

Supporting Information

Rec. Nat. Prod. 11:4 (2017) 401-405

Fatty Acid Composition and Biological Activities of *Tanacetum zahlbruckneri* (Náb.) Grierson Growing in Turkey **Pinar Caglar-Eyol¹, Nazli Boke Sarikahya², Omer C. Karakoc³, Ayhan Gokce⁴, Fatih Demirci⁵, Suheyla Kirmizigul² and Nezhun Goren¹**

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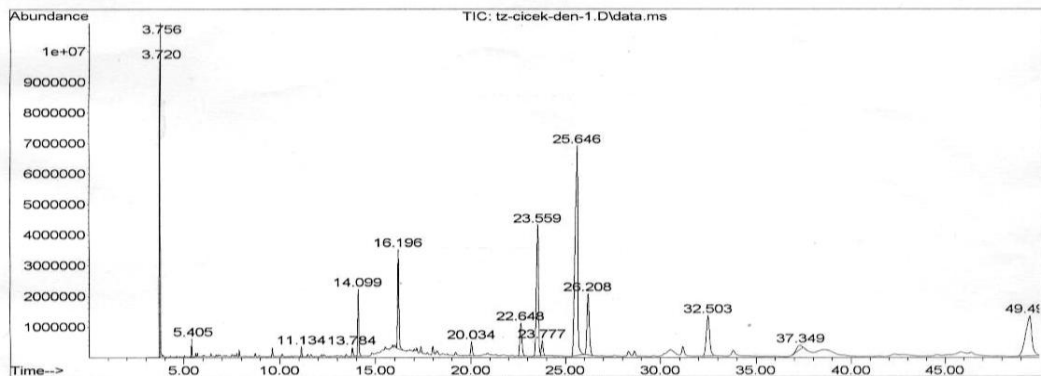
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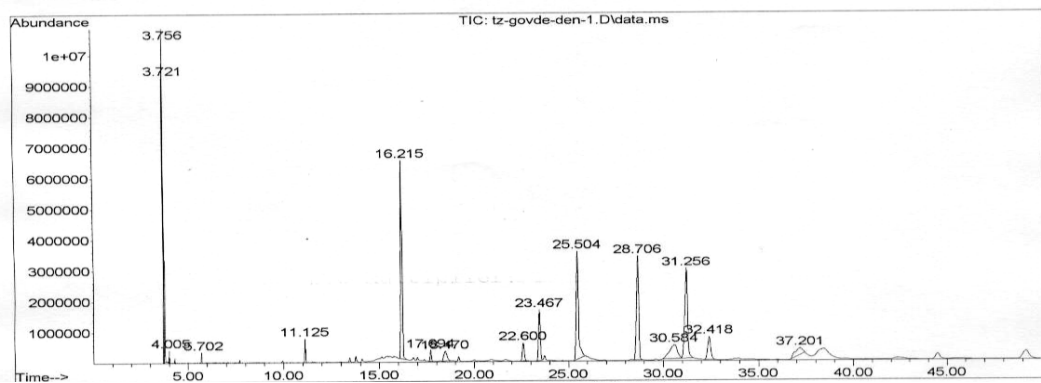
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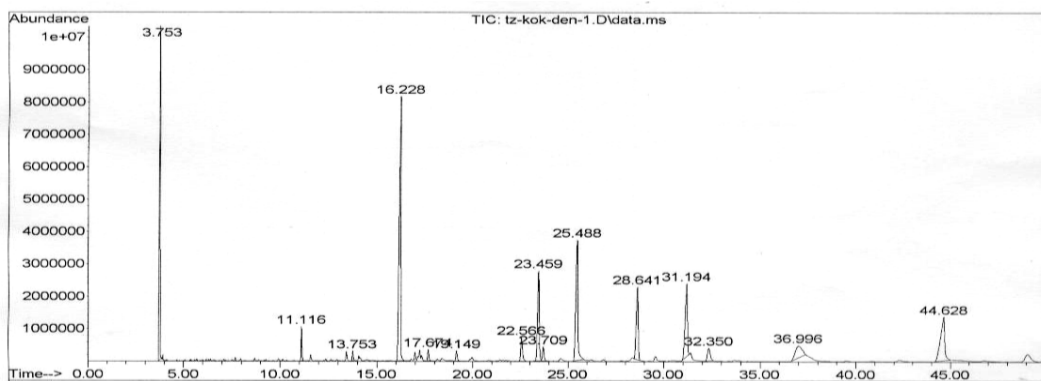
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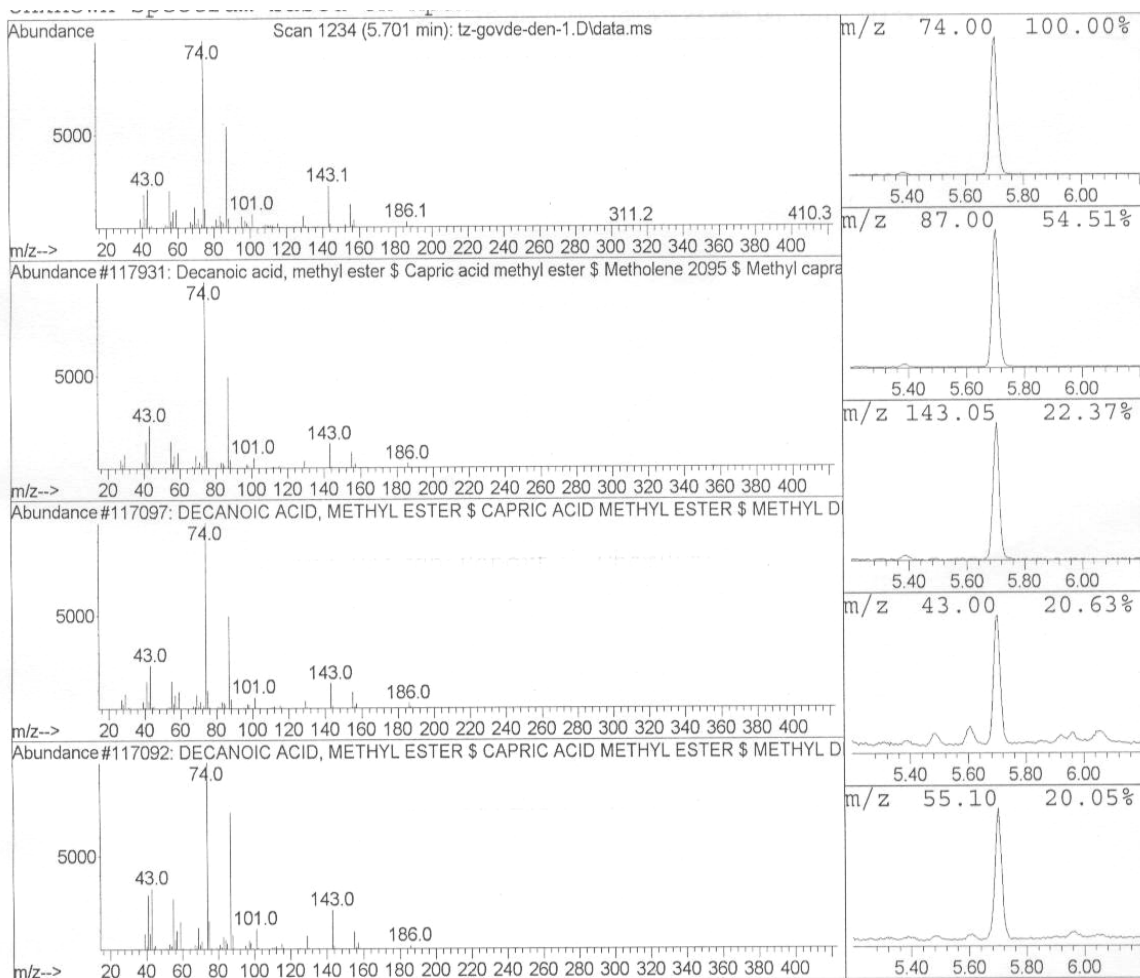
S1: GC-MS Chromatogram of *n*-hexane extract of Flowers



