

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
 Data File : BF132009.D
 Acq On : 10 Jan 2023 22:05
 Operator : CG\JU
 Sample : 01076-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BU-03-010923

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_F\Methods\8270-BF010923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132009.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	487	492	509	rVB	465651	596898	6.30%	2.092%
2	5.399	559	563	584	rVB	1491196	1439334	15.19%	5.044%
3	6.428	734	738	749	rBV	1433812	1459001	15.39%	5.113%
4	6.781	795	798	802	rVB	494695	390269	4.12%	1.368%
5	7.357	891	896	899	rBV	966138	955392	10.08%	3.348%
6	8.075	1014	1018	1021	rVB	498202	444476	4.69%	1.558%
7	9.151	1196	1201	1204	rBV	1786971	1536954	16.22%	5.386%
8	9.834	1313	1317	1320	rVB	604651	464260	4.90%	1.627%
9	10.628	1448	1452	1455	rBV	894442	743074	7.84%	2.604%
10	11.328	1567	1571	1573	rBV	475737	437129	4.61%	1.532%
11	11.722	1634	1638	1641	rBV	3141713	2490198	26.28%	8.726%
12	12.422	1751	1757	1759	rBV	7071389	9477144	100.00%	33.210%
13	12.445	1759	1761	1766	rVV	5376582	4750685	50.13%	16.648%
14	12.516	1770	1773	1776	rVV	1293362	1036505	10.94%	3.632%
15	12.545	1776	1778	1782	rVB	204531	162098	1.71%	0.568%
16	12.775	1815	1817	1826	rVB	177165	153779	1.62%	0.539%
17	12.922	1838	1842	1845	rBV	1413025	1166888	12.31%	4.089%
18	13.816	1991	1994	2002	rVB2	102156	128453	1.36%	0.450%
19	13.974	2017	2021	2024	rBV2	400648	419983	4.43%	1.472%
20	15.445	2267	2271	2275	rBV	227278	284070	3.00%	0.995%

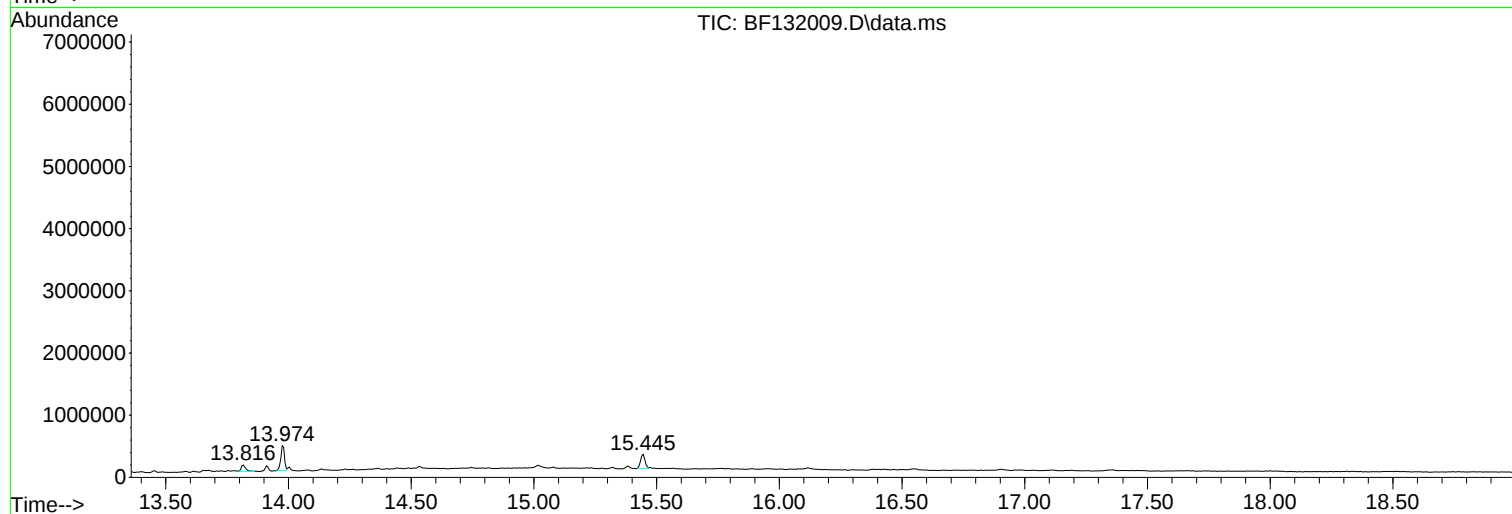
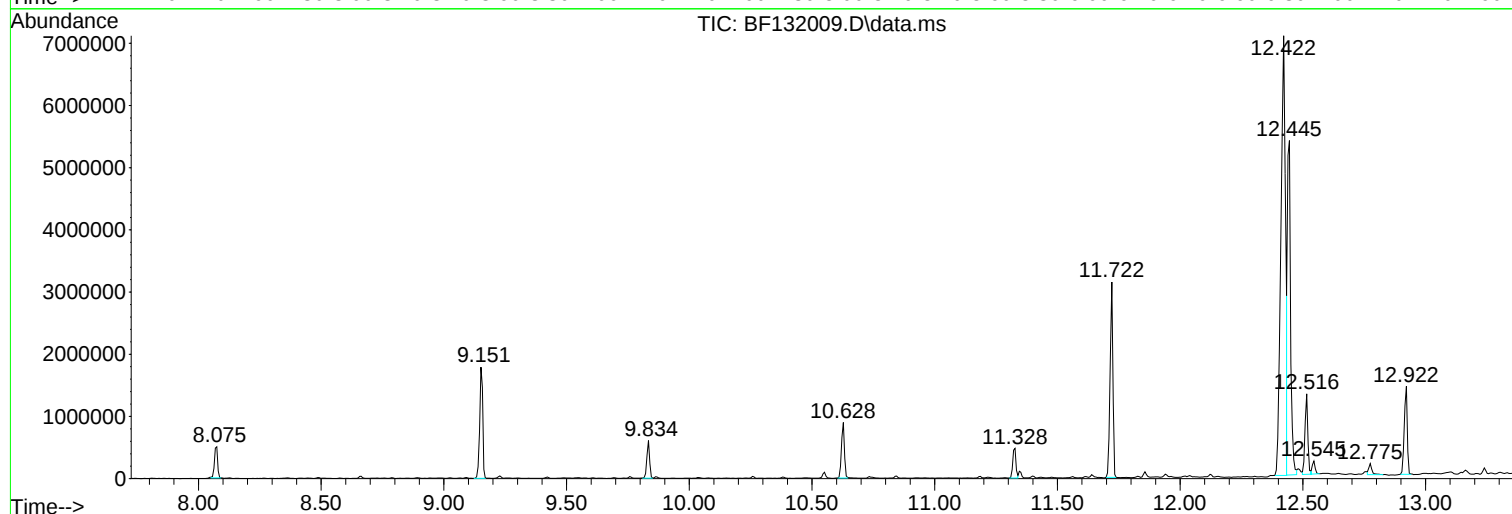
