

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101923\
 Data File : BF135890.D
 Acq On : 19 Oct 2023 17:09
 Operator : CG\JU
 Sample : 04905-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LSS-B4-COMP-101323

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-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135890.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.963	485	489	508	rBV	451055	643892	34.81%	5.075%
2	5.381	556	560	585	rBV	1589739	1692932	91.52%	13.342%
3	5.757	621	624	630	rBV	22171	24499	1.32%	0.193%
4	6.393	728	732	749	rBV	1557423	1699285	91.86%	13.392%
5	6.593	764	766	774	rBV	14645	30720	1.66%	0.242%
6	6.734	787	790	798	rBV	351431	290266	15.69%	2.288%
7	7.304	883	887	905	rBV	1161531	1107790	59.88%	8.731%
8	8.016	1005	1008	1024	rVB	414113	389240	21.04%	3.068%
9	9.092	1187	1191	1194	rBV	2288209	1849873	100.00%	14.579%
10	9.210	1208	1211	1219	rVB	40579	39297	2.12%	0.310%
11	9.769	1303	1306	1319	rVB	466077	424207	22.93%	3.343%
12	10.569	1439	1442	1453	rBV	1244348	1192096	64.44%	9.395%
13	10.698	1461	1464	1471	rVB	17989	24403	1.32%	0.192%
14	11.269	1557	1561	1569	rBV	503866	426032	23.03%	3.358%
15	11.804	1649	1652	1664	rBV	258402	275962	14.92%	2.175%
16	12.592	1783	1786	1797	rBV	58219	80465	4.35%	0.634%
17	12.869	1828	1833	1836	rBV	1635497	1604291	86.72%	12.644%
18	13.804	1987	1992	2007	rVB5	31756	99485	5.38%	0.784%
19	13.933	2011	2014	2022	rBV	333842	327927	17.73%	2.584%
20	15.027	2197	2200	2207	rVB	25774	32282	1.75%	0.254%
21	15.410	2260	2265	2274	rBV	292504	398095	21.52%	3.137%
22	15.839	2333	2338	2344	rVB2	19280	35376	1.91%	0.279%

