09 Jun 2021 23:05
 Operator : CG/JU
 Sample : M2613-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 18-B12(102-106)

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-BM060921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM030355.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.434	392	399	416	rBV	4962835	7458007	36.82%	8.968%
2	7.010	659	667	676	rBV	5049464	8235007	40.66%	9.902%
3	7.846	803	809	817	rBV	836760	1346650	6.65%	1.619%
4	9.004	997	1006	1023	rBV	2999096	4997890	24.67%	6.010%
5	10.640	1276	1284	1294	rBV	1129086	1920701	9.48%	2.310%
6	13.098	1694	1702	1714	rBV	8327163	12339544	60.92%	14.838%
7	14.469	1928	1935	1945	rBV	1913675	2788709	13.77%	3.353%
8	15.957	2178	2188	2205	rBV	7237746	10189973	50.31%	12.253%
9	17.204	2391	2400	2412	rBV	2449756	3446700	17.02%	4.145%
10	18.092	2544	2551	2562	rBV	551458	848706	4.19%	1.021%
11	19.251	2739	2748	2761	rBV2	369794	895873	4.42%	1.077%
12	19.368	2763	2768	2785	rVB	536666	840956	4.15%	1.011%
13	19.821	2838	2845	2850	rBV	16183483	20255320	100.00%	24.356%
14	21.074	3054	3058	3068	rBV3	274896	486940	2.40%	0.586%
15	21.362	3102	3107	3116	rBV	2984555	3755384	18.54%	4.516%
16	23.645	3488	3495	3508	rVB2	1702475	3355789	16.57%	4.035%

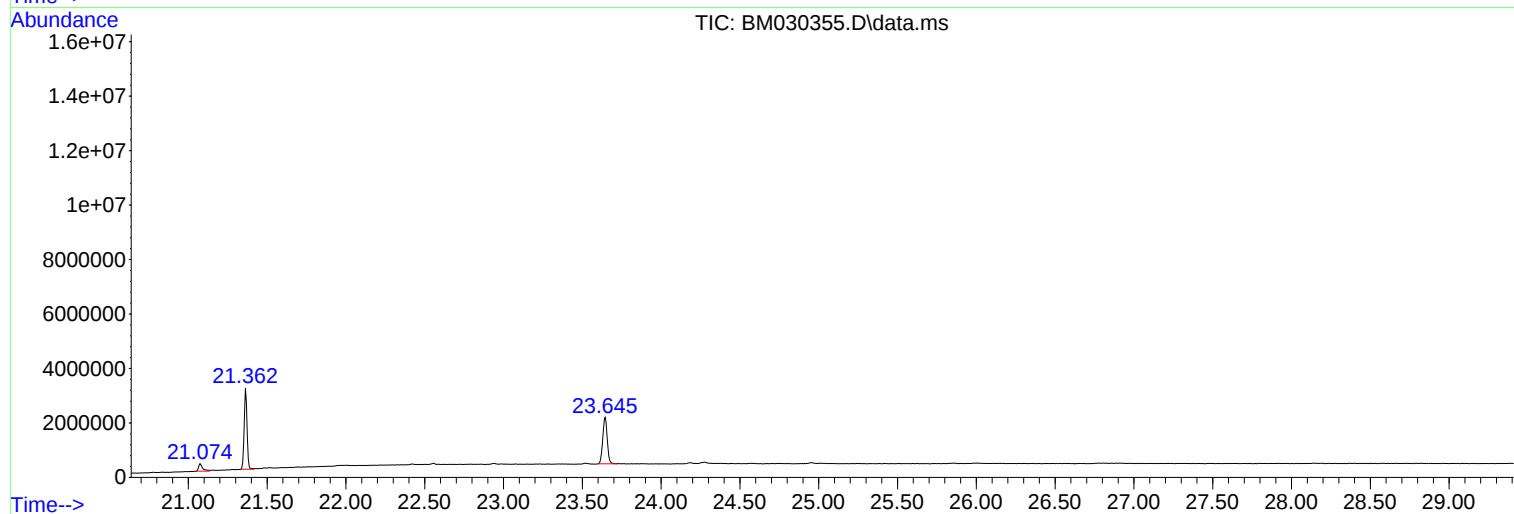
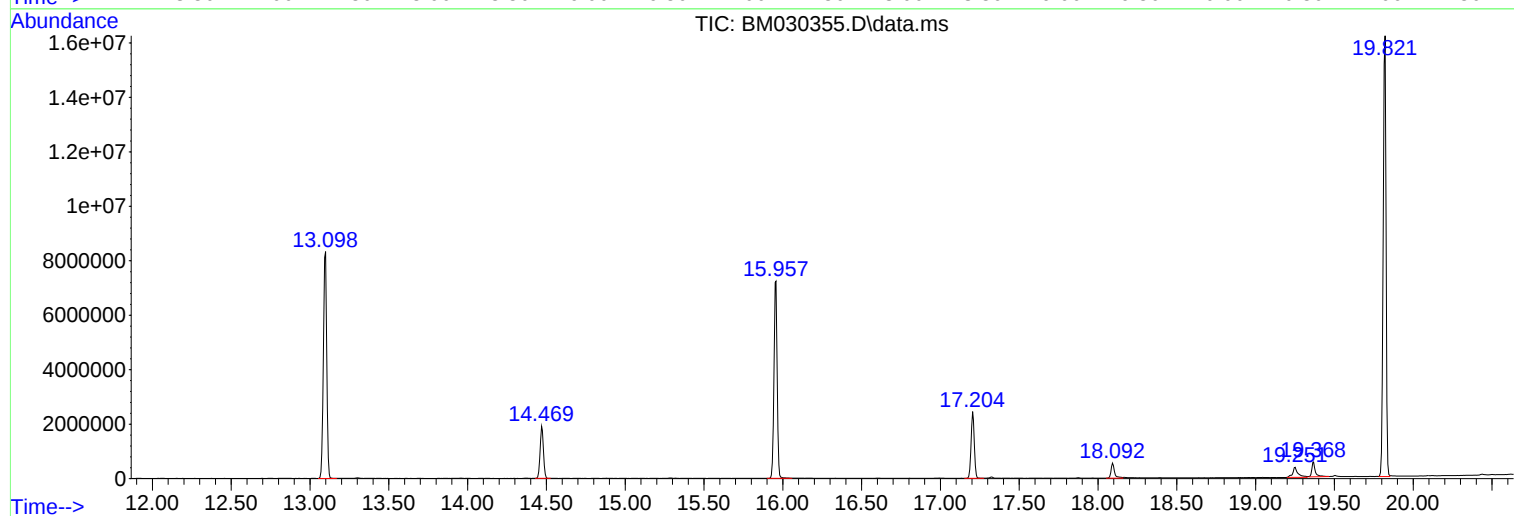
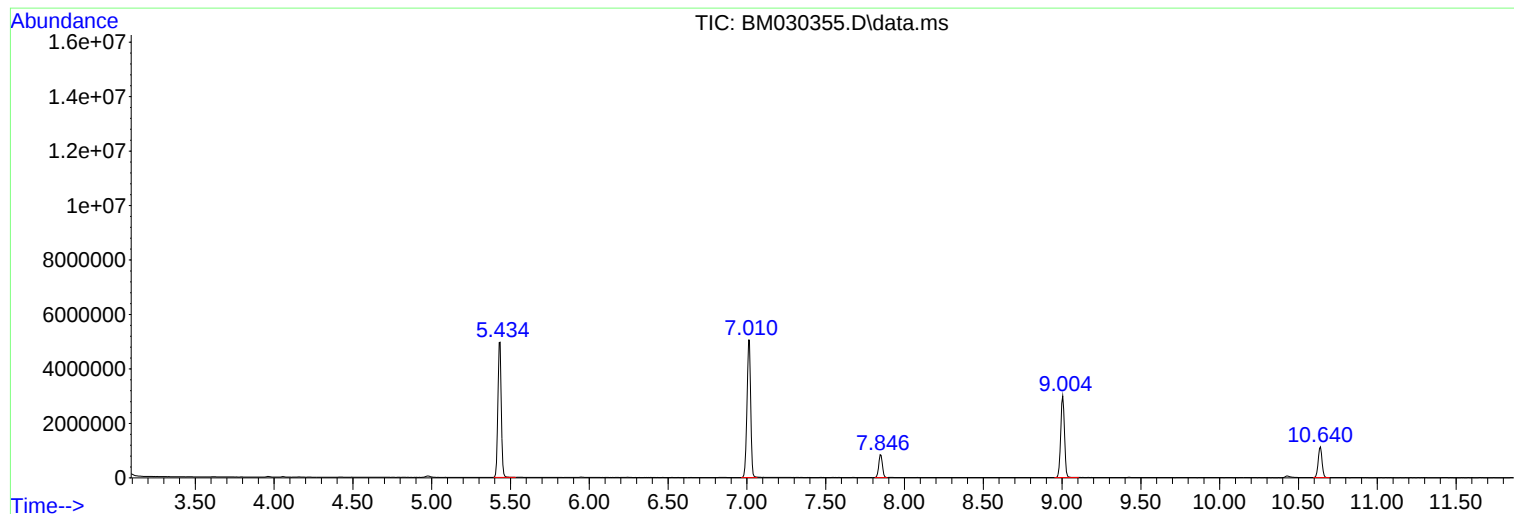
Sum of corrected areas: 83162149

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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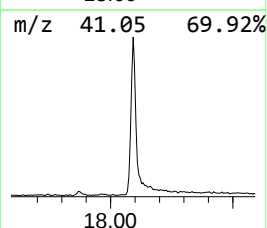
