H/F Replacement in secondary alcohols of sydnones as examples of isostructural OH····O=C hydrogen bonded dimer structures

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-=SUPPLEMENTARY MATERIAL=-

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1. Relevant secondary alcohol dimers from the literature

| | | | | ANG1 | ANG2 | DIST1 | DIST2 |
|-------|----------|-------|----------|---------|---------|---|---------------------|
| | | | | 0-H…0 | 0-H…0 | H···O | Н…О |
| Index | CCD Ref. | DIMER | Fragment | >150° | >150° | <vdw< th=""><th><vdw< th=""></vdw<></th></vdw<> | <vdw< th=""></vdw<> |
| 1 | ADOHUY | YES | 1 | 175.498 | 173.071 | 1.937 | 1.933 |
| | ADUNAP | NO | 1 | 173.506 | 168.773 | 1.923 | 1.917 |
| 2 | ADUNAP | NO | 2 | 173.506 | 151.576 | 1.923 | 2.031 |
| | ADUNAP | NO | 3 | 151.576 | 168.773 | 2.031 | 1.917 |
| 3 | AKUFIX | NO | 1 | 160.313 | 178.159 | 1.993 | 1.951 |
| 4 | ARAFPY10 | NO | 1 | 158.146 | 154.245 | 1.947 | 1.991 |
| 5 | AZELAV | NO | 1 | 177.711 | 154.421 | 1.969 | 1.934 |
| 6 | BARJOX | NO | 1 | 163.534 | 154.156 | 2.006 | 2.024 |
| 7 | BUQDIC | NO | 1 | 160.662 | 160.103 | 2.009 | 2.09 |
| 8 | BUVFAA | NO | 1 | 169.063 | 158.963 | 2.033 | 1.913 |
| 9 | CAQRUH | NO | 1 | 164.587 | 173.054 | 2.012 | 1.948 |
| 10 | CEHDAX | NO | 1 | 152.591 | 172.274 | 2.036 | 2.008 |
| 11 | COBQEP | NO | 1 | 158.045 | 167.558 | 2.036 | 1.982 |
| | COKKIY | | 1 | 170.713 | 159.461 | 2.088 | 2.02 |
| 12 | COKKIY | | 2 | 170.62 | 159.461 | 2.051 | 2.02 |
| | COKKIY | YES | 3 | 170.62 | 170.713 | 2.051 | 2.088 |
| 13 | CUQJII | NO | 1 | 173.469 | 169.002 | 1.948 | 1.987 |
| | DUNFEY | NO | 1 | 171.677 | 155.669 | 1.922 | 2.095 |
| | DUNFEY | NO | 2 | 154.725 | 171.677 | 2.04 | 1.922 |
| 14 | DUNFEY | NO | 3 | 154.725 | 155.669 | 2.04 | 2.095 |
| | EBOPOE | NO | 1 | 153.469 | 156.929 | 1.972 | 1.931 |
| | EBOPOE | NO | 2 | 155.407 | 153.469 | 2.241 | 1.972 |
| | EBOPOE | NO | 3 | 155.407 | 156.929 | 2.241 | 1.931 |
| 15 | EDEMOR | YES | 1 | 153.18 | 162.555 | 2.028 | 1.975 |
| 16 | EGALAB | YES | 1 | 172.271 | 178.141 | 1.942 | 1.923 |
| 17 | ELEJUB01 | YES | 1 | 164.113 | 174.283 | 1.897 | 1.864 |
| 18 | ELEKAI01 | YES | 1 | 179.295 | 177.757 | 1.83 | 1.83 |
| 19 | EZEPEF | YES | 1 | 152.996 | 150.364 | 2.105 | 2.179 |
| | FELNIU | NO | 1 | 168.236 | 168.524 | 1.927 | 1.89 |
| 20 | FELNIU | NO | 2 | 168.236 | 164.13 | 1.927 | 1.99 |
| | FELNIU | NO | 3 | 164.13 | 168.524 | 1.99 | 1.89 |
| 21 | FIBMIQ | NO | 1 | 174.141 | 176.153 | 1.977 | 1.936 |
| 22 | FIDSES | NO | 1 | 154.691 | 177.031 | 1.999 | 2.104 |
| 23 | FIQDOZ | YES | 1 | 150.797 | 150.797 | 2.244 | 2.244 |
| 24 | FLOCOS | NO | 1 | 154.383 | 154.383 | 2.21 | 2.21 |
| 25 | FUHYAL | YES | 1 | 168.845 | 178.438 | 2.022 | 1.992 |
| 26 | GEGRAP | NO | 1 | 166.971 | 158.007 | 2.001 | 2.108 |
| 27 | GEJPUH | NO | 1 | 166.812 | 161.227 | 2.049 | 2.049 |
| 28 | GOGQEZ | NO | 1 | 164.571 | 163.096 | 2 | 2.064 |
| 29 | HBMHPO10 | YES | 1 | 153.947 | 156.697 | 2.316 | 2.182 |
| 30 | HIJBEK | NO | 1 | 170.71 | 174.596 | 1.973 | 1.969 |
| 31 | HIKWEG | YES | 1 | 166.685 | 160.122 | 1.916 | 1.982 |
| | HIWREM | NO | 1 | 169.477 | 169.258 | 1.947 | 1.929 |
| | HIWREM | NO | 2 | 169.477 | 167.815 | 1.947 | 1.963 |
| | HIWREM | NO | 3 | 169 258 | 167 815 | 1 929 | 1 963 |

Table 1S. Secondary alcohols identified through CCDC search and dimeric -like structures identified

