

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080122\
 Data File : BF129474.D
 Acq On : 01 Aug 2022 15:30
 Operator : CG\JU
 Sample : N3977-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MS-TOTE-0729

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-BF072522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129474.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.099	475	478	486	rVB	56878	66721	1.25%	0.251%
2	5.510	544	548	562	rBV	2007770	1801221	33.61%	6.778%
3	6.522	716	720	729	rBV	1219748	1081747	20.19%	4.071%
4	6.875	776	780	783	rBV	1226267	1031467	19.25%	3.881%
5	7.440	871	876	879	rBV	3255687	3063344	57.16%	11.527%
6	8.157	994	998	1001	rBV	1677040	1347100	25.14%	5.069%
7	8.681	1083	1087	1089	rBV	67193	76922	1.44%	0.289%
8	8.916	1125	1127	1130	rVB	86016	64276	1.20%	0.242%
9	9.234	1176	1181	1184	rBV	6005181	5358816	100.00%	20.165%
10	9.475	1220	1222	1225	rBV	70061	66241	1.24%	0.249%
11	9.587	1236	1241	1245	rBV6	70024	133647	2.49%	0.503%
12	9.910	1293	1296	1302	rVB	1544246	1458177	27.21%	5.487%
13	10.134	1331	1334	1338	rBV	248124	249152	4.65%	0.938%
14	10.710	1427	1432	1435	rBV	3182256	3003564	56.05%	11.302%
15	11.081	1492	1495	1499	rVB4	118124	137012	2.56%	0.516%
16	11.404	1547	1550	1553	rVB	1469786	1162815	21.70%	4.376%
17	11.933	1637	1640	1650	rVB2	342255	402625	7.51%	1.515%
18	12.710	1770	1772	1778	rVB	129136	148276	2.77%	0.558%
19	12.986	1815	1819	1823	rBV	3795103	3687628	68.81%	13.877%
