**Supplementary data**

Evaluation of antimicrobial activity by marine *Nocardiopsis dassonvillei* against foodborne *Listeria* *monocytogenes* and Shiga toxin-producing *Escherichia coli*

Siyanda S. Ngema1, Solomuzi H. Khumalo1, Michael C. Ojo1, Ofentse J. Pooe2, Tsolanku S. Malilehe3, Albert K. Basson1 and Evelyn Madoroba1\*

|  |
| --- |
| **Citation:** To be added by editorial staff during production.  Academic Editor: Firstname Lastname  Received: date  Accepted: date  Published: date  **Publisher’s Note:** MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.    **Copyright:** © 2022 by the authors. Submitted for possible open access publication under the terms and conditions of the Creative Commons Attribution (CC BY) license (https://creativecommons.org/licenses/by/4.0/). |

1 Department of Biochemistry and Microbiology; ngemasiyanda05@gmail.com; [elsherawy7@gmail.com](mailto:elsherawy7@gmail.com); mikekonyegwachie2015@gmail.com; BassonA@unizulu.ac.za; evelyn.madoroba@gmail.com; MadorobaE@unizulu.ac.za

2 Discipline of Biochemistry, School of Life Sciences, University of KwaZulu-Natal, Durban, South Africa PooeO@ukzn.ac.za

3 Department of Water and Sanitation, University of Limpopo, Private Bag X1106, Polokwane, 0727, South Africa tsolanku.maliehe@ul.ac.za