| 32 HIWREM NO 5 163.33 167.815 2.004 1.943 BAQEL NO 1 151.872 156.975 2.32 2.33 BAQEL NO 2 151.872 155.538 2.32 2.33 BAQEL NO 3 155.538 1.56.975 2.229 2.33 JARADE NO 1 160.0758 168.136 2.029 1.839 35 IRAGEP NO 1 170.403 168.492 1.939 1.995 36 ISAFEQ YES 1 171.083 165.432 2.121 2.157 36 ISAFEQ YES 1 176.343 154.582 2.121 2.157 40 KEBTUK NO 1 154.433 154.582 2.027 4.035 1.81 1.993 2.012 42 KIMPAL YES 1 175.387 1.58.1 1.072 2.012 4.193 43 KIWPAL | | HIWREM | NO | 4 | 163.33 | 169.258 | 2.004 | 1.929 |
|--|-----|----------|-----|---|---------|---------|-------|-------|
| HIWREM NO 6 163.33 169.477 2.004 1.947 BAQEL NO 1 151.872 156.975 2.32 2.33 BAQEL NO 2 151.872 155.538 2.32 2.33 33 ILAROF NO 1 162.033 158.672 1.973 1.977 34 IQONIO NO 1 160.758 168.136 2.029 1.839 35 IRAGEP NO 1 160.758 166.117 1.953 2.08 37 JEVPAF NO 1 154.333 154.582 2.121 1.176 38 JONZUJ NO 1 153.433 154.582 2.121 2.157 39 JUXKAR NO 1 173.742 166.247 1.969 2.233 41 KESTUK NO 1 173.742 165.345 1.871 1.927 KIWPAL YES 1 175.851 1.022 <td< td=""><td>32</td><td>HIWREM</td><td>NO</td><td>5</td><td>163.33</td><td>167.815</td><td>2.004</td><td>1.963</td></td<> | 32 | HIWREM | NO | 5 | 163.33 | 167.815 | 2.004 | 1.963 |
| BAQEL NO 1 151.872 156.975 2.32 2.33 BAQEL NO 2 151.872 155.538 2.32 2.269 33 ILAROF NO 3 155.538 156.975 2.269 1.839 35 IRAGEP NO 1 160.758 168.136 2.029 1.839 35 IRAGEP NO 1 160.758 168.492 1.939 1.995 36 ISAFEQ YES 1 171.043 168.492 1.939 1.995 36 ISAFEQ YES 1 171.043 168.492 1.939 1.953 37 JEVPAF NO 1 154.333 154.582 2.121 2.157 38 JONZUJ NO 1 173.742 166.247 1.969 2.233 41 KEXNFA YES 1 176.458 164.030 1.871 1.927 KIWPAL 2 152.897 158.1 | | HIWREM | NO | 6 | 163.33 | 169.477 | 2.004 | 1.947 |
| BAQEL NO 2 151.872 155.538 2.32 2.269 BAQEL NO 3 155.538 156.975 2.269 2.3 33 ILAROF NO 1 162.603 158.672 1.973 1.973 34 IQONIO NO 1 160.758 168.136 2.029 1.839 35 IRAGEP NO 1 170.403 168.492 1.939 1.995 36 ISAFEQ YES 1 171.085 161.617 1.953 2.083 37 JEVPAF NO 1 153.433 154.582 2.121 2.157 39 JUXKAR NO 1 173.742 166.247 1.969 2.253 41 KEXSIS YES 1 175.895 1.81 1.927 KIWPAL YES 1 150.345 159.895 2.002 1.077 KIWPAL YES 1 172.658 158.1 2.092 | | IBAOEL – | NO | 1 | 151.872 | 156.975 | 2.32 | 2.3 |
| IBAQEL NO 3 155.538 156.975 2.269 2.3 33 ILAROF NO 1 162.603 158.672 1.973 1.977 34 IQONIO NO 1 160.758 168.136 2.029 1.839 35 IRAGEP NO 1 170.403 168.492 1.933 2.08 37 JEVPAF NO 1 169.297 170.141 1.952 1.946 38 JONZU NO 1 153.33 154.582 2.12 2.157 39 JUXKAR NO 1 153.341 70.954 2.032 2.23 41 KESTUK NO 1 153.857 158.1 1.993 2.012 KIWPAL YES 1 176.458 164.305 1.871 1.927 43 KIWPAL 2 152.897 158.1 2.002 2.001 KIWPAL 5 150.345 158.1 2.002 | | IBAOEL | NO | 2 | 151.872 | 155.538 | 2.32 | 2.269 |
| 33 ILAROF NO 1 162.603 158.672 1.973 1.977 34 IQONIO NO 1 160.758 168.136 2.029 1.839 35 IRAGEP NO 1 170.403 168.492 1.939 1.995 36 ISAFEQ YES 1 171.1085 161.617 1.953 2.08 37 JEVPAF NO 1 154.333 154.582 2.121 2.157 39 JUXKAR NO 1 173.742 166.247 1.969 2.253 41 KEXSIS YES 1 179.895 1.881 1.927 KIWPAL 2 152.897 158.1 1.993 2.012 KIWPAL 3 152.897 158.1 2.022 2.077 KIWPAL 5 150.345 159.895 2.071 1.993 KIWPAL 6 150.345 158.1 2.022 2.077 KIWPAL 1 | | IBAOEL | NO | 3 | 155.538 | 156.975 | 2.269 | 2.3 |
| 34 IQONIO NO 1 160.758 168.136 2.029 1.839 35 IRAGEP NO 1 170.403 168.492 1.939 1.995 36 ISAFEQ YES 1 171.085 161.617 1.953 2.08 37 IEVPAF NO 1 159.297 170.141 1.952 1.946 38 JONZUJ NO 1 153.433 154.582 2.121 2.157 39 JUXKAR NO 1 173.742 166.247 1.969 2.253 41 KEXSIS YES 1 176.458 164.305 1.871 1.927 KIWPAL YES 1 159.895 158.1 1.993 2.022 2.012 43 KIWPAL 4 152.897 158.41 2.022 2.012 44 KUPAOM YES 1 170.92 160.577 1.869 1.859 LAGQES NO 1 <t< td=""><td>33</td><td>ILAROF</td><td>NO</td><td>1</td><td>162.603</td><td>158.672</td><td>1.973</td><td>1.977</td></t<> | 33 | ILAROF | NO | 1 | 162.603 | 158.672 | 1.973 | 1.977 |
| Signed Point NO 1 170.403 168.492 1.939 1.935 36 ISAFEQ YES 1 171.085 161.617 1.953 2.08 37 JEVPAF NO 1 169.297 170.141 1.952 1.946 38 JONZUJ NO 1 154.333 154.582 2.121 2.157 39 JUXKAR NO 1 173.742 166.247 1.969 2.253 41 KEXSIS YES 1 176.458 164.305 1.871 1.927 KIWPAL YES 1 159.895 158.1 1.993 2.012 KIWPAL 2 152.897 150.345 1.2022 2.012 KIWPAL 5 150.345 158.1 2.07 1.993 LAGQES NO 1 170.92 174.707 1.869 1.859 LAGQES NO 2 170.72 1.74.909 1.866 1.999 LA | 34 | IOONIO | NO | 1 | 160.758 | 168.136 | 2.029 | 1.839 |
| 36 ISAFEQ YES 1 171.085 161.617 1.953 2.08 37 JEVPAF NO 1 169.297 170.141 1.952 1.946 38 JONZUJ NO 1 154.333 154.582 2.121 2.157 39 JUXKAR NO 1 173.42 166.247 1.969 2.253 41 KEXSIS YES 1 178.354 170.954 2.035 2.23 42 KIWPAL YES 1 179.895 158.1 1.993 2.012 KIWPAL YES 1 179.895 2.022 2.012 KIWPAL 4 152.897 158.1 2.007 1.993 43 KIWPAL 6 150.345 159.895 2.07 1.993 KIWPAL 6 150.345 158.1 2.07 2.012 44 KUPYOM YES 1 172.655 170.026 2.069 2.048 | 35 | IRAGEP | NO | 1 | 170.403 | 168.492 | 1.939 | 1.995 |
| 37 FEVPAF NO 1 169.297 170.141 1.952 1.946 38 JONZUJ NO 1 154.333 154.582 2.121 2.157 39 JUXKAR NO 1 150.414 162.309 2.288 2.027 40 KEBTUK NO 1 173.742 166.247 1.969 2.253 41 KEXSIS YES 1 176.458 164.305 1.871 1.927 KIWPAL YES 1 159.895 150.345 2.022 2.012 KIWPAL 4 152.897 159.495 2.022 2.07 KIWPAL 5 150.345 158.1 2.07 1.993 KIWPAL 5 150.345 1.07 2.012 1.072 4 KUPYOM YES 1 172.655 170.026 2.069 2.048 LAGQES NO 2 174.707 1.869 1.859 LAGQES NO | 36 | ISAFEO | YES | 1 | 171.085 | 161.617 | 1.953 | 2.08 |
| 38 JONZUJ NO 1 154.333 154.582 2.121 2.157 39 JUXKAR NO 1 150.414 162.309 2.288 2.027 40 KEBTUK NO 1 173.742 166.247 1.969 2.253 41 KEXSIS YES 1 176.458 164.305 1.871 1.927 KIWPAL YES 1 159.895 158.1 1.993 2.012 KIWPAL YES 1 152.897 150.345 1.202 2.017 KIWPAL 4 152.897 150.345 1.202 2.017 KIWPAL 5 150.345 158.1 2.07 1.993 KIWPAL 6 170.92 174.002 1.60.577 1.869 1.858 LAGQES NO 1 170.92 174.007 1.869 1.858 LAGQES NO 4 174.909 1.869 1.858 LAGQES NO 6 <td>37</td> <td>JEVPAF</td> <td>NO</td> <td>1</td> <td>169.297</td> <td>170.141</td> <td>1.952</td> <td>1.946</td> | 37 | JEVPAF | NO | 1 | 169.297 | 170.141 | 1.952 | 1.946 |
| 39 JUXKAR NO 1 150.414 162.309 2.288 2.027 40 KEBTUK NO 1 173.742 166.247 1.969 2.233 41 KEXSIS YES 1 178.354 170.954 2.035 2.233 42 KIMPAL YES 1 176.458 164.305 1.871 1.927 KIWPAL YES 1 159.895 158.1 1.922 2.012 KIWPAL 3 152.897 158.1 2.022 2.017 KIWPAL 4 152.897 158.1 2.022 2.077 KIWPAL 5 150.345 158.1 2.07 2.012 44 KUPYOM YES 1 172.655 170.026 2.069 2.048 LAQES NO 1 170.92 174.707 1.869 1.859 LAGQES NO 5 174.707 1.60.577 1.859 1.858 LAQES NO | 38 | JONZUJ | NO | 1 | 154.333 | 154.582 | 2.121 | 2.157 |
| 40 KEBTUK NO 1 173.742 166.247 1.969 2.253 41 KEXSIS YES 1 178.354 170.954 2.035 2.23 42 KHNOF YES 1 176.458 164.305 1.871 1.927 KIWPAL YES 1 159.895 158.1 1.993 2.012 KIWPAL 2 152.897 159.345 2.022 2.007 KIWPAL 4 152.897 150.345 2.022 2.007 KIWPAL 5 150.345 159.895 2.07 1.993 KIWPAL 6 150.345 158.1 2.07 2.012 44 KUPYOM YES 1 172.655 170.02 2.069 2.048 LAGQES NO 2 170.92 160.577 1.869 1.859 LAGQES NO 5 174.707 160.577 1.859 1.858 LAGQES NO 1 173.678< | 39 | JUXKAR | NO | 1 | 150.414 | 162.309 | 2.288 | 2.027 |
| 41 KEXSIS YES 1 178.354 170.954 2.035 2.23 42 KIMPAL YES 1 176.458 164.305 1.871 1.927 KIWPAL YES 1 159.895 158.1 1.993 2.012 KIWPAL YES 1 152.897 159.895 2.022 2.012 KIWPAL 4 152.897 150.345 2.022 2.012 KIWPAL 5 150.345 158.1 2.07 1.993 KIWPAL 6 177.655 170.026 2.069 2.048 LAGQES NO 1 172.655 170.026 2.069 2.048 LAGQES NO 2 170.92 174.707 1.869 1.858 LAGQES NO 3 170.92 174.707 1.869 1.858 LAGQES NO 6 174.707 1.66.577 1.859 1.858 LAGQES NO 1 173.678 <th1< td=""><td>40</td><td>KEBTUK</td><td>NO</td><td>1</td><td>173.742</td><td>166.247</td><td>1.969</td><td>2.253</td></th1<> | 40 | KEBTUK | NO | 1 | 173.742 | 166.247 | 1.969 | 2.253 |
| 11 11 176.458 164.305 1.871 1.927 12 KIWPAL YES 1 159.895 158.1 1.993 2.012 KIWPAL 2 152.897 159.895 2.022 1.993 13 KIWPAL 3 152.897 158.1 2.022 2.012 KIWPAL 5 150.345 158.1 2.022 2.077 KIWPAL 5 150.345 158.1 2.07 2.012 KIWPAL 5 150.345 158.1 2.07 2.012 44 KUPYOM YES 1 172.655 170.026 2.069 2.048 LAGQES NO 1 170.92 160.577 1.869 1.858 LAGQES NO 2 173.678 169.477 1.869 1.858 LAGQES NO 5 174.707 160.577 1.859 1.858 LAGQES NO 6 174.707 160.577 1.969 1.858 LAGQES NO 1 173.678 170.579 1.911 | 41 | KEXSIS | YES | 1 | 178 354 | 170 954 | 2.035 | 2.23 |
