

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110423\
 Data File : BM042589.D
 Acq On : 04 Nov 2023 13:41
 Operator : MA/JU
 Sample : 05243-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-11-AT-4.5-5.0

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-BM103023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042589.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.446	377	384	400	rBV	696455	1038274	56.56%	9.246%
2	7.081	655	662	674	rBV	638940	1044392	56.89%	9.301%
3	7.516	731	736	742	rBV3	10251	21029	1.15%	0.187%
4	7.910	797	803	811	rBV	201773	316204	17.22%	2.816%
5	9.110	1001	1007	1020	rVB	403724	662454	36.08%	5.900%
6	10.733	1275	1283	1290	rBV	219783	380928	20.75%	3.392%
7	13.186	1693	1700	1713	rBV	820181	1206619	65.73%	10.746%
8	13.410	1732	1738	1745	rVB	30129	47694	2.60%	0.425%
9	14.563	1928	1934	1941	rVB	318892	451241	24.58%	4.019%
10	16.057	2182	2188	2199	rBV	733253	1042999	56.81%	9.288%
11	17.315	2396	2402	2409	rBV	379463	530128	28.88%	4.721%
12	18.168	2540	2547	2570	rBV	424893	706540	38.49%	6.292%
13	19.445	2759	2764	2783	rBV	175217	306831	16.71%	2.732%
14	19.927	2841	2846	2856	rBV	1488209	1835856	100.00%	16.349%
15	21.162	3051	3056	3063	rBV	133819	212493	11.57%	1.892%
16	21.497	3108	3113	3118	rBV	538864	676419	36.84%	6.024%
17	23.915	3518	3524	3533	rVB	385683	748856	40.79%	6.669%

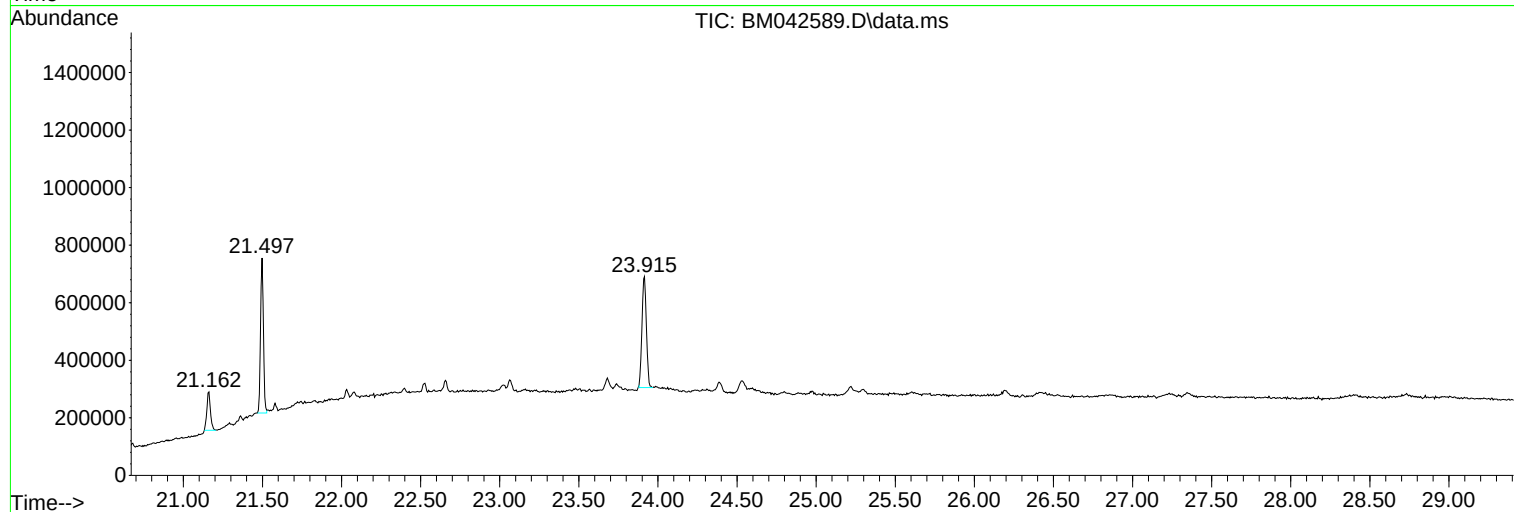
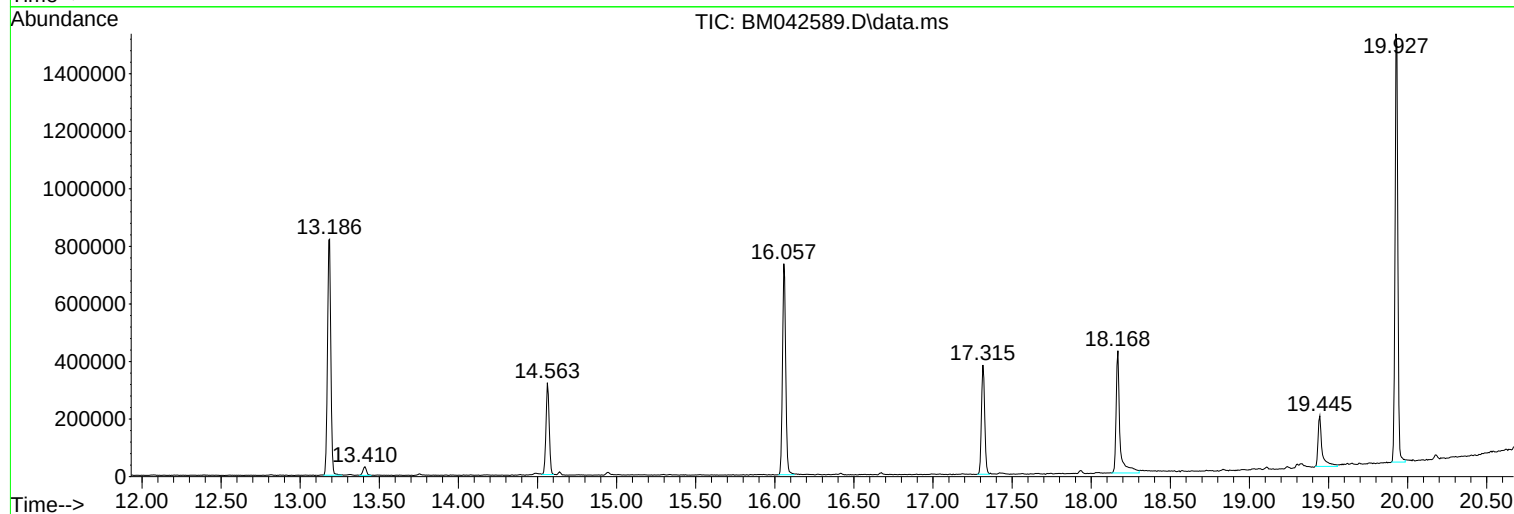
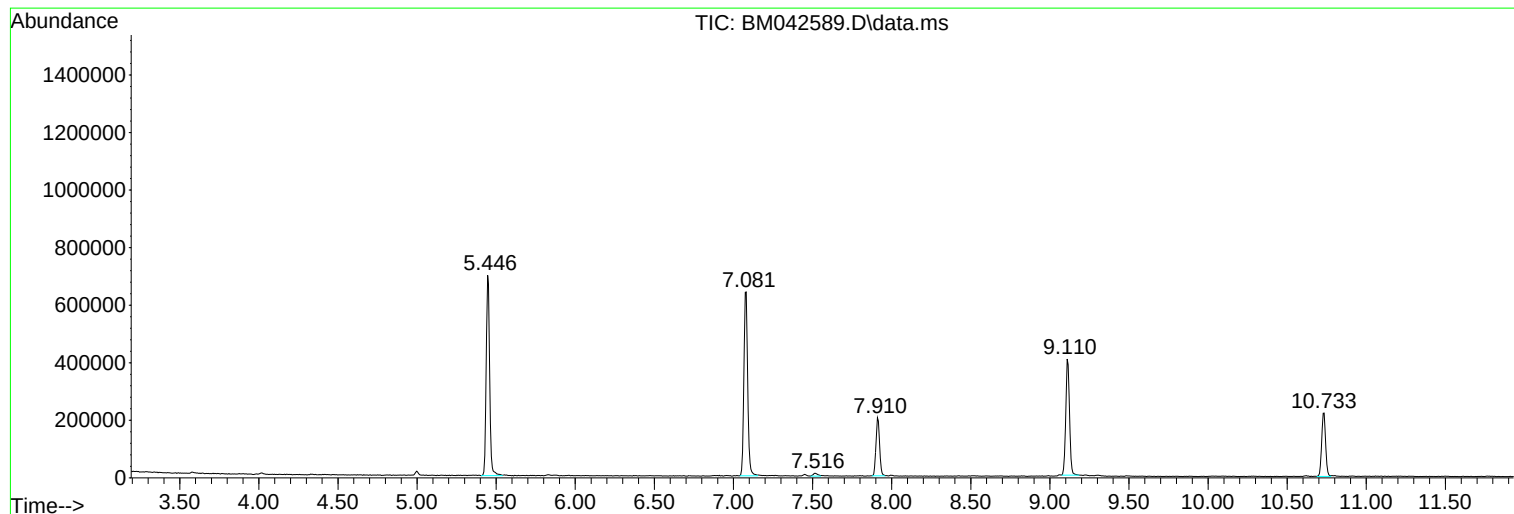
Sum of corrected areas: 11228957

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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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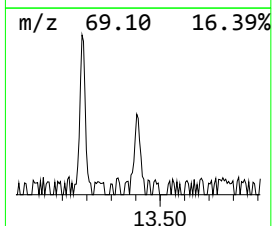