20	13.874	1968	1970	1981	rVB2	131289	172945	3.23%	0.651%
21	14.045	1996	1999	2003	rVB	1091278	938647	17.52%	3.532%
22	15.533	2247	2252	2261	rVB	857174	1122134	20.94%	4.223%

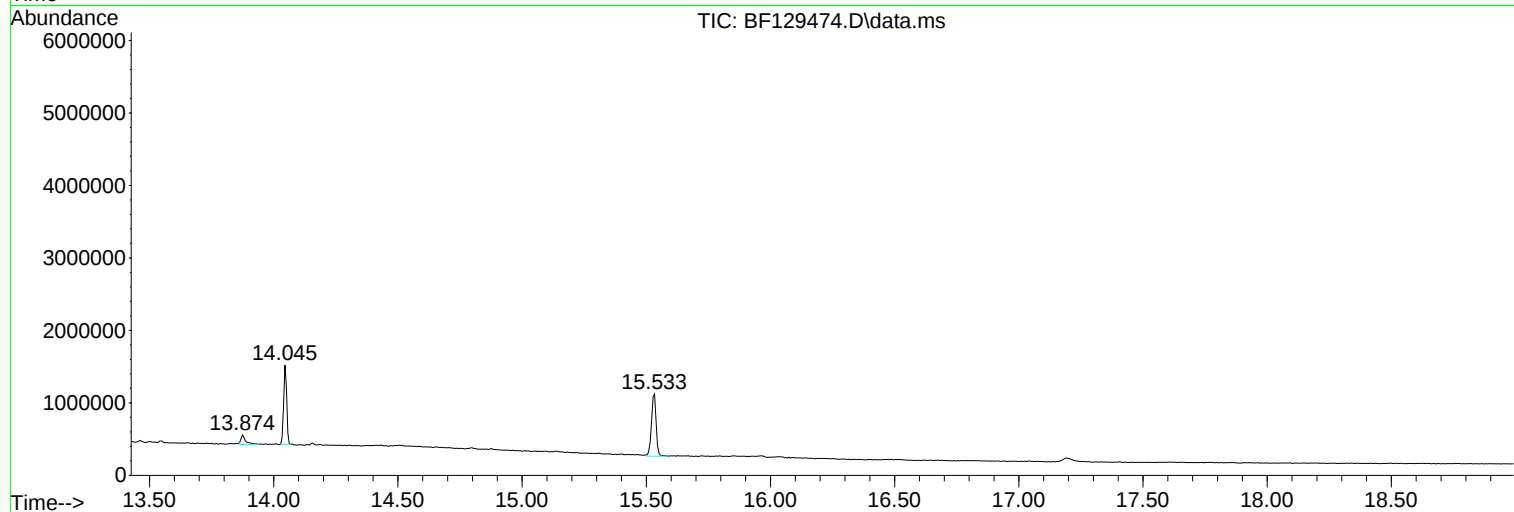
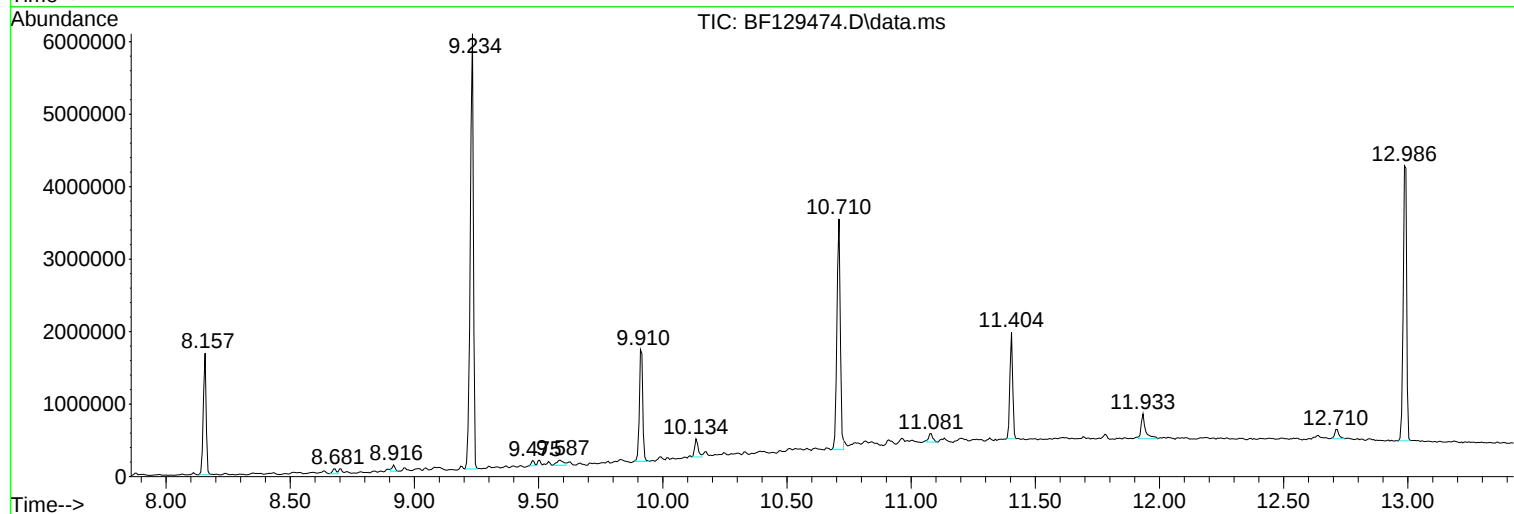
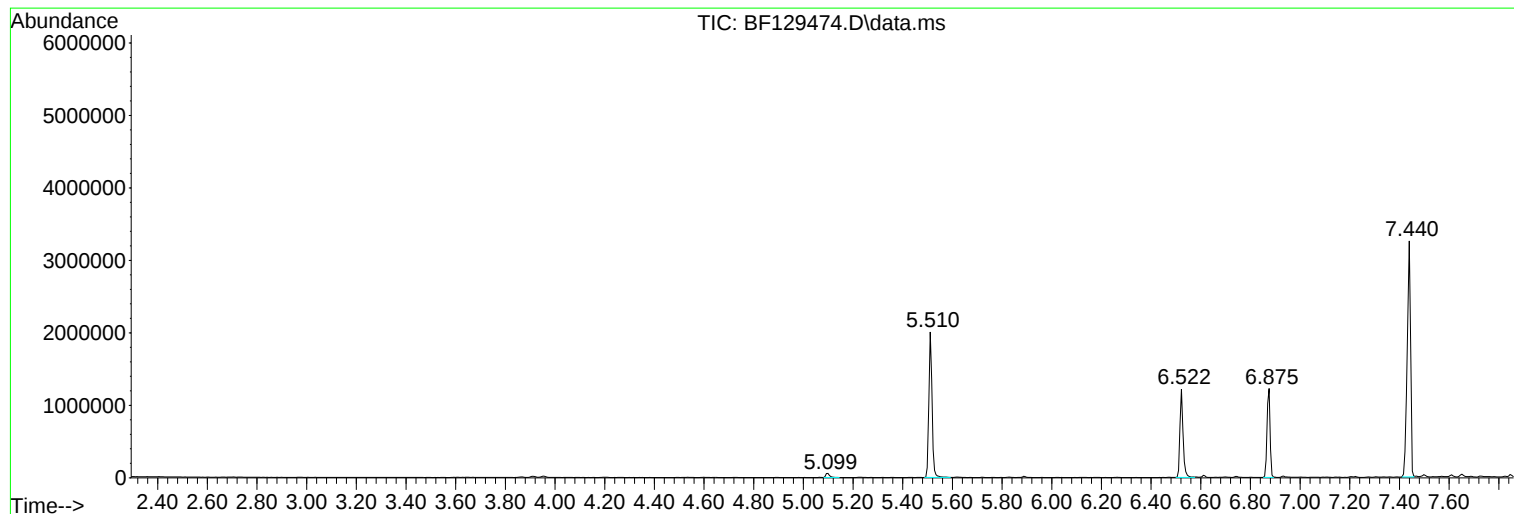
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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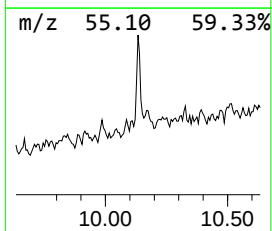
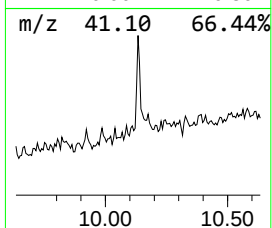
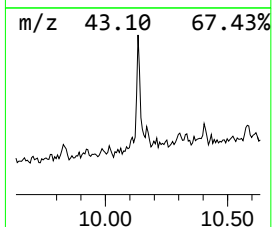
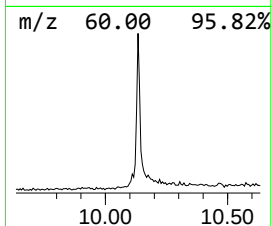
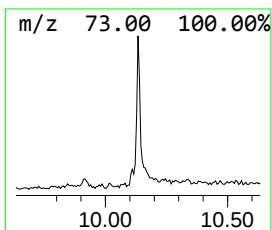
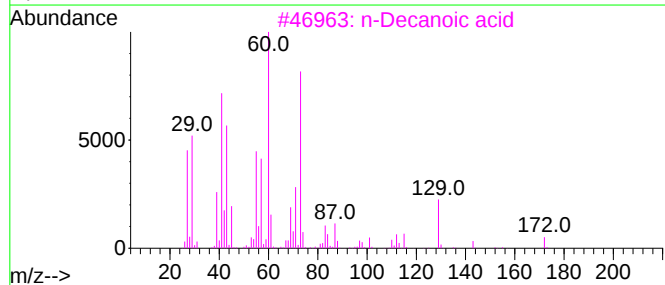
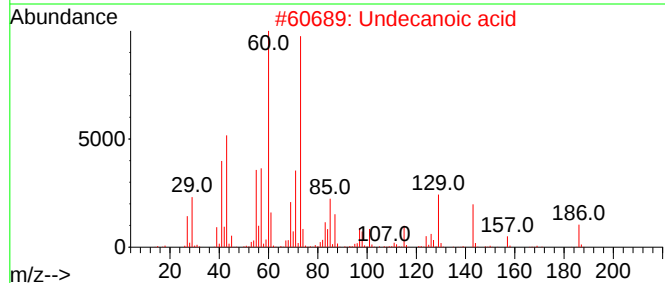