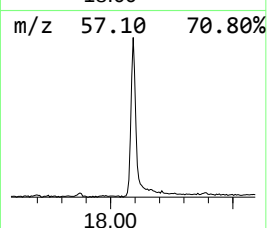
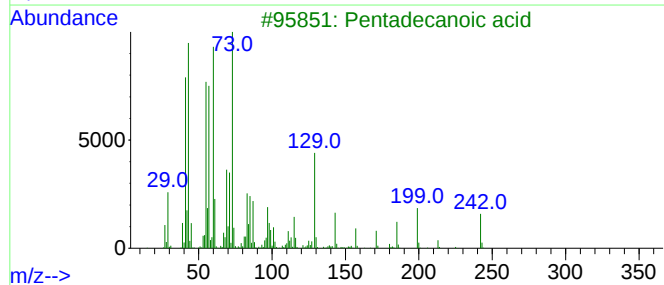
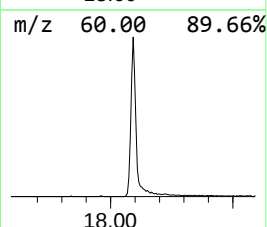
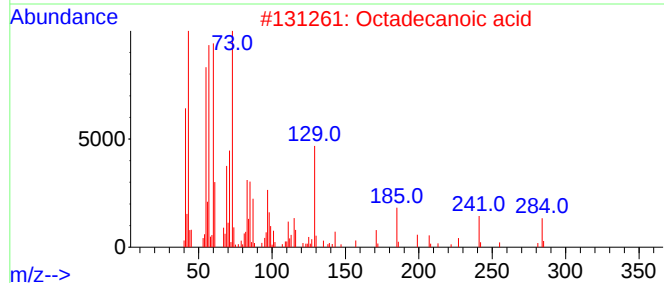
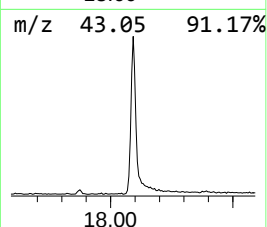
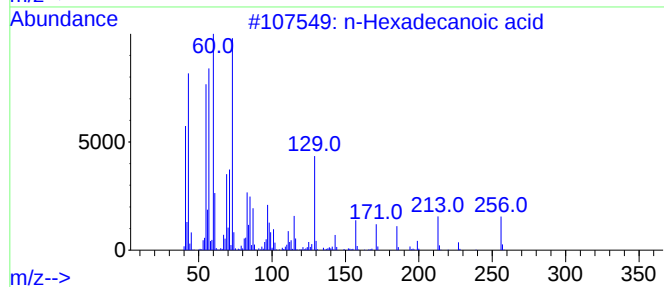
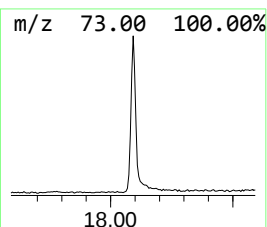
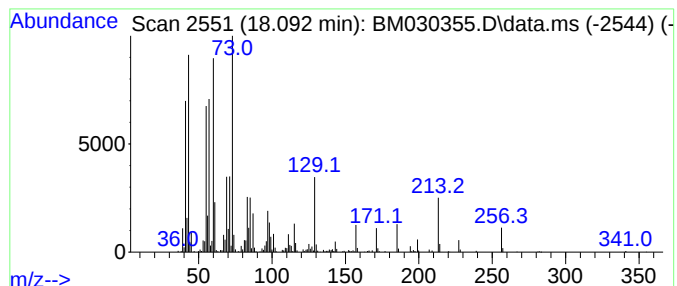
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	4.92 ng	848706	Phenanthrene-d10	17.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	86
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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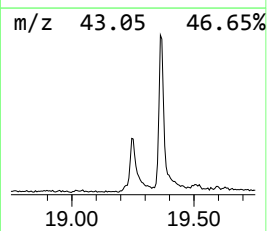
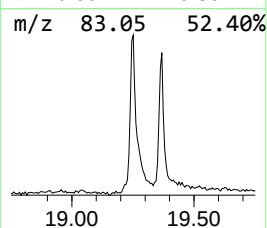
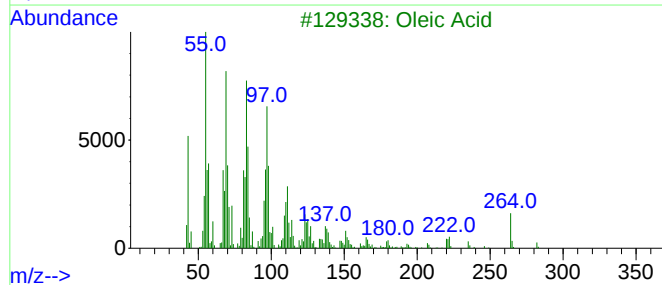
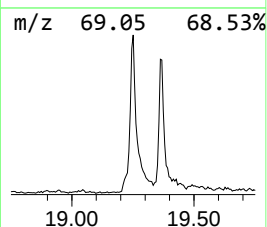