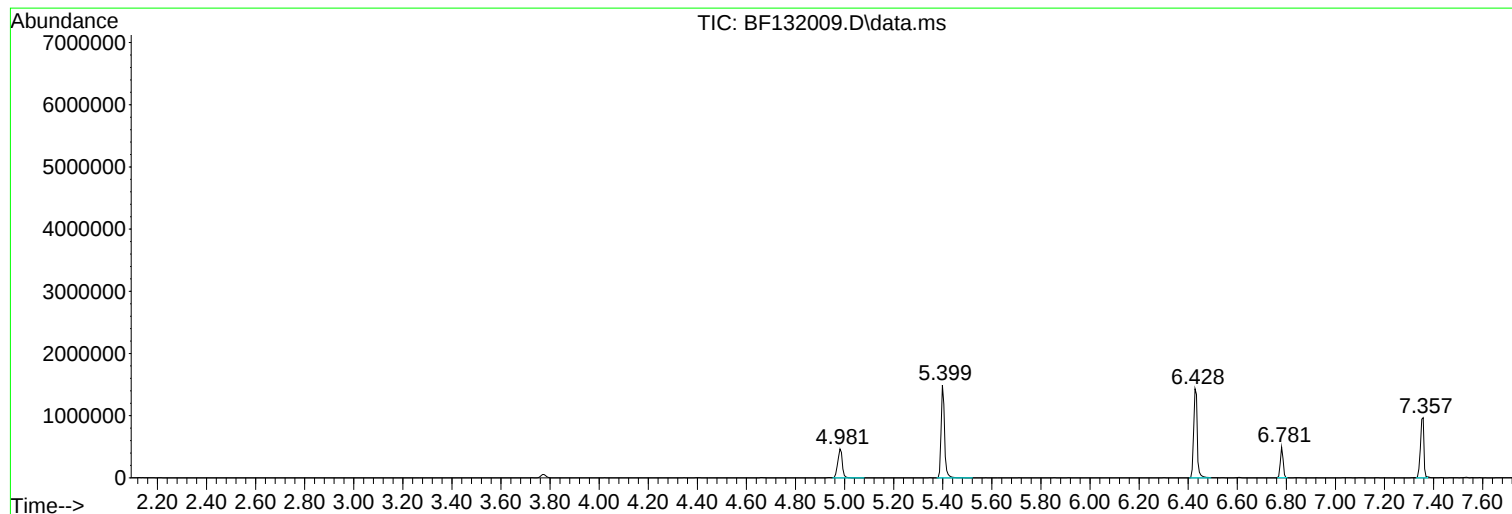
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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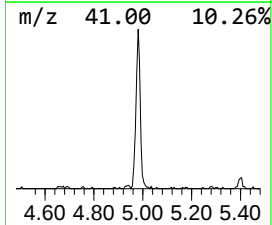
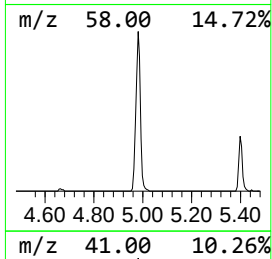
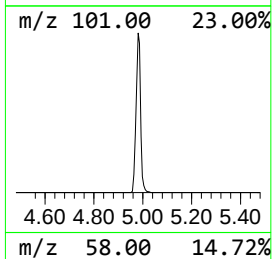
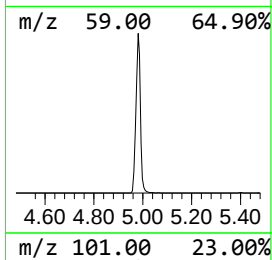
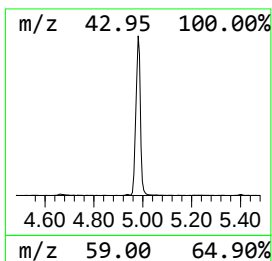
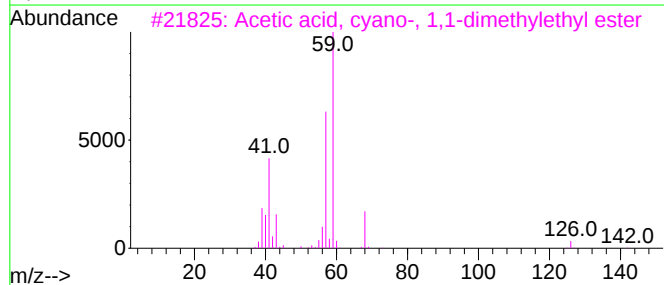
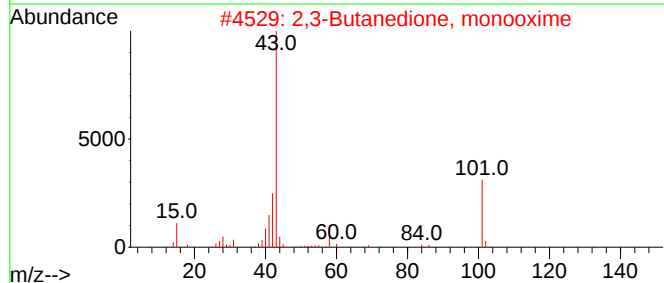
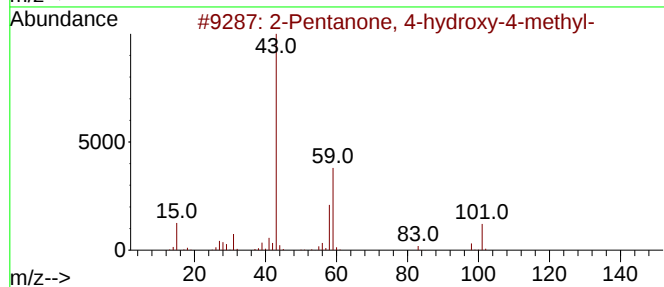
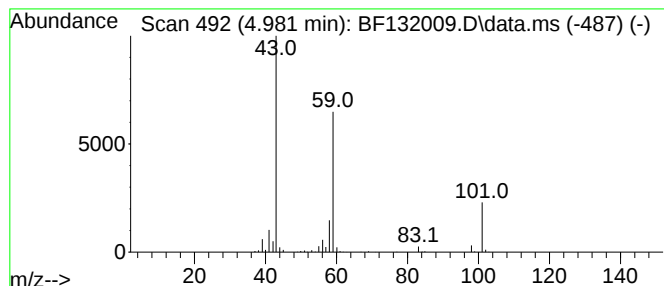
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	30.59 ng	596898	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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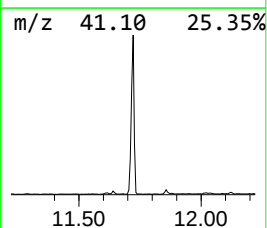
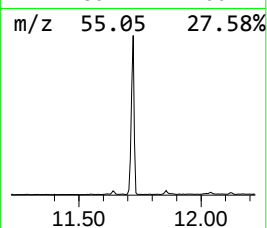
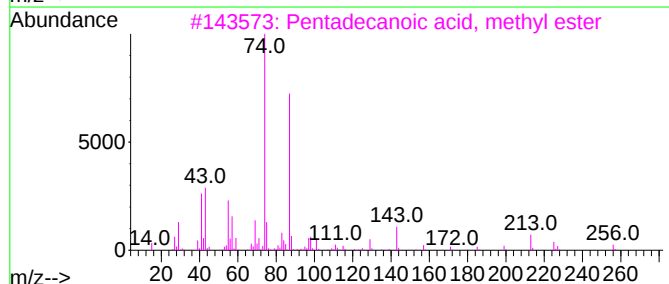