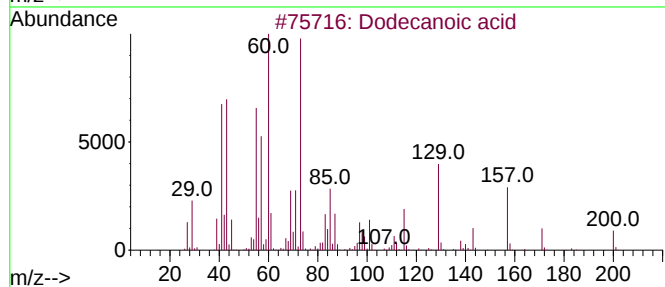
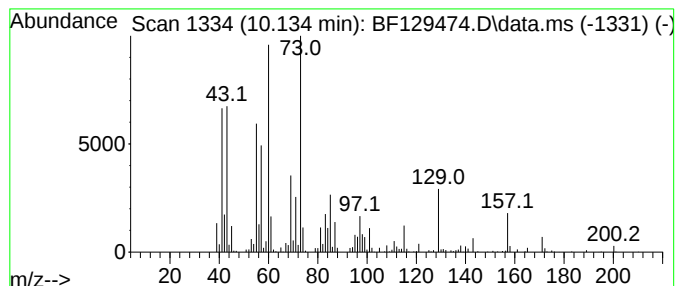
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.134	3.42 ng	249152	Acenaphthene-d10	9.910

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecanoic acid	200	C12H24O2	000143-07-7	98
2		Undecanoic acid	186	C11H22O2	000112-37-8	80
3		n-Decanoic acid	172	C10H20O2	000334-48-5	74
4		Nonanoic acid	158	C9H18O2	000112-05-0	58
5		Heptanoic acid	130	C7H14O2	000111-14-8	46



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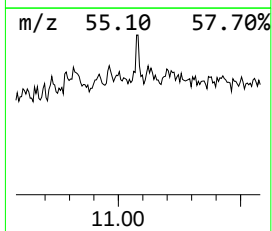
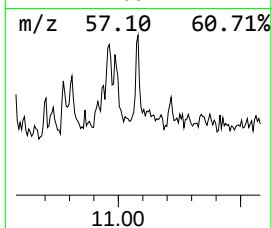
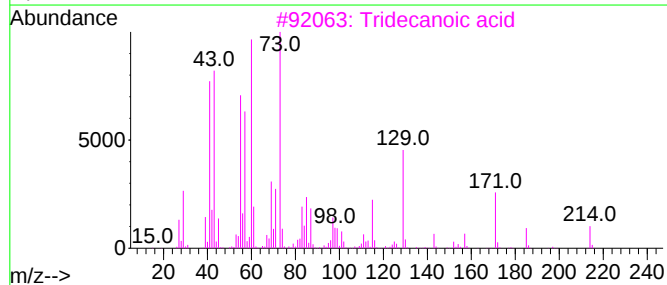
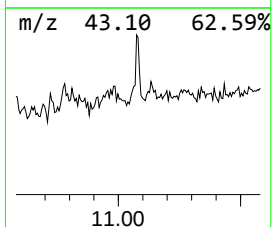
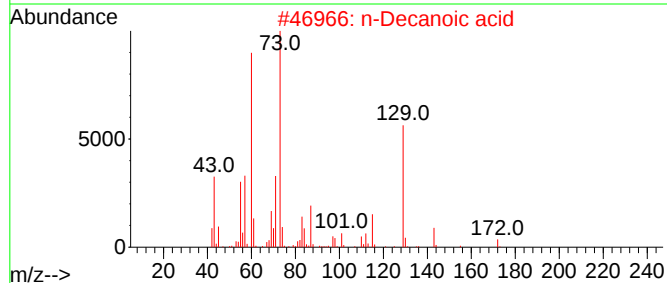