| KIWPAL YES 1 159.895 158.1 1.993 2.012 43 KIWPAL 2 152.897 159.895 2.022 1.993 43 KIWPAL 3 152.897 158.1 2.022 2.012 KIWPAL 4 152.897 150.345 2.022 2.07 KIWPAL 5 150.345 158.1 2.07 2.012 KIWPAL 5 150.345 158.1 2.07 1.993 KIWPAL 6 150.345 158.1 2.07 2.012 44 KUPYOM YES 1 172.655 170.026 2.069 2.048 LAGQES NO 2 170.92 174.909 1.869 1.858 LAGQES NO 5 174.707 160.577 1.869 1.858 LAGQES NO 6 174.707 174.909 1.969 1.858 LAPDEO NO 1 173.678 170.579 1.906 1. | 42 | KIHNOF | YES | 1 | 176.458 | 164.305 | 1.871 | 1.927 |
| KIWPAL 2 152.897 159.895 2.022 1.993 43 KIWPAL 3 152.897 158.1 2.022 2.012 KIWPAL 5 150.345 159.895 2.07 1.993 KIWPAL 5 150.345 159.895 2.07 1.993 KIWPAL 5 150.345 158.1 2.07 2.012 44 KUPYOM YES 1 172.655 170.026 2.069 2.048 LAGQES NO 1 172.655 170.026 2.069 2.048 LAGQES NO 2 170.92 174.707 1.869 1.859 LAGQES NO 4 174.909 160.577 1.859 1.858 LAGQES NO 5 174.707 160.577 1.859 1.858 LAGQES NO 6 174.707 170.579 1.911 1.946 LAPDEO NO 1 172.561 172.246 2.167 | | KIWPAL | YES | 1 | 159.895 | 158.1 | 1.993 | 2.012 |
| 43 KIWPAL 3 152.897 158.1 2.022 2.012 KIWPAL 4 152.897 158.1 2.022 2.07 KIWPAL 5 150.345 159.895 2.07 1.993 KIWPAL 6 150.345 158.1 2.07 2.012 44 KUPYOM YES 1 177.2655 170.026 2.069 2.048 LAGQES NO 2 170.92 174.909 1.869 1.859 LAGQES NO 2 170.92 174.707 1.869 1.858 LAGQES NO 3 170.92 174.707 1.869 1.858 LAGQES NO 5 174.707 160.577 1.859 1.858 LAGQES NO 6 174.707 174.909 1.966 1.911 LAPDEO NO 1 173.678 170.579 1.906 1.946 LEQUE NO 1 172.205 155.546 1.957 2.107 44 LIGVUT NO 1 162.498 | | KIWPAL | 110 | 2 | 152.897 | 159 895 | 2.022 | 1 993 |
| KIWPAL 4 152.87 150.345 2.022 2.071 KIWPAL 5 150.345 150.345 2.002 2.012 KIWPAL 6 150.345 158.1 2.07 1.993 KIWPAL 6 150.345 158.1 2.07 2.012 44 KUPYOM YES 1 172.655 170.026 2.069 2.048 LAGQES NO 2 170.92 174.707 1.869 1.859 LAGQES NO 3 170.92 174.707 1.869 1.858 LAGQES NO 4 174.909 160.577 1.859 1.858 LAGQES NO 5 174.707 160.577 1.969 1.858 LAPDEO NO 1 173.678 169.447 1.906 1.911 LAPDEO NO 1 172.205 155.546 1.957 2.107 44 LEGEK NO 1 172.205 2.033 2.0 | 43 | KIWPAL | | 3 | 152.897 | 159.099 | 2.022 | 2.012 |
| RINNIAL TOUST 1 TOUST 1 <t< td=""><td>15</td><td>KIWPAL</td><td></td><td>4</td><td>152.027</td><td>150 345</td><td>2.022</td><td>2.012</td></t<> | 15 | KIWPAL | | 4 | 152.027 | 150 345 | 2.022 | 2.012 |
| INVERAL 6 150.545 150.545 1207 2012 44 KUPYOM YES 1 172.655 170.026 2.069 2.048 LAGQES NO 1 170.92 160.577 1.869 1.859 LAGQES NO 2 170.92 174.707 1.869 1.859 LAGQES NO 4 174.909 160.577 1.869 1.859 LAGQES NO 4 174.909 160.577 1.869 1.859 LAGQES NO 5 174.707 160.577 1.969 1.858 LAGQES NO 6 174.707 160.577 1.969 1.859 LAGQES NO 2 173.678 169.447 1.906 1.911 LAGQES NO 1 172.656 1.957 2.107 44 LEOPEK NO 1 172.561 172.246 2.167 2.168 48 LIGVUT NO 1 | | KIWPAL | | 5 | 150 345 | 159 895 | 2.022 | 1 993 |
| HILL Instruction Instruction <thinstruction< th=""> <thin< td=""><td></td><td>KIWPAL</td><td></td><td>6</td><td>150.345</td><td>158.1</td><td>2.07</td><td>2.012</td></thin<></thinstruction<> | | KIWPAL | | 6 | 150.345 | 158.1 | 2.07 | 2.012 |
| Intervent Intervent <thintervent< th=""> <thintervent< th=""> <thi< td=""><td>44</td><td>KUPYOM</td><td>VES</td><td>1</td><td>172 655</td><td>170.026</td><td>2.67</td><td>2.012</td></thi<></thintervent<></thintervent<> | 44 | KUPYOM | VES | 1 | 172 655 | 170.026 | 2.67 | 2.012 |
| LAGQES NO 1 170.92 174.909 1.869 1.859 LAGQES NO 3 170.92 174.909 1.869 1.859 LAGQES NO 4 174.909 160.577 1.869 1.859 LAGQES NO 5 174.707 160.577 1.969 1.858 LAGQES NO 6 174.707 160.577 1.969 1.859 LAGQES NO 6 174.707 174.909 1.969 1.859 LAGQES NO 6 174.707 174.909 1.969 1.859 LAGQES NO 2 173.678 170.579 1.911 1.946 LAPDEO NO 1 172.205 155.546 1.957 2.107 47 LETNOR NO 1 166.183 167.225 2.033 2.056 LONVUI NO 1 163.136 1.64.581 2.012 2.009 LONVUI NO 2< | ••• | LAGOES | NO | 1 | 170.92 | 160 577 | 1 869 | 1 858 |
| LAGQES NO 3 170.92 174.707 1.869 1.969 LAGQES NO 4 174.909 160.577 1.859 1.858 45 LAGQES NO 5 174.707 160.577 1.969 1.858 LAGQES NO 6 174.707 174.909 1.969 1.859 LAGQES NO 6 174.707 174.909 1.969 1.859 LAGQES NO 6 174.707 174.909 1.969 1.859 LAPDEO NO 2 173.678 170.579 1.906 1.946 LAPDEO NO 3 169.447 170.579 1.911 1.946 46 LEOGEK NO 1 172.266 172.246 2.167 2.168 48 LIGVUT NO 1 163.136 164.581 2.012 2.009 LONVUI NO 2 171.122 163.136 1.943 2.007 10 <td></td> <td>LAGOES</td> <td>NO</td> <td>2</td> <td>170.92</td> <td>174 909</td> <td>1.869</td> <td>1.859</td> | | LAGOES | NO | 2 | 170.92 | 174 909 | 1.869 | 1.859 |
| Indeques No 4 174.909 160.577 1.859 1.858 45 LAGQES NO 5 174.707 160.577 1.859 1.858 LAGQES NO 5 174.707 160.577 1.859 1.859 LAGQES NO 6 174.707 174.909 1.969 1.859 LAPDEO NO 1 173.678 169.447 1.906 1.911 LAPDEO NO 2 173.678 170.579 1.911 1.946 LAPDEO NO 1 172.205 155.546 1.957 2.107 47 LETNOR NO 1 172.261 172.246 2.167 2.168 48 LIGVUT NO 1 163.136 164.581 2.012 2.009 LONVUI NO 2 171.122 164.581 2.012 2.009 LONVUI NO 3 160.109 164.581 2.077 2.012 LON | | LAGOES | NO | 3 | 170.92 | 174 707 | 1.869 | 1 969 |
| 45 LAGQES NO 5 174.707 160.577 1.969 1.858 LAGQES NO 6 174.707 174.909 1.969 1.859 LAPDEO NO 1 173.678 169.447 1.906 1.911 LAPDEO NO 2 173.678 170.579 1.906 1.946 LAPDEO NO 3 169.447 170.579 1.911 1.946 46 LEDGEK NO 1 172.205 155.546 1.957 2.107 47 LETNOR NO 1 172.561 172.246 2.167 2.168 48 LIGVUT NO 1 156.498 159.741 2.04 2.012 49 LISSUE YES 1 168.183 167.225 2.033 2.056 LONVUI NO 2 171.122 164.581 2.012 2.009 LONVUI NO 3 160.109 163.136 2.077 2.012 </td <td></td> <td>LAGOES</td> <td>NO</td> <td>4</td> <td>174.909</td> <td>160.577</td> <td>1.859</td> <td>1.858</td> | | LAGOES | NO | 4 | 174.909 | 160.577 | 1.859 | 1.858 |
| LAGQES NO 6 174.707 174.907 1705 1859 LAPDEO NO 1 173.678 169.447 1.906 1.911 LAPDEO NO 2 173.678 170.579 1.906 1.946 LAPDEO NO 2 173.678 170.579 1.906 1.946 LAPDEO NO 3 169.447 170.579 1.911 1.946 46 LEDGEK NO 1 172.205 155.546 1.957 2.107 47 LETNOR NO 1 172.561 172.246 2.167 2.168 48 LIGVUT NO 1 163.136 164.581 2.042 2.012 49 LISSUE YES 1 168.183 167.225 2.033 2.056 LONVUL NO 2 171.122 164.581 2.012 2.009 50 LONVUL NO 5 160.109 1.943 2.012 | 45 | LAGOES | NO | 5 | 174.707 | 160.577 | 1.969 | 1.858 |
| LAPDEO NO 1 173.678 169.447 1.905 1.057 LAPDEO NO 2 173.678 170.579 1.906 1.911 LAPDEO NO 2 173.678 170.579 1.906 1.946 LAPDEO NO 3 169.447 170.579 1.911 1.946 46 LEDGEK NO 1 172.205 155.546 1.957 2.107 47 LETNOR NO 1 172.561 172.246 2.167 2.168 48 LIGVUT NO 1 163.136 164.581 2.012 2.009 49 LISSUE YES 1 163.136 164.581 2.012 2.009 40 NO 2 171.122 164.581 2.017 2.009 50 LONVUI NO 3 160.109 163.136 1.943 2.012 LONVUI NO 5 160.109 1.943 2.077 2.012 | 10 | LAGOES | NO | 6 | 174 707 | 174 909 | 1 969 | 1.859 |
| LAPDEO NO 2 173.678 170.579 1.906 1.946 LAPDEO NO 3 169.447 170.579 1.911 1.946 46 LEDGEK NO 1 172.205 155.546 1.957 2.107 47 LETNOR NO 1 172.561 172.246 2.167 2.168 48 LIGVUT NO 1 156.498 159.741 2.04 2.012 49 LISSUE YES 1 168.183 167.225 2.033 2.056 LONVUI NO 1 163.136 164.581 2.012 2.009 LONVUI NO 2 171.122 164.581 2.012 2.009 LONVUI NO 3 160.109 164.581 2.077 2.009 LONVUI NO 4 171.122 163.136 1.943 2.012 LONVUI NO 5 160.109 163.136 2.077 2.012 <t< td=""><td></td><td>LAPDEO</td><td>NO</td><td>1</td><td>173 678</td><td>169 447</td><td>1 906</td><td>1 911</td></t<> | | LAPDEO | NO | 1 | 173 678 | 169 447 | 1 906 | 1 911 |
| LAPDEO NO 3 169.447 170.579 1.911 1.946 46 LEDGEK NO 1 172.205 155.546 1.957 2.107 47 LETNOR NO 1 172.205 155.546 1.957 2.107 47 LETNOR NO 1 172.561 172.246 2.167 2.168 48 LIGVUT NO 1 156.498 159.741 2.04 2.012 49 LISSUE YES 1 168.183 167.225 2.033 2.056 LONVUI NO 2 171.122 164.581 2.012 2.009 LONVUI NO 2 171.122 164.581 2.077 2.009 LONVUI NO 4 171.122 163.136 1.943 2.012 LONVUI NO 5 160.109 163.136 2.077 2.012 LONVUI NO 1 175.718 171.487 1.881 2.017 </td <td></td> <td>LAPDEO</td> <td>NO</td> <td>2</td> <td>173.678</td> <td>170.579</td> <td>1.906</td> <td>1.946</td> | | LAPDEO | NO | 2 | 173.678 | 170.579 | 1.906 | 1.946 |