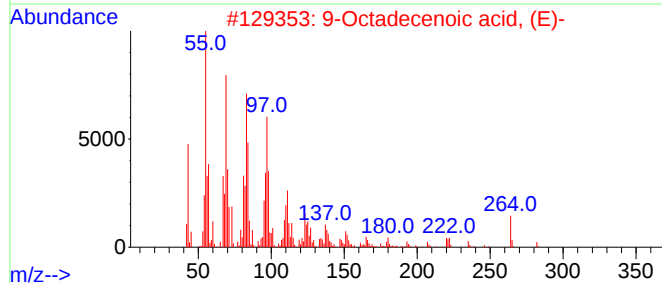
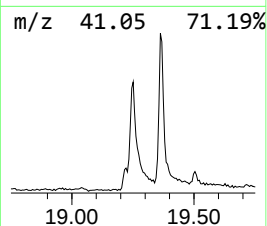
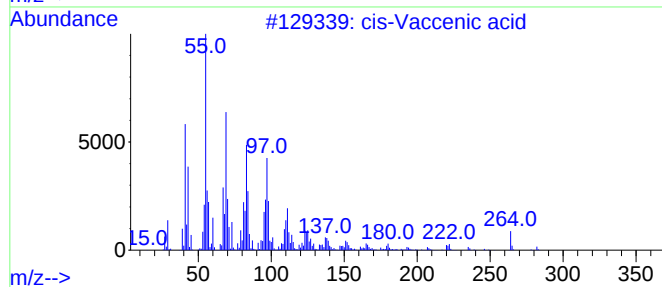
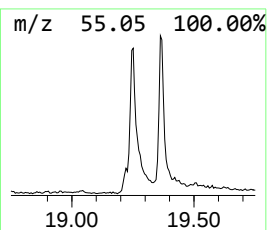
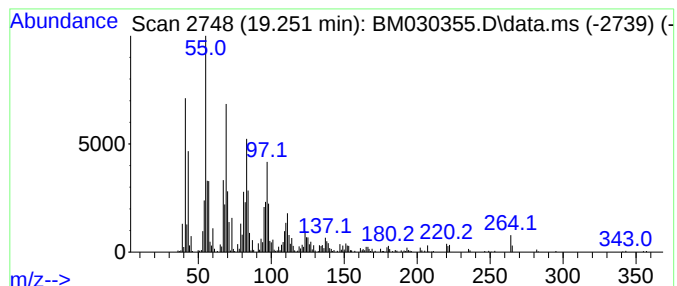
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TIC Integration Parameters: LSCINT.P

Peak Number 2 cis-Vaccenic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.251	5.20 ng	895873	Phenanthrene-d10	17.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	98
2			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	98
3			Oleic Acid	282	C18H34O2	000112-80-1	98
4			6-Octadecenoic acid	282	C18H34O2	1000336-66-8	97
5			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	97



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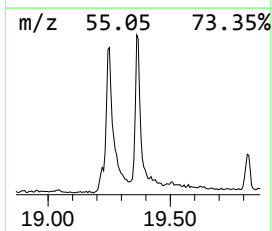
