

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010824\
 Data File : BF136995.D
 Acq On : 08 Jan 2024 13:47
 Operator : CG\JU
 Sample : P1042-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-303-20240104

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136995.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	494	498	506	rBV	61162	72043	3.71%	0.718%
2	5.428	565	568	581	rBV	625595	613449	31.62%	6.110%
3	6.434	735	739	753	rBV	328329	350968	18.09%	3.496%
4	6.781	795	798	802	rBV	479208	378842	19.53%	3.773%
5	7.345	889	894	897	rBV	1048357	1021707	52.67%	10.177%
6	8.057	1011	1015	1019	rBV	573309	482405	24.87%	4.805%
7	9.139	1193	1199	1202	rBV	2175404	1939780	100.00%	19.321%
8	9.816	1310	1314	1318	rBV	623889	523781	27.00%	5.217%
9	10.616	1445	1450	1464	rBV	1146578	1131864	58.35%	11.274%
10	11.310	1564	1568	1571	rBV	645676	525004	27.07%	5.229%
11	11.839	1653	1658	1663	rBV	78710	85510	4.41%	0.852%
12	12.551	1774	1779	1788	rBV	36424	56942	2.94%	0.567%
13	12.633	1789	1793	1805	rVB2	46892	68148	3.51%	0.679%
14	12.780	1811	1818	1824	rVB6	10593	25491	1.31%	0.254%
15	12.910	1835	1840	1843	rBV	1872085	1781661	91.85%	17.746%
16	13.621	1954	1961	1967	rBV3	18507	36265	1.87%	0.361%
17	13.968	2016	2020	2029	rVB	473122	431604	22.25%	4.299%
18	14.251	2061	2068	2072	rBV2	22097	41050	2.12%	0.409%
19	14.780	2154	2158	2162	rBV3	18402	29203	1.51%	0.291%
20	15.457	2267	2273	2282	rBV	318735	444127	22.90%	4.424%

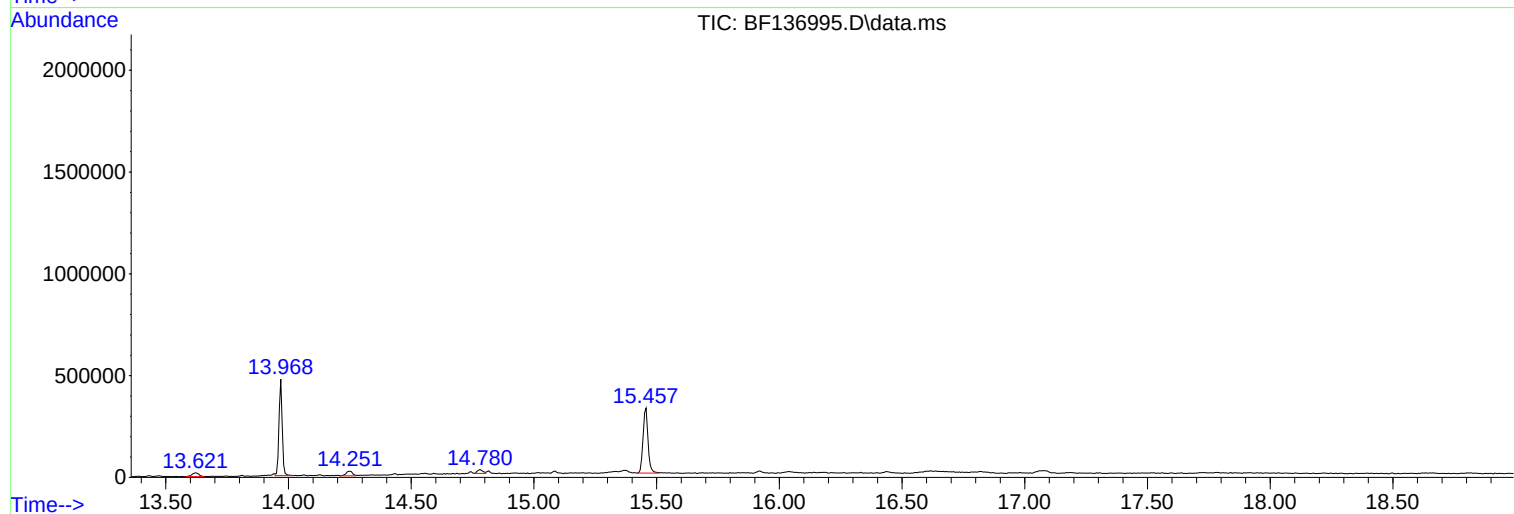
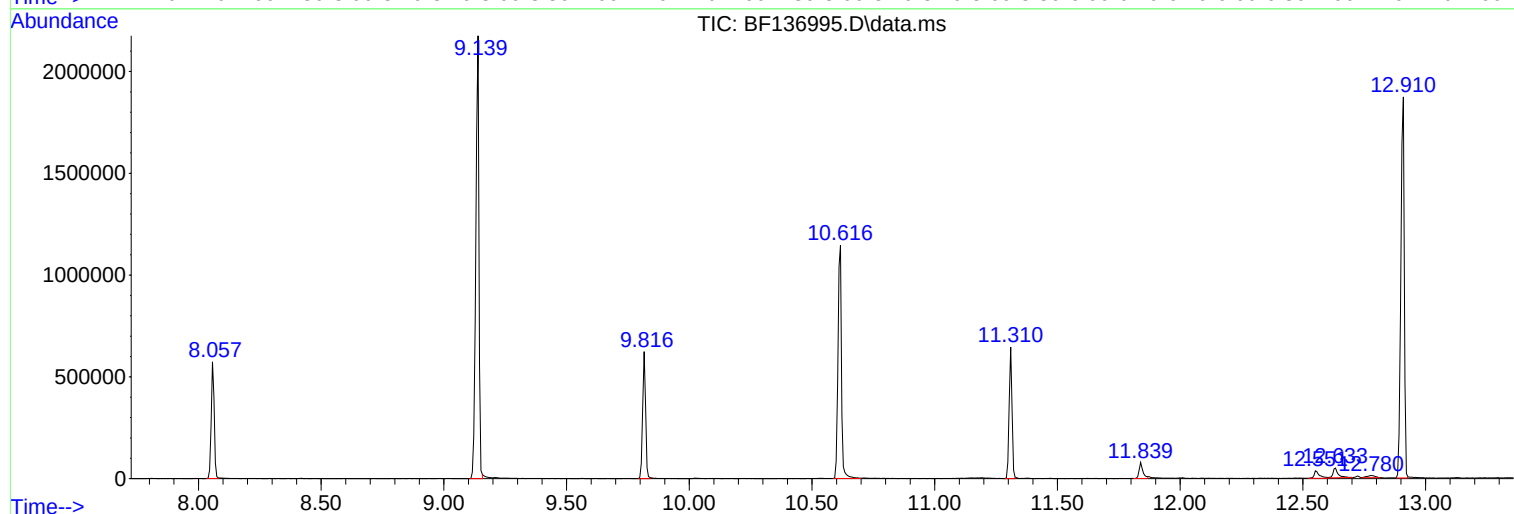
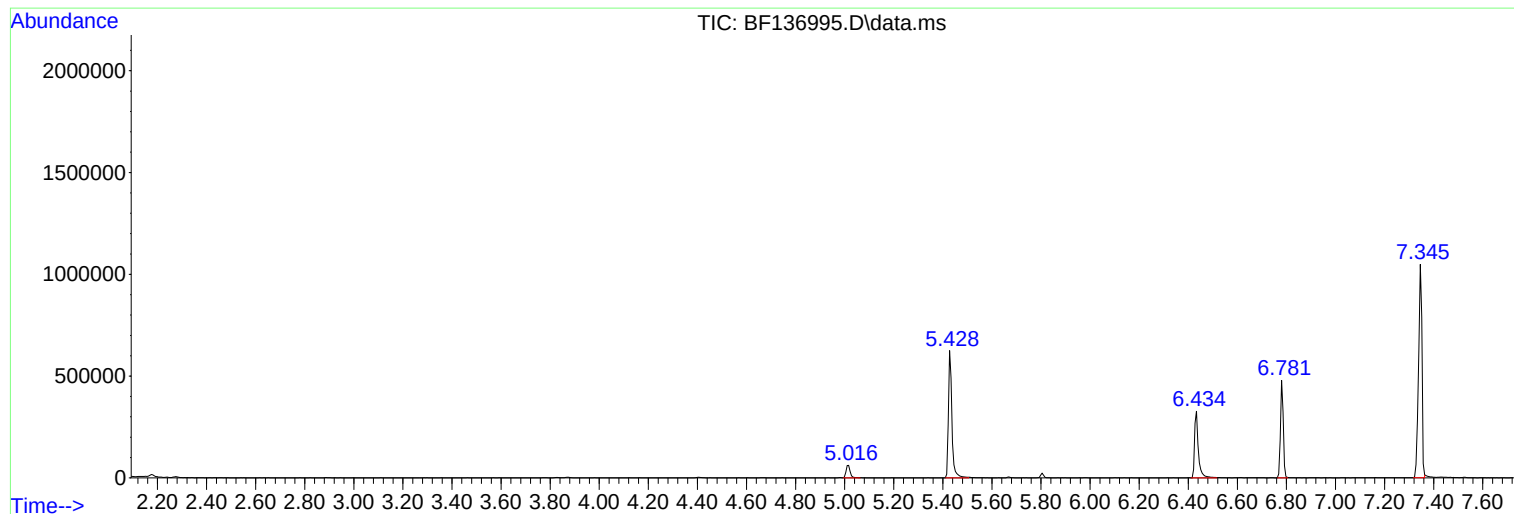
Sum of corrected areas: 10039844