S2: GC-MS Chromatogram of *n*-hexane extract of Stem



S3: GC-MS Chromatogram of *n*-hexane extract of Root



Data File: C:\msdchem\1\5975\tz-govde-den-1.D
 Sample : tz govde

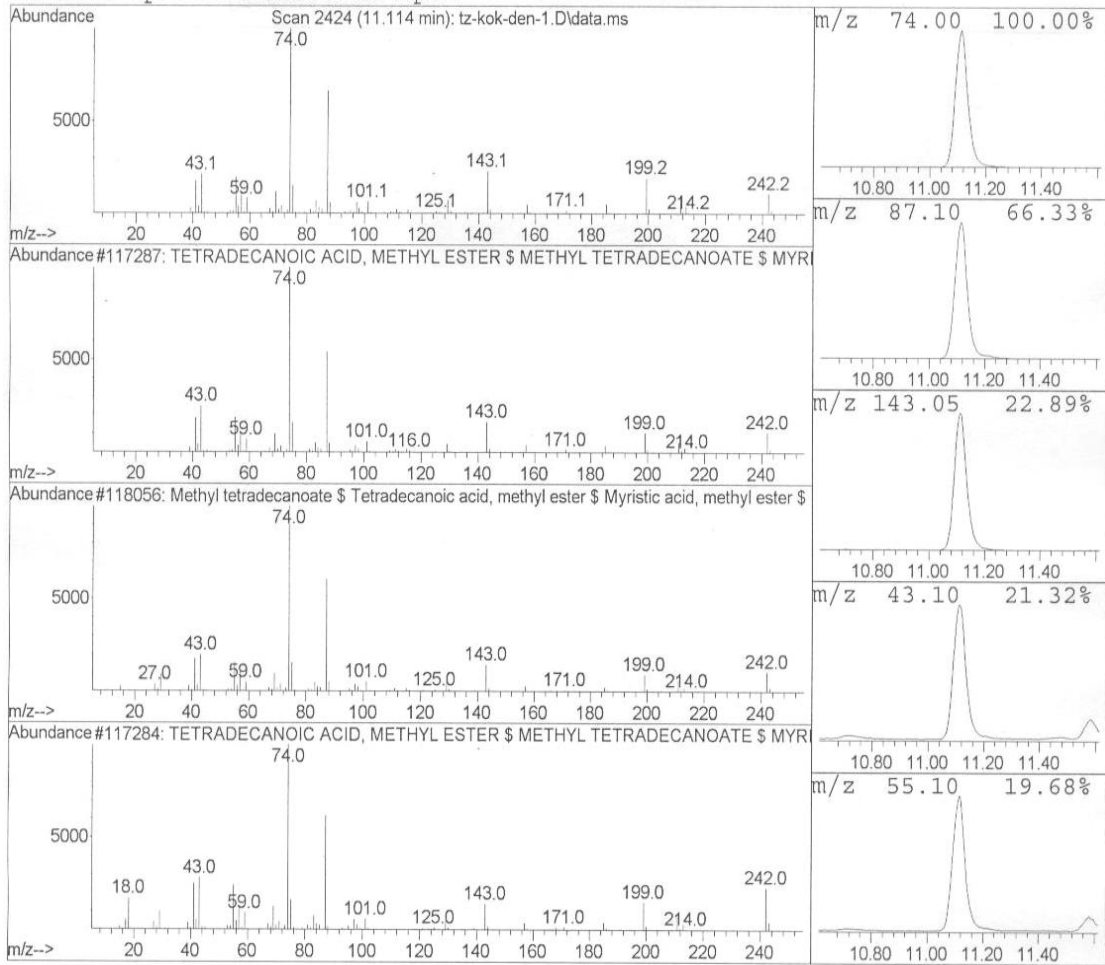
Peak Number: 4 at 5.701 min Area: 5744292 Area % 0.28

The 3 best hits from each library.			
	Ref\#	CAS\#	Qual

C:\Database\Wiley8NST.L			
1 Decanoic acid, methyl ester \$ Ca...	117931	000110-42-9	96
2 DECANOIC ACID, METHYL ESTER \$ CA...	117097	000110-42-9	96
3 DECANOIC ACID, METHYL ESTER \$ CA...	117092	000110-42-9	95

S4: Mass Spectrum of Decanoic Acid ME

m/z : 186 ($C_{11}H_{22}O_2$) $[M]^+$, 143 $[M-C_3H_7]^+$, 101 $[143-C_3H_6]^+$, 74 $[CH_3O-C(OH)=CH_2]^+$ (Mc Lafferty Rearrangement).



Data File: C:\msdchem\1\5975\tz-kok-den-1.D
 Sample : tz kok

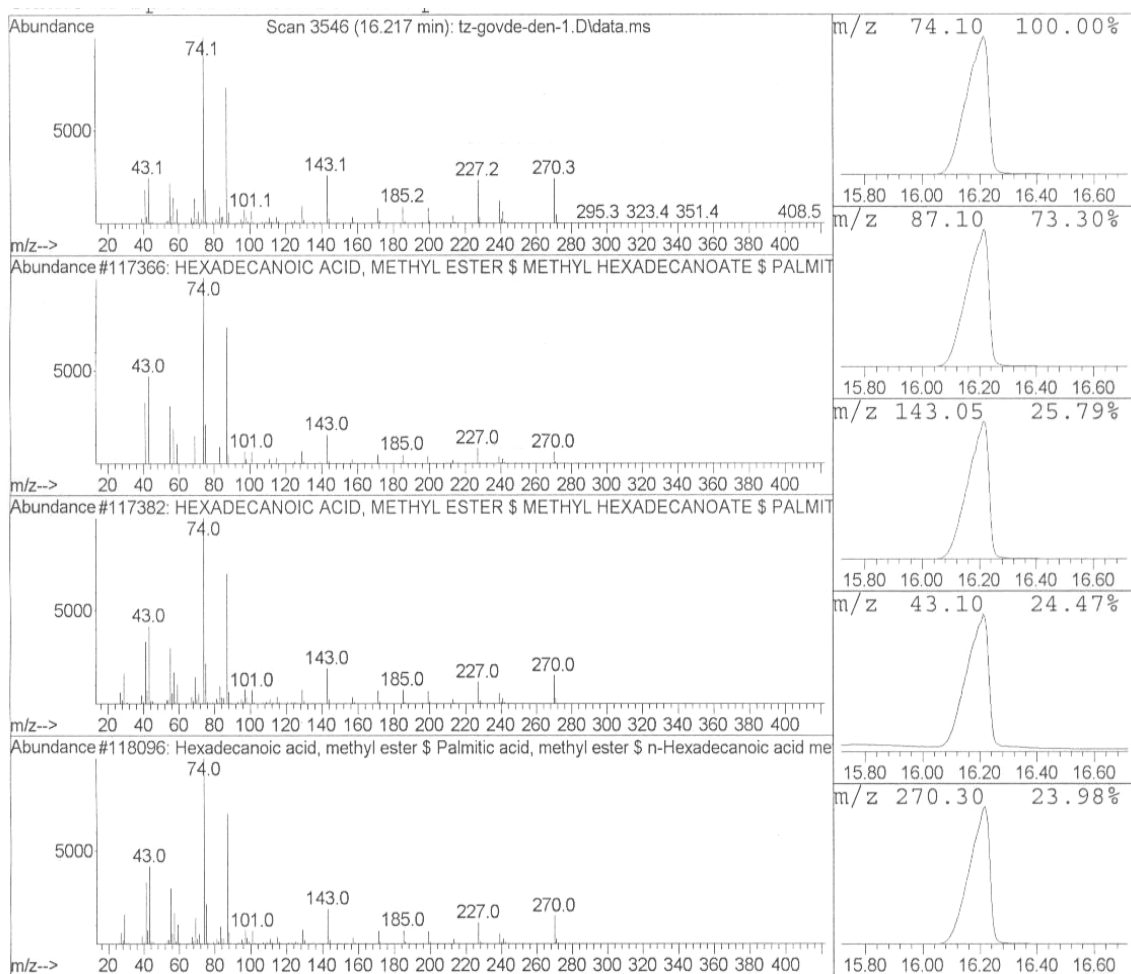
Peak Number: 2 at 11.114 min Area: 32636333 Area % 1.57

The 3 best hits from each library.