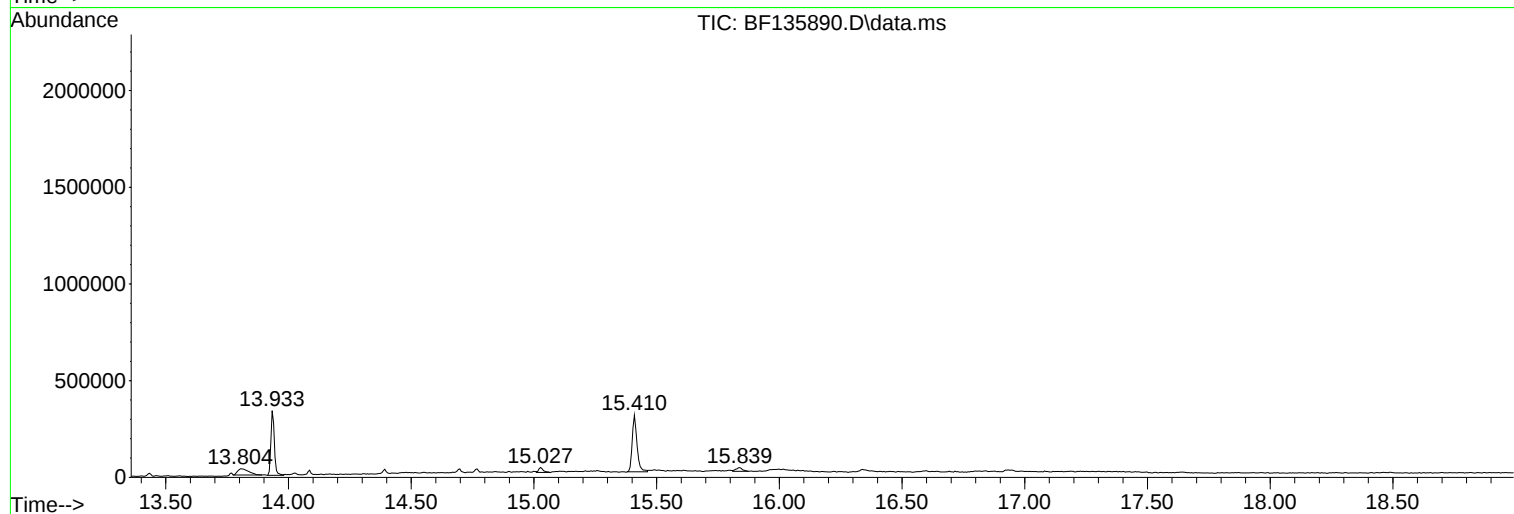
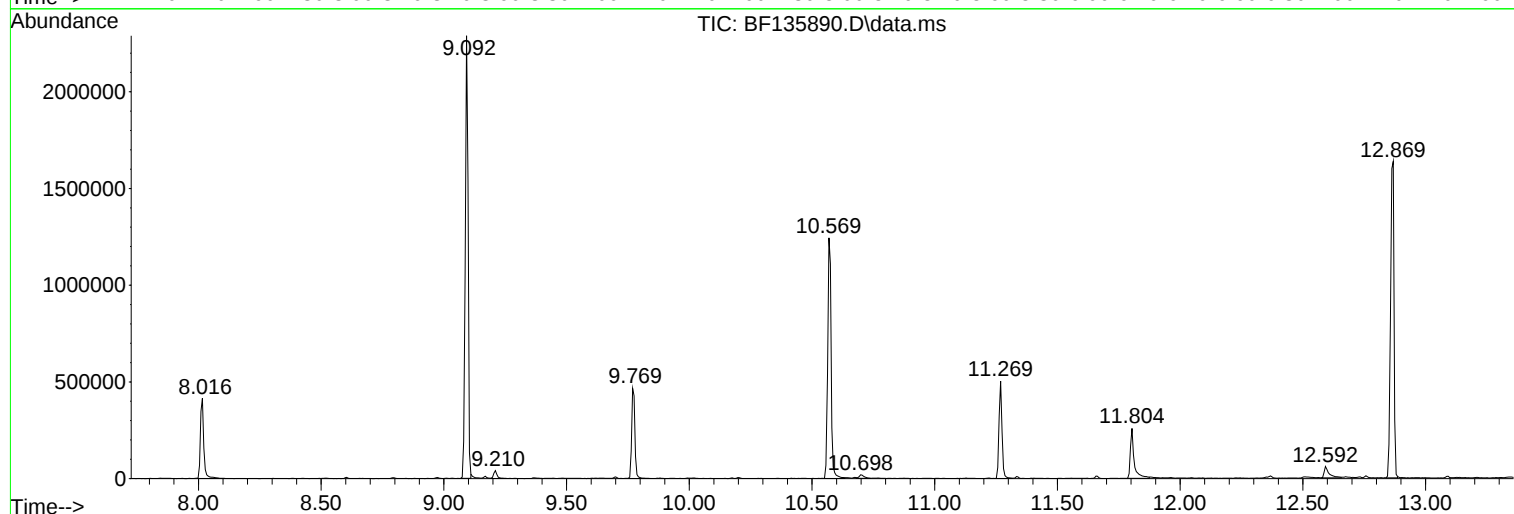
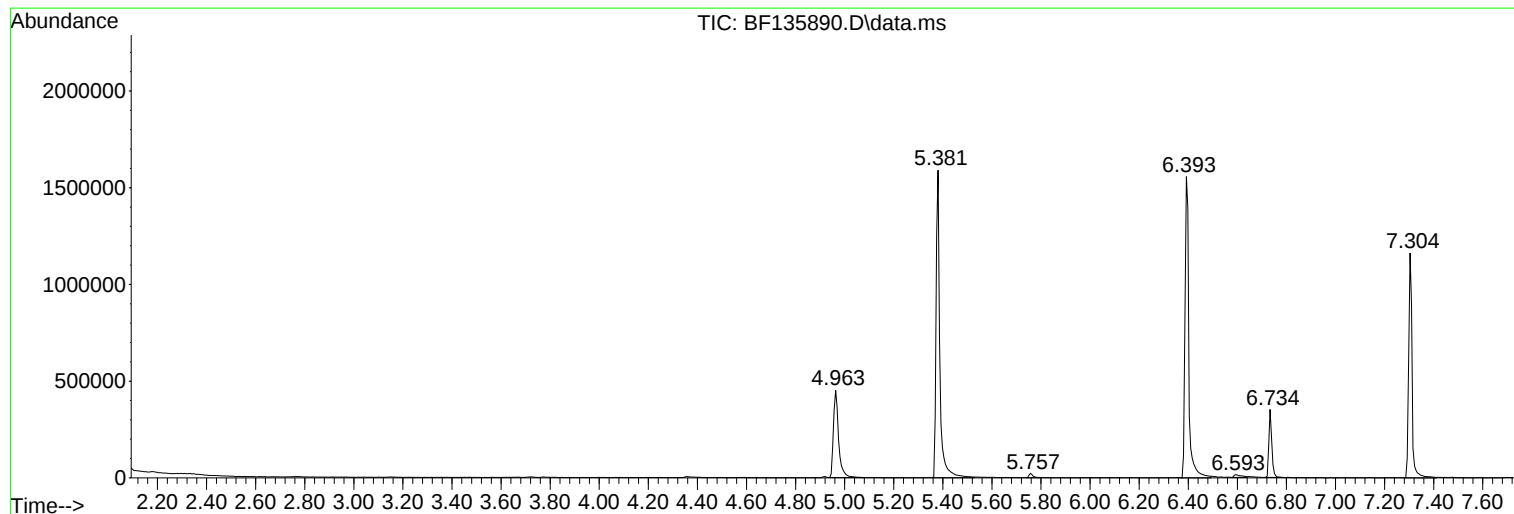
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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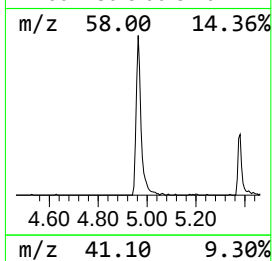
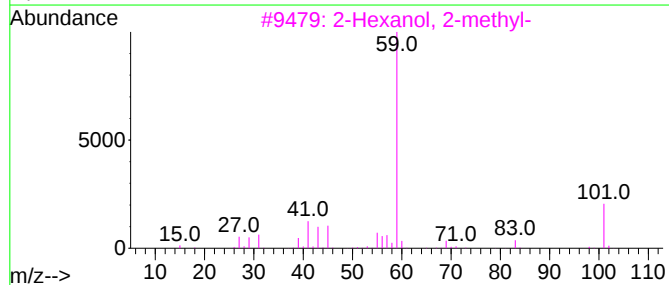
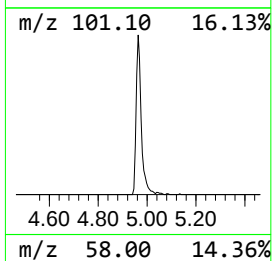
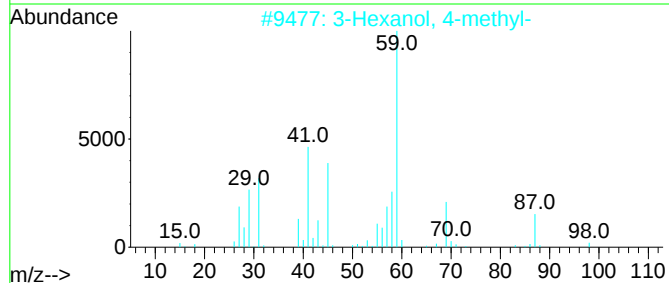
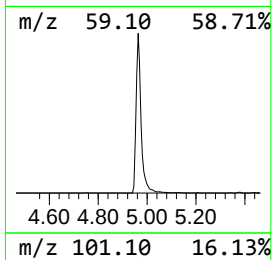
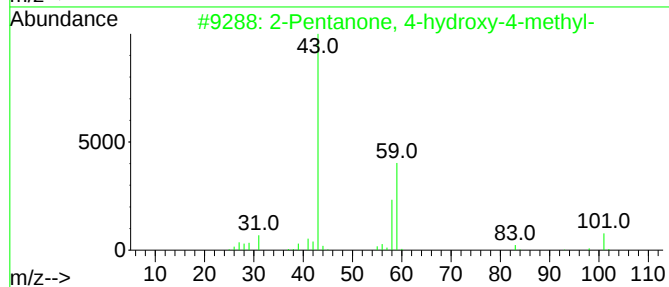
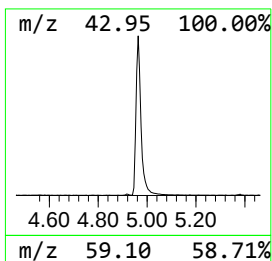
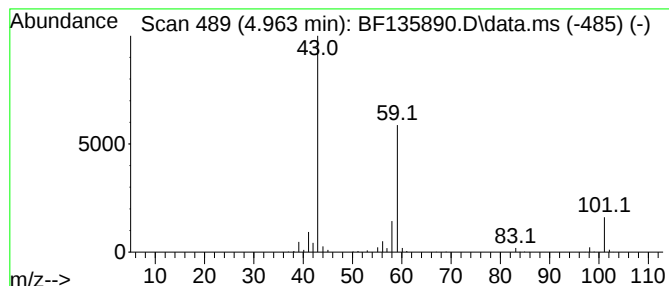
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.963	44.37 ng	643892	1,4-Dichlorobenzene-d4			6.734
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	16



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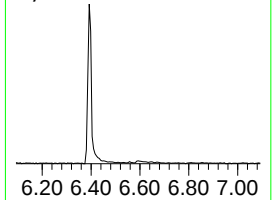
