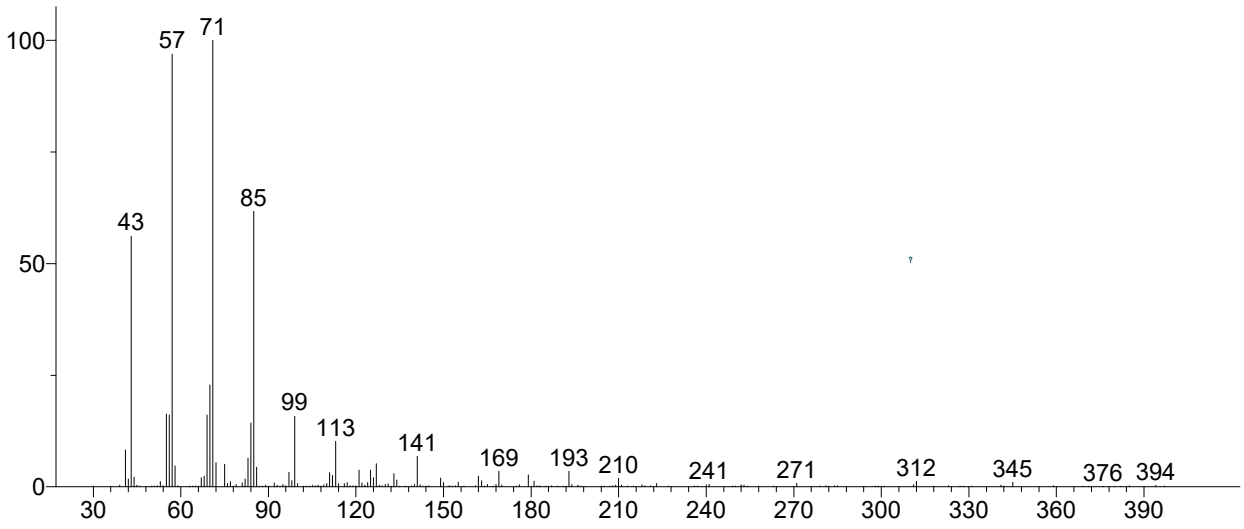
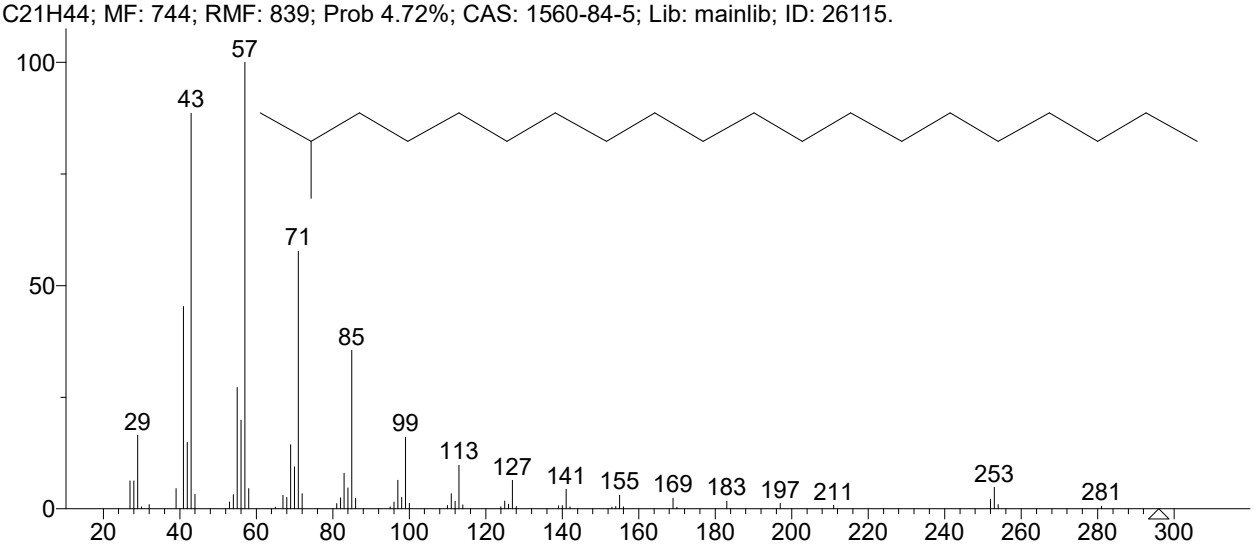
Unknown; InLib=-1103



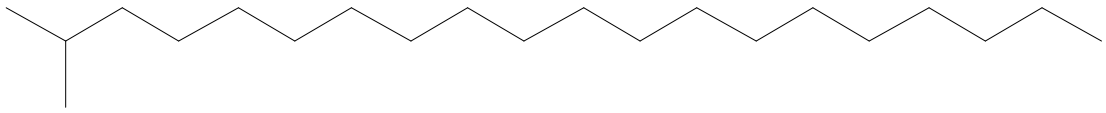
(Text File) +EI Scan (rt: 6.215-6.271 min, 21 scans) Frag=70.0V NC64A 1.D Subtract

Name: +EI Scan (rt: 6.215-6.271 min, 21 scans) Frag=70.0V NC64A 1.D Subtract
MW: N/A ID#: 591 DB: Text File
10 largest peaks:
71 999 | 57 968 | 85 616 | 43 561 | 70 227 | 55 162 | 56 160 | 69 160 | 99 159 | 84 142 |
Synonyms:
no synonyms.

Hit 1 : Eicosane, 2-methyl-
C21H44; MF: 744; RMF: 839; Prob 4.72%; CAS: 1560-84-5; Lib: mainlib; ID: 26115.

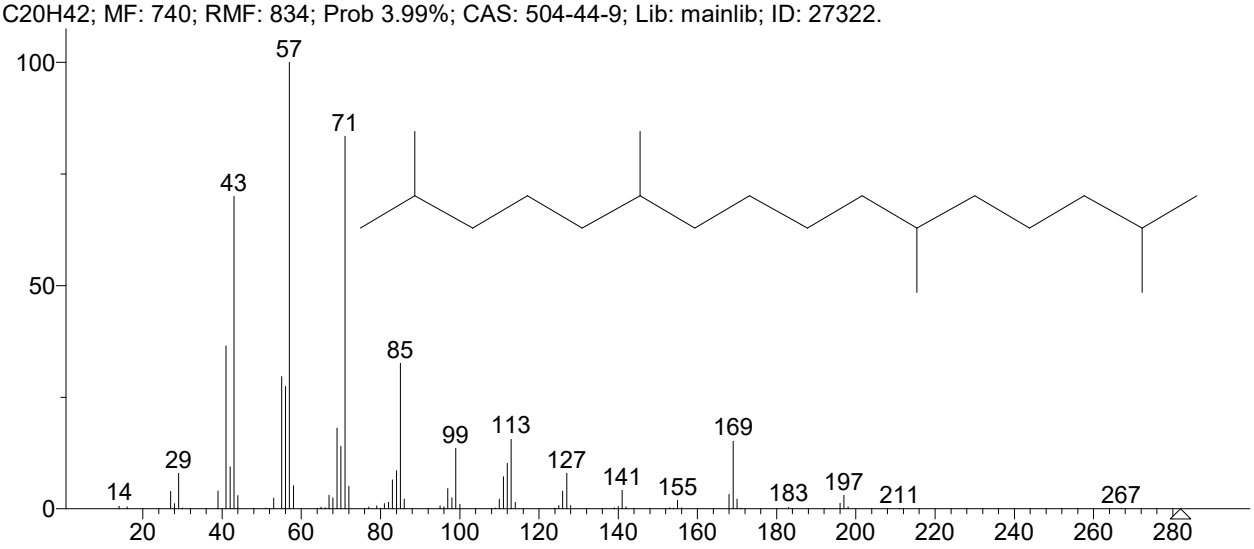


(mainlib) Eicosane, 2-methyl-

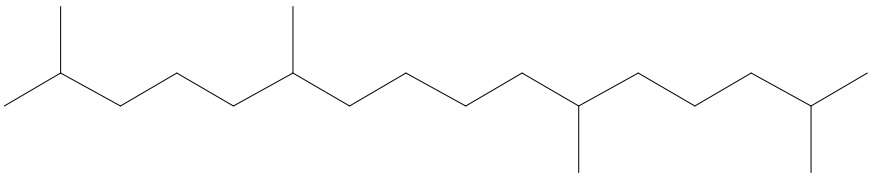


Name: Eicosane, 2-methyl-
Formula: $C_{21}H_{44}$
MW: 296 Exact Mass: 296.344301 CAS#: 1560-84-5 NIST#: 113884 ID#: 26115 DB: mainlib
Other DBs: None
Contributor: NIST Mass Spectrometry Data Center, 1990.
InChIKey: MLKZKPUBHSWMNA-UHFFFAOYSA-N Non-stereo
10 largest peaks:
57 999 | 43 885 | 71 577 | 41 452 | 85 355 | 55 271 | 56 198 | 29 164 | 99 161 | 42 148 |
Synonyms:
1.2-Methyleicosane
2.2-Methylicosane #

Hit 2 : Hexadecane, 2,6,11,15-tetramethyl-
C20H42; MF: 740; RMF: 834; Prob 3.99%; CAS: 504-44-9; Lib: mainlib; ID: 27322.