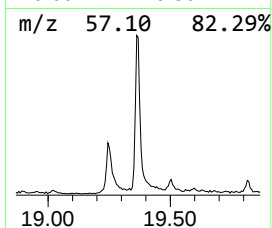
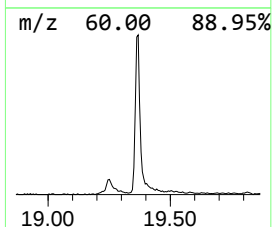
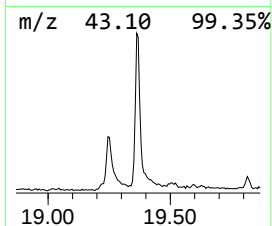
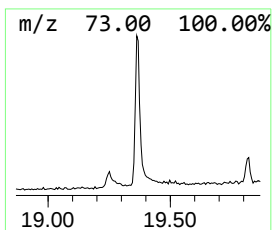
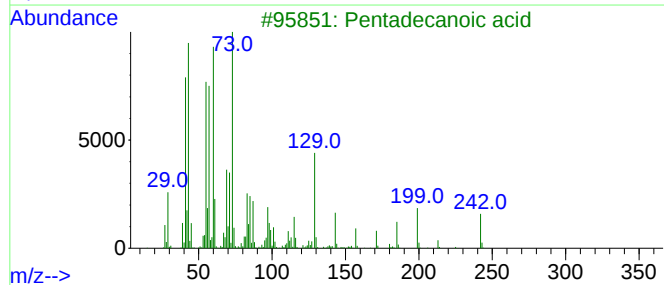
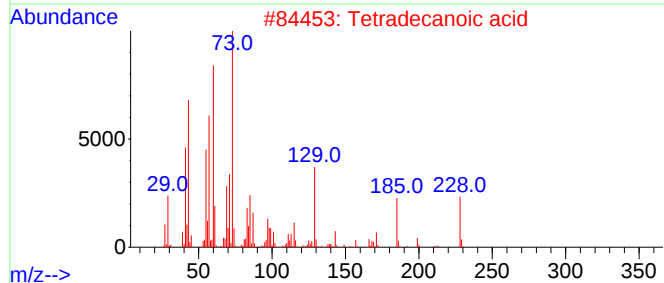
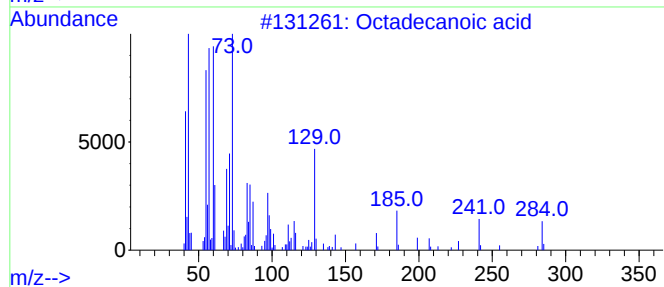
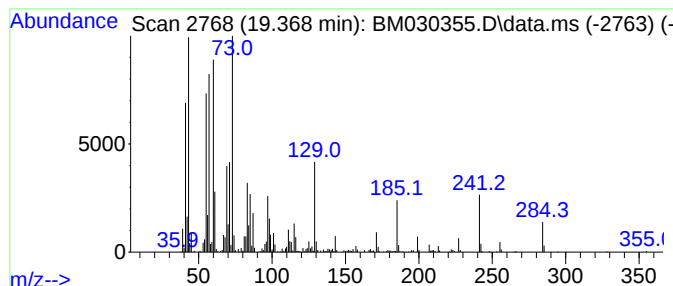
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Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.368	4.48 ng	840956	Chrysene-d12	21.362

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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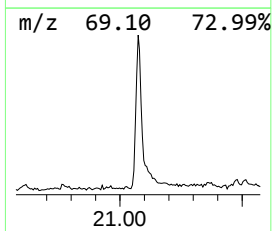
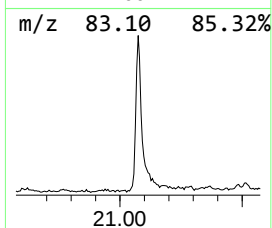
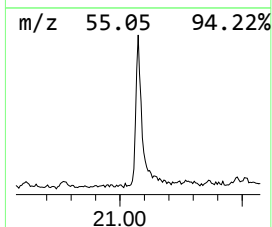