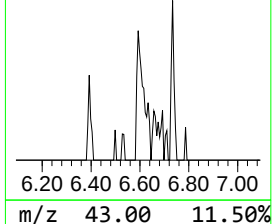
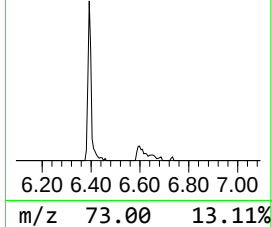
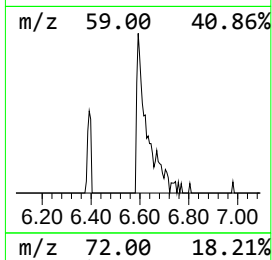
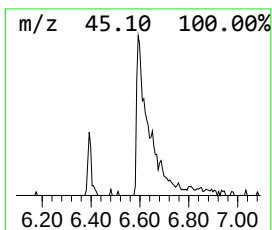
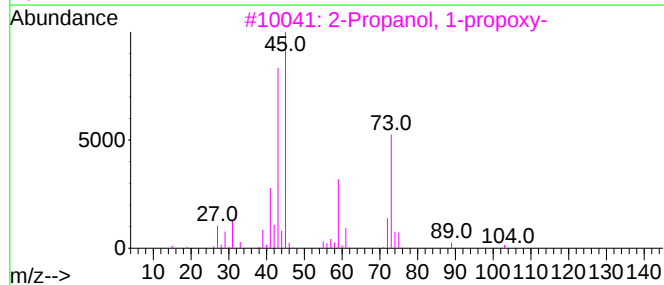
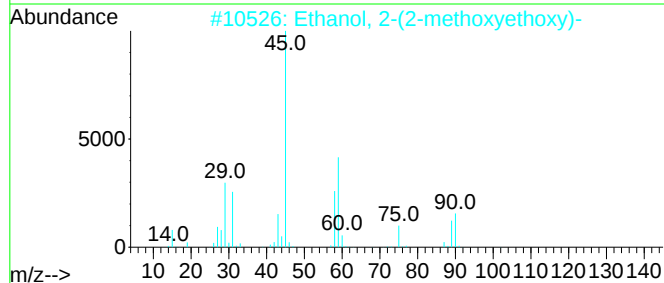
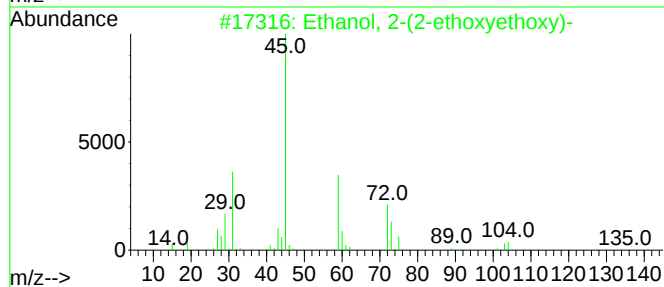
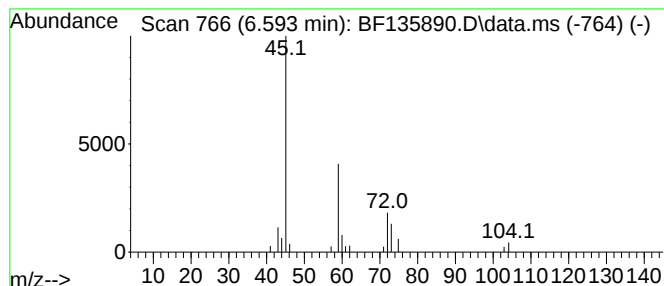
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.593	2.12 ng	30720	1,4-Dichlorobenzene-d4	6.734

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	78
2		Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	50
3		2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	39
4		Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	38
5		2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38



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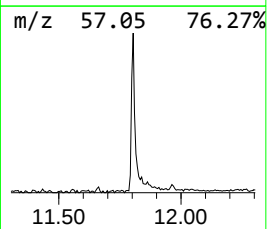