	Ref\#	CAS\#	Qual
C:\Database\Wiley8NST.L			
1 TETRADECANOIC ACID, METHYL ESTER...	117287	000124-10-7	98
2 Methyl tetradecanoate \$ Tetradec...	118056	000124-10-7	98
3 TETRADECANOIC ACID, METHYL ESTER...	117284	000124-10-7	98

S5: Mass Spectrum of Tetradecanoic Acid ME

m/z : 242 ($C_{15}H_{30}O_2$) $[M]^+$, 199 $[M-C_3H_7]^+$, 171 $[199-C_2H_4]^+$, 143 $[171-C_2H_4]^+$, 125 $[143-C_2H_4]^+$, 74 $[CH_3O-C(OH)=CH_2]^+$. (Mc Lafferty Rearrangement).



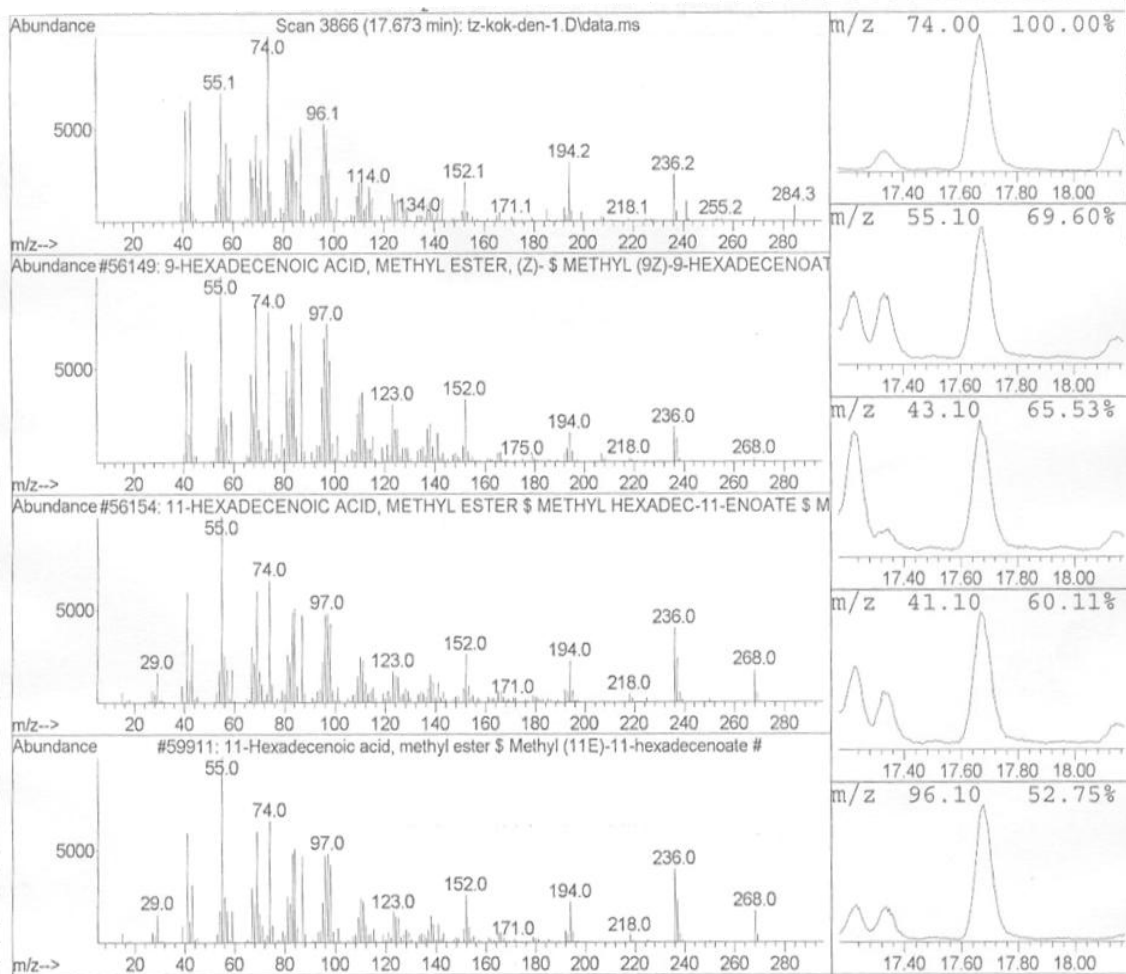
Data File: C:\msdchem\1\5975\tz-govde-den-1.D
 Sample : tz govde

Peak Number: 6 at 16.217 min Area: 339340746 Area % 16.76

The 3 best hits from each library.	Ref\#	CAS\#	Qual
C:\Database\Wiley8NST.L			
1 HEXADECANOIC ACID, METHYL ESTER ...	117366	000112-39-0	99
2 HEXADECANOIC ACID, METHYL ESTER ...	117382	000112-39-0	98
3 Hexadecanoic acid, methyl ester ...	118096	000112-39-0	98

S6: Mass Spectrum of Hexadecanoic Acid ME

m/z : 270 (C₁₇H₃₄O₂) [M]⁺, 227 [M-C₃H₇]⁺, 185 [M-C₆H₁₃]⁺, 143 [185-C₃H₆]⁺, 101 [143-C₃H₆]⁺, 74 [CH₃O-C(OH)=CH₂]⁺ (Mc Lafferty Rearrangement), 43 [C₃H₇]⁺.



Data File: C:\msdchem\1\5975\tz-kok-den-1.D
 Sample : tz kok

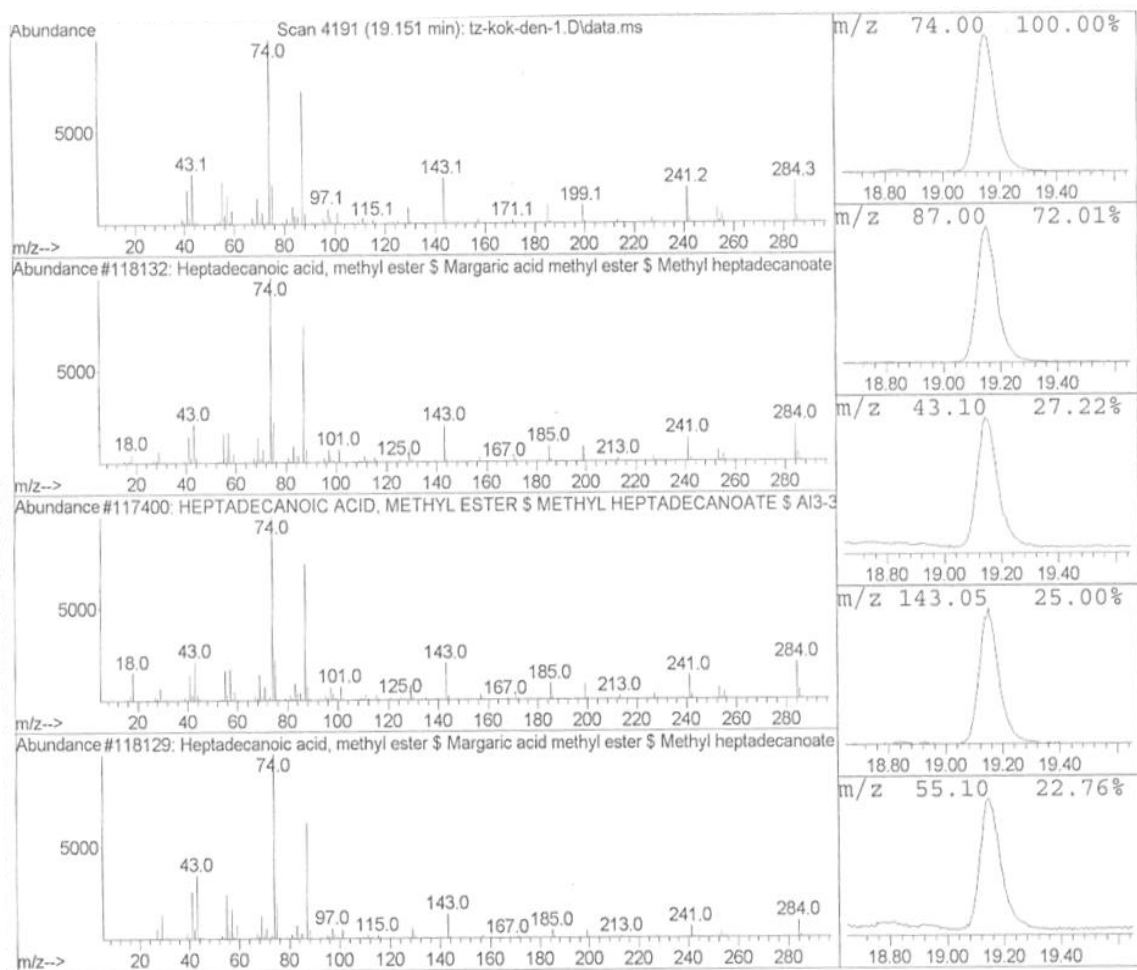
Peak Number: 5 at 17.673 min Area: 15345932 Area % 0.74

The 3 best hits from each library.