| 46 LEDGEK NO 1 172.205 155.546 1.957 2.107 47 LETNOR NO 1 172.205 155.546 1.957 2.107 47 LETNOR NO 1 172.561 172.246 2.167 2.168 48 LIGVUT NO 1 156.498 159.741 2.04 2.012 49 LISSUE YES 1 168.183 167.225 2.033 2.056 LONVUI NO 2 171.122 164.581 2.012 2.009 LONVUI NO 2 171.122 164.581 2.017 2.009 LONVUI NO 3 160.109 164.581 2.077 2.009 50 LONVUI NO 4 171.122 163.136 1.943 2.012 LONVUI NO 5 160.109 163.136 2.077 2.012 LONVUI NO 1 175.718 171.487 1.881 | | LAPDEO | NO | 3 | 169.447 | 170.579 | 1.911 | 1.946 |
| 47 LETNOR NO 1 172.561 172.246 2.167 2.168 48 LIGVUT NO 1 156.498 159.741 2.04 2.012 49 LISSUE YES 1 168.183 167.225 2.033 2.056 LONVUI NO 1 163.136 164.581 2.012 2.009 LONVUI NO 2 171.122 164.581 2.012 2.009 LONVUI NO 2 171.122 164.581 2.012 2.009 LONVUI NO 2 171.122 164.581 2.012 2.009 LONVUI NO 3 160.109 164.581 2.077 2.009 50 LONVUI NO 4 171.122 163.136 1.943 2.012 LONVUI NO 5 160.109 163.136 2.077 2.012 LONVUI NO 1 175.718 171.487 1.881 2.018 52 LUYHAR NO 1 173.418 173.488 1.965 < | 46 | LEDGEK | NO | 1 | 172.205 | 155.546 | 1.957 | 2.107 |
| 48 LIGVUT NO 1 156.498 159.741 2.04 2.012 49 LISSUE YES 1 168.183 167.225 2.033 2.056 LONVUI NO 1 163.136 164.581 2.012 2.009 LONVUI NO 2 171.122 164.581 2.012 2.009 LONVUI NO 2 171.122 164.581 2.012 2.009 50 LONVUI NO 3 160.109 164.581 2.077 2.009 50 LONVUI NO 4 171.122 163.136 1.943 2.012 LONVUI NO 4 171.122 163.136 2.077 2.009 50 LONVUI NO 5 160.109 163.136 2.077 2.012 LONVUI NO 6 171.122 160.109 1.943 2.077 51 LUQHUD NO 1 175.718 171.487 1.881 2.018 52 LUYHAR NO 1 173.418 173.4 | 47 | LETNOR | NO | 1 | 172.561 | 172.246 | 2.167 | 2.168 |
| 49 LISSUE YES 1 168.183 167.225 2.033 2.056 LONVUI NO 1 163.136 164.581 2.012 2.009 LONVUI NO 2 171.122 164.581 2.012 2.009 LONVUI NO 2 171.122 164.581 2.012 2.009 LONVUI NO 2 171.122 164.581 2.077 2.009 50 LONVUI NO 3 160.109 164.581 2.077 2.009 50 LONVUI NO 4 171.122 163.136 1.943 2.012 LONVUI NO 5 160.109 163.136 2.077 2.012 LONVUI NO 6 171.122 163.136 2.077 2.012 LONVUI NO 1 153.35 163.566 1.996 1.901 52 LUZHUD NO 1 175.718 171.487 1.881 2.018 53 LUZJUL YES 1 151.001 2.193 2.193 <td>48</td> <td>LIGVUT</td> <td>NO</td> <td>1</td> <td>156.498</td> <td>159.741</td> <td>2.04</td> <td>2.012</td> | 48 | LIGVUT | NO | 1 | 156.498 | 159.741 | 2.04 | 2.012 |
| LONUL NO 1 163.136 164.581 2.012 2.009 LONVUI NO 2 171.122 164.581 2.012 2.009 LONVUI NO 2 171.122 164.581 1.943 2.009 50 LONVUI NO 3 160.109 164.581 2.077 2.009 50 LONVUI NO 4 171.122 163.136 1.943 2.012 LONVUI NO 4 171.122 163.136 1.943 2.012 LONVUI NO 5 160.109 163.136 2.077 2.012 LONVUI NO 6 171.122 160.109 1.943 2.077 51 LUQHUD NO 1 153.35 163.566 1.996 1.901 52 LUYHAR NO 1 175.718 171.487 1.881 2.018 53 LUZJUL YES 1 151.001 2.193 2.193 | 49 | LISSUE | YES | 1 | 168,183 | 167.225 | 2.033 | 2.056 |
| LONVUI NO 2 171.122 164.581 1.943 2.009 LONVUI NO 3 160.109 164.581 2.077 2.009 50 LONVUI NO 4 171.122 163.136 1.943 2.012 LONVUI NO 4 171.122 163.136 1.943 2.012 LONVUI NO 4 171.122 163.136 2.077 2.012 LONVUI NO 5 160.109 163.136 2.077 2.012 LONVUI NO 6 171.122 160.109 1.943 2.077 51 LUQHUD NO 1 153.35 163.566 1.996 1.901 52 LUYHAR NO 1 175.718 171.487 1.881 2.018 53 LUZJUL YES 1 151.001 151.001 2.193 2.193 54 MEHNPQ NO 1 173.418 173.488 1.965 1.956 </td <td>.,</td> <td>LONVUI</td> <td>NO</td> <td>1</td> <td>163.136</td> <td>164.581</td> <td>2.012</td> <td>2.009</td> | ., | LONVUI | NO | 1 | 163.136 | 164.581 | 2.012 | 2.009 |
| LONVUI NO 3 160.109 164.581 2.077 2.009 50 LONVUI NO 4 171.122 163.136 1.943 2.012 LONVUI NO 5 160.109 163.136 1.943 2.012 LONVUI NO 5 160.109 163.136 2.077 2.012 LONVUI NO 6 171.122 160.109 1.943 2.077 51 LUQHUD NO 6 171.122 160.109 1.943 2.077 51 LUQHUD NO 1 153.35 163.566 1.996 1.901 52 LUYHAR NO 1 175.718 171.487 1.881 2.018 53 LUZJUL YES 1 151.001 151.001 2.193 2.193 54 MEHNPQ NO 1 173.418 173.488 1.965 1.956 55 MEQCEU NO 1 172.647 168.294 | | LONVUI | NO | 2 | 171.122 | 164.581 | 1.943 | 2.009 |
| 50 LONVUI NO 4 171.122 163.136 1.943 2.012 LONVUI NO 5 160.109 163.136 2.077 2.012 LONVUI NO 6 171.122 160.109 1.943 2.077 51 LUQHUD NO 6 171.122 160.109 1.943 2.077 51 LUQHUD NO 1 153.35 163.566 1.996 1.901 52 LUYHAR NO 1 175.718 171.487 1.881 2.018 53 LUZJUL YES 1 151.001 151.001 2.193 2.193 54 MEHNPQ NO 1 173.418 173.488 1.965 1.956 55 MEQCEU NO 1 163.359 164.122 1.95 2.19 56 MIDMUK NO 1 172.647 168.294 2.188 2.097 57 MOJPUW YES 1 1 | | LONVUI | NO | 3 | 160.109 | 164.581 | 2.077 | 2.009 |
| LONVUI NO 5 160.109 163.136 2.077 2.012 LONVUI NO 6 171.122 160.109 1.943 2.077 51 LUQHUD NO 1 153.35 163.566 1.996 1.901 52 LUYHAR NO 1 175.718 171.487 1.881 2.018 53 LUZJUL YES 1 151.001 151.001 2.193 2.193 54 MEHNPQ NO 1 173.418 173.488 1.965 1.956 55 MEQCEU NO 1 163.359 164.122 1.95 2.19 56 MIDMUK NO 1 172.647 168.294 2.188 2.097 57 MOJPUW YES 1 153.171 157.485 2.116 2.211 58 MOYPUO NO 1 158.33 174.119 2.081 1.989 60 NOQKIO NO 1 15 | 50 | LONVUI | NO | 4 | 171.122 | 163.136 | 1.943 | 2.012 |
| LONVUINO6171.122160.1091.9432.07751LUQHUDNO1153.35163.5661.9961.90152LUYHARNO1175.718171.4871.8812.01853LUZJULYES1151.001151.0012.1932.19354MEHNPQNO1173.418173.4881.9651.95655MEQCEUNO1163.359164.1221.952.1956MIDMUKNO1172.647168.2942.1882.09757MOJPUWYES1153.171157.4852.1162.21158MOYPUONO1158.33174.1192.0811.98960NOQKIONO1179.118168.2451.8771.857 | | LONVUI | NO | 5 | 160.109 | 163.136 | 2.077 | 2.012 |
| 51 LUQHUD NO 1 153.35 163.566 1.996 1.901 52 LUYHAR NO 1 175.718 171.487 1.881 2.018 53 LUZJUL YES 1 151.001 151.001 2.193 2.193 54 MEHNPQ NO 1 173.418 173.488 1.965 1.956 55 MEQCEU NO 1 163.359 164.122 1.95 2.19 56 MIDMUK NO 1 172.647 168.294 2.188 2.097 57 MOJPUW YES 1 153.171 157.485 2.116 2.211 58 MOYPUO NO 1 158.19 168.659 1.963 2.017 59 NANFOB NO 1 158.33 174.119 2.081 1.989 60 NOQKIO NO 1 179.118 168.245 1.877 1.857 | | LONVUI | NO | 6 | 171.122 | 160.109 | 1.943 | 2.077 |
| 52 LUYHAR NO 1 175.718 171.487 1.881 2.018 53 LUZJUL YES 1 151.001 151.001 2.193 2.193 54 MEHNPQ NO 1 173.418 173.488 1.965 1.956 55 MEQCEU NO 1 163.359 164.122 1.95 2.19 56 MIDMUK NO 1 172.647 168.294 2.188 2.097 57 MOJPUW YES 1 153.171 157.485 2.116 2.211 58 MOYPUO NO 1 158.19 168.659 1.963 2.017 59 NANFOB NO 1 158.33 174.119 2.081 1.989 60 NOQKIO NO 1 179.118 168.245 1.877 1.857 | 51 | LUOHUD | NO | 1 | 153.35 | 163.566 | 1.996 | 1.901 |
| 53 LUZJUL YES 1 151.001 151.001 2.193 2.193 54 MEHNPQ NO 1 173.418 173.488 1.965 1.956 55 MEQCEU NO 1 163.359 164.122 1.95 2.19 56 MIDMUK NO 1 172.647 168.294 2.188 2.097 57 MOJPUW YES 1 153.171 157.485 2.116 2.211 58 MOYPUO NO 1 158.19 168.659 1.963 2.017 59 NANFOB NO 1 158.33 174.119 2.081 1.989 60 NOQKIO NO 1 179.118 168.245 1.877 1.857 | 52 | LUYHAR | NO | 1 | 175.718 | 171.487 | 1.881 | 2.018 |
| 54MEHNPQNO1173.418173.4881.9651.95655MEQCEUNO1163.359164.1221.952.1956MIDMUKNO1172.647168.2942.1882.09757MOJPUWYES1153.171157.4852.1162.21158MOYPUONO1158.19168.6591.9632.01759NANFOBNO1158.33174.1192.0811.98960NOQKIONO1179.118168.2451.8771.857 | 53 | LUZJUL | YES | 1 | 151.001 | 151.001 | 2.193 | 2.193 |
| 55MEQCEUNO1163.359164.1221.952.1956MIDMUKNO1172.647168.2942.1882.09757MOJPUWYES1153.171157.4852.1162.21158MOYPUONO1158.19168.6591.9632.01759NANFOBNO1158.33174.1192.0811.98960NOQKIONO1179.118168.2451.8771.857 | 54 | MEHNPO | NO | 1 | 173.418 | 173.488 | 1.965 | 1.956 |
| 56 MIDMUK NO 1 172.647 168.294 2.188 2.097 57 MOJPUW YES 1 153.171 157.485 2.116 2.211 58 MOYPUO NO 1 158.19 168.659 1.963 2.017 59 NANFOB NO 1 158.33 174.119 2.081 1.989 60 NOQKIO NO 1 179.118 168.245 1.877 1.857 | 55 | MEOCEU | NO | 1 | 163.359 | 164.122 | 1.95 | 2.19 |
| 57 MOJPUW YES 1 153.171 157.485 2.116 2.211 58 MOYPUO NO 1 158.19 168.659 1.963 2.017 59 NANFOB NO 1 158.33 174.119 2.081 1.989 60 NOOKIO NO 1 179.118 168.245 1.877 1.857 | 56 | MIDMUK | NO | 1 | 172.647 | 168.294 | 2.188 | 2.097 |
| 58 MOYPUO NO 1 158.19 168.659 1.963 2.017 59 NANFOB NO 1 158.33 174.119 2.081 1.989 60 NOOKIO NO 1 179.118 168.245 1.877 1.857 | 57 | MOJPUW | YES | 1 | 153.171 | 157.485 | 2.116 | 2.211 |
| 59 NANFOB NO 1 158.33 174.119 2.081 1.989 60 NOQKIO NO 1 179.118 168.245 1.877 1.857 | 58 | MOYPUO | NO | 1 | 158.19 | 168.659 | 1.963 | 2.017 |
| 60 NOOKIO NO 1 179.118 168.245 1.877 1.857 | 59 | NANFOB | NO | 1 | 158.33 | 174.119 | 2.081 | 1.989 |
| | 60 | NOQKIO | NO | 1 | 179.118 | 168.245 | 1.877 | 1.857 |