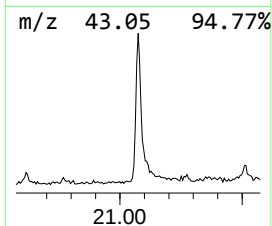
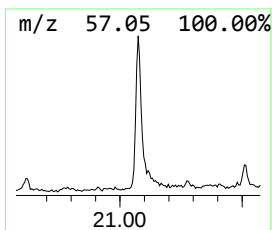
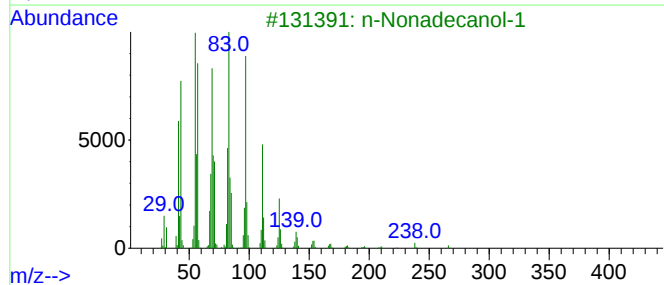
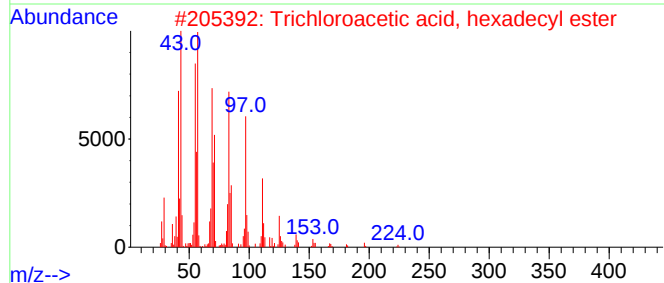
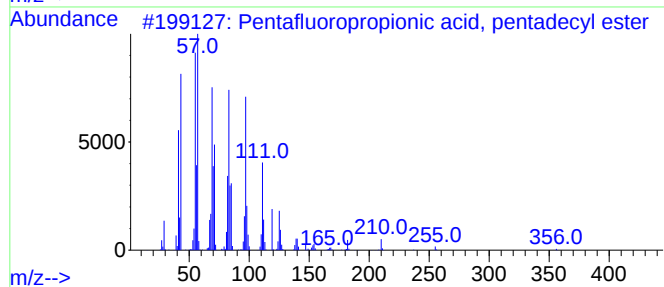
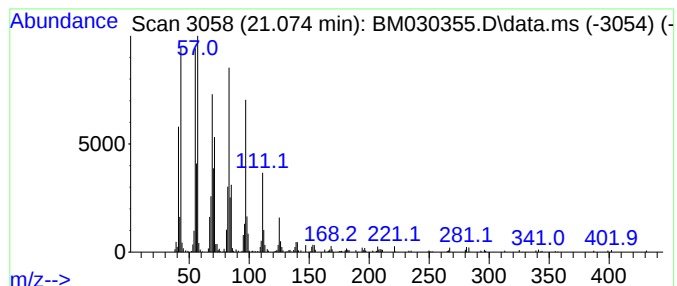
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Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.074	2.59 ng	486940	Chrysene-d12	21.362

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4			1-Tricosene	322	C23H46	018835-32-0	91
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.092	4.9	ng	848706	4	17.204	3446700	20.0
cis-Vaccenic acid	19.251	5.2	ng	895873	4	17.204	3446700	20.0
Octadecanoic acid	19.368	4.5	ng	840956	5	21.362	3755380	20.0
Pentafluoroprop...	21.074	2.6	ng	486940	5	21.362	3755380	20.0