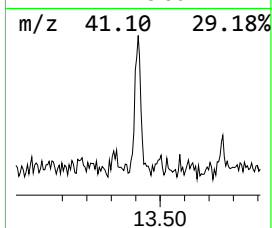
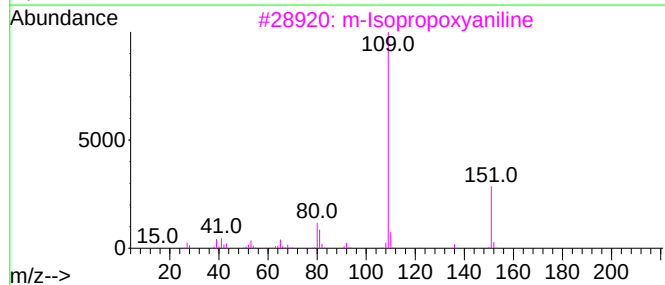
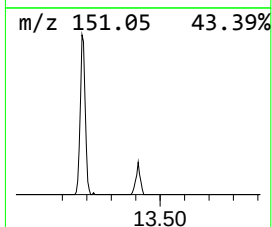
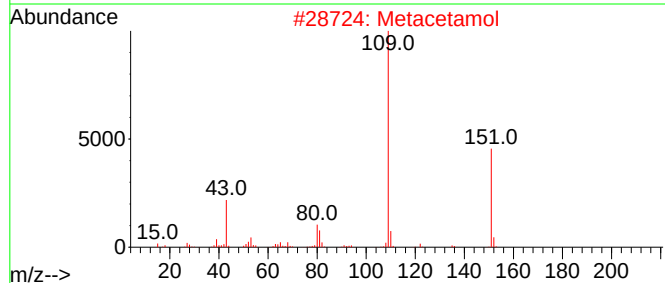
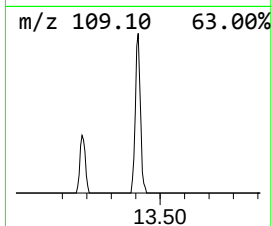
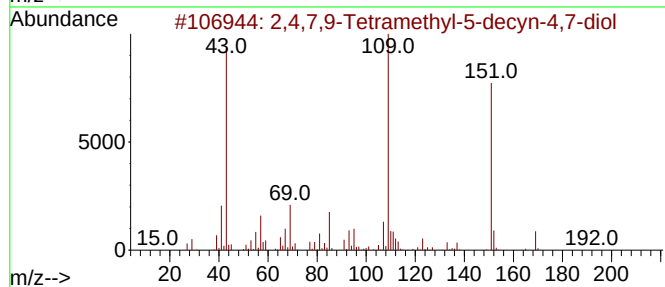
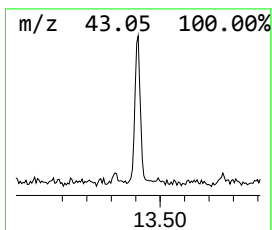
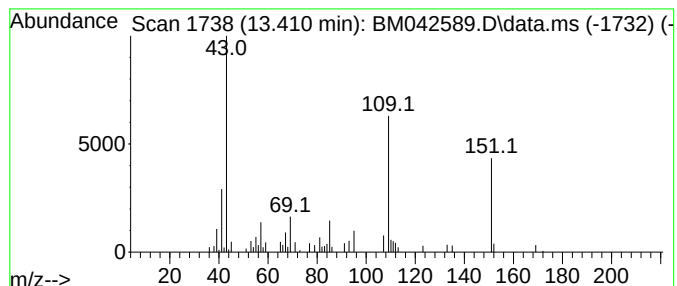
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.410	2.11 ng	47694	Acenaphthene-d10	14.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	64		
2	Metacetamol	151	C8H9NO2	000621-42-1	58		
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	58		
4	Acetaminophen	151	C8H9NO2	000103-90-2	53		
5	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	32		



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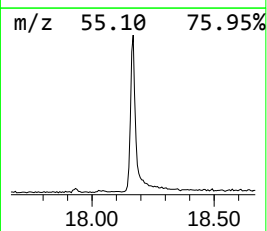