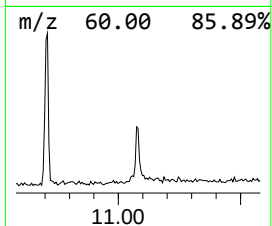
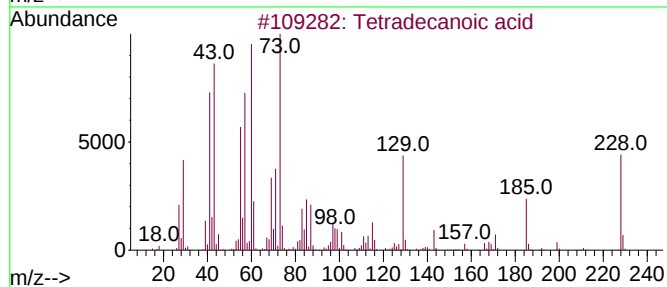
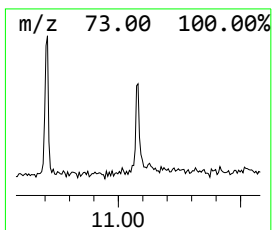
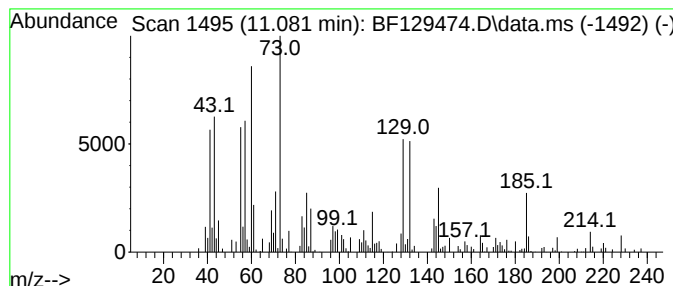
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.081	2.36 ng	137012	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
2			n-Decanoic acid	172	C10H20O2	000334-48-5	95
3			Tridecanoic acid	214	C13H26O2	000638-53-9	94
4			Dodecanoic acid	200	C12H24O2	000143-07-7	50
5			Undecanoic acid	186	C11H22O2	000112-37-8	46



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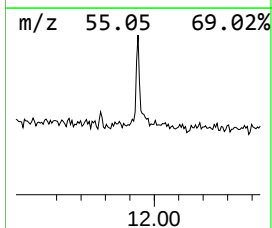
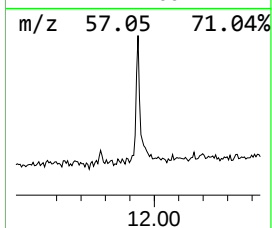
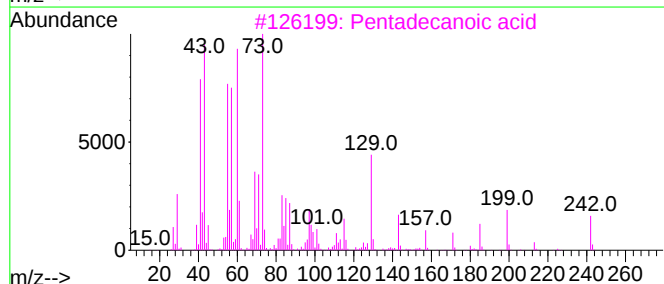
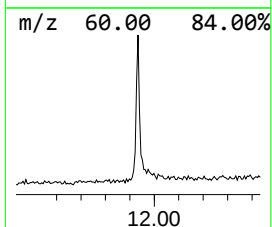