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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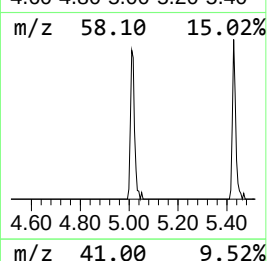
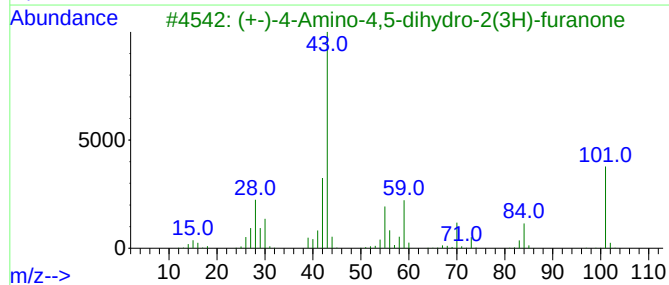
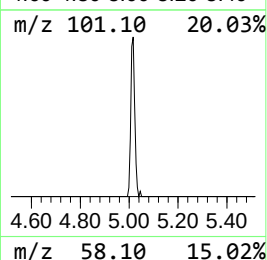
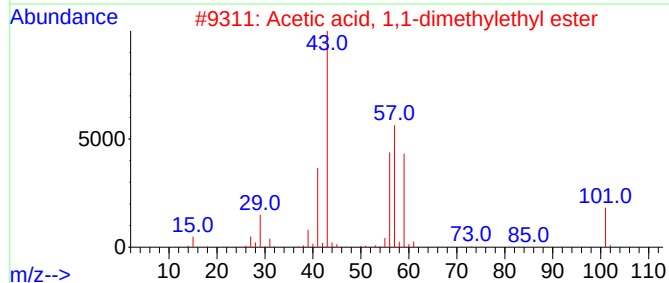
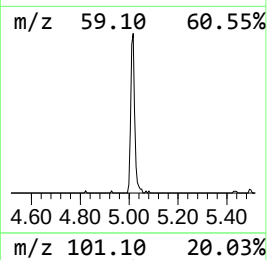
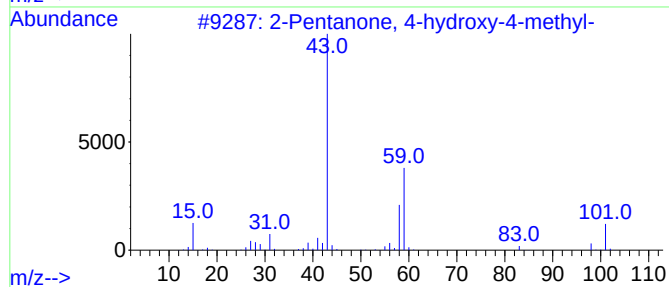
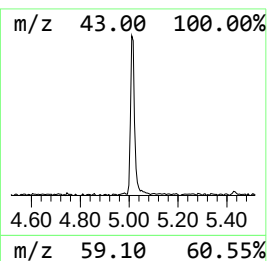
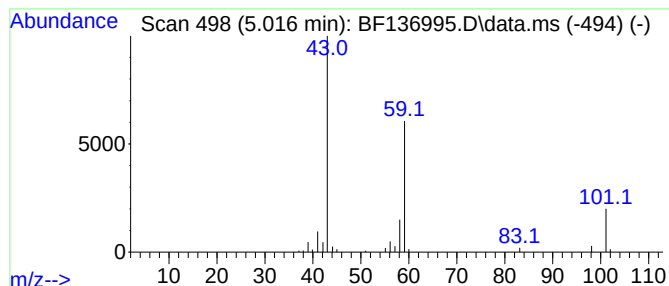
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	3.80 ng	72043	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	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		
4	Butane	58	C4H10	000106-97-8	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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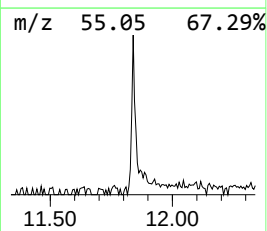