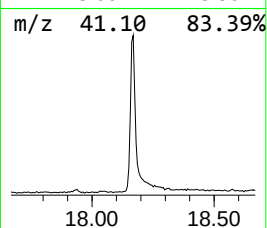
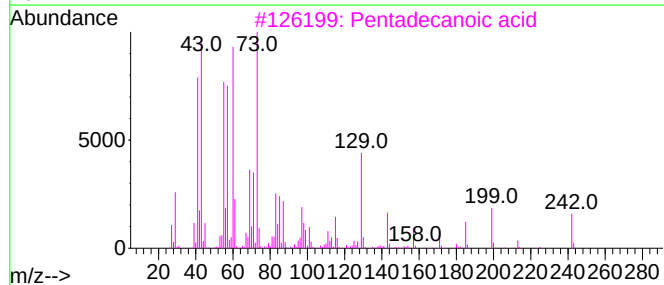
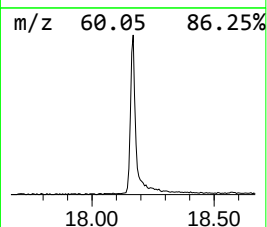
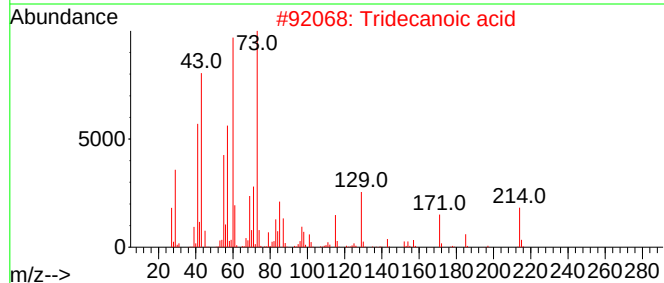
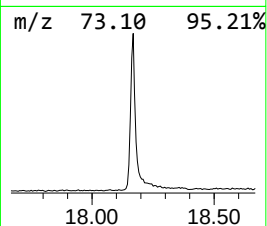
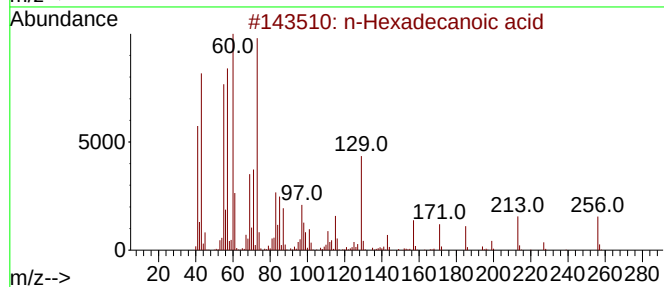
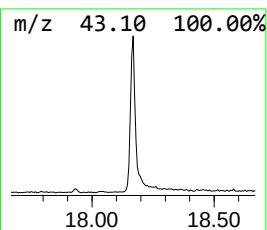
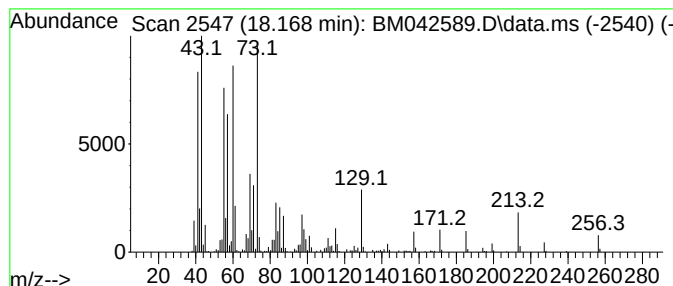
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.168	26.66 ng	706540	Phenanthrene-d10	17.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Nonanoic acid	158	C9H18O2	000112-05-0	64



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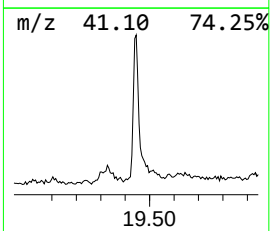
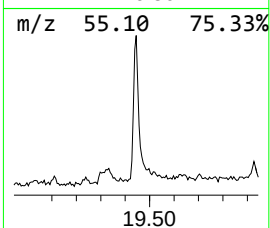
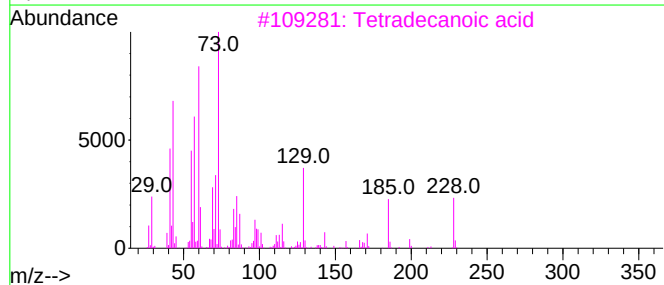
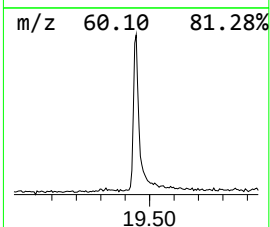
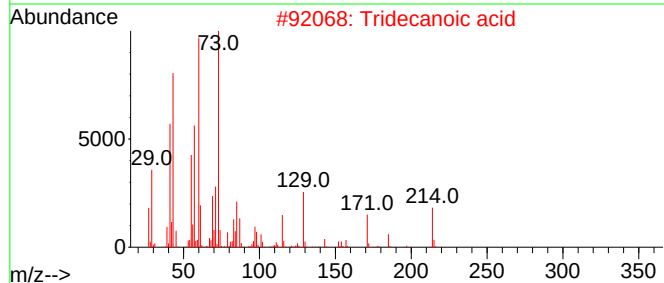
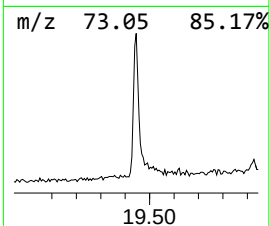