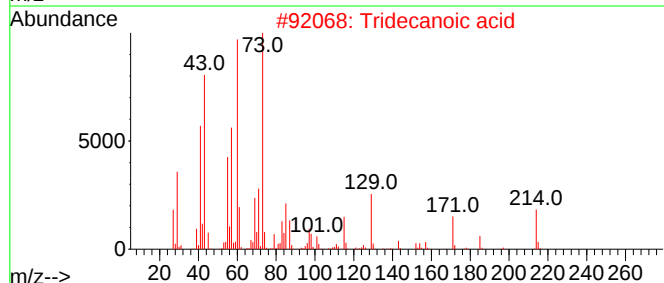
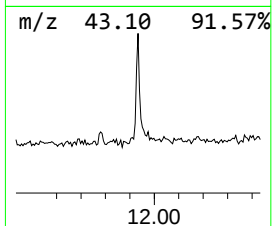
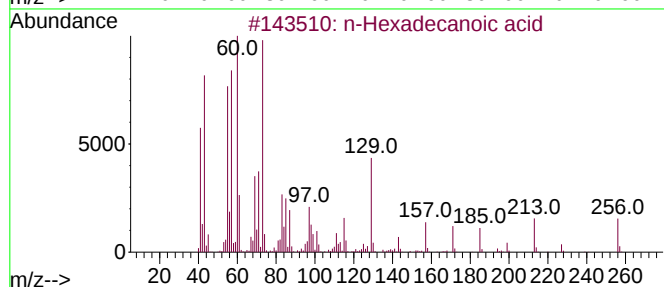
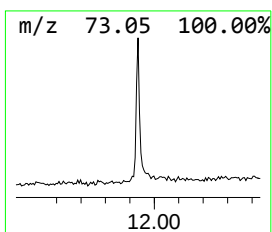
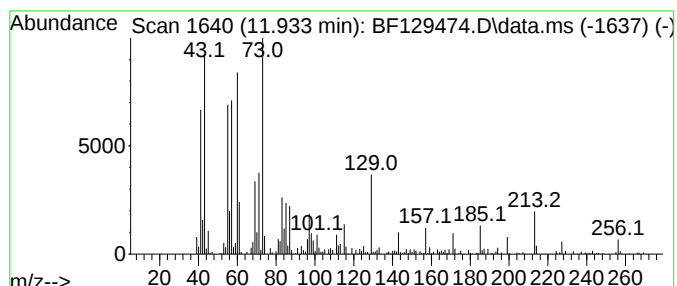
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	6.93 ng	402625	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



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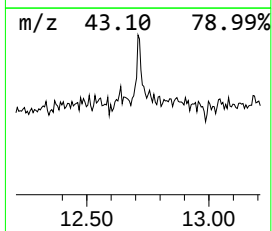
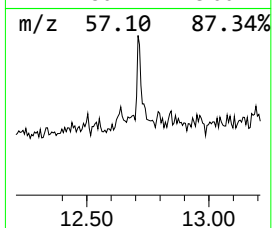
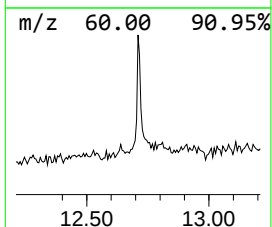
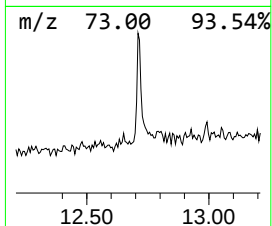
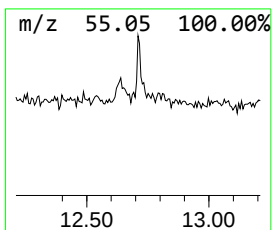
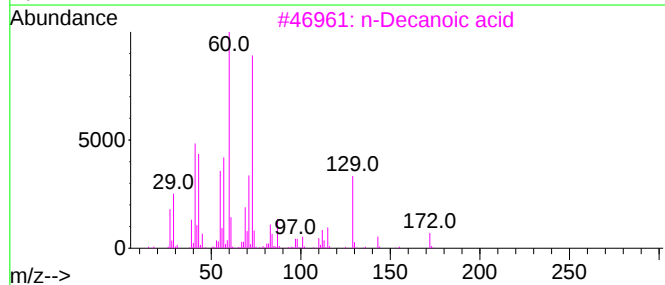
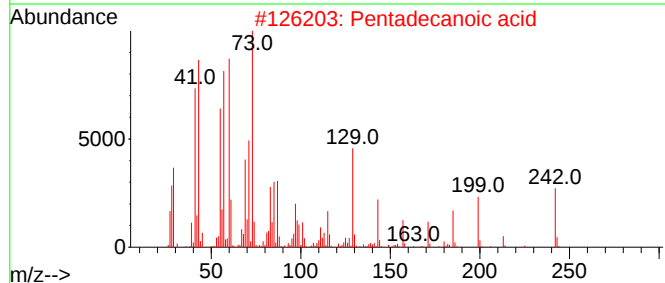
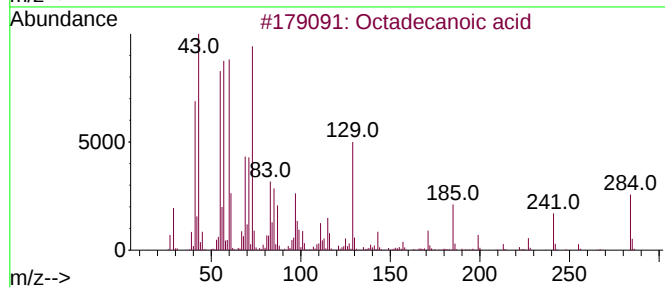