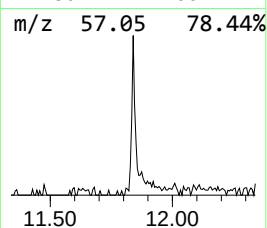
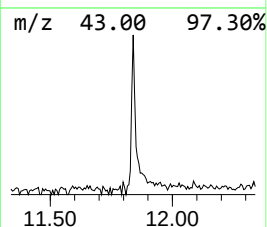
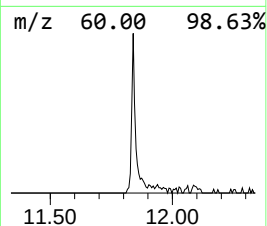
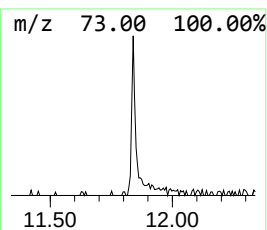
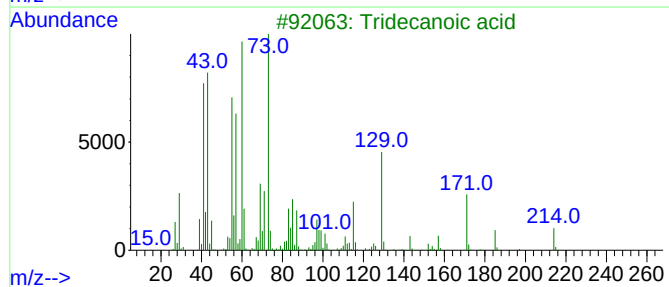
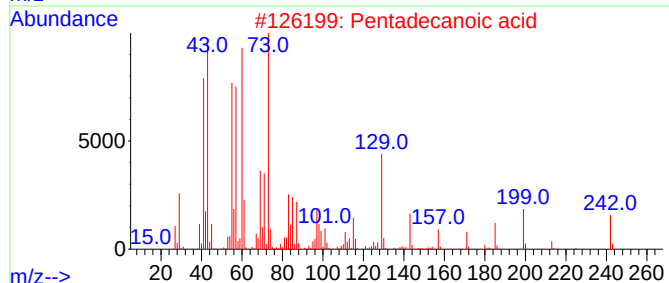
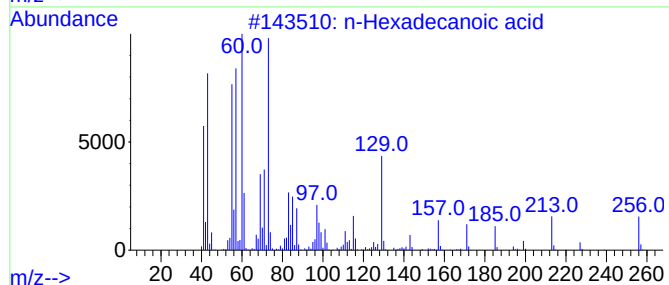
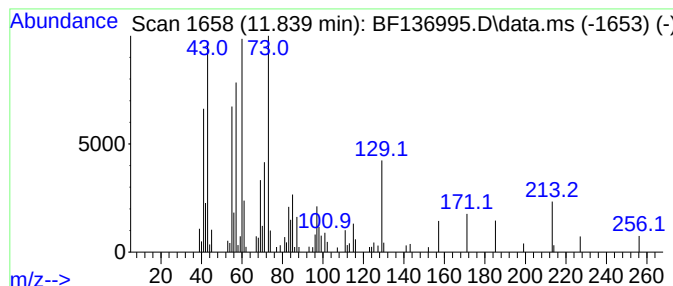
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	3.26 ng	85510	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3			Tridecanoic acid	214	C13H26O2	000638-53-9	30
4			Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25
5			Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	18



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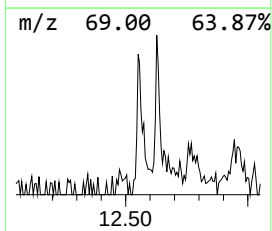
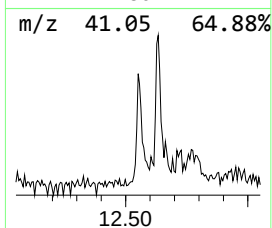