	Ref\#	CAS\#	Qual
C:\Database\Wiley8NST.L			
1 9-HEXADECENOIC ACID, METHYL ESTE...	56149	001120-25-8	93
2 11-HEXADECENOIC ACID, METHYL EST...	56154	055000-42-5	90
3 11-Hexadecenoic acid, methyl est...	59911	055000-42-5	90

S7: Mass Spectrum of 9-Hexadecenoic Acid ME

m/z : 268($C_{17}H_{32}O_2$) $[M]^+$, 236 $[M-CH_3OH]^+$, 194 $[M-74]^+$, 152 $[194-(CH_2)_3]^+$, 97 $[194-C_7H_{13}]^+$, 74 $[CH_3O-C(OH)=CH_2]^+$ (Mc Lafferty Rearrangement), 55 $[97-(CH_2)_3]^+$.



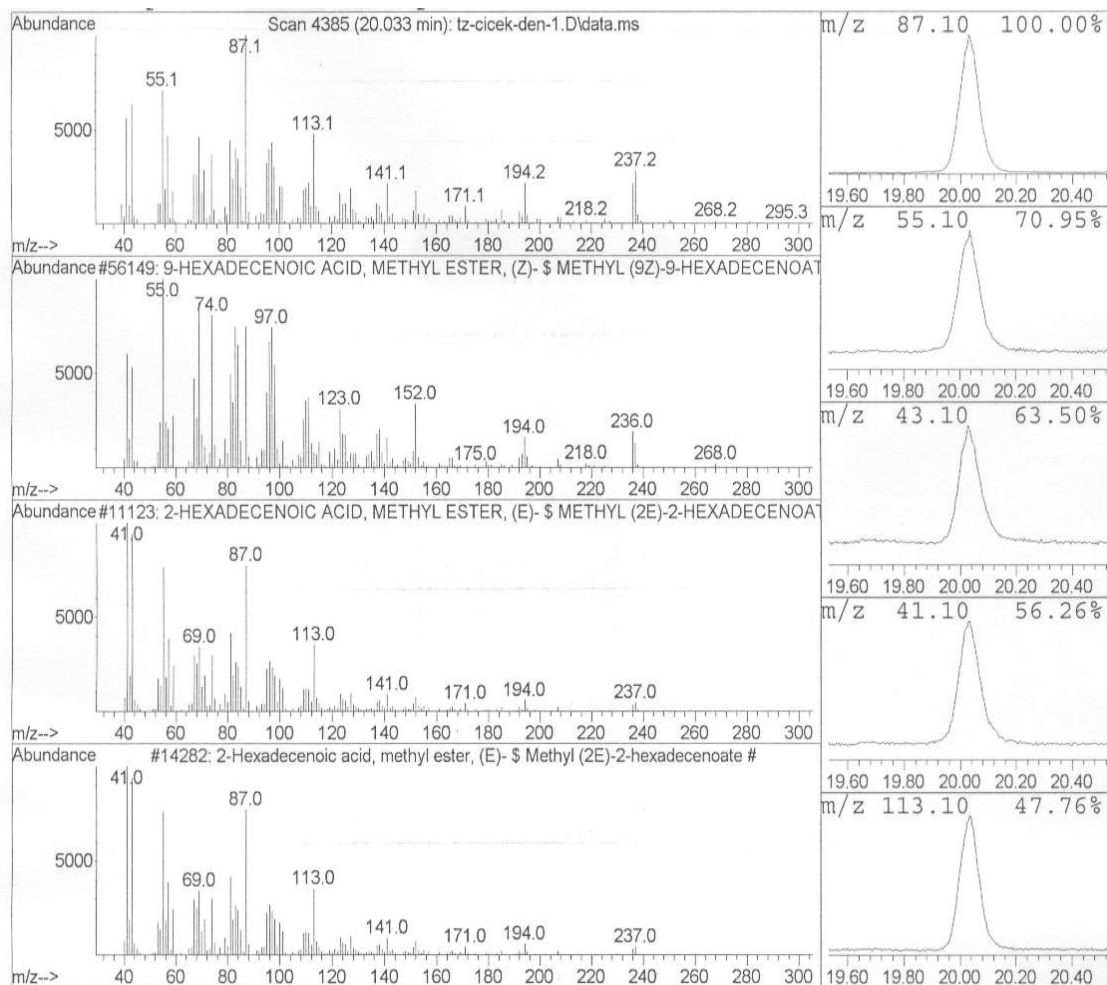
Data File: C:\msdchem\1\5975\tz-kok-den-1.D
 Sample : tz kok

Peak Number: 6 at 19.151 min Area: 15439802 Area % 0.74

The 3 best hits from each library.			
	Ref\#	CAS\#	Qual
C:\Database\Wiley8NST.L			
1 Heptadecanoic acid, methyl ester...	118132	001731-92-6	99
2 HEPTADECANOIC ACID, METHYL ESTER...	117400	001731-92-6	99
3 Heptadecanoic acid, methyl ester...	118129	001731-92-6	98

S8: Mass Spectrum of Heptadecanoic Acid ME

m/z : 284 ($C_{18}H_{36}O_2$) $[M]^+$, 241 $[M-C_3H_7]^+$, 199 $[M-C_3H_7]^+$, 171 $[199-C_2H_4]^+$, 143 $[171-C_2H_4]^+$, 115 $[143-C_2H_4]^+$, 74 $[CH_3O-C(OH)=CH_2]^+$ (Mc Lafferty rearrangement), 43 $[C_3H_7]^+$.