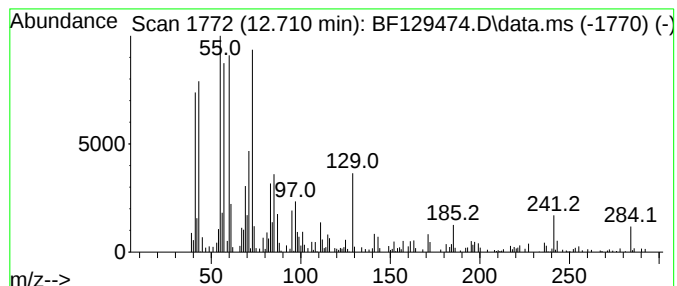
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	2.55 ng	148276	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			n-Decanoic acid	172	C10H20O2	000334-48-5	58
4			Tridecane	184	C13H28	000629-50-5	44
5			Oxalic acid, pentadecyl propyl e...	342	C20H38O4	1000309-26-8	35



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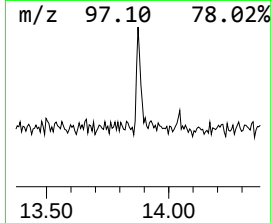
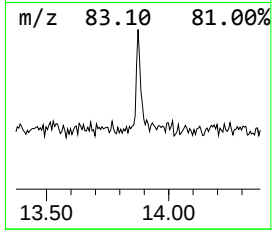
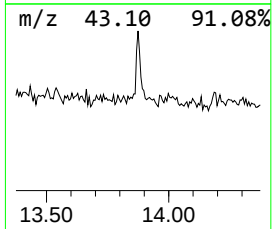
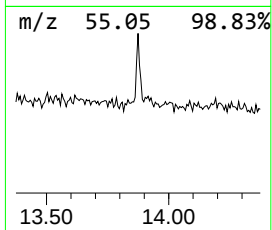
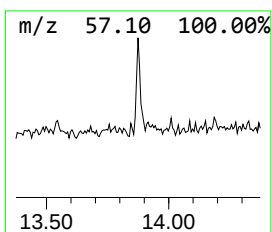
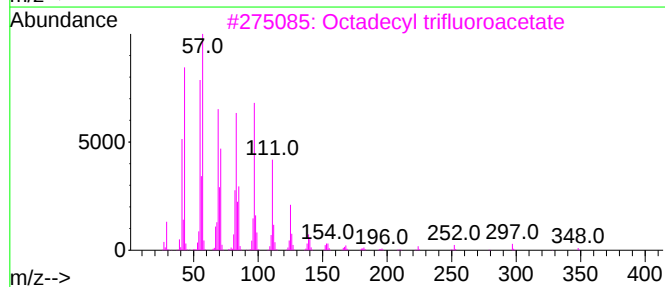
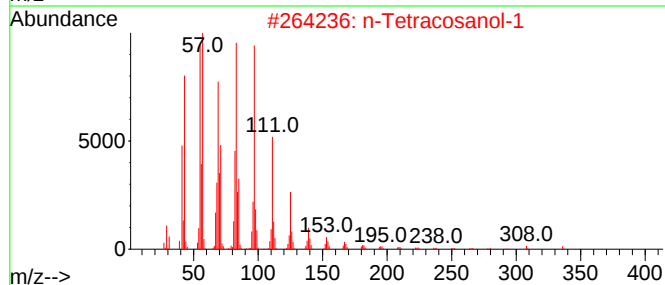
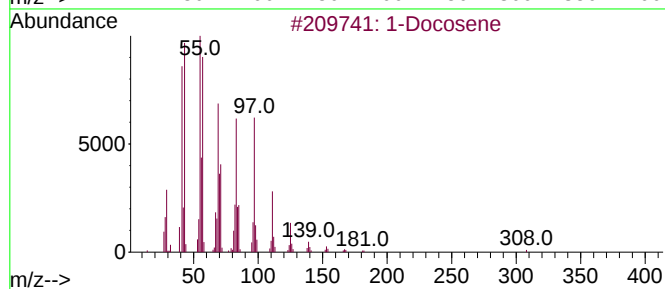