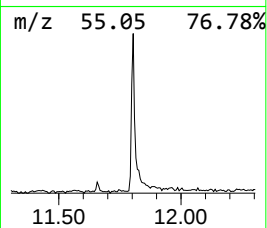
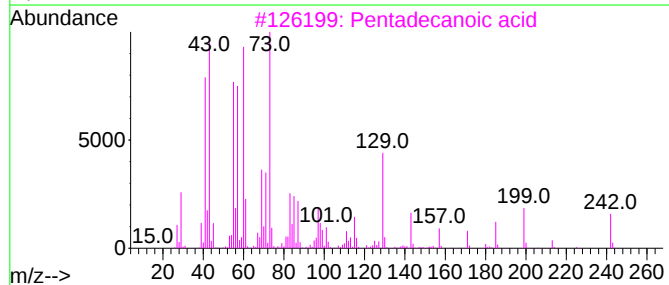
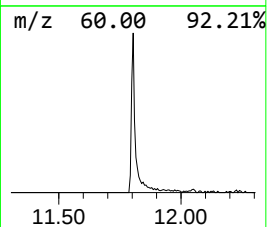
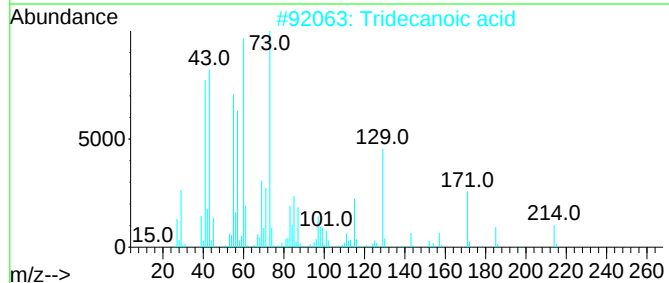
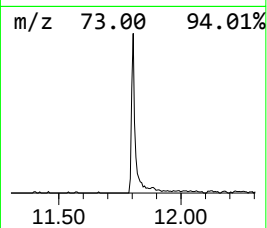
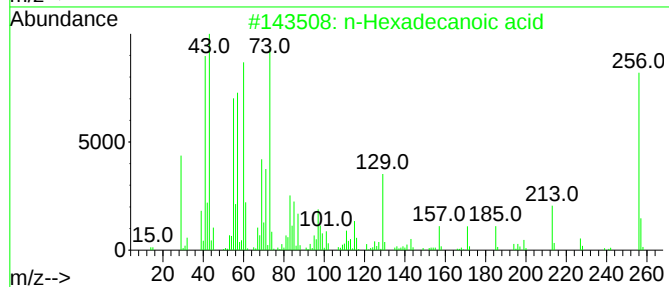
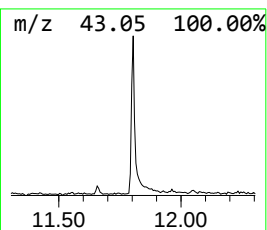
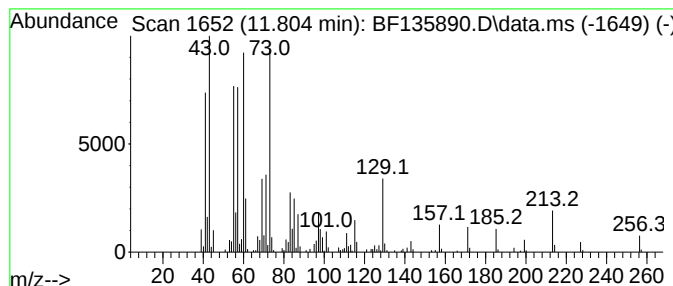
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	12.96 ng	275962	Phenanthrene-d10	11.269

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	59



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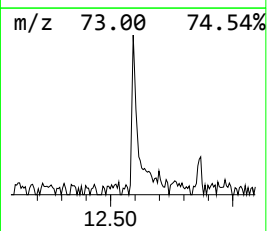
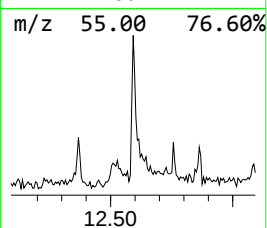
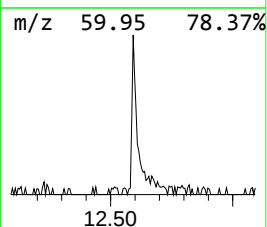
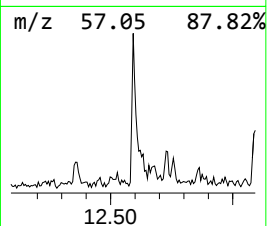
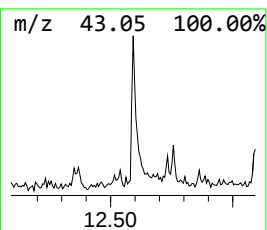