Data File: C:\msdchem\1\5975\tz-cicek-den-1.D
 Sample : tz cicek

Peak Number: 8 at 20.033 min Area: 24898576 Area % 1.05

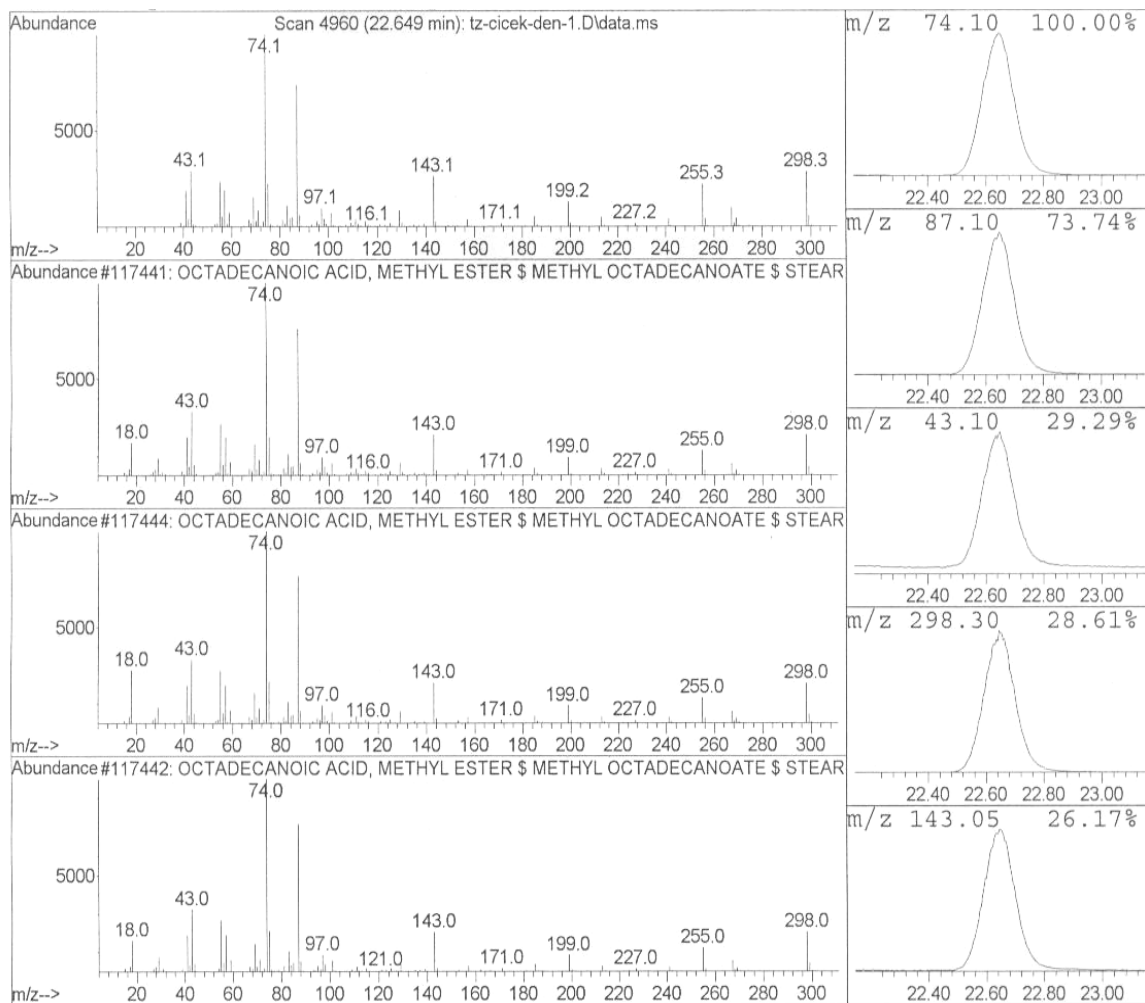
The 3 best hits from each library.

	Ref\#	CAS\#	Qual

C:\Database\Wiley8NST.L			
1	9-HEXADECENOIC ACID, METHYL ESTE...	56149 001120-25-8	93
2	2-HEXADECENOIC ACID, METHYL ESTE...	11123 002825-81-2	87
3	2-Hexadecenoic acid, methyl este...	14282 002825-81-2	87

S9: Mass Spectrum of 2-Hexadecenoic Acid ME

m/z: 268 (C₁₇H₃₂O₂) [M]⁺, 237 [M-OCH₃]⁺, 194 [C₃H₇]⁺, 87[CH₃OCOCH₂CH₂]⁺, 55 [87-CH₃OH]⁺.



Data File: C:\msdchem\1\5975\tz-cicek-den-1.D
 Sample : tz cicek

Peak Number: 9 at 22.649 min Area: 81790109 Area % 3.46

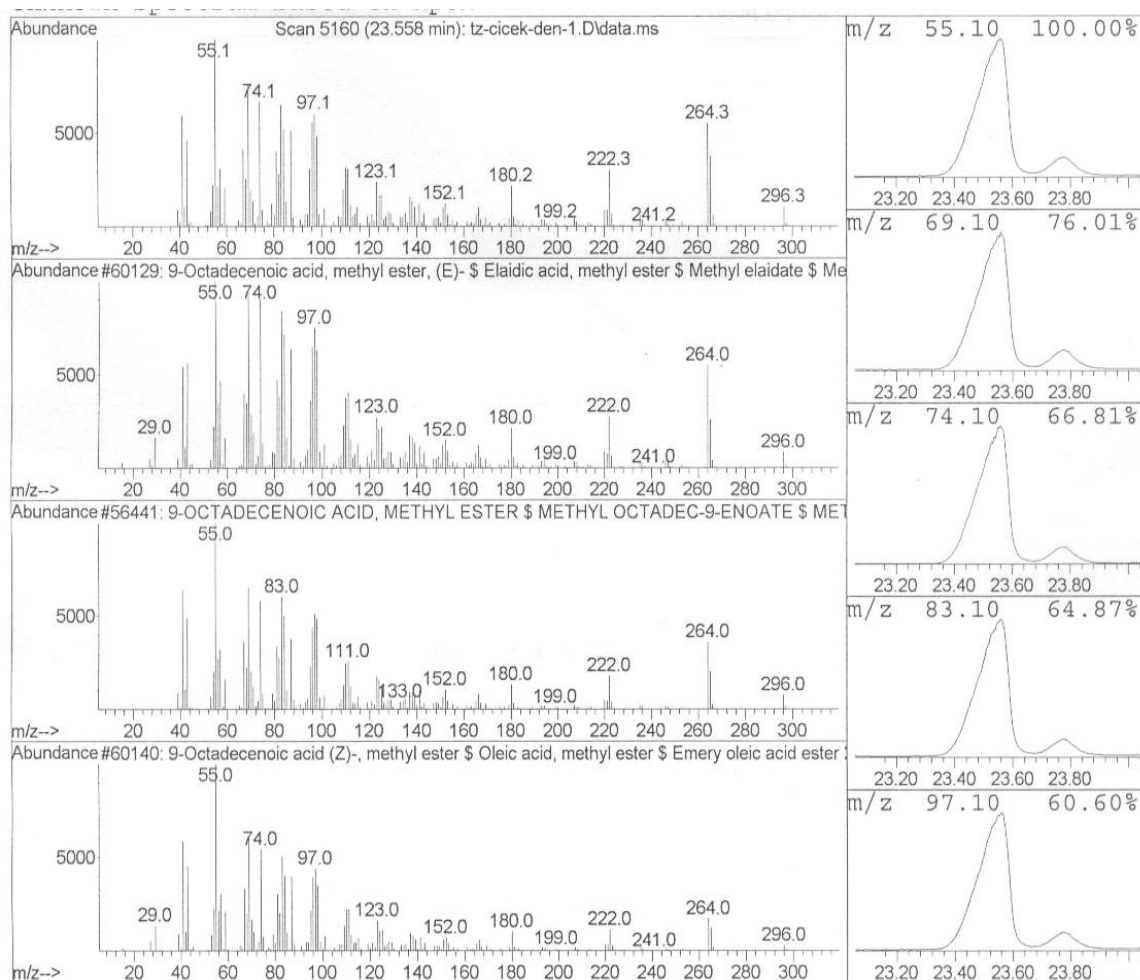
The 3 best hits from each library.

	Ref\#	CAS\#	Qual

C:\Database\Wiley8NST.L			
1 OCTADECANOIC ACID, METHYL ESTER ...	117441	000112-61-8	99
2 OCTADECANOIC ACID, METHYL ESTER ...	117444	000112-61-8	99
3 OCTADECANOIC ACID, METHYL ESTER ...	117442	000112-61-8	99

S10: Mass Spectrum of Octadecanoic Acid ME

m/z : 296 (C₁₉H₃₈O₂) [M]⁺, 255[M-C₃H₇]⁺, [M-C₃H₇]⁺, 171 [199-C₂H₄]⁺, 143 [171-C₂H₄]⁺, 74 [CH₃O-C(OH)=CH₂]⁺ (Mc Lafferty Rearrangement), 43 [C₃H₇]⁺.