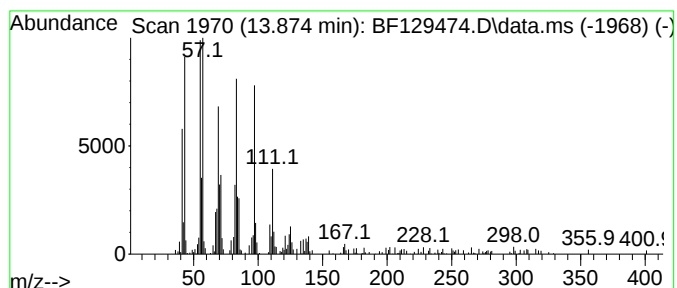
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Docosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	3.68 ng	172945	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	93
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87
4			17-Pentatriacontene	491	C35H70	006971-40-0	83
5			1-Tricosene	322	C23H46	018835-32-0	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dodecanoic acid	10.134	3.4	ng	249152	3	9.910	1458180	20.0
Tetradecanoic acid	11.081	2.4	ng	137012	4	11.404	1162820	20.0
n-Hexadecanoic ...	11.933	6.9	ng	402625	4	11.404	1162820	20.0
Octadecanoic acid	12.710	2.5	ng	148276	4	11.404	1162820	20.0
1-Docosene	13.874	3.7	ng	172945	5	14.045	938647	20.0