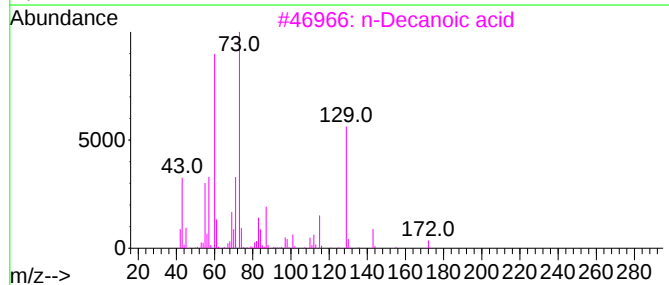
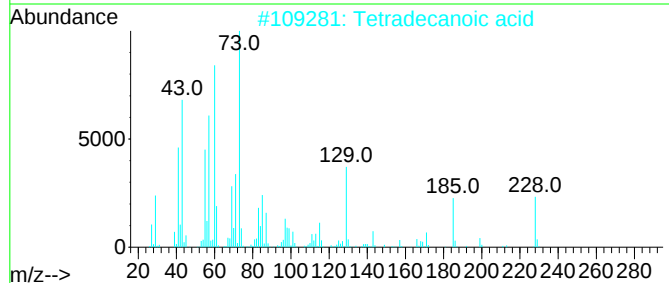
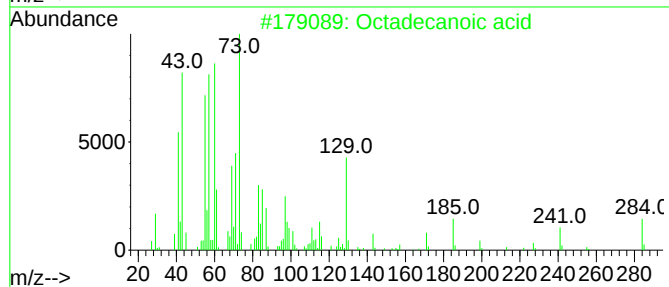
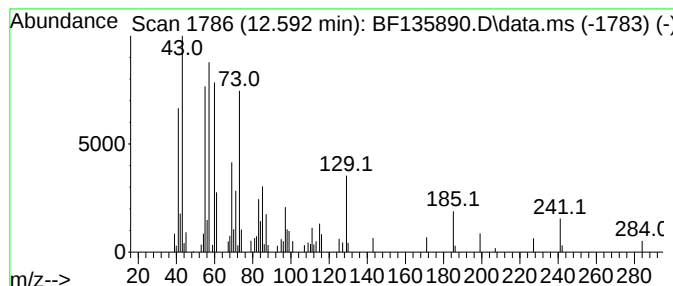
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.592	3.78 ng	80465	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	83
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3			n-Decanoic acid	172	C10H20O2	000334-48-5	47
4			Isoamyl nitrite	117	C5H11NO2	000110-46-3	22
5			Hexacosyl isobutyl ether	438	C30H62O	1000406-33-3	11



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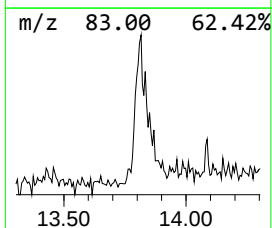
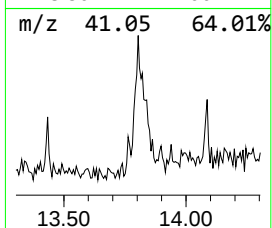
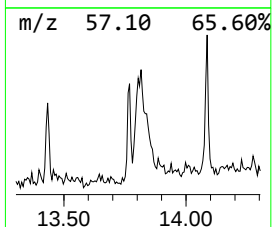
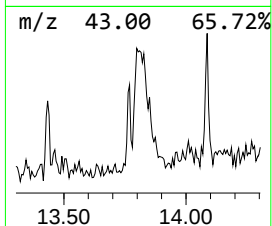
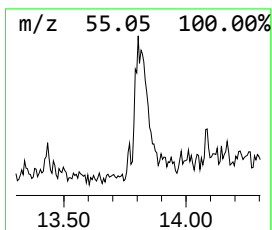
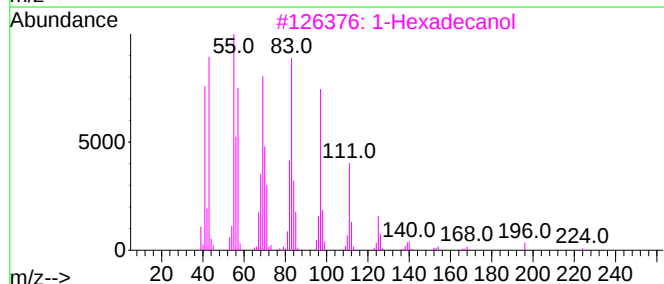