**\*** Correspondence: evelyn.madoroba@gmail.com; [MadorobaE@unizulu.ac.za](mailto:MadorobaE@unizulu.ac.za)

**Table S1.** Compounds identified by GC-MS in the chloroform extract of *N. dassonvillei* SOD(B)ST2SA2

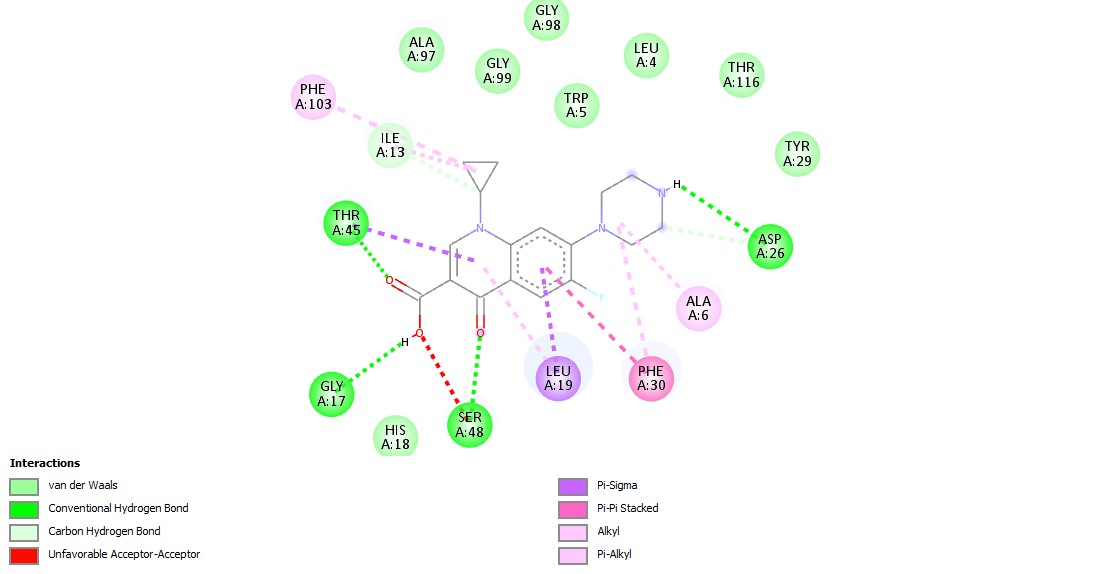
|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Peak# | R.Time | Area | Area% | Height | Height% | Name |
| 1 | 9.130 | 211980 | 0.23 | 65206 | 0.28 | Acetamide, N-(.beta.-mercaptoethyl)- |
| 2 | 9.175 | 373287 | 0.40 | 86963 | 0.38 | 1,2,4,5-Tetrazine, hexahydro-1,2,4,5-tetramethy |
| 3 | 9.250 | 206326 | 0.22 | 76562 | 0.33 | 2-Heptanone, 5-methyl- |
| 4 | 9.300 | 35784 | 0.04 | 64479 | 0.28 | Cyclohexan-1,4,5-triol-3-one-1-carboxylic acid |
| 5 | 9.315 | 146328 | 0.16 | 64669 | 0.28 | Butanamine, 2,2-dinitro-N-methyl- |
| 6 | 9.380 | 139656 | 0.15 | 60365 | 0.26 | (3s)-Pentanol, 4,4-dimethyl-(2s)-[(tert.butyloxy |
| 7 | 9.430 | 307005 | 0.33 | 50129 | 0.22 | dl-3-Aminoisobutyric acid, N-methyl-, methyl e |
| 8 | 10.110 | 175018 | 0.19 | 70704 | 0.31 | 2,4(1H,3H)-Pyrimidinedione, dihydro-5-hydrox |
| 9 | 10.155 | 226458 | 0.25 | 86358 | 0.38 | Tetraacetyl-d-xylonic nitrile |
| 10 | 10.190 | 225361 | 0.24 | 105667 | 0.46 | 2-Acetylamino-3-hydroxy-propionic acid |
| 11 | 10.220 | 267666 | 0.29 | 132157 | 0.58 | Ethylamine, 2-(adamantan-1-yl)-1-methyl- |
| 12 | 10.260 | 123177 | 0.13 | 147519 | 0.64 | Acetamide, 2,2,2-trichloro- |
| 13 | 10.320 | 884208 | 0.96 | 211519 | 0.92 | n-Hexadecanoic acid |
| 14 | 10.365 | 229977 | 0.25 | 197549 | 0.86 | 3-Hexene-2,5-diol |
| 15 | 10.395 | 377728 | 0.41 | 243640 | 1.06 | (+-)-2-Hydroxyoctanoic acid, acetate |
| 16 | 10.410 | 683729 | 0.74 | 262216 | 1.14 | Propanedioic acid, propyl- |
| 17 | 10.475 | 991521 | 1.07 | 314815 | 1.37 | Acetic acid, [(aminocarbonyl)amino]oxo- |
| 18 | 10.523 | 1462876 | 1.58 | 347052 | 1.51 | Acetic acid, mercapto-, hexyl ester |
| 19 | 10.580 | 381422 | 0.41 | 337616 | 1.47 | 2-Amino-1,3-propanediol |
| 20 | 10.600 | 2008032 | 2.17 | 326741 | 1.42 | 3-Butenamide |
| 21 | 10.745 | 496823 | 0.54 | 254460 | 1.11 | Pterin-6-carboxylic acid |
| 22 | 10.780 | 487622 | 0.53 | 234248 | 1.02 | Dec-9-en-6-oxo-1-ylamide |
| 23 | 10.795 | 1216371 | 1.32 | 240812 | 1.05 | Tetraacetyl-d-xylonic nitrile |
| 24 | 11.396 | 183148 | 0.20 | 68991 | 0.30 | Carbonochloridic acid, decyl ester |
| 25 | 12.263 | 363340 | 0.39 | 197357 | 0.86 | 2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dim |
| 26 | 12.672 | 347074 | 0.38 | 79378 | 0.35 | 1b,4a-Epoxy-2H-cyclopenta[3,4]cyclopropa[8, |
| 27 | 12.793 | 537547 | 0.58 | 197146 | 0.86 | Phenol, 2,4-bis(1,1-dimethylethyl)- |
| 28 | 12.840 | 141944 | 0.15 | 66831 | 0.29 | Methyl 4,6-di-O-acetyl-2,3-diacetamido-2,3-di |
| 29 | 12.880 | 148018 | 0.16 | 56144 | 0.24 | 4H-1,3,4-Triazol-3-amine, N-dimethylaminome |
| 30 | 13.505 | 355849 | 0.39 | 183223 | 0.80 | 1-Pentadecene |
| 31 | 13.575 | 3170477 | 3.43 | 1224825 | 5.33 | Diethyl Phthalate |
| 32 | 13.700 | 259201 | 0.28 | 126006 | 0.55 | 4,5-Dicarboxy-1,2,3-triazole |
| 33 | 13.731 | 641870 | 0.69 | 128624 | 0.56 | 2H-Azepine-2-thione, hexahydro- |
| 34 | 14.543 | 1021053 | 1.10 | 209437 | 0.91 | 1H-Pyrrolo[2,3-b]pyridine-2,6-dione, 3,3a,4,5- |
| 35 | 14.650 | 93480 | 0.10 | 73437 | 0.32 | Cyclopentanecarboxylic acid, 2-acetyl-5-methy |
| 36 | 14.701 | 357455 | 0.39 | 126085 | 0.55 | Acetamide, N-(2,4-dimethylphenyl)- |
| 37 | 14.811 | 771031 | 0.83 | 296529 | 1.29 | Phenol, 4-(1,1,3,3-tetramethylbutyl)- |
| 38 | 14.886 | 1046732 | 1.13 | 336573 | 1.47 | 1-(2,6-Dimethyl-4-propoxyphenyl)propan-1-on |
| 39 | 14.936 | 446275 | 0.48 | 229748 | 1.00 | N-(Chroman-5-yl)acetamide |
| 40 | 15.003 | 1315900 | 1.42 | 296823 | 1.29 | 1,3-Cyclopentadiene, 2,3,4,5-tetramethyl-1-(4- |
| 41 | 15.110 | 393725 | 0.43 | 193558 | 0.84 | Benzestrol |
| 42 | 15.135 | 285726 | 0.31 | 114745 | 0.50 | Phenol, 3,5-diethyl- |
| 43 