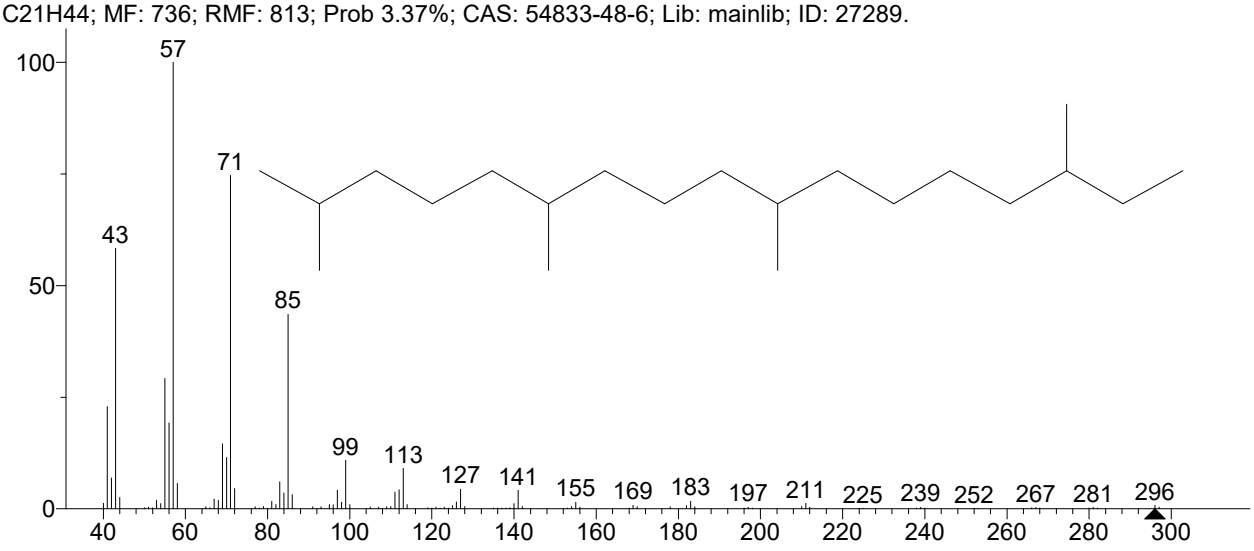


(mainlib) Hexadecane, 2,6,11,15-tetramethyl-

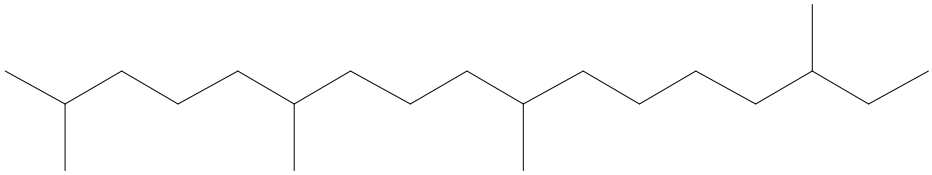


Name: Hexadecane, 2,6,11,15-tetramethyl-
Formula: $C_{20}H_{42}$
MW: 282 Exact Mass: 282.328651 CAS#: 504-44-9 NIST#: 114255 ID#: 27322 DB: mainlib
Other DBs: IRDB
Contributor: NIST Mass Spectrometry Data Center, 1990.
InChIKey: KKFZXXATNGJPJS-UHFFFAOYSA-N Non-stereo
10 largest peaks:
57 999 | 71 833 | 43 699 | 41 364 | 85 325 | 55 295 | 56 273 | 69 180 | 113 157 | 169 152 |
Synonyms:
1.Crocetane
2.2,6,11,15-Tetramethylhexadecane

Hit 3 : Heptadecane, 2,6,10,15-tetramethyl-
C21H44; MF: 736; RMF: 813; Prob 3.37%; CAS: 54833-48-6; Lib: mainlib; ID: 27289.

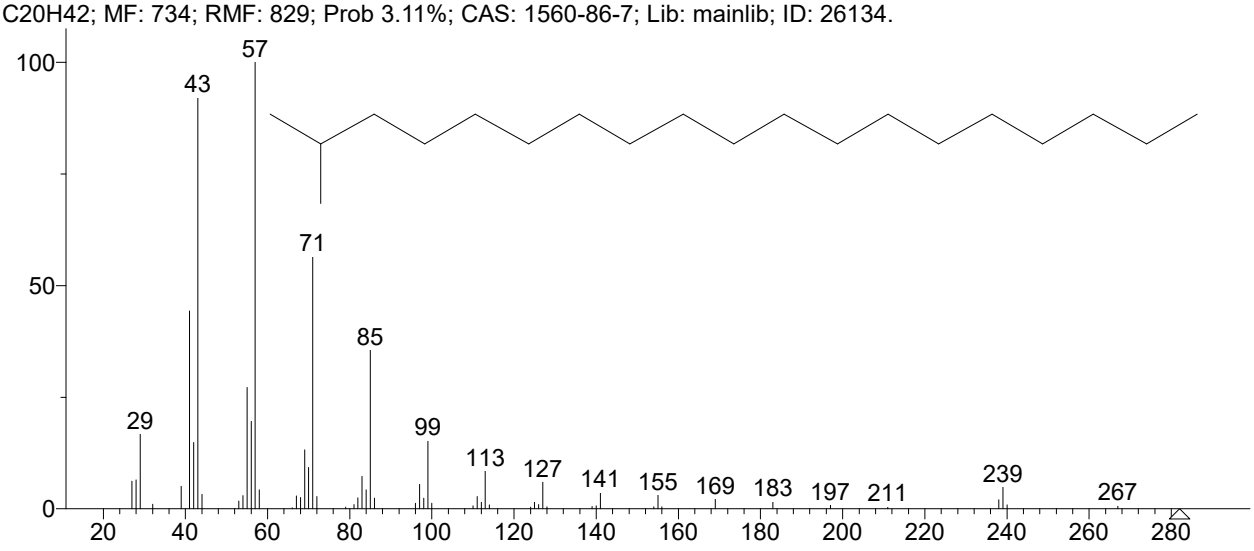


(mainlib) Heptadecane, 2,6,10,15-tetramethyl-

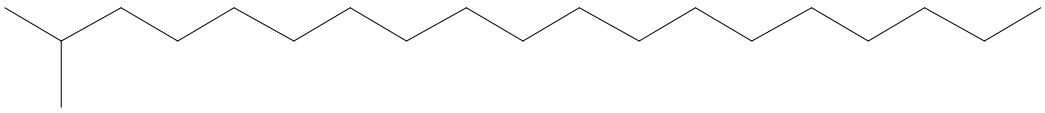


Name: Heptadecane, 2,6,10,15-tetramethyl-
Formula: $C_{21}H_{44}$
MW: 296 Exact Mass: 296.344301 CAS#: 54833-48-6 NIST#: 14103 ID#: 27289 DB: mainlib
Other DBs: None
Contributor: W. VAN HOEVEN, UNIV. OF CALIFORNIA, BERKELEY, USA
InChIKey: ZZEQNXPBKOFTBG-UHFFFAOYSA-N Non-stereo
10 largest peaks:
57 999 | 71 745 | 43 582 | 85 436 | 55 291 | 41 228 | 56 191 | 69 145 | 70 114 | 99 109 |
Synonyms:
1.2,6,10,15-Tetramethylheptadecane #

Hit 4 : Nonadecane, 2-methyl-
C20H42; MF: 734; RMF: 829; Prob 3.11%; CAS: 1560-86-7; Lib: mainlib; ID: 26134.