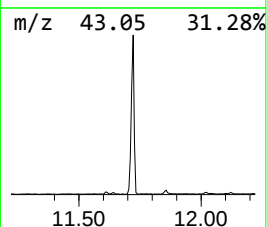
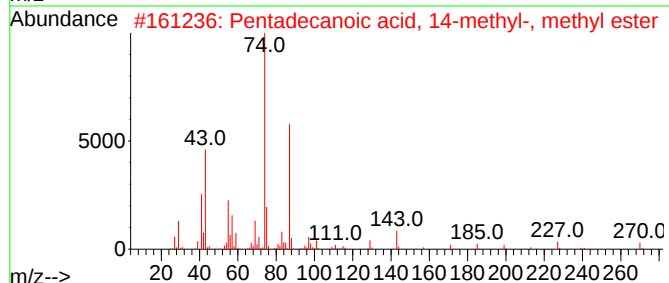
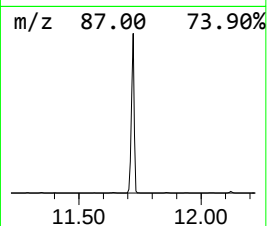
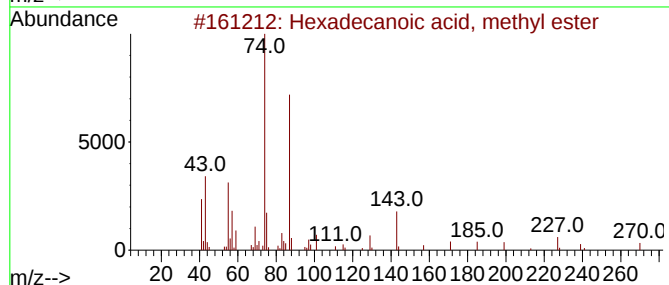
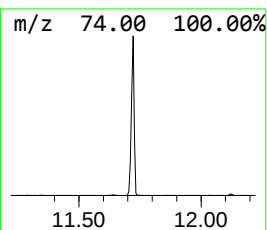
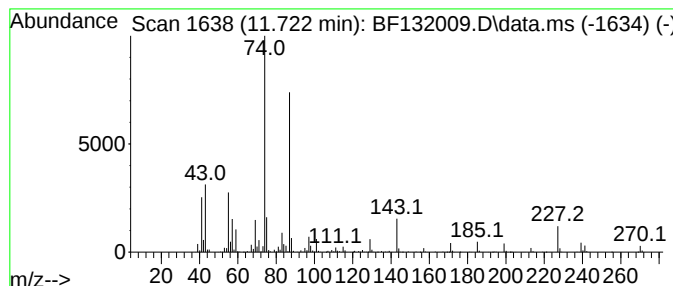
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.722	113.93 ng	2490200	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	92
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	83
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	83



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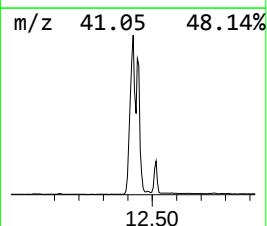
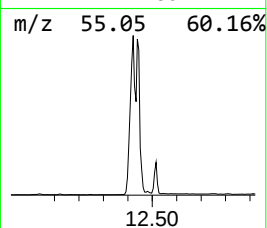
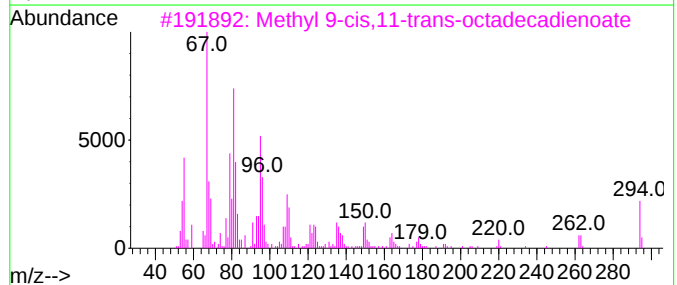
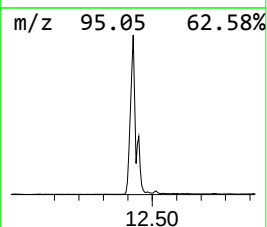
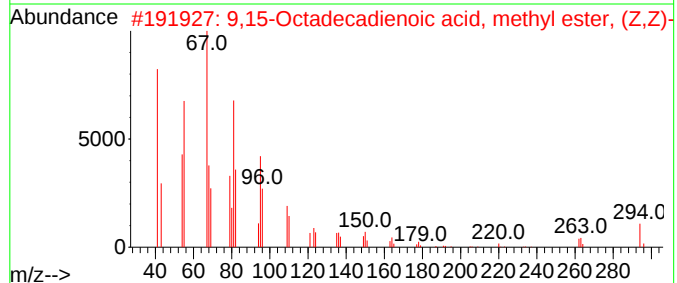
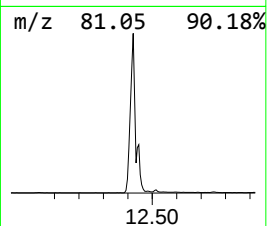