Data File: C:\msdchem\1\5975\tz-cicek-den-1.D
 Sample : tz cicek

Peak Number: 10 at 23.558 min Area: 313960780 Area % 13.28

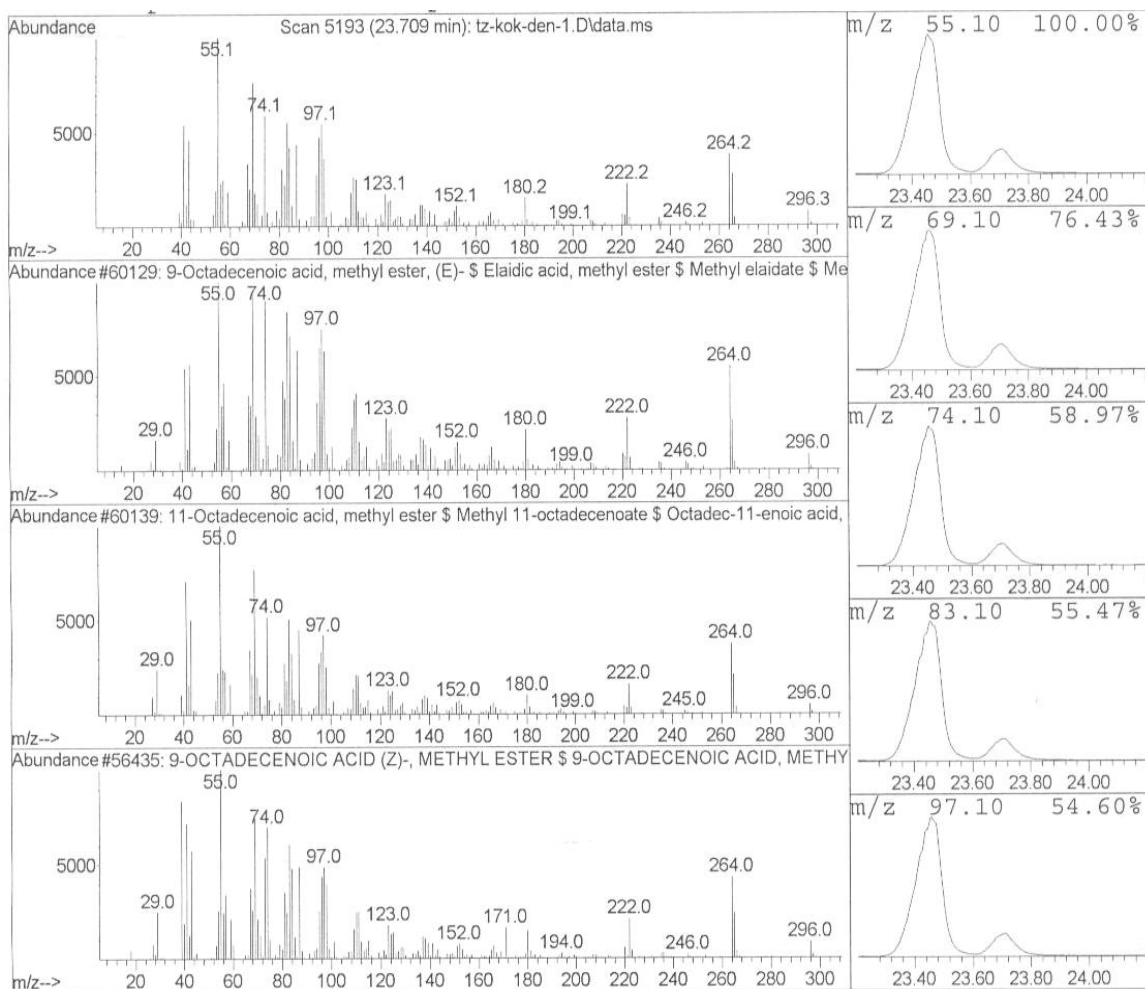
The 3 best hits from each library.

	Ref\#	CAS\#	Qual

C:\Database\Wiley8NST.L			
1 9-Octadecenoic acid, methyl este...	60129	001937-62-8	99
2 9-OCTADECENOIC ACID, METHYL ESTE...	56441	002462-84-2	99
3 9-Octadecenoic acid (Z)-, methyl...	60140	000112-62-9	99

S11: Mass Spectrum of 9-Octadecenoic Acid ME

m/z 296 ($C_{19}H_{38}O_2$) $[M]^+$, 264 $[M-CH_3OH]^+$, 222 $[M-74]^+$, 180 $[222-C_3H_6]^+$, 152 $[180-C_2H_4]^+$, 74 $[CH_3O-C(OH)=CH_2]^+$ (Mc Lafferty Rearrangement).



Data File: C:\msdchem\1\5975\tz-kok-den-1.D
 Sample : tz kok

Peak Number: 9 at 23.709 min Area: 23881124 Area % 1.15

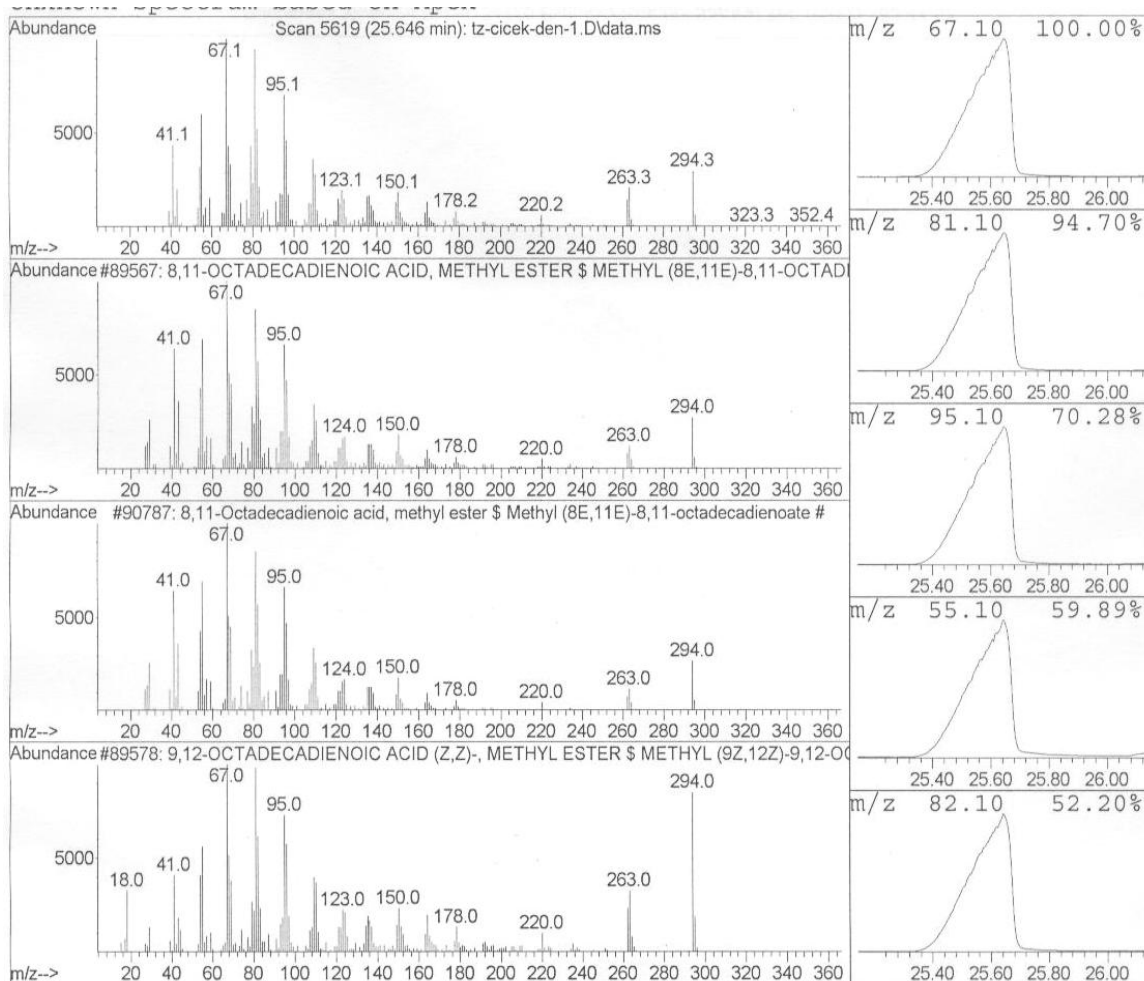
The 3 best hits from each library.

	Ref\#	CAS\#	Qual

C:\Database\Wiley8NST.L			
1 9-Octadecenoic acid, methyl este...	60129	001937-62-8	99
2 11-Octadecenoic acid, methyl est...	60139	052380-33-3	99
3 9-OCTADECENOIC ACID (Z)-, METHYL...	56435	000112-62-9	99

S12: Mass Spectrum of 11-Octadecenoic Acid ME

m/z 296 (C₁₉H₃₈O₂) [M]⁺, 264 [M-CH₃OH]⁺, 222 [M-74]⁺, 180 [222-C₃H₆]⁺, 152 [180-C₂H₄]⁺, 74 [CH₃O-C(OH)=CH₂]⁺ (Mc Lafferty rearrangement).