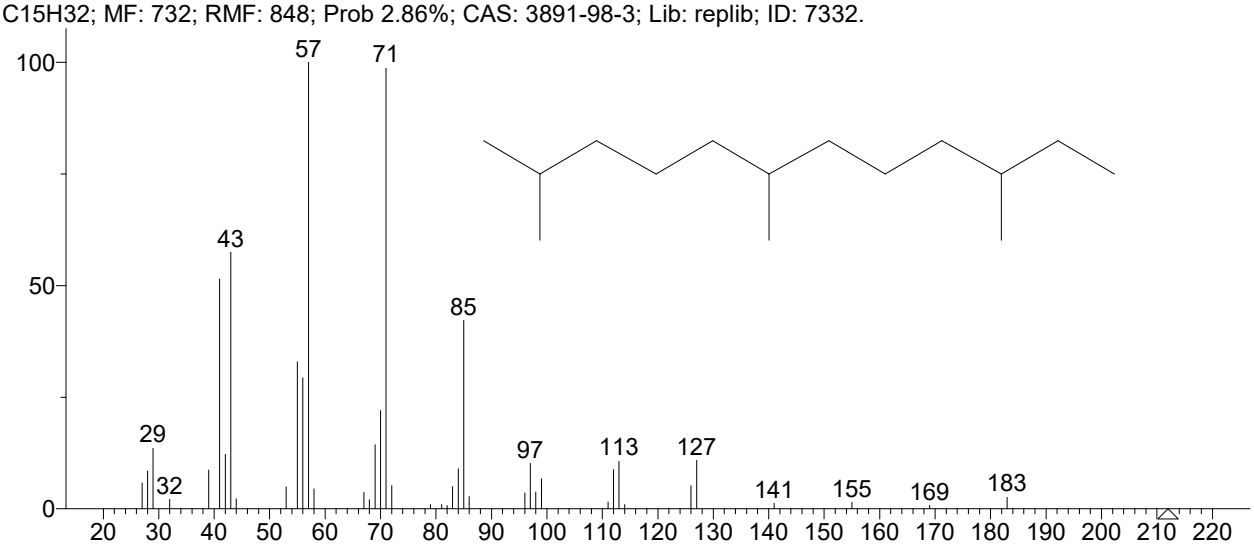


(mainlib) Nonadecane, 2-methyl-

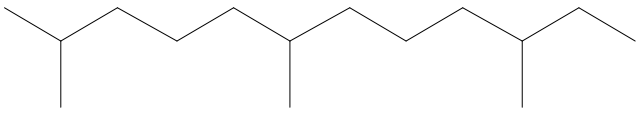


Name: Nonadecane, 2-methyl-
Formula: $C_{20}H_{42}$
MW: 282 Exact Mass: 282.328651 CAS#: 1560-86-7 NIST#: 113882 ID#: 26134 DB: mainlib
Other DBs: IRDB
Contributor: NIST Mass Spectrometry Data Center, 1990.
InChIKey: LEEDMQGKBNGPDN-UHFFFAOYSA-N Non-stereo
10 largest peaks:
57 999 | 43 919 | 71 563 | 41 442 | 85 355 | 55 271 | 56 195 | 29 167 | 99 152 | 42 148 |
Synonyms:
1.2-Methylnonadecane

Hit 5 : Dodecane, 2,6,10-trimethyl-
C15H32; MF: 732; RMF: 848; Prob 2.86%; CAS: 3891-98-3; Lib: replib; ID: 7332.

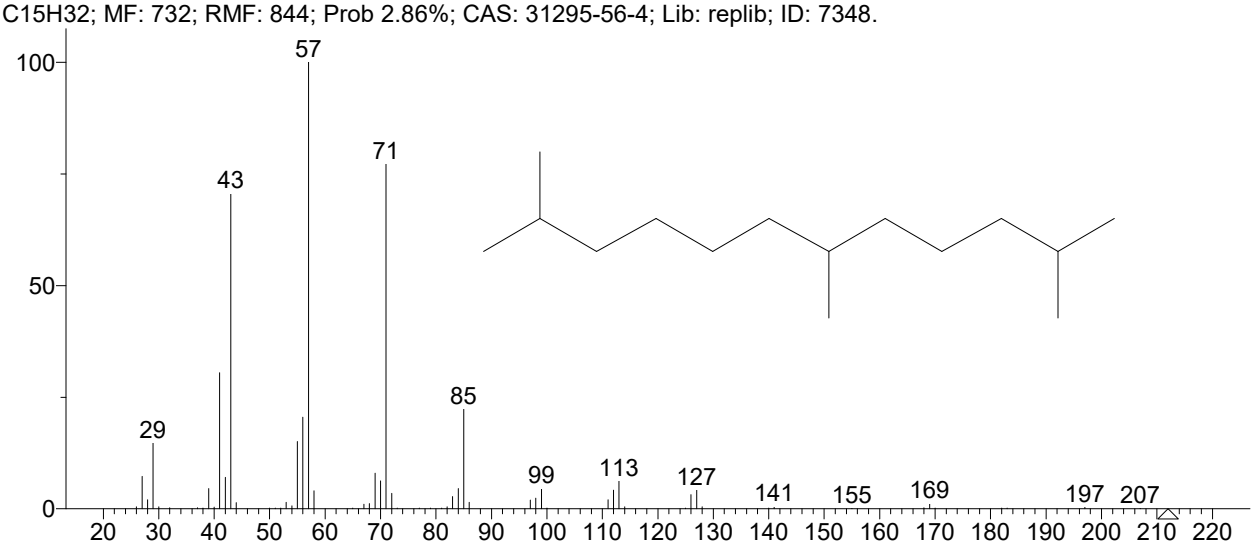


(replib) Dodecane, 2,6,10-trimethyl-

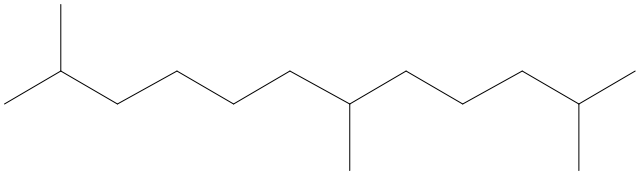


Name: Dodecane, 2,6,10-trimethyl-
Formula: $C_{15}H_{32}$
MW: 212 Exact Mass: 212.2504015 CAS#: 3891-98-3 NIST#: 114045 ID#: 7332 DB: replib
Other DBs: Fine, IRDB
Contributor: NIST Mass Spectrometry Data Center, 1990.
InChIKey: YFHFHLSMISYUAQ-UHFFFAOYSA-N Non-stereo
10 largest peaks:
57 999 | 71 986 | 43 573 | 41 513 | 85 421 | 55 328 | 56 292 | 70 219 | 69 143 | 29 136 |
Synonyms:
1.Farnesan
2.Farnesane
3.2,6,10-Trimethyldodecane

Hit 6 : Dodecane, 2,6,11-trimethyl-
C15H32; MF: 732; RMF: 844; Prob 2.86%; CAS: 31295-56-4; Lib: replib; ID: 7348.

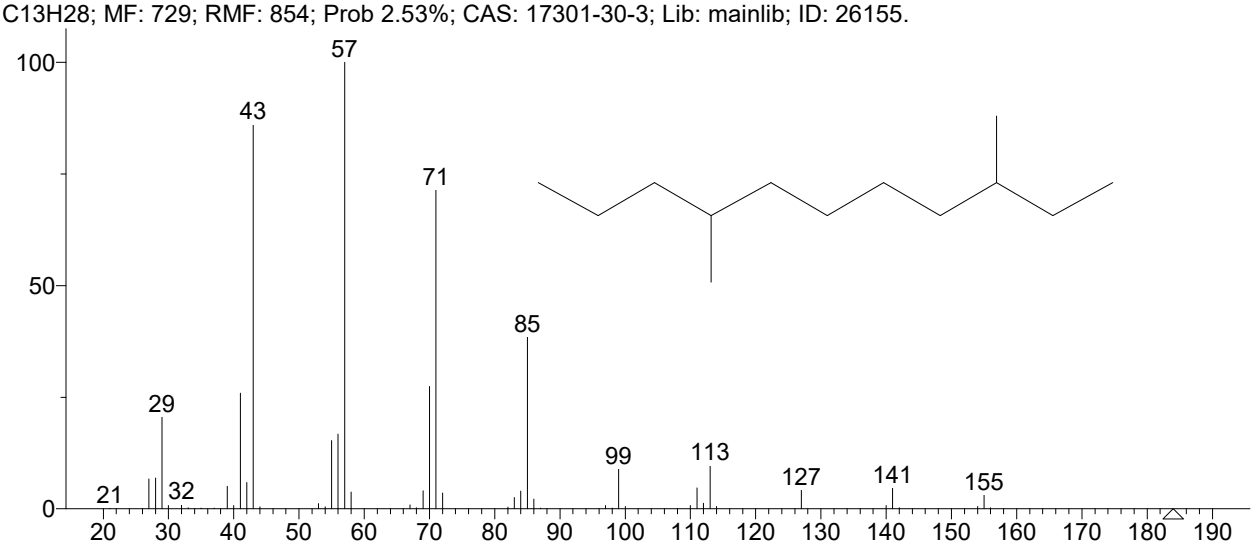


(replib) Dodecane, 2,6,11-trimethyl-

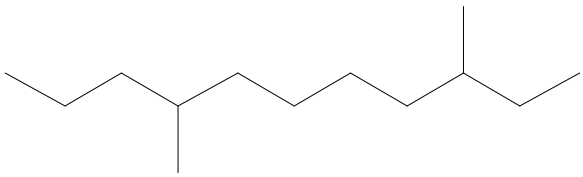


Name: Dodecane, 2,6,11-trimethyl-
Formula: $C_{15}H_{32}$
MW: 212 Exact Mass: 212.2504015 CAS#: 31295-56-4 NIST#: 62130 ID#: 7348 DB: replib
Other DBs: HODOC, IRDB
Contributor: D.HENNEBERG, MAX-PLANCK INSTITUTE, MULHEIM, WEST GERMANY
InChIKey: FONXOARHSFUBAN-UHFFFAOYSA-N Non-stereo
10 largest peaks:
57 999 | 71 770 | 43 704 | 41 304 | 85 222 | 56 204 | 55 150 | 29 147 | 69 79 | 27 72 |
Synonyms:
1.2,6,11-Trimethyldodecane

Hit 7 : Undecane, 3,8-dimethyl-
C13H28; MF: 729; RMF: 854; Prob 2.53%; CAS: 17301-30-3; Lib: mainlib; ID: 26155.