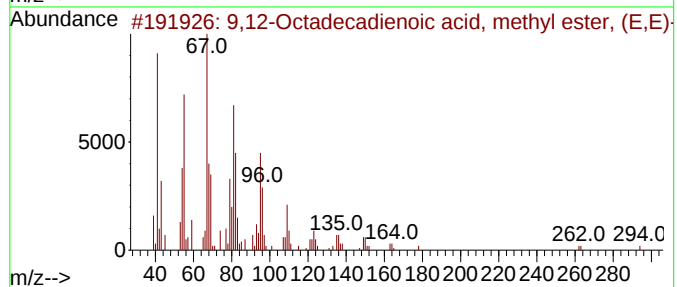
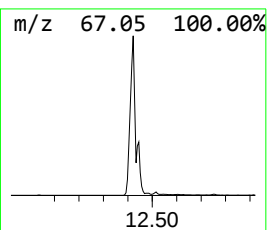
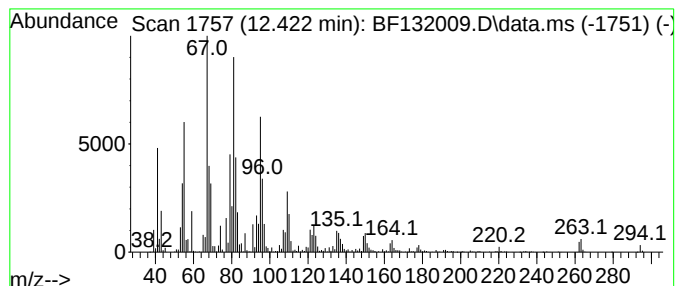
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Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.422	433.61 ng	9477140	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
2			9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	97
3			Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	96
4			11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	96
5			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95



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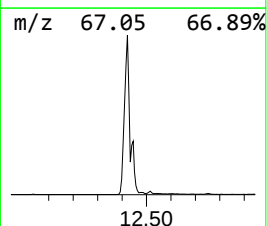
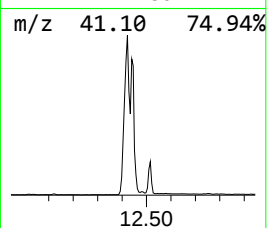
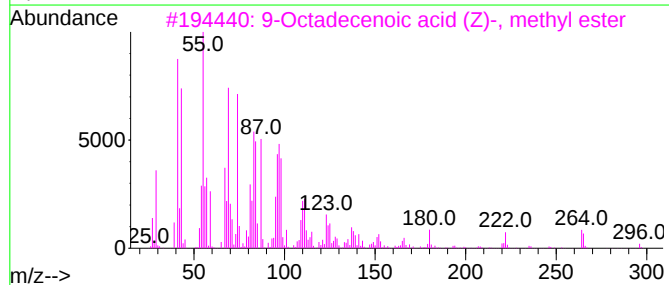
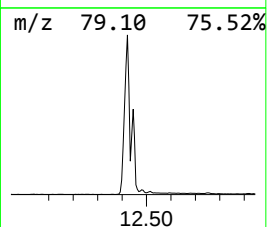