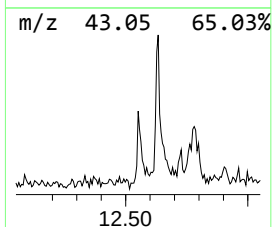
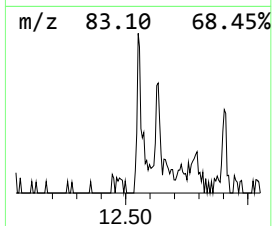
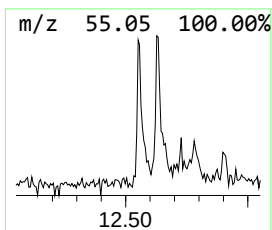
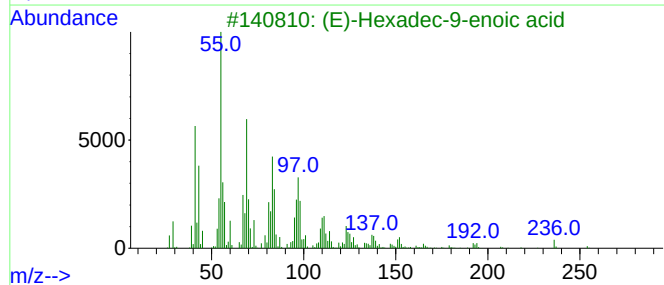
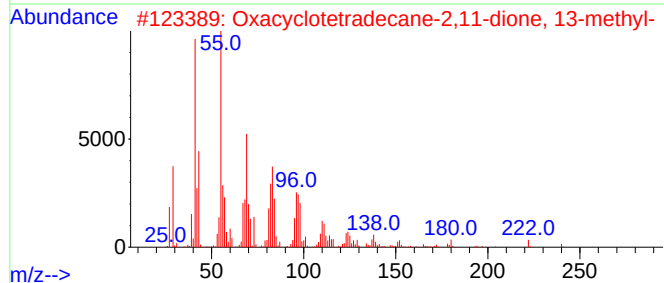
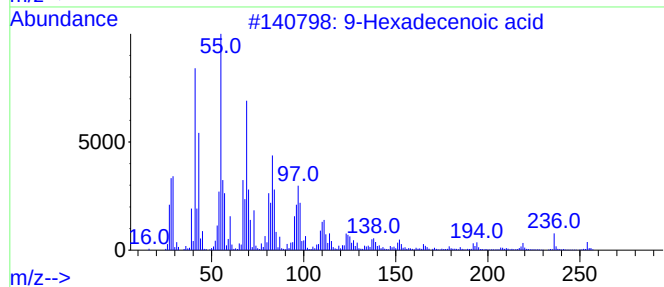
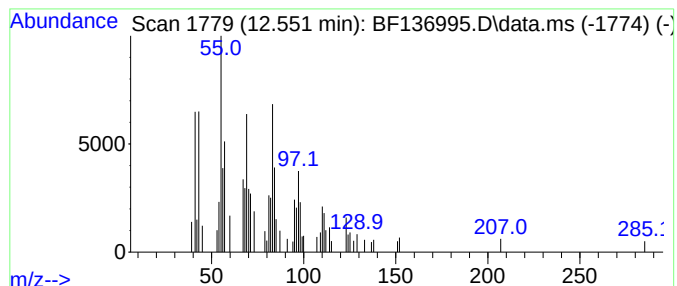
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 9-Hexadecenoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.551	2.17 ng	56942	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	87		
2	Oxacyclotetradecane-2,11-dione, ...	240	C14H24O3	074685-36-2	74		
3	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	74		
4	cis-Vaccenic acid	282	C18H34O2	000506-17-2	68		
5	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	68		



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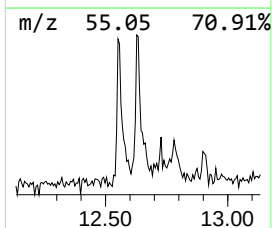