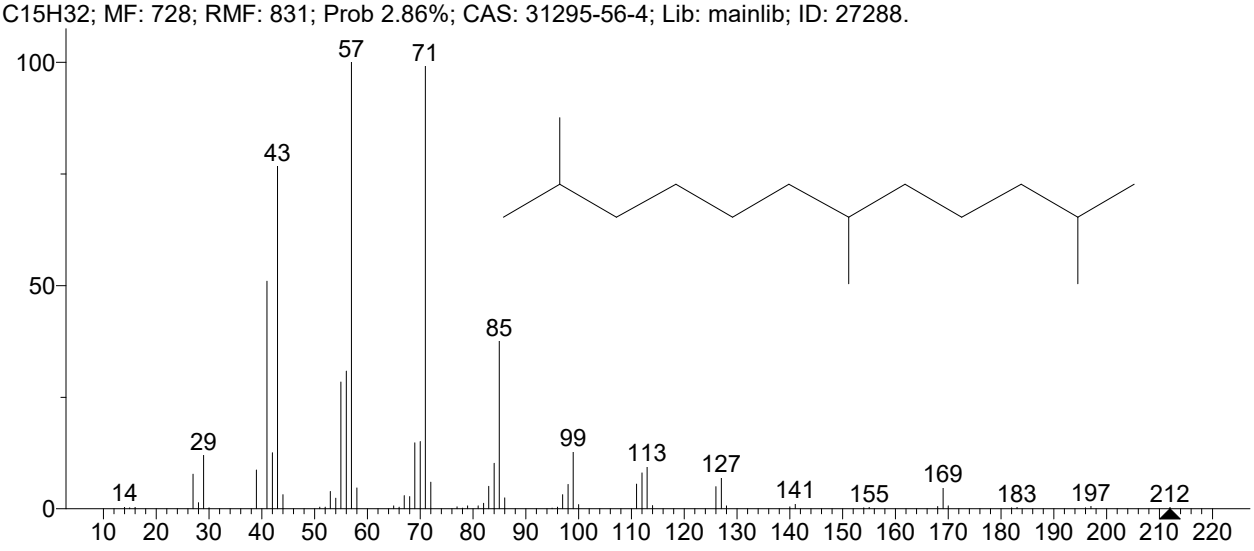


(mainlib) Undecane, 3,8-dimethyl-

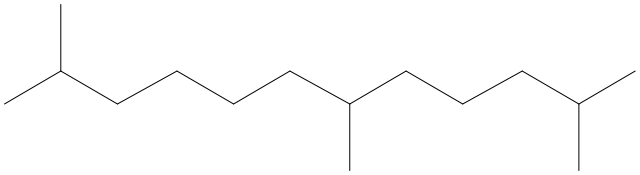


Name: Undecane, 3,8-dimethyl-
Formula: $C_{13}H_{28}$
MW: 184 Exact Mass: 184.219101 CAS#: 17301-30-3 NIST#: 60745 ID#: 26155 DB: mainlib
Other DBs: None
Contributor: D.HENNEBERG, MAX-PLANCK INSTITUTE, MULHEIM, WEST GERMANY
InChIKey: WOGVWUCXENBLIV-UHFFFAOYSA-N Non-stereo
10 largest peaks:
57 999 | 43 859 | 71 712 | 85 383 | 70 273 | 41 258 | 29 205 | 56 166 | 55 152 | 113 96 |
Synonyms:
1.3,8-Dimethylundecane #

Hit 8 : Dodecane, 2,6,11-trimethyl-
C15H32; MF: 728; RMF: 831; Prob 2.86%; CAS: 31295-56-4; Lib: mainlib; ID: 27288.

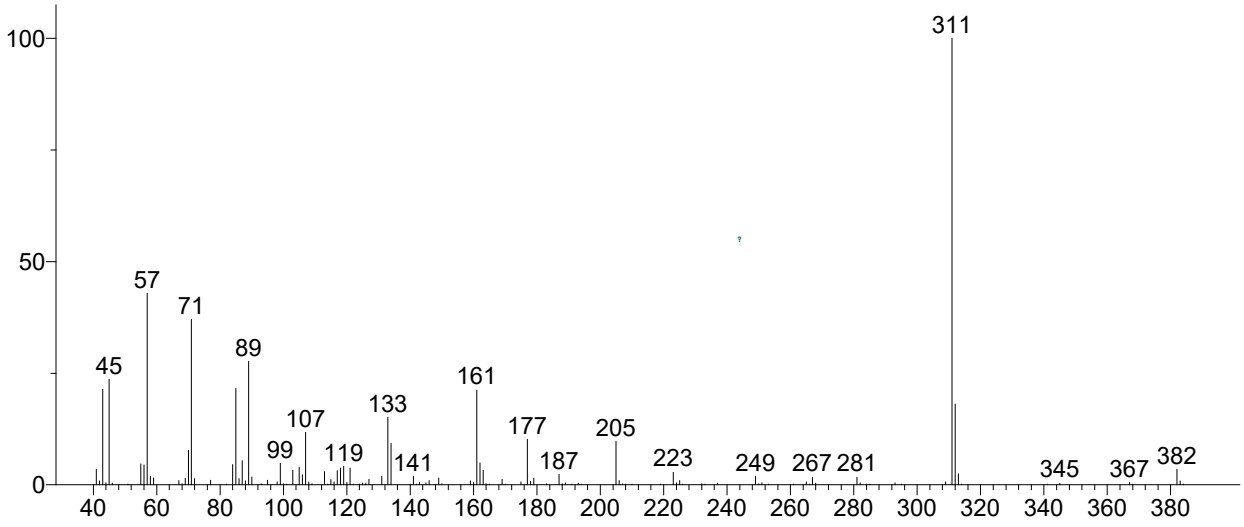


(mainlib) Dodecane, 2,6,11-trimethyl-



Name: Dodecane, 2,6,11-trimethyl-
Formula: $C_{15}H_{32}$
MW: 212 Exact Mass: 212.2504015 CAS#: 31295-56-4 NIST#: 114223 ID#: 27288 DB: mainlib
Other DBs: HODOC, IRDB
Contributor: NIST Mass Spectrometry Data Center, 1990.
InChIKey: FONXOARHSFUBAN-UHFFFAOYSA-N Non-stereo
10 largest peaks:
57 999 | 71 989 | 43 766 | 41 508 | 85 375 | 56 307 | 55 283 | 70 150 | 69 147 | 99 128 |
Synonyms:
1.2,6,11-Trimethyldodecane

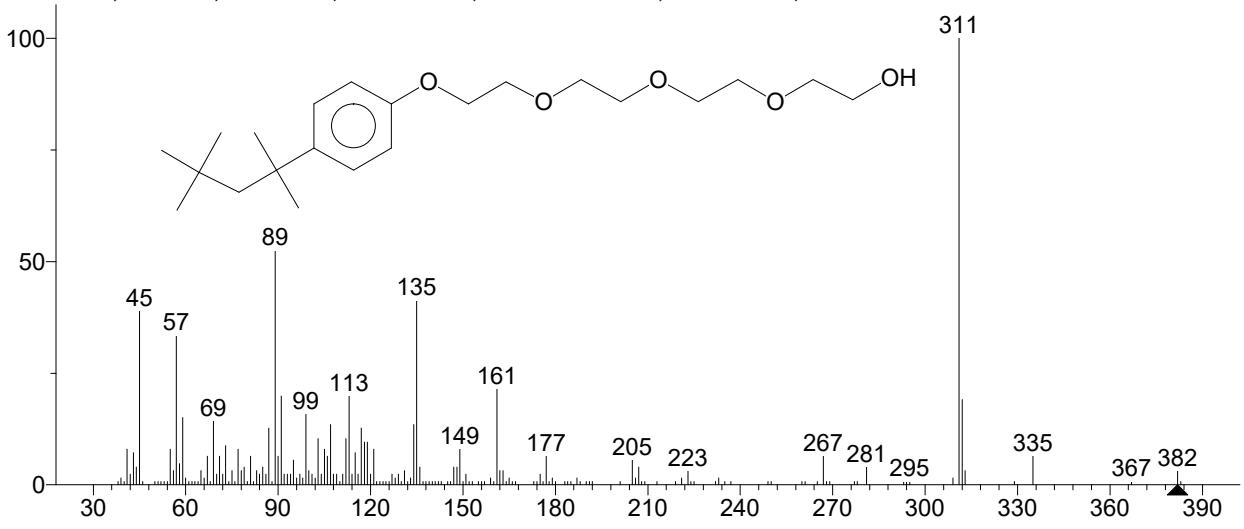
Unknown; InLib=-383



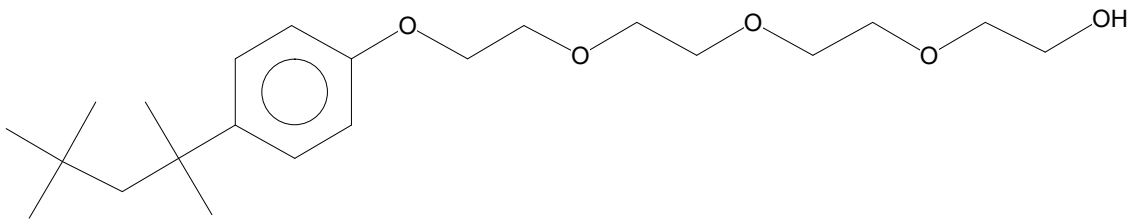
(Text File) +EI Scan (rt: 6.205-6.270 min, 24 scans) Frag=70.0V Negative Control 1.D Subtract (2)

Name: +EI Scan (rt: 6.205-6.270 min, 24 scans) Frag=70.0V Negative Control 1.D Subtract (2)
MW: N/A ID#: 590 DB: Text File
10 largest peaks:
311 999 | 57 428 | 71 371 | 89 276 | 45 236 | 85 215 | 43 213 | 161 213 | 312 180 | 133 151 |
Synonyms:
no synonyms.

Hit 1 : Ethanol, 2-[2-[2-[2-[p-(1,1,3,3-tetramethylbutyl)phenoxy]ethoxy]ethoxy]ethoxy]-
C22H38O5; MF: 682; RMF: 686; Prob 67.1%; CAS: 2315-63-1; Lib: mainlib; ID: 250209.

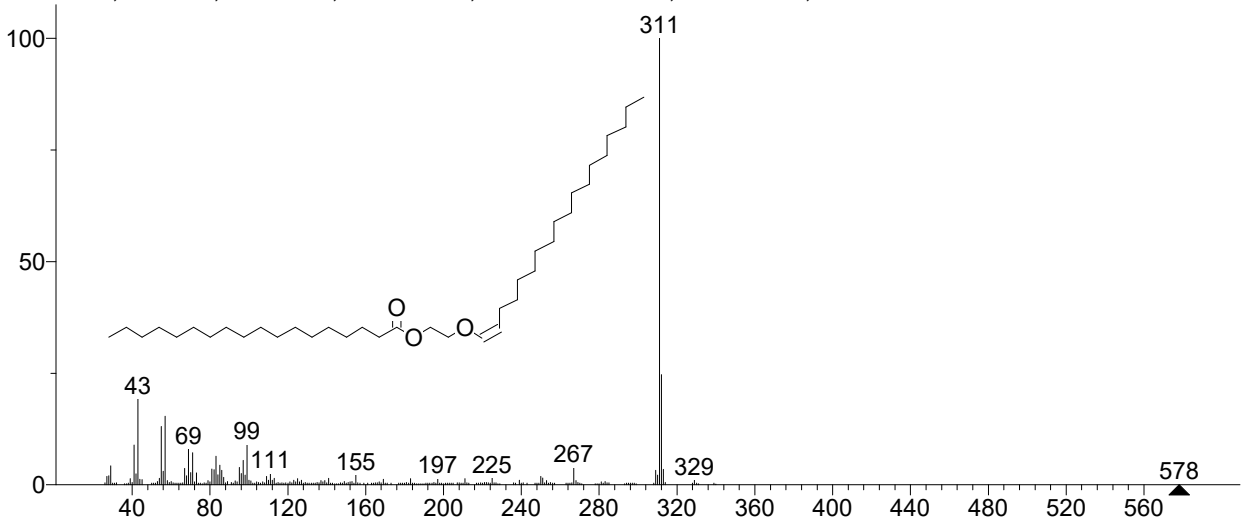


(mainlib) Ethanol, 2-[2-[2-[2-[p-(1,1,3,3-tetramethylbutyl)phenoxy]ethoxy]ethoxy]ethoxy]-

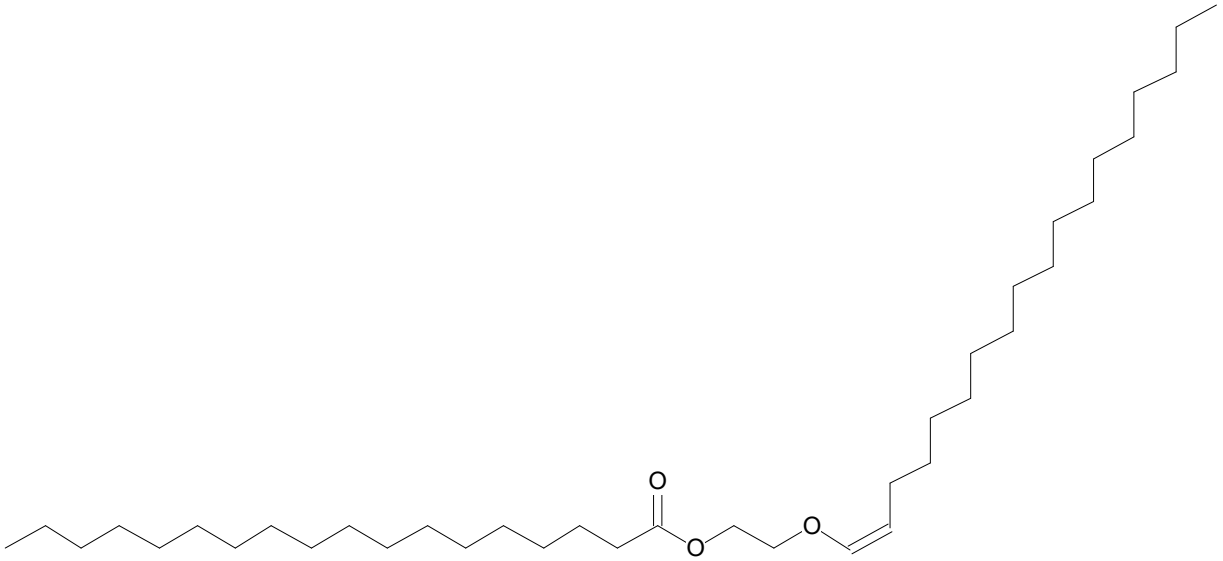


Name: Ethanol, 2-[2-[2-[2-[p-(1,1,3,3-tetramethylbutyl)phenoxy]ethoxy]ethoxy]ethoxy]-
Formula: $C_{22}H_{38}O_5$
MW: 382 Exact Mass: 382.271925 CAS#: 2315-63-1 NIST#: 59549 ID#: 250209 DB: mainlib
Other DBs: None
Contributor: R.A. HITES, MIT, CAMBRIDGE, MASS, USA.
InChIKey: UYDLBVPAAFVANX-UHFFFAOYSA-N Non-stereo
10 largest peaks:
311 999 | 89 523 | 135 412 | 45 388 | 57 333 | 161 214 | 91 198 | 113 198 | 312 190 | 99 158 |
Synonyms:
1.2-[2-(2-(2-[4-(1,1,3,3-Tetramethylbutyl)phenoxy]ethoxy)ethoxy)ethoxy]ethanol #

Hit 2 : Stearic acid, 2-(1-octadecenyloxy)ethyl ester, (Z)-
C38H74O3; MF: 601; RMF: 618; Prob 7.11%; CAS: 30760-05-5; Lib: mainlib; ID: 250317.

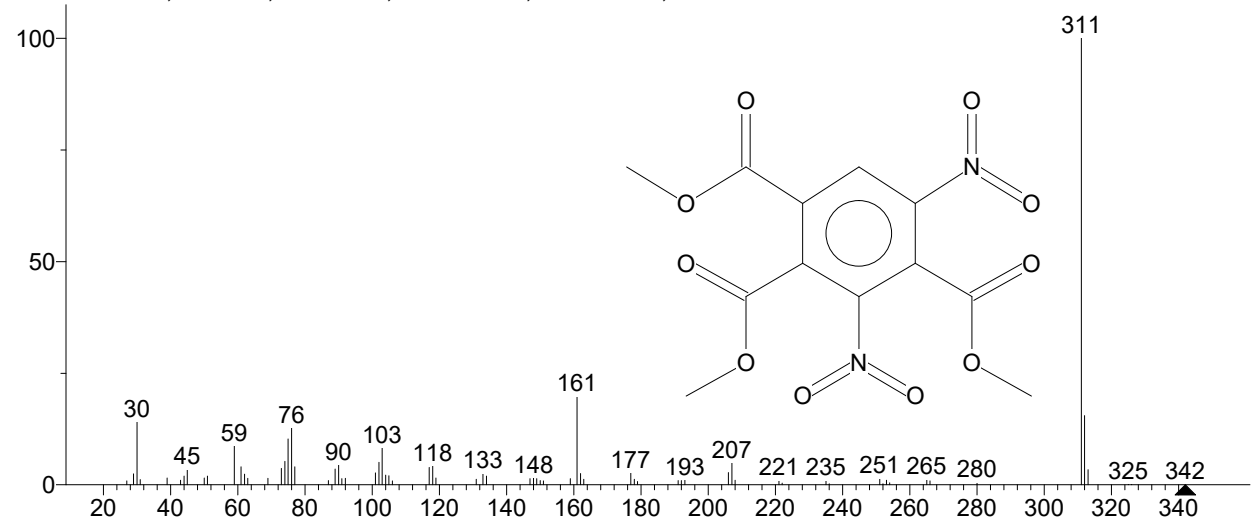


(mainlib) Stearic acid, 2-(1-octadecenyloxy)ethyl ester, (Z)-

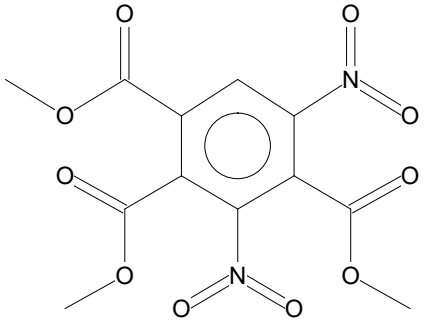


Name: Stearic acid, 2-(1-octadecenyloxy)ethyl ester, (Z)-
Formula: $C_{38}H_{74}O_3$
MW: 578 Exact Mass: 578.563797 CAS#: 30760-05-5 NIST#: 36287 ID#: 250317 DB: mainlib
Other DBs: None
Contributor: R.T.HOLMAN,UNIVERSITY OF MINNESOTA
InChIKey: SNTPMLQNCPCOIJ-OAPYJULQSA-N Non-stereo
10 largest peaks:
311 999 | 312 246 | 43 192 | 57 153 | 55 130 | 99 90 | 41 88 | 69 79 | 71 71 | 83 63 |
Synonyms:
1.2-[(1Z)-1-Octadecenyloxy]ethyl stearate #

Hit 3 : 1,2,4-Benzenetricarboxylic acid, 3,5-dinitro-, trimethyl ester
C12H10N2O10; MF: 600; RMF: 751; Prob 6.83%; Lib: mainlib; ID: 250243.

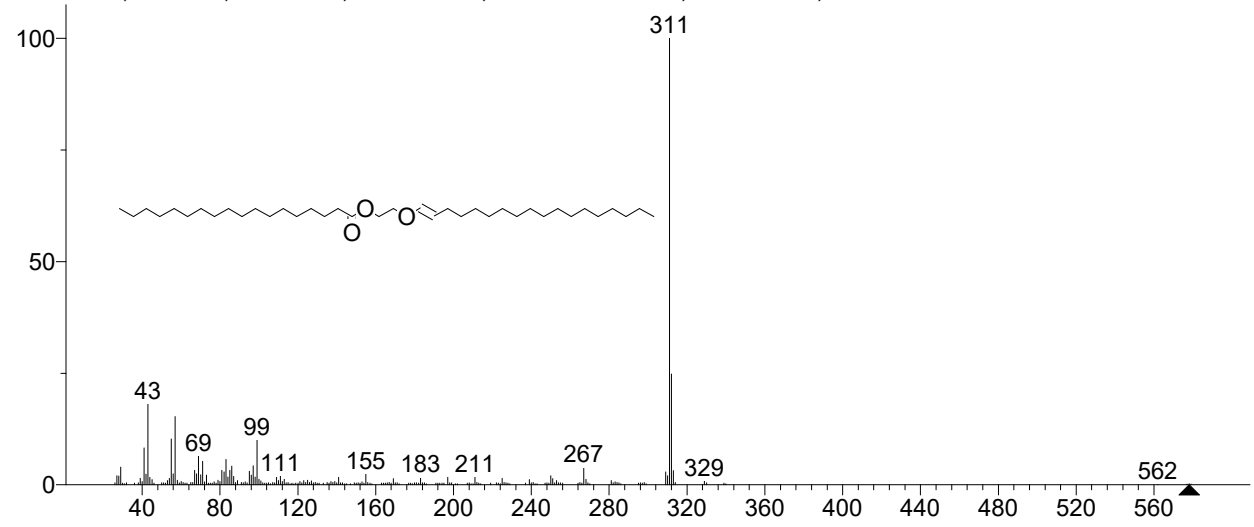


(mainlib) 1,2,4-benzenetricarboxylic acid, 3,5-dinitro-, trimethyl ester

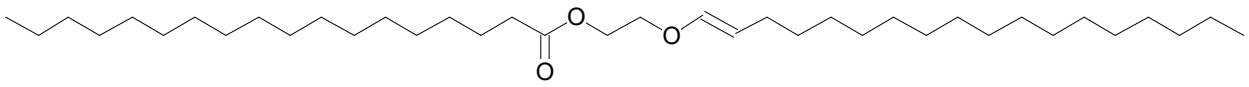


Name: 1,2,4-benzenetricarboxylic acid, 3,5-dinitro-, trimethyl ester
Formula: $C_{12}H_{10}N_2O_{10}$
MW: 342 Exact Mass: 342.033545 NIST#: 398225 ID#: 250243 DB: mainlib
Contributor: J. Little, Eastman chemical company.
InChIKey: QMPATDFNKWPHGV-UHFFFAOYSA-N Non-stereo
10 largest peaks:
311 999 | 161 197 | 312 154 | 30 140 | 76 127 | 75 102 | 59 87 | 103 82 | 74 52 | 102 50 |
Synonyms:
1.trimethyl 3,5-dinitrobenzene-1,2,4-tricarboxylate

Hit 4 : Stearic acid, 2-(1-octadecenyloxy)ethyl ester, (E)-
C38H74O3; MF: 584; RMF: 643; Prob 3.93%; CAS: 30760-06-6; Lib: mainlib; ID: 250318.

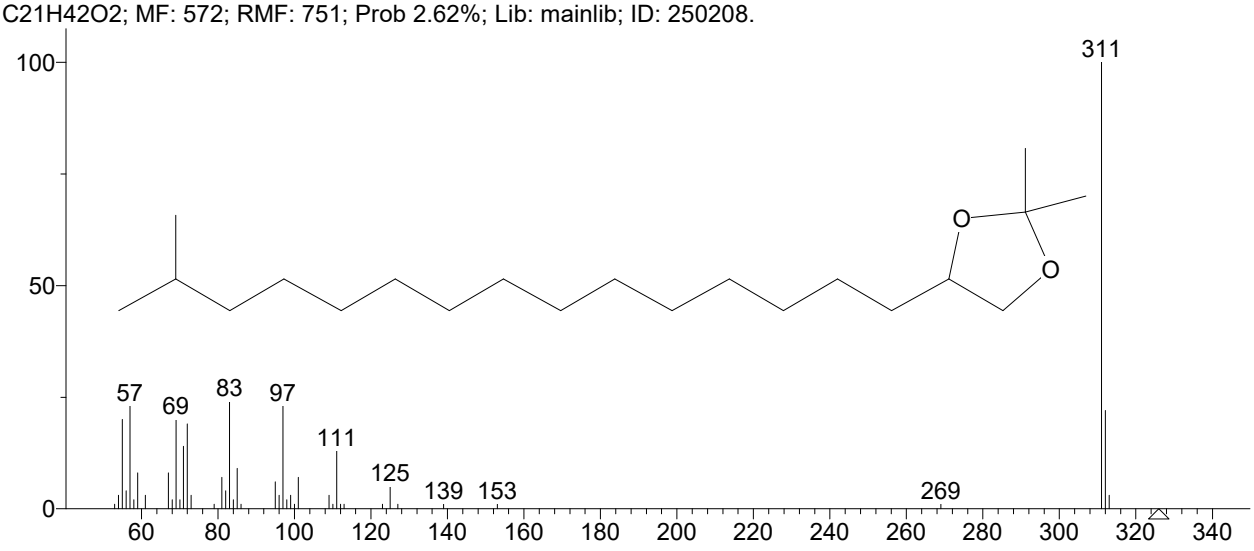


(mainlib) Stearic acid, 2-(1-octadecenyloxy)ethyl ester, (E)-

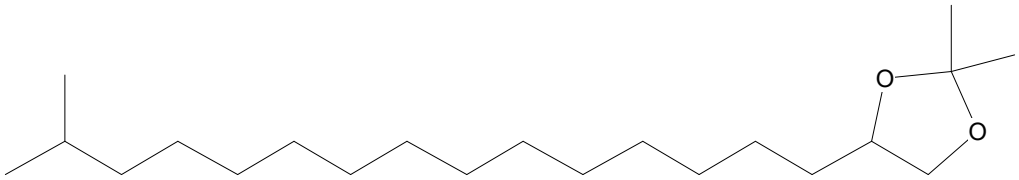


Name: Stearic acid, 2-(1-octadecenyloxy)ethyl ester, (E)-
Formula: $C_{38}H_{74}O_3$
MW: 578 Exact Mass: 578.563797 CAS#: 30760-06-6 NIST#: 36286 ID#: 250318 DB: mainlib
Other DBs: None
Contributor: R.T.HOLMAN,UNIVERSITY OF MINNESOTA
InChIKey: SNTPMLQNCPCOIJ-LAPDZXRHSA-N Non-stereo
10 largest peaks:
311 999 | 312 247 | 43 180 | 57 152 | 55 102 | 99 100 | 41 82 | 69 63 | 83 56 | 71 52 |
Synonyms:
1.2-[(1E)-1-Octadecenyloxy]ethyl stearate #

Hit 5 : 16-Methyl-heptadecane-1,2-diol, isopropylidene derivative
C21H42O2; MF: 572; RMF: 751; Prob 2.62%; Lib: mainlib; ID: 250208.

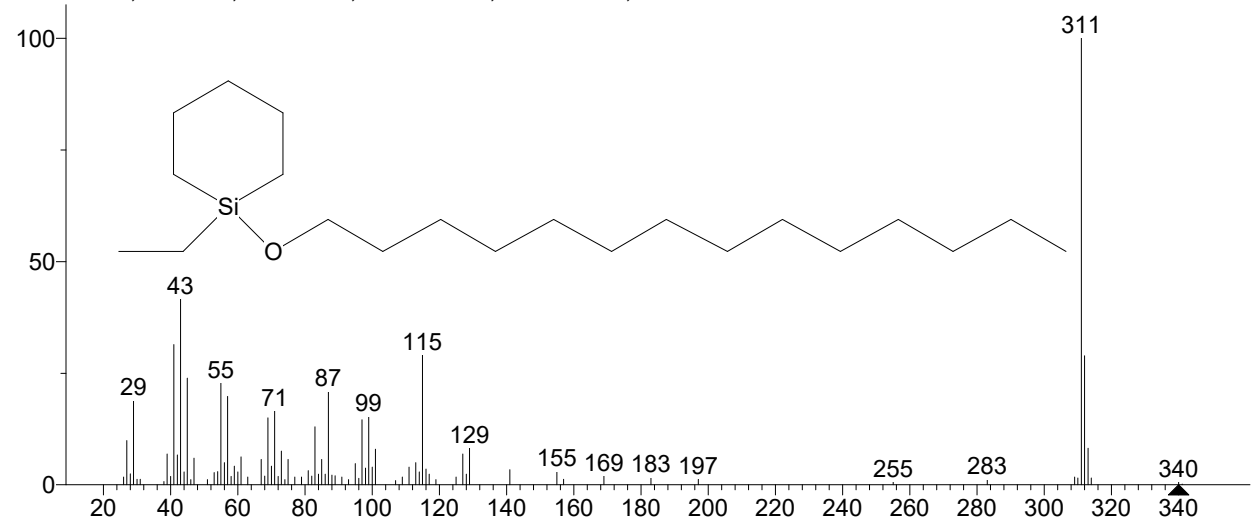


(mainlib) 16-Methyl-heptadecane-1,2-diol, isopropylidene derivative

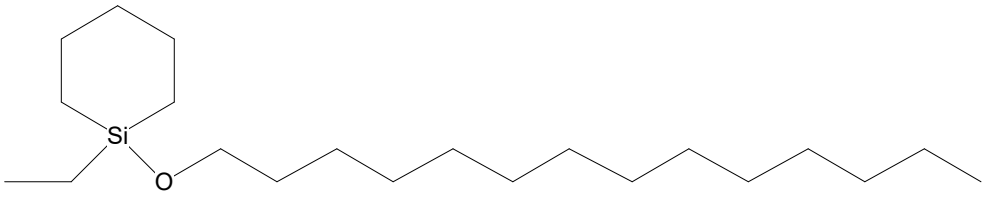


Name: 16-Methyl-heptadecane-1,2-diol, isopropylidene derivative
Formula: $C_{21}H_{42}O_2$
MW: 326 Exact Mass: 326.318481 NIST#: 336669 ID#: 250208 DB: mainlib
Contributor: William W. Christie, Mylnefield Lipid Analysis, Invergowrie, Dundee, Scotland, UK
InChIKey: KEEBDRWAHRUZHX-UHFFFAOYSA-N Non-stereo
10 largest peaks:
311 999 | 83 239 | 57 229 | 97 229 | 312 219 | 55 199 | 69 199 | 72 189 | 71 139 | 111 129 |
Synonyms:
no synonyms.

Hit 6 : 1-Ethyl-1-tetradecyloxy-1-silacyclohexane
C21H44OSi; MF: 558; RMF: 685; Prob 1.64%; Lib: mainlib; ID: 250182.

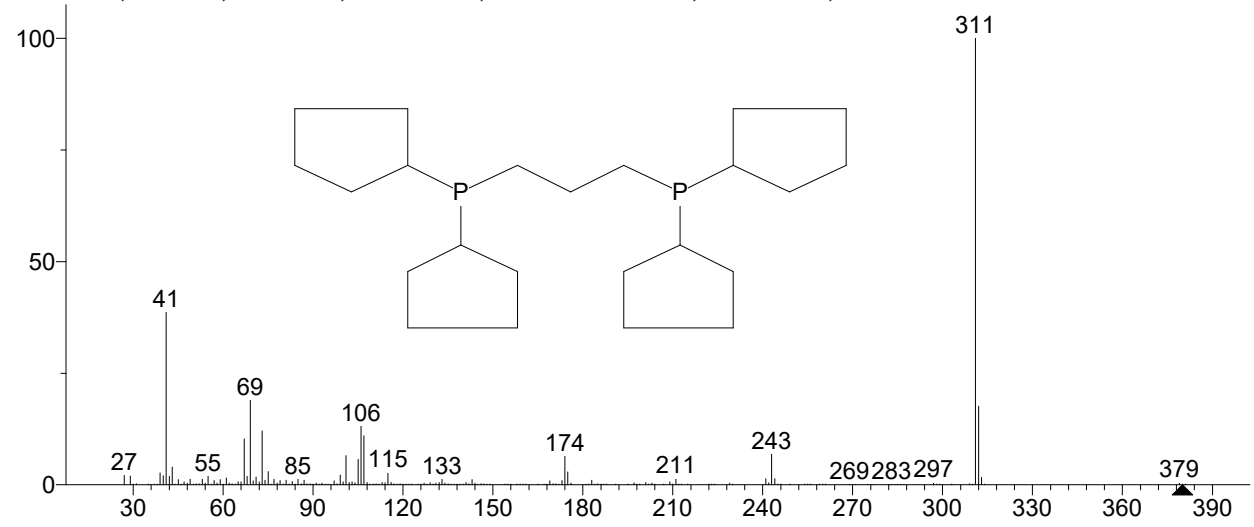


(mainlib) 1-Ethyl-1-tetradecyloxy-1-silacyclohexane

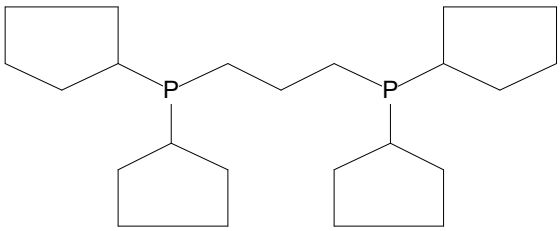


Name: 1-Ethyl-1-tetradecyloxy-1-silacyclohexane
Formula: $C_{21}H_{44}OSi$
MW: 340 Exact Mass: 340.316143 NIST#: 279384 ID#: 250182 DB: mainlib
Contributor: V.G.Zaikin, TIPS RAS, Moscow, Russia
InChIKey: MVQXXWLQNRLPCH-UHFFFAOYSA-N Non-stereo
10 largest peaks:
311 999 | 43 415 | 41 313 | 115 289 | 312 288 | 45 238 | 55 228 | 87 208 | 57 197 | 29 188 |
Synonyms:
1.1-Ethyl-1-(tetradecyloxy)silinane #

Hit 7 : Propane, 1,3-bis(dicyclopentylphosphino)-
C23H42P2; MF: 558; RMF: 636; Prob 1.64%; CAS: 149081-88-9; Lib: mainlib; ID: 250178.

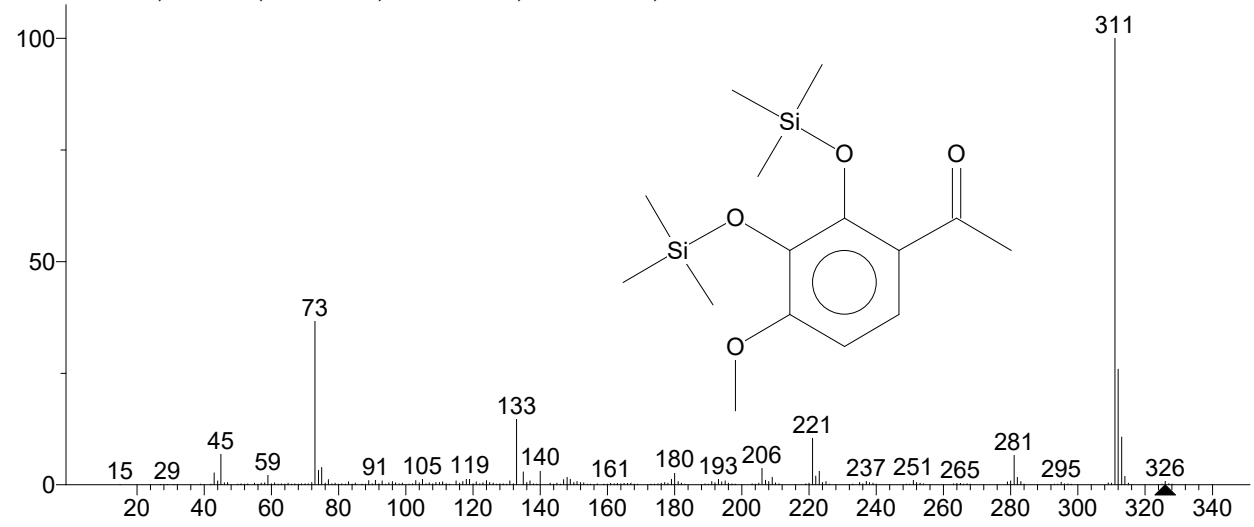


(mainlib) Propane, 1,3-bis(dicyclopentylphosphino)-

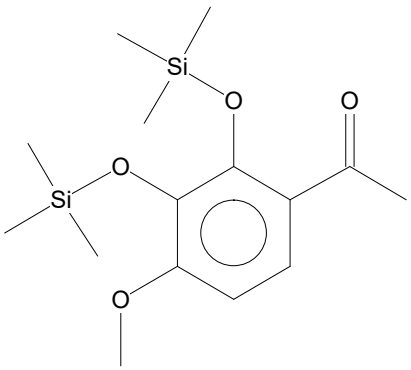


Name: Propane, 1,3-bis(dicyclopentylphosphino)-
Formula: $C_{23}H_{42}P_2$
MW: 380 Exact Mass: 380.276175 CAS#: 149081-88-9 NIST#: 161296 ID#: 250178 DB: mainlib
Other DBs: None
Contributor: Chemical Concepts
InChIKey: XNDWOYYSZZBBEJ-UHFFFAOYSA-N Non-stereo
10 largest peaks:
311 999 | 41 385 | 69 189 | 312 175 | 106 131 | 73 120 | 107 109 | 67 102 | 243 69 | 101 65 |
Synonyms:
1.Dicyclopentyl[3-(dicyclopentylphosphino)propyl]phosphine #

Hit 8 : Gallacetophenone-4'-methylether, bis(trimethylsilyl) ether
C15H26O4Si2; MF: 557; RMF: 577; Prob 1.57%; Lib: mainlib; ID: 250200.

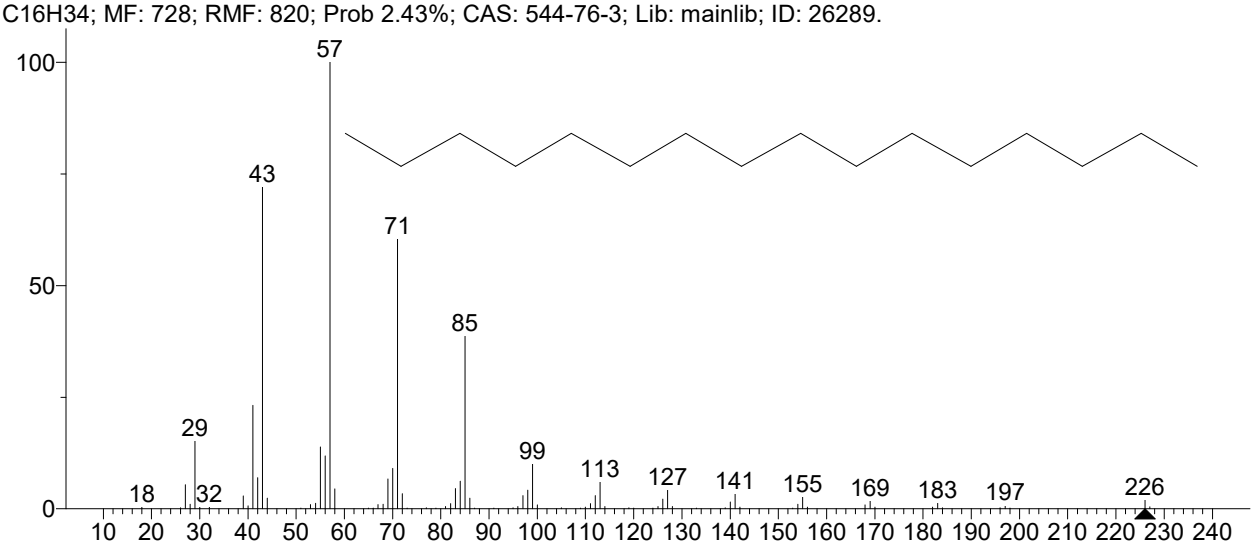


(mainlib) Gallacetophenone-4'-methylether, bis(trimethylsilyl) ether

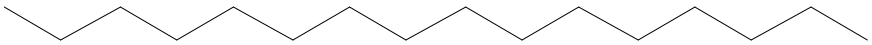


Name: Gallacetophenone-4'-methylether, bis(trimethylsilyl) ether
Formula: $C_{15}H_{26}O_4Si_2$
MW: 326 Exact Mass: 326.136963 NIST#: 462955 ID#: 250200 DB: mainlib
Contributor: NIST Mass Spectrometry Data Center, 2016
InChIKey: UALJQPKMVPEAMK-UHFFFAOYSA-N Non-stereo
10 largest peaks:
311 999 | 73 366 | 312 258 | 133 146 | 313 106 | 221 104 | 45 69 | 281 66 | 75 38 | 206 37 |
Synonyms:
no synonyms.

Hit 9 : Hexadecane
C16H34; MF: 728; RMF: 820; Prob 2.43%; CAS: 544-76-3; Lib: mainlib; ID: 26289.

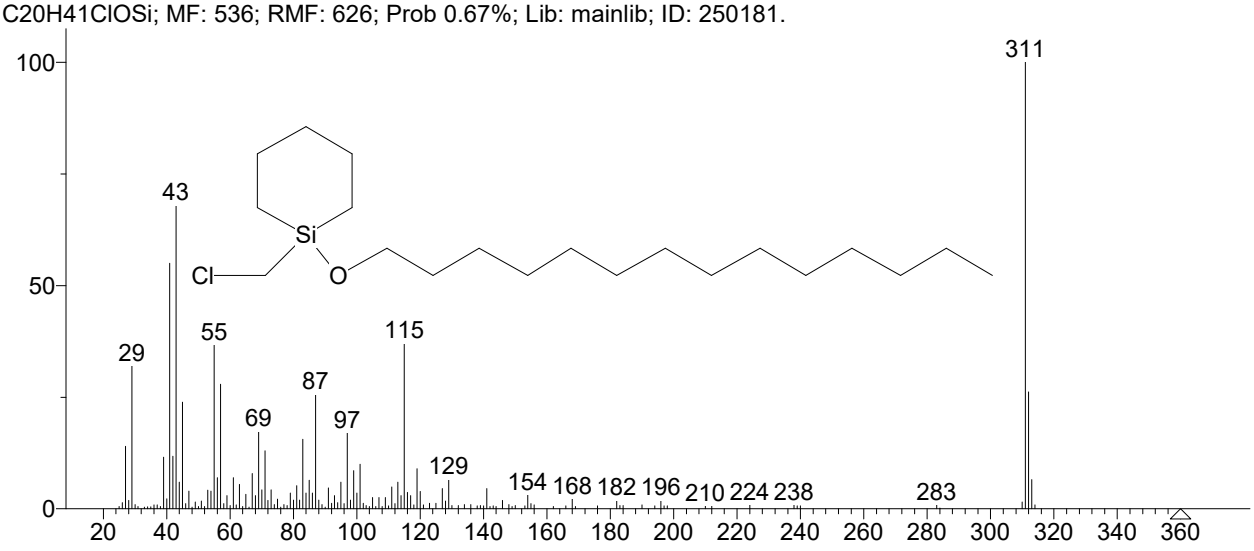


(mainlib) Hexadecane

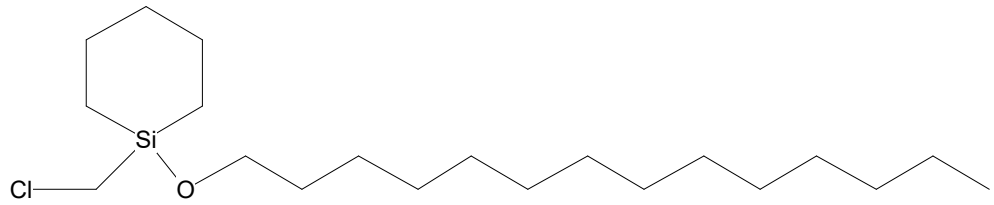


Name: Hexadecane
Formula: $C_{16}H_{34}$
MW: 226 Exact Mass: 226.266051 CAS#: 544-76-3 NIST#: 228773 ID#: 26289 DB: mainlib
Other DBs: Fine, TSCA, RTECS, EPA, HODOC, NIH, EINECS, IRDB
Contributor: Japan AIST/NIMC Database- Spectrum MS-NW-1507
InChIKey: DCAYPVUWAIABOU-UHFFFAOYSA-N Non-stereo
10 largest peaks:
57 999 | 43 719 | 71 603 | 85 385 | 41 231 | 29 151 | 55 138 | 56 118 | 99 100 | 70 90 |
Synonyms:
1.n-Cetane
2.n-Hexadecane
3.Cetane

Hit 9 : 1-Chloromethyl-1-tetradecyloxy-1-silacyclohexane
C20H41ClOSi; MF: 536; RMF: 626; Prob 0.67%; Lib: mainlib; ID: 250181.



(mainlib) 1-Chloromethyl-1-tetradecyloxy-1-silacyclohexane



Name: 1-Chloromethyl-1-tetradecyloxy-1-silacyclohexane
Formula: $C_{20}H_{41}ClOSi$
MW: 360 Exact Mass: 360.26152 NIST#: 279342 ID#: 250181 DB: mainlib
Contributor: V.G.Zaikin, TIPS RAS, Moscow, Russia
InChIKey: ITXLGLXYHPJQCH-UHFFFAOYSA-N Non-stereo
10 largest peaks:
311 999 | 43 678 | 41 548 | 115 369 | 55 365 | 29 319 | 57 278 | 312 261 | 87 255 | 45 238 |
Synonyms:
1.1-(Chloromethyl)-1-(tetradecyloxy)silinane #