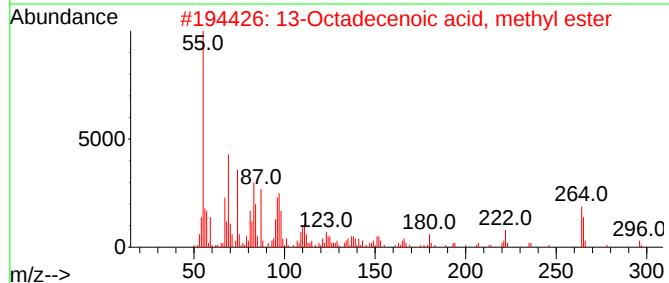
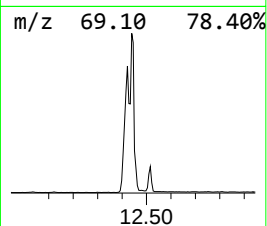
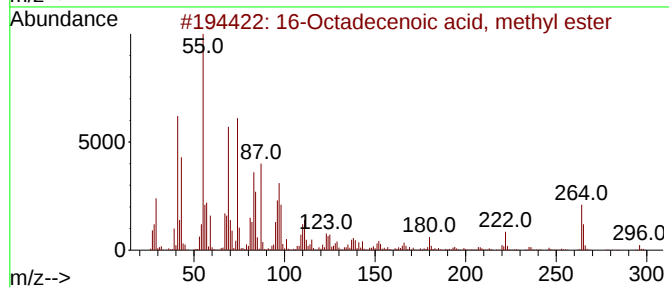
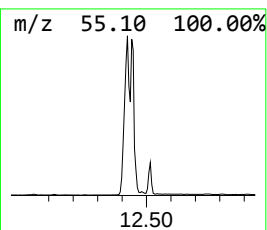
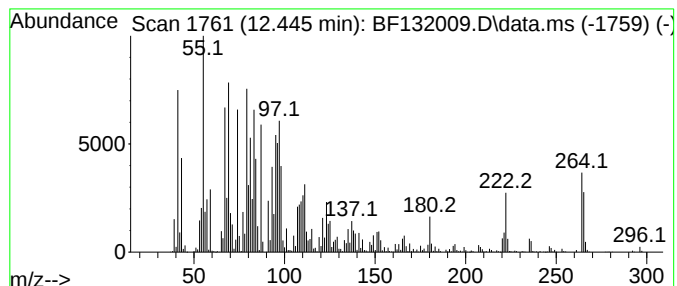
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Peak Number 4 16-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.445	217.36 ng	4750690	Phenanthrene-d10	11.328	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	97
4	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91



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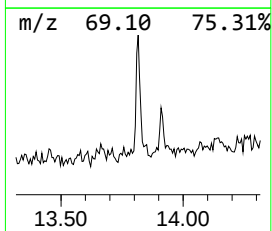
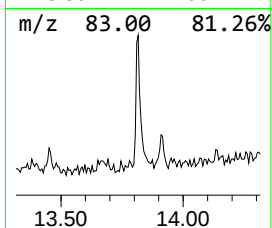
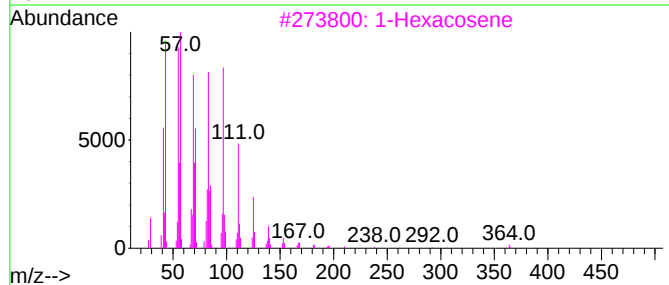
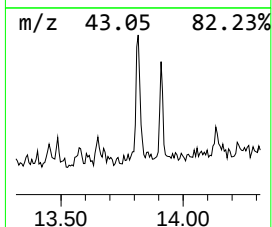
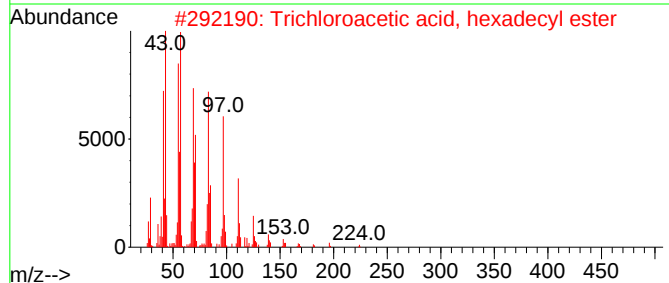
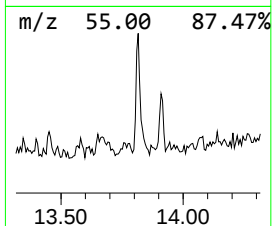
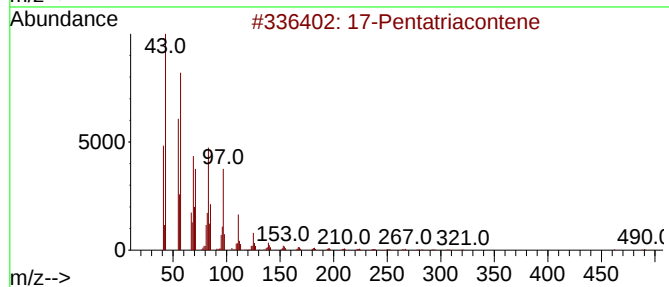