| 61 | OGIXIO | NO | 1 | 167.028 | 159.771 | 1.967 | 1.987 |
|-------------------|----------|-----|----|---------|---------|-------|-------|
| 62 | OHUKIO | NO | 1 | 174.923 | 174.773 | 1.975 | 1.934 |
| 63 | OMAFEP | YES | 1 | 172.359 | 172.085 | 1.989 | 1.964 |
| 64 | PAVQEI | NO | 1 | 176.158 | 178.751 | 1.846 | 1.913 |
| 65 | PESPOT | NO | 1 | 168.206 | 175.445 | 2.148 | 2.088 |
| | QETZUL | NO | 1 | 152.467 | 156.298 | 1.943 | 2.002 |
| | QETZUL | NO | 2 | 152.467 | 164.434 | 1.943 | 1.975 |
| 66 | QETZUL | NO | 3 | 152.467 | 164.576 | 1.943 | 1.989 |
| | QETZUL | NO | 4 | 156.298 | 164.434 | 2.002 | 1.975 |
| | QETZUL | NO | 5 | 164.576 | 156.298 | 1.989 | 2.002 |
| | QETZUL | NO | 6 | 164.576 | 164.434 | 1.989 | 1.975 |
| 67 | QOMBUS | NO | 1 | 156.679 | 161.65 | 2.097 | 1.874 |
| 68 | QULBII | NO | 1 | 165.907 | 168.249 | 2.042 | 2.005 |
| 69 | QUWZEQ | NO | 1 | 150.846 | 159.578 | 2.194 | 2.154 |
| 70 | RAGDEM | NO | 1 | 172.31 | 165.237 | 2.086 | 2.031 |
| 71 | REPDEX | YES | 1 | 169.627 | 169.627 | 1.889 | 1.889 |
| 72 | REXHEI | NO | 1 | 172.477 | 169.539 | 2.002 | 2.071 |
| 73 | RUVSOS | NO | 1 | 175.306 | 175.847 | 1.898 | 2.108 |
| 74 | RUVSOS01 | NO | 1 | 167.71 | 176.547 | 2.101 | 1.885 |
| 75 | RUVVEL | NO | 1 | 179.731 | 173.373 | 2.131 | 1.975 |
| 76 | SAKJOG | NO | 1 | 166.899 | 171.21 | 1.924 | 1.869 |
| 77 | SAKKAT | NO | 1 | 163.959 | 172.888 | 1.916 | 1.927 |
| 78 | SAZRUK | NO | 1 | 173.774 | 177.79 | 1.954 | 1.953 |
| 79 | SEHLEA | NO | 1 | 167.812 | 164.378 | 2.021 | 2.078 |
| 80 | SELTEM | YES | 1 | 173.587 | 175.25 | 1.97 | 1.862 |
| 81 | SEWFAD | NO | 1 | 162.661 | 162.661 | 2.038 | 2.038 |
| 82 | SIMDUR | NO | 1 | 162.888 | 159.881 | 2.208 | 2.395 |
| 83 | SIMKAE | NO | 1 | 159.653 | 166.154 | 1.996 | 2.019 |
| 84 | SUOBIR | NO | 1 | 172.554 | 178.027 | 1.959 | 2.066 |
| 85 | SUOBUD | NO | 1 | 174.527 | 176.254 | 1.974 | 2.252 |
| 86 | TANFUJ | YES | 1 | 152.333 | 150.407 | 2.031 | 2.153 |
| 87 | TESTON10 | NO | 1 | 167.368 | 163.324 | 1.993 | 1.805 |
| | TUDSOD | NO | 1 | 156.036 | 160.699 | 2.037 | 2.015 |
| | TUDSOD | NO | 2 | 159.683 | 160.699 | 2.059 | 2.015 |
| | TUDSOD | NO | 3 | 159.683 | 156.036 | 2.059 | 2.037 |
| | UMAHAT | NO | 1 | 158.59 | 157.93 | 1.954 | 1.959 |
| | UMAHAT | NO | 2 | 158.59 | 151.965 | 1.954 | 1.964 |
| | UMAHAT | NO | 3 | 151.965 | 157.93 | 1.964 | 1.959 |
| 88 | UMAHAT | NO | 4 | 155.613 | 158.59 | 1.974 | 1.954 |
| | UMAHAT | NO | 5 | 155.613 | 157.93 | 1.974 | 1.959 |
| | UMAHAT | NO | 6 | 155.613 | 151.965 | 1.974 | 1.964 |
| | UMAHAT | NO | 7 | 152.498 | 158.59 | 1.975 | 1.954 |
| | UMAHAT | NO | 8 | 152.498 | 157.93 | 1.975 | 1.959 |
| | UMAHAT | NO | 9 | 152.498 | 151.965 | 1.975 | 1.964 |
| | UMAHAT | NO | 10 | 152.498 | 155.613 | 1.975 | 1.974 |
| 89 | UTILUG | NO | 1 | 156.55 | 169.581 | 2.108 | 1.869 |
| 90 | UVEMOA | NO | 1 | 167.727 | 167.064 | 2.067 | 2.037 |
| 91 | UYOOAB | NO | 1 | 151.568 | 158.035 | 2.038 | 2.042 |
| <i>,</i> , | UZIPIF | NO | 1 | 155.614 | 160.608 | 2.084 | 2.002 |
| 92 | UZIPIF | NO | 2 | 155,614 | 150.688 | 2.084 | 2,166 |
| | UZIPIF | NO | 3 | 150,688 | 160,608 | 2.166 | 2.002 |
| 93 | VAHCOZ | NO | 1 | 167.597 | 164.638 | 1.972 | 1.986 |
| | | · - | - | | | ··· | |