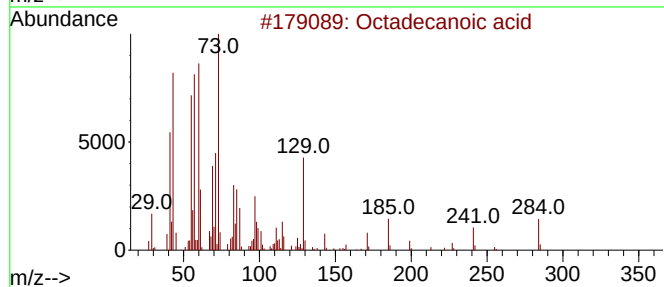
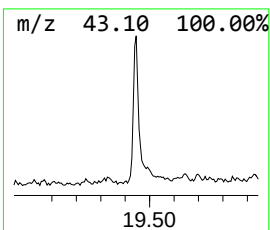
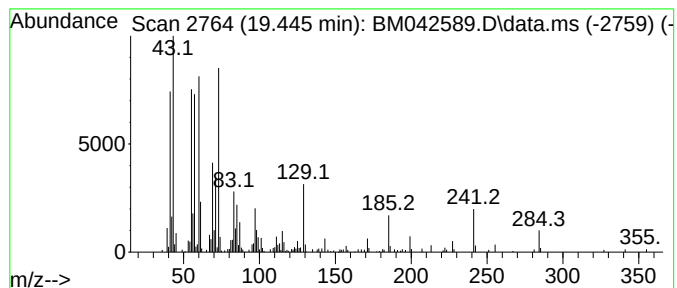
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Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	9.07 ng	306831	Chrysene-d12	21.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	64
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	59
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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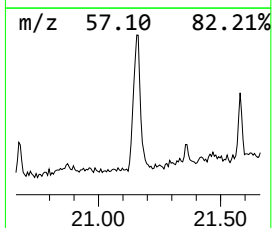
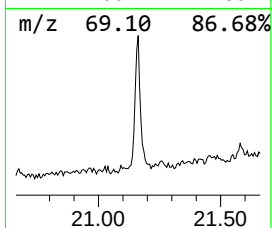
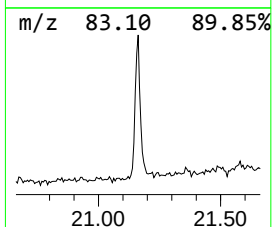
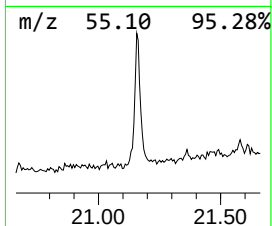
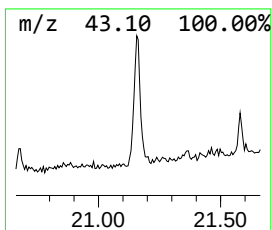
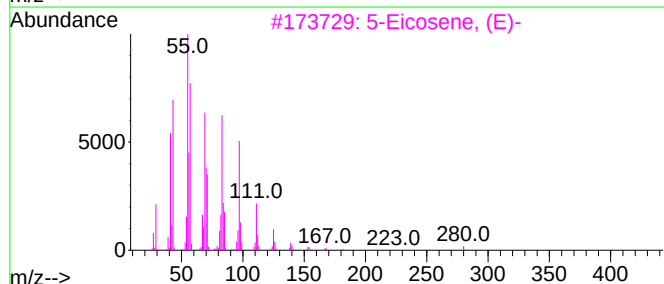
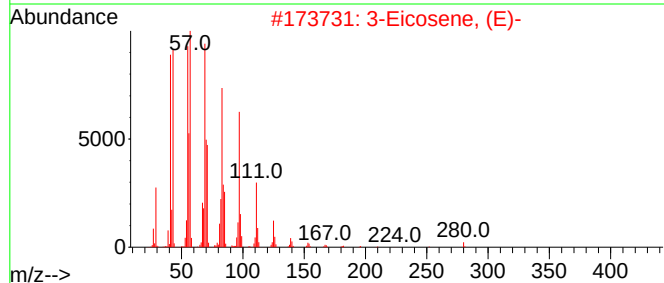
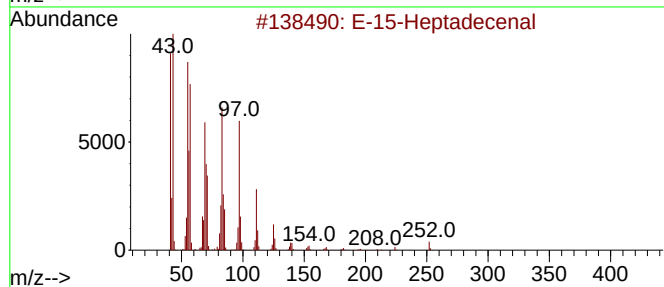