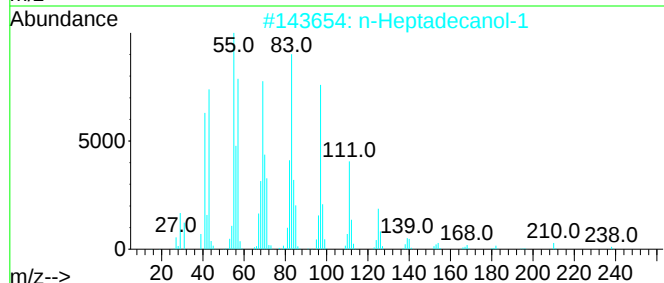
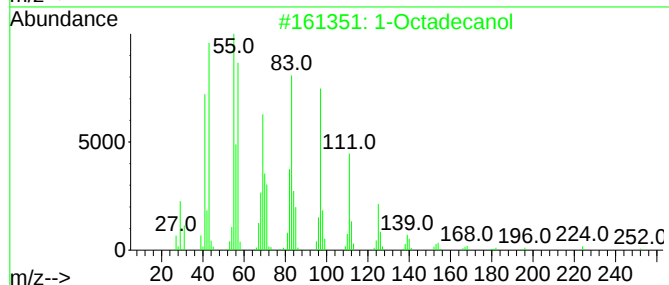
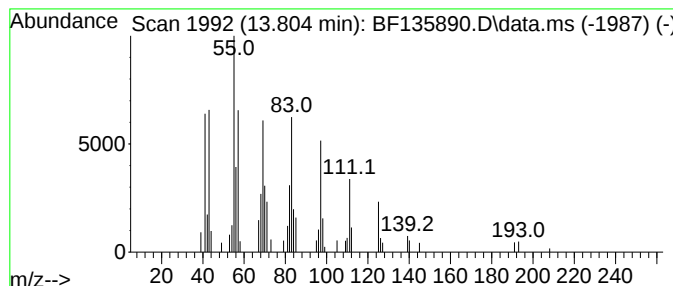
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Octadecanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.804	6.07 ng	99485	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanol	270	C18H38O	000112-92-5	91
2			n-Heptadecanol-1	256	C17H36O	001454-85-9	91
3			1-Hexadecanol	242	C16H34O	036653-82-4	91
4			1-Nonadecene	266	C19H38	018435-45-5	91
5			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.963	44.4	ng	643892	1	6.734	290266	20.0
Ethanol, 2-(2-e...	6.593	2.1	ng	30720	1	6.734	290266	20.0
n-Hexadecanoic ...	11.804	13.0	ng	275962	4	11.269	426032	20.0
Octadecanoic acid	12.592	3.8	ng	80465	4	11.269	426032	20.0
1-Octadecanol	13.804	6.1	ng	99485	5	13.933	327927	20.0