| 94 | VAWMUF | YES | 1 | 158.743 | 159.337 | 2.049 | 2.109 |
|-----|----------|-----|---|---------|---------|-------|-------|
| 95 | VEMNUA | NO | 1 | 174.254 | 159.785 | 1.985 | 1.974 |
| 96 | VIQQUK | NO | 1 | 164.847 | 173.271 | 2.016 | 2.037 |
| 97 | VUYYUJ | YES | 1 | 165.327 | 166.589 | 1.908 | 1.902 |
| 98 | WAKWIQ | NO | 1 | 175.416 | 172.22 | 1.94 | 1.955 |
| 99 | WAQYUI | NO | 1 | 156.392 | 164.152 | 1.957 | 1.933 |
| 100 | WEGLON | NO | 1 | 166.39 | 167.065 | 1.942 | 1.942 |
| 101 | WIMLEL | NO | 1 | 171.104 | 163.447 | 2.022 | 2.043 |
| 102 | WIPVOG | YES | 1 | 166.45 | 173.316 | 2.142 | 1.99 |
| 103 | XIDZES | NO | 1 | 175.446 | 172.468 | 2.02 | 1.983 |
| 104 | XIFSIP | NO | 1 | 155.345 | 159.686 | 1.975 | 2.029 |
| 105 | XODQAL | NO | 1 | 151.498 | 154.53 | 2.112 | 2.067 |
| 106 | YOFWEW | NO | 1 | 155.35 | 172.702 | 1.808 | 1.646 |
| 107 | YOWPAE | NO | 1 | 179.44 | 177.965 | 1.955 | 2.148 |
| 108 | ZEPZEB | NO | 1 | 164.303 | 157.868 | 1.845 | 1.969 |
| 109 | ZIBTEN | NO | 1 | 150.853 | 157.537 | 2.058 | 2.013 |
| 110 | ZIBTUB | NO | 1 | 171.072 | 168.115 | 2.06 | 2.014 |
| 111 | ZICZEQ | NO | 1 | 168.909 | 164.796 | 1.705 | 1.831 |
| 112 | ZOYMOP03 | NO | 1 | 170.911 | 170.671 | 2.068 | 1.912 |
| | ZUDKAM | NO | 1 | 158.352 | 157.084 | 2.044 | 2.047 |
| | ZUDKAM | | 2 | 158.352 | 157.802 | 2.044 | 2.052 |
| 113 | ZUDKAM | | 3 | 157.433 | 158.352 | 2.045 | 2.044 |
| | ZUDKAM | | 4 | 157.433 | 157.084 | 2.045 | 2.047 |
| | ZUDKAM | | 5 | 157.433 | 157.802 | 2.045 | 2.052 |
| | ZUDKAM | | 6 | 157.084 | 157.802 | 2.047 | 2.052 |
| 114 | ZUKRUS | NO | 1 | 165.281 | 168.839 | 1.94 | 1.817 |
| 115 | JOCVAC | YES | 1 | 154.769 | 163.307 | 2.053 | 1.936 |
| 116 | KUHRIR | NO | | | | | |
| 117 | TIMFAA | NO | | | | | |
| 118 | UFABUC | NO | | | | | |
| 119 | UHUDAD | NO | | | | | |
| 120 | UZIPEB | NO | | | | | |
| 121 | XEJAO | NO | | | | | |