Data File: C:\msdchem\1\5975\tz-cicek-den-1.D
 Sample : tz cicek

Peak Number: 12 at 25.646 min Area: 657115223 Area % 27.79

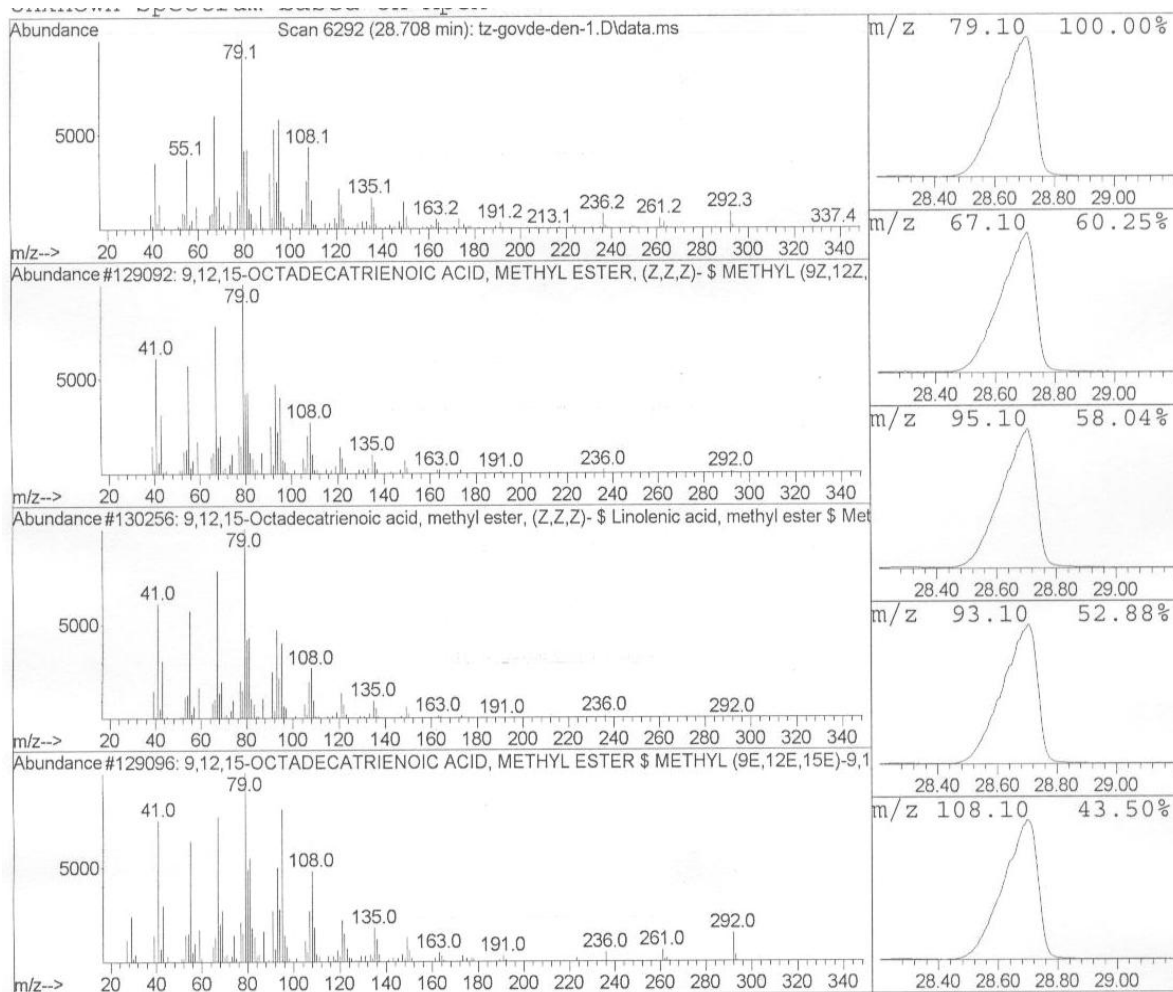
The 3 best hits from each library.

	Ref\#	CAS\#	Qual

C:\Database\Wiley8NST.L			
1	89567	056599-58-7	99
2	90787	056599-58-7	99
3	89578	000112-63-0	99

S13: Mass Spectrum of 9,12-Octadecadienoic Acid ME

m/z: 294 ($C_{19}H_{34}O_2$) $[M]^+$, 263 $[M-OCH_3]^+$, 220 $[M-74]^+$, 178 $[220 - (CH_2)_3]^+$, 150 $[178-CH_2]^+$, 95 $[C_7H_{11}]^+$ (C_{10} β -rearrangement), 67 $[96-C_2H_5]^+$.



Data File: C:\msdchem\1\5975\tz-govde-den-1.D
 Sample : tz govde

Peak Number: 12 at 28.708 min Area: 276002986 Area % 13.63

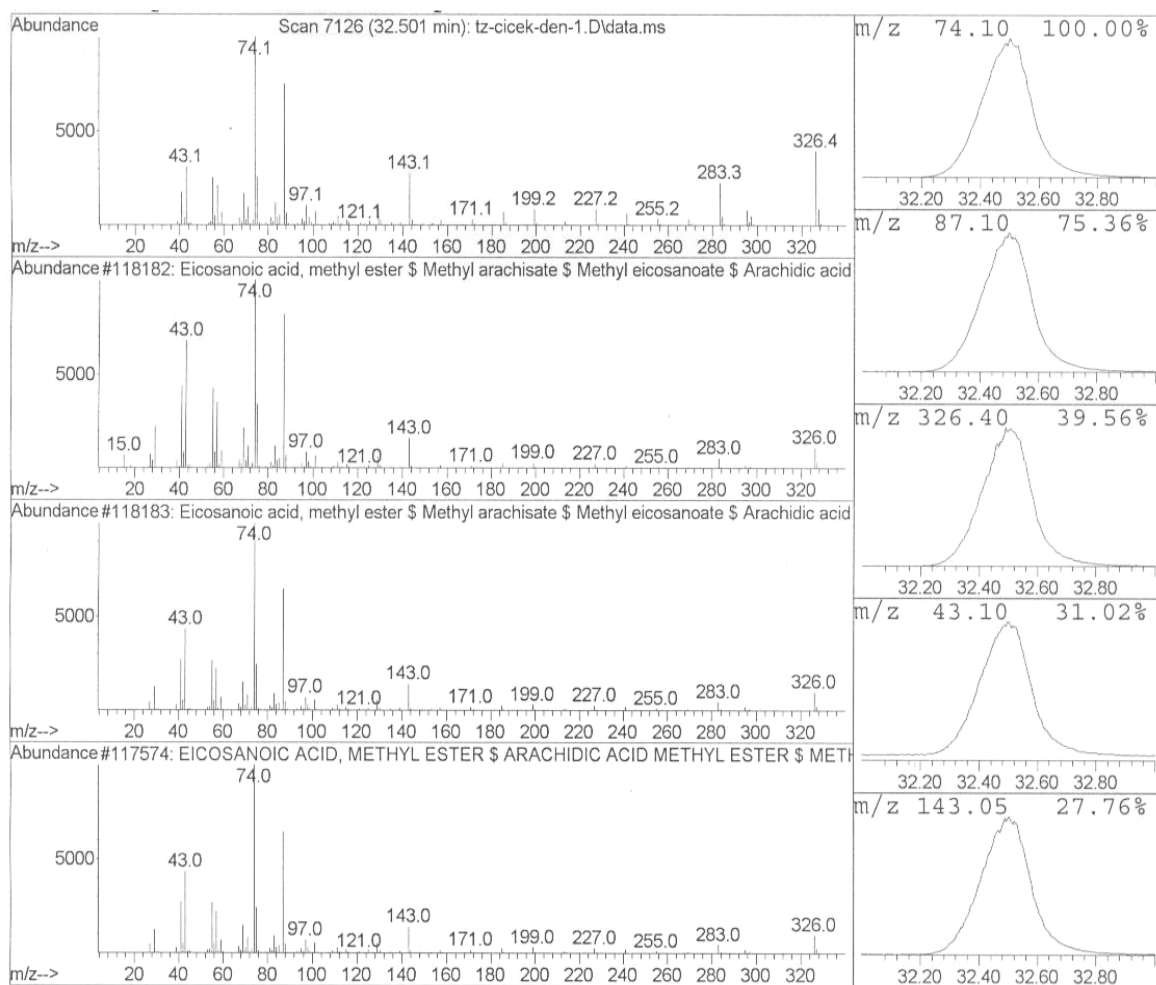
The 3 best hits from each library.