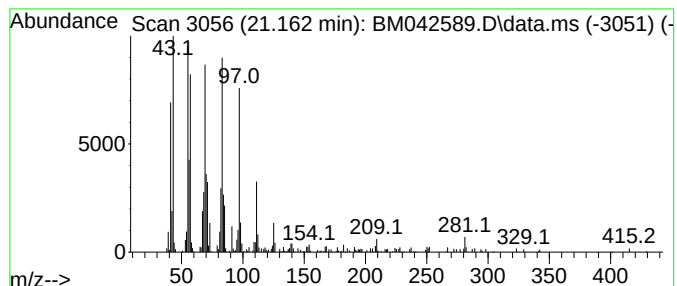
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Peak Number 4 E-15-Heptadecenal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.162	6.28 ng	212493	Chrysene-d12	21.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			E-15-Heptadecenal	252	C17H32O	1000130-97-9	99
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	98
3			5-Eicosene, (E)-	280	C20H40	074685-30-6	96
4			3-Octadecene, (E)-	252	C18H36	007206-19-1	92
5			Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1010348-57-1	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,4,7,9-Tetrame...	13.410	2.1	ng	47694	3	14.563	451241	20.0
n-Hexadecanoic ...	18.168	26.7	ng	706540	4	17.315	530128	20.0
Octadecanoic acid	19.445	9.1	ng	306831	5	21.497	676419	20.0
E-15-Heptadecenal	21.162	6.3	ng	212493	5	21.497	676419	20.0