Identified separately from the search

122 XEZJES

123 YIQMUJ

124 YOVWOX

NO

YES

NO

2. IR spectroscopy revealing the O-H····O=C interaction

The ATR-IR spectra for compounds Alc-1, Alc-2, Keto-1 and Keto-2 show that the CO exocyclic group in the sydnone presents a redshift in the frequency from 1752-1771 cm⁻¹ (Figure 1S) in ketones down to 1722 cm^{-1} for Alc-2 and 1719 cm^{-1} Alc-1.



Figure 1S. ATR-IR Spectra of Alc-1, Alc-2, Keto-1 and Keto-2 (from top)

Table 2S also confirms such a trend with literature IR data. However, to gain more insight we performed DFT simulated spectra for Alc-1 and Keto-1 as models. For the purpose of the calculation we have employed the monomer of Keto-1 and for Alc-1 we have envisaged three scenarios: monomer extracted from the .cif file (optimized or used as is), the O-H···O=C H bonded dimer (optimized or used as is) and the most stable configuration presenting an intramolecular H-bond between the O-H and C=O groups of the sydnone.

| 1 | No. | Ketone | Other | CO | Alcohol | OH | CO |
|---|-----|--|----------------------|------------------------------|--|-------------------|-------------------|
| 1 | | N^{N} Me | 3060 1426 1053 | 1780 1662 1793 1665 | + OH N ^{·N} Me O O ⁻ | 3402* | 1719* |
| 2 | | Me + O N ^{:N} Me | 2933 1509 1316 | 1771* 1783 1686 | | <mark>3436</mark> | <mark>1770</mark> |
| 3 | | | 1050 N/A | 1780 | | <mark>3418</mark> | <mark>1725</mark> |
| 4 | | | N/A | 1780 1658 | | <mark>3412</mark> | <mark>1734</mark> |
| 5 | | OEt | N/A | 1792 1660 | | <mark>3442</mark> | <mark>1725</mark> |
| 6 | | $N \rightarrow Me$ $O \rightarrow O^-$ Br $+ \dots O$ | N/A | 1790 1655 | | <mark>3406</mark> | <mark>1731</mark> |
| 7 | | N MeO^-COMeO | - N/A | <mark>1762</mark> 1664 | | <mark>3394</mark> | <mark>1728</mark> |
| 8 | | $\overset{+}{O}$ $\overset{-}{O}$ $\overset{-}{O}$ | N/A | 1791 1734 1668 | | <mark>3340</mark> | <mark>1707</mark> |
| 9 | | + O N O O F | 1752* | | | 3394* | 1722* |

Synth. Commun. 1996, 26, 2757-2764

Table 2S. Literature data-mining on the IR spectra of certain ketones and analogous alcohols

Figure 2S presents the stacked simulated spectra. The band at 1791 cm⁻¹ for the Keto-1 corresponds to the 1752-1771 cm⁻¹ range for ATR IR spectra (**Keto-1** and **Keto-2**). All the alcohol configurations, in either monomer or dimeric forms, present the CO sydnone vibration at a lower frequency confirming that IR vibration is correlated with the H-bond. For the optimized monomer and the intramolecular H-bonded monomer the CO bond vibrates at a higher frequency due to more relaxed configuration obtained by optimization. For the dimer form (either optimized or not) and monomer (non-optimized) the CO band ranges from 1692.5 to 1703.7 cm⁻¹. All three structures adopt the configurations constrained by the crystalline packing. These bands are analogous to the 1722 cm⁻¹ bands from the ATR IR spectra. The conclusion is that historically the H-bonds between OH and sydnone CO could be predicted by IR spectroscopy and are confirmed by X-ray diffraction analysis.



wavenumber/cm⁻¹

Figure 2S. Calculated IR spectra of **Alc-1 and Keto-1**: Alc1- dimeric form as extracted from the X-Ray spectra (solid red) , **Alc1**-dimeric form as extracted from the X-ray spectra – optimized (solid dark gray), **Alc-1** monomer as extracted from X-ray spectra (solid green), Alc-1-monomer as extracted from X-Ray spectra – optimized (dash green), **Alc1**-monomer – proposed structure to form intramolecular H bond - optimized (solid blue), **Keto-1** monomer as extracted from the X-Ray optimized (solid purple).

For the calculation of the IR spectra, the CAM-B3LYP [1] functional was used. This is one of the functionals that was proved reliable for the simulation of the IR spectra [2,3]. A scaling factor of 0.95 was applied to the calculated spectra [4]. Besides the conformations provided by the X-ray spectra, we have investigated a monomer conformation that provides an intramolecular hydrogen bonding.

[1] Yanai, T.; Tew, D. P.; Handy, N. C. A new hybrid exchange–correlation functional using the Coulomb-attenuating method (CAM-B3LYP) *Chem. Phys. Lett.* **2004**, *393*, 51-57. <u>https://doi.org/10.1016/j.cplett.2004.06.011</u>

^[2] Srivastava, R.; Al-Omary, F.A.M.; El-Emam, A.A.; Pathak, S.K.; Karabacak, M.; Narayan, V.; Chand, S.; Prasad, O.; Sinha, L. A combined experimental and theoretical DFT (B3LYP, CAM-B3LYP and M06-2X) study on electronic structure, hydrogen bonding, solvent effects and spectral features of methyl 1H-indol-5-carboxylate *J. Mol. Struct.* **2017**, *1137*, 725-741. https://doi.org/10.1016/j.molstruc.2017.02.084

^[3] Komjati, B.; Urai, A.; Hosztafi, S.; Kokosi, J.; Kovats, B.; Nagy, J.; Horvath, P. Systematic study on the TD-DFT calculated electronic circular dichroism spectra of chiral aromatic nitro compounds: A comparison of B3LYP and CAM-B3LYP *Spectrochim. Acta A* **2016**, *155*, 95-102. <u>https://doi.org/10.1016/j.saa.2015.11.002</u>

^[4] Jarota, A.; Drwal, D.; Pieta, J.; Pastorczak, E. Wide-range IR spectra of diarylethene derivatives and their simulation using the density functional theory *Sci. Rep.* **2022**, *12*, 16834. <u>https://doi.org/10.1038/s41598-022-20264-x</u>

3. Condensed sydnones with tertiary alcohol structure generating O-H···O=C dimers



Figure 3S. OH…O=C dimers of *ABELID* [5] (two independent molecules)



Figure 4S. OH····O=C dimers of TAPJUP [6]

^[5] Riddle, G.B.; Grossie, D.A.; Turnbull, K. The sydnone compound 4-hydroxy-4-benzyl-sydno-[3,4-a]-indole Acta Cryst. E 2004, 60, o1568-o1570. <u>https://doi.org/10.1107/S1600536804020082</u>

^[6] Grossie, D.A.; Turnbull, K. 5-Hydroxy-5-methylsydno[3,4-a]indole Acta Cryst. C 1992, 48, 377-379. https://doi.org/10.1107/S0108270191009125

4. Primary interactions in 4-acetylsydnones deposited in the CSD



Figure 5S. Known CCDC 4-acetylsydnones: a. *ERUCAW*-four independent molecules-highlight $O \cdots \pi$ contact; b. *FIXPIL* – Examples of H-bonds involving the C=O bonds; c. *MIHTUU* – Contacts involving the O atoms in the sydnone and acetyl moiety.