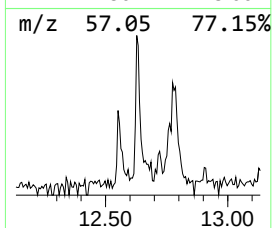
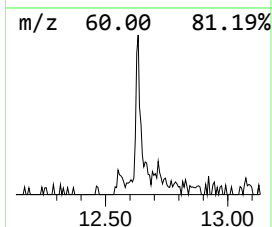
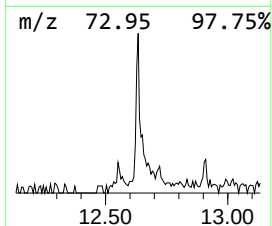
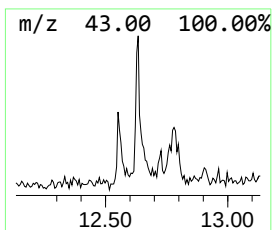
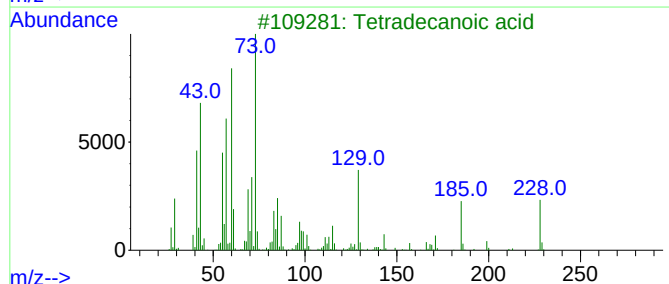
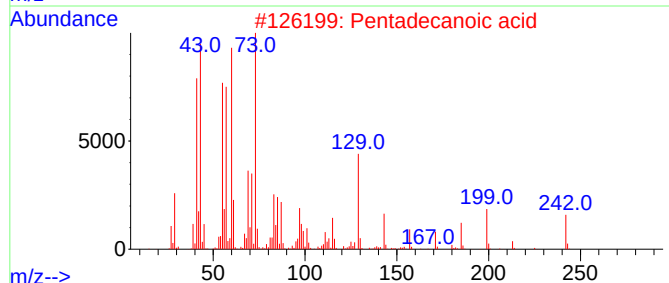
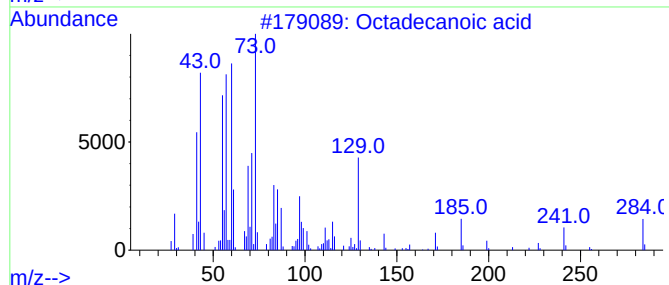
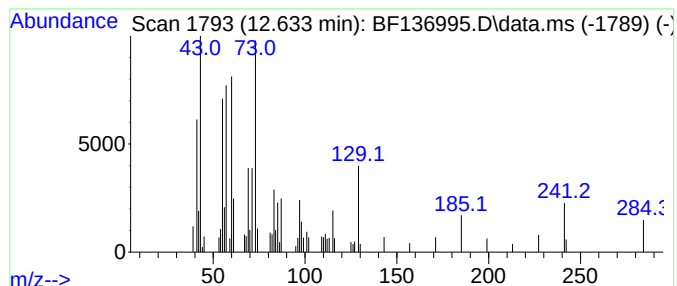
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	2.60 ng	68148	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			n-Decanoic acid	172	C10H20O2	000334-48-5	53
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.016	3.8	ng	72043	1	6.781	378842	20.0
n-Hexadecanoic ...	11.839	3.3	ng	85510	4	11.310	525004	20.0
9-Hexadecenoic ...	12.551	2.2	ng	56942	4	11.310	525004	20.0
Octadecanoic acid	12.633	2.6	ng	68148	4	11.310	525004	20.0