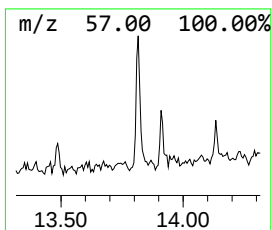
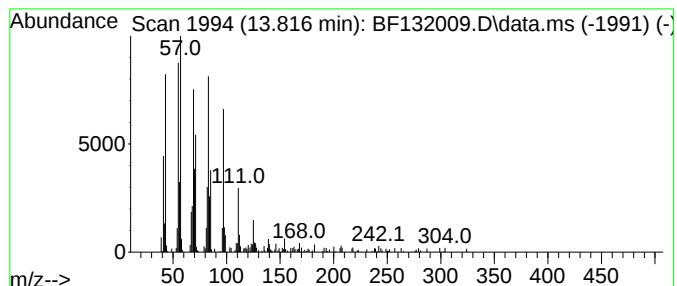
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Peak Number 5 17-Pentatriacontene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	6.12 ng	128453	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	91
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
3			1-Hexacosene	364	C26H52	018835-33-1	81
4			Cyclododecane	168	C12H24	000294-62-2	78
5			Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.981	30.6	ng	596898	1	6.781	390269	20.0
Hexadecanoic ac...	11.722	113.9	ng	2490200	4	11.328	437129	20.0
9,12-Octadecadi...	12.422	433.6	ng	9477140	4	11.328	437129	20.0
16-Octadecenoic...	12.445	217.4	ng	4750690	4	11.328	437129	20.0
17-Pentatriacon...	13.816	6.1	ng	128453	5	13.974	419983	20.0