	Ref\#	CAS\#	Qual

C:\Database\Wiley8NST.L			
1	9,12,15-OCTADECATRIENOIC ACID, M...	129092 000301-00-8	99
2	9,12,15-Octadecatrienoic acid, m...	130256 000301-00-8	99
3	9,12,15-OCTADECATRIENOIC ACID, M...	129096 007361-80-0	98

S14: Mass Spectrum of 9,12,15-Octadecatrienoic Acid ME

m/z: 292 ($C_{19}H_{32}O_2$) $[M]^+$, 261 $[292-OCH_3]^+$, 108 (C_{10} β -rearrangement), 79 $[108-CH_3CH_2]^+$,
 55 $[CH_3CH_2CH=CH]^+$ (C_{13} β -rearrangement).



Data File: C:\msdchem\1\5975\tz-cicek-den-1.D
 Sample : tz cicek

Peak Number: 14 at 32.501 min Area: 156995904 Area % 6.64

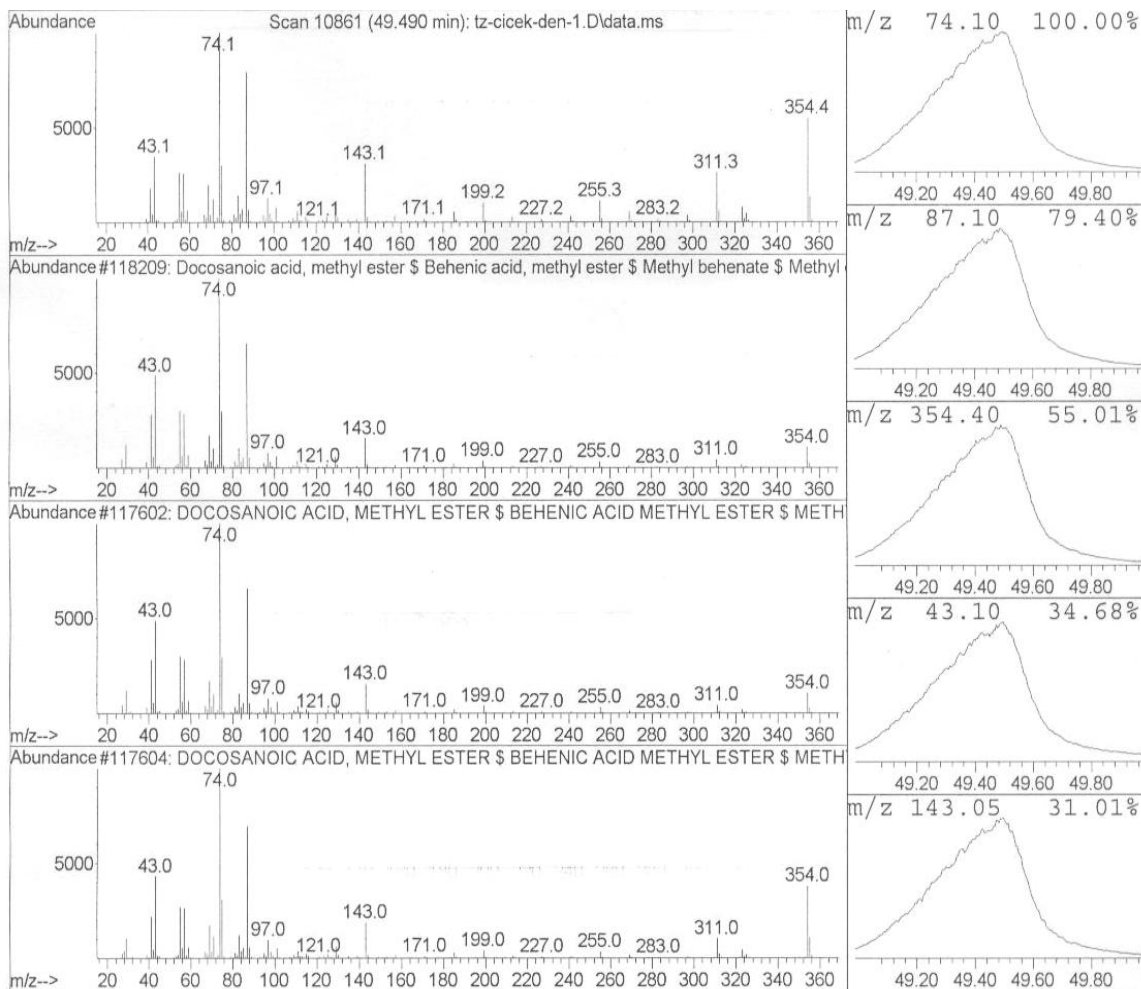
The 3 best hits from each library.

	Ref\#	CAS\#	Qual

C:\Database\Wiley8NST.L			
1 Eicosanoic acid, methyl ester \$...	118182	001120-28-1	99
2 Eicosanoic acid, methyl ester \$...	118183	001120-28-1	99
3 EICOSANOIC ACID, METHYL ESTER \$...	117574	001120-28-1	99

S15: Mass Spectrum of Eicosanoic Acid ME

m/z: 326 (C₂₁H₄₂O₂) [M]⁺, 283 [M-C₃H₇]⁺, 255 [283-C₂H₄]⁺, 227 [255-C₂H₄]⁺, 199 [227-C₂H₄]⁺, 171 [199-C₂H₄]⁺, 143 [171-C₂H₄]⁺, 74 [CH₃O-C(OH)=CH₂]⁺ (Mc Lafferty Rearrangement), 43 [C₃H₇]⁺.



Data File: C:\msdchem\1\5975\tz-cicek-den-1.D
 Sample : tz cicek

Peak Number: 16 at 49.490 min Area: 298194937 Area % 12.61

The 3 best hits from each library.			
	Ref\#	CAS\#	Qual

C:\Database\Wiley8NST.L			
1 Docosanoic acid, methyl ester \$...	118209	000929-77-1	99
2 DOCOSANOIC ACID, METHYL ESTER \$...	117602	000929-77-1	99
3 DOCOSANOIC ACID, METHYL ESTER \$...	117604	000929-77-1	99

S16: Mass Spectrum of Docosanoic Acid ME

m/z: 254 (C₂₃H₄₆O₂) [M]⁺, 311 [M-C₃H₇]⁺, 283 [311-C₂H₄]⁺, 255[283-C₂H₄]⁺, 227 [255-C₂H₄]⁺, 199 [227-C₂H₄]⁺, 171 [199-C₂H₄]⁺, 143 [171-C₂H₄]⁺, 74[CH₃O-C(OH)=CH₂]⁺ (McLafferty rearrangement), 43 [C₃H₇]⁺.

Microorganism	Root	Flower	Stem	Reference
Gram positive bacteria				Chloramphenicol
<i>Staphylococcus aureus</i>	1.250	1.250	1.250	0.0156
<i>Staphylococcus epidermidis</i>	0.625	1.250	1.250	0.0156
<i>Bacillus subtilis</i>	1.250	0.625	1.250	0.0156
<i>Meth. Resist. S. aureus MRSA</i>	1.250	0.625	0.625	0.0156
Gram negative bacteria				Chloramphenicol
<i>Escherichia coli</i>	2.500	2.500	2.500	0.06250
<i>Proteus vulgaris</i>	2.500	2.500	2.500 <	0.03125
Candida sp.				Ketoconazole
<i>Candida parapsilosis</i>	1.250	0.156	1.250	1.25
<i>Candida albicans</i>	1.250	0.156	0.625	1.25

S17: Microdilution activity results (concentration values were given in mg/mL)