5. X-Ray-Diffraction supplementary data for Alc-1,2 and Keto-1,2

| Alc-1 | | | Alc-2 | | | | |
|---|--|---|---|--|---|--|---|
| Atom-Atom | Length/Å | Atom-Atom | Length/Å | Atom-Atom | Length/Å | Atom-Atom | Length/Å |
| O1-N2 | 1.378(2) | C1-C6 | 1.366(3) | F1-C4 | 1.347(3) | C1-C6 | 1.370(3) |
| O1-C8 | 1.402(3) | C2-C3 | 1.373(4) | O1-N2 | 1.377(3) | C2-C3 | 1.373(4) |
| O2-C8 | 1.223(3) | C3-C4 | 1.359(4) | O1-C8 | 1.398(3) | C3-C4 | 1.360(4) |
| O3-C9 | 1.419(3) | C4-C5 | 1.374(3) | O2-C8 | 1.228(3) | C4-C5 | 1.363(4) |
| N1-N2 | 1.311(3) | C5-C6 | 1.371(3) | O3-C9 | 1.424(3) | C5-C6 | 1.377(4) |
| N1-C1 | 1.448(3) | C7-C8 | 1.396(3) | N1-N2 | 1.313(3) | C7-C8 | 1.402(3) |
| N1-C7 | 1.346(3) | C7-C9 | 1.496(3) | N1-C1 | 1.445(3) | C7-C9 | 1.502(4) |
| C1-C2 | 1.369(3) | C9-C10 | 1.511(3) | N1-C7 | 1.341(3) | C9-C10 | 1.507(4) |
| | | | | C1-C2 | 1.366(3) | - | |
| | Ke | to-1 | | | Ke | to-2 | |
| Atom-Atom | Length/Å | Atom-Atom | Length/Å | Atom-Atom | Length/Å | Atom-Atom | Length/Å |
| O1-N2 | 1.351(10) | C1-C6 | 1.367(12) | F1-C4 | 1.362(2) | C1-C6 | 1.373(3) |
| O1-C8 | 1.432(11) | C2-C3 | 1.367(13) | 01-N2 | 1.370(2) | $C_2 C_3$ | 1.381(3) |
| O2-C8 | | | | 01112 | 1.570(2) | C2-CJ | 1.001(0) |
| | 1.173(10) | C3-C4 | 1.369(17) | 01-C8 | 1.419(3) | C2-C3 C3-C4 | 1.358(3) |
| O3-C9 | 1.173(10) 1.220(9) | C3-C4 C4-C5 | 1.369(17) 1.377(16) | O1-C8 O2-C8 | 1.376(2) 1.419(3) 1.206(2) | C2-C3 C3-C4 C4-C5 | 1.358(3) 1.372(3) |
| O3-C9 N1-N2 | 1.173(10) 1.220(9) 1.307(9) | C3-C4 C4-C5 C5-C6 | 1.369(17) 1.377(16) 1.365(14) | 01-C8 02-C8 03-C9 | 1.376(2) $1.419(3)$ $1.206(2)$ $1.215(2)$ | C3-C4 C4-C5 C5-C6 | 1.358(3) 1.372(3) 1.383(3) |
| O3-C9 N1-N2 N1-C1 | 1.173(10) 1.220(9) 1.307(9) 1.448(10) | C3-C4 C4-C5 C5-C6 C7-C8 | 1.369(17) 1.377(16) 1.365(14) 1.445(11) | 01-C8 02-C8 03-C9 N1-N2 | $\begin{array}{c} 1.376(2) \\ 1.419(3) \\ 1.206(2) \\ 1.215(2) \\ 1.307(2) \end{array}$ | C3-C4 C4-C5 C5-C6 C7-C8 | $\begin{array}{c} 1.358(3) \\ 1.372(3) \\ 1.383(3) \\ 1.418(3) \end{array}$ |
| O3-C9 N1-N2 N1-C1 N1-C7 | $\begin{array}{c} 1.173(10) \\ 1.220(9) \\ 1.307(9) \\ 1.448(10) \\ 1.345(9) \end{array}$ | C3-C4 C4-C5 C5-C6 C7-C8 C7-C9 | $\begin{array}{c} 1.369(17)\\ 1.377(16)\\ 1.365(14)\\ 1.445(11)\\ 1.458(10)\end{array}$ | 01-C8 02-C8 03-C9 N1-N2 N1-C1 | $\begin{array}{c} 1.376(2) \\ 1.419(3) \\ 1.206(2) \\ 1.215(2) \\ 1.307(2) \\ 1.447(2) \end{array}$ | C2-C3 C3-C4 C4-C5 C5-C6 C7-C8 C7-C9 | $\begin{array}{c} 1.358(3) \\ 1.372(3) \\ 1.383(3) \\ 1.418(3) \\ 1.459(3) \end{array}$ |
| O3-C9 N1-N2 N1-C1 N1-C7 C1-C2 | $\begin{array}{c} 1.173(10) \\ 1.220(9) \\ 1.307(9) \\ 1.448(10) \\ 1.345(9) \\ 1.379(11) \end{array}$ | C3-C4 C4-C5 C5-C6 C7-C8 C7-C9 C9-C10 | $\begin{array}{c} 1.369(17)\\ 1.377(16)\\ 1.365(14)\\ 1.445(11)\\ 1.458(10)\\ 1.495(12)\end{array}$ | 01-C8 02-C8 03-C9 N1-N2 N1-C1 N1-C7 | $\begin{array}{c} 1.376(2) \\ 1.419(3) \\ 1.206(2) \\ 1.215(2) \\ 1.307(2) \\ 1.447(2) \\ 1.358(2) \end{array}$ | C3-C4 C3-C4 C4-C5 C5-C6 C7-C8 C7-C9 C9-C10 | $\begin{array}{c} 1.358(3) \\ 1.372(3) \\ 1.383(3) \\ 1.418(3) \\ 1.459(3) \\ 1.500(3) \end{array}$ |

Table 3S. Bond lengths in crystals of the investigated compounds



Figure 6S. View of 1D supramolecular chain showing the role of C-H---O hydrogen bonds in the crystal structure of keto-1. H-bond parameters (Å, °): C5-H---O2 [C5-H 0.930, H---O2 2.63, C5---O2(-0.5 + x, 1.5 - y, z - 0.5) 3.43(1), \angle C5HO2 145.2].



Figure 7S. View of 1D supramolecular chain showing the role of C-H---O hydrogen bonds in the crystal structure of keto-2. H-bond parameters (Å, °): C2-H---O2 [C2-H 0.952, H---O2 2.37, C2---O2(-0.5 + x, y, 0.5 - z) 3.191(2), \angle C2HO2 144.8].

6. Hirshfeld surface analysis of keto-1 and keto-2



Figure 8S. $-O-\cdots C=O$, $CO\cdots \pi$, $CH\cdots \pi$ and $C=O\cdots H(para)$ contacts in Keto-1



Figure 9S. $-O-\cdots C=O$, $CO\cdots \pi$, and $C=O\cdots H(ortho)$ contacts in Keto-2



Figure 10S. HF surface Shape index mode presents complementarity surfaces indicating a $\pi \cdots \pi$ interaction. However, $C_g \cdots C_g$ distances of 4.22 Å and interplanar angles for benzene ring planes of 17° are not favorable



Figure 11S. Measurements of possible C=O··· π interactions to justify increased O···C contacts in Keto-2 (more favorable angle and vdW contact distance < 3.22 Å)

| Keto-1 | | | | | | |
|--------|----------|-----------|-------------|------------|--|-----------|
| | All | С…Н 20.3% | H···H 30.4% | N···H 8.1% | O···C 5.4% | O…H 20.9% |
| | | | | | | |
| | O…N 3.9% | | | | | |
| Keto-2 | | | | | 22 22 20 18 16 10 10 10 10 10 10 10 10 10 10 10 10 10 | |
| | All | С…Н 7.1% | H···H 23.1% | N···H 8.8% | O…C 9.6% | O…H 22.0% |
| | | | | | | |
| | O…N 3.1% | C…C 4.0% | F…H 14.8% | | | |

 Table 4S. Fingerprint plots for ketones Keto-1 and Keto-2 and percentage interactions



7. Crystal features and analysis of Alc-3

Table 5S. Complete crystal data refinement for Alc-3



| Reflections collected | 30898 |
|--------------------------------------|---|
| Independent reflections | $6826 [R_{int} = 0.1163, R_{sigma} = 0.0644]$ |
| Data/restraints/parameters | 6826/0/550 |
| Goodness-of-fit on F ² | 1.093 |
| Final R indexes $[I \ge 2\sigma(I)]$ | $R_1 = 0.1196, wR_2 = 0.2986$ |
| Final R indexes [all data] | $R_1 = 0.1703$, $wR_2 = 0.3425$ |
| Largest diff. peak/hole / e Å-3 | 0.67/-0.35 |

8. ISOS output diagram for isostructurality search

shI_3445_FlDu.res vs. shI_3473_FlDu.res



Figure 12S. ISOS output with superposition of 15 atoms with search mode ON



Figure 13S - Molecular graphs of HB dimeric complexes (-O-H···O-), showing positions of the two attractors (purple spheres) linking the bond paths (BPs) and the corresponding bond critical points (BCP) (yellow spheres) for **Alc-1** and **Alc-2**, obtained with M06-D3/6-311++G**. The orange mid-point represents the ring critical point. Graphs were performed with the aid of the QTAIM extension available in Avogadro



Figure 14S - Molecular graphs of HB dimeric complexes (C=O···H-C/C-H···H-C/C-F···H-C), showing positions of the two attractors (purple spheres) linking the bond paths (BPs) and the corresponding bond critical points (BCP) (yellow spheres) for Alc-1 and Alc-2, obtained with M06-D3/6-311++G**. Graphs were performed with the aid of the QTAIM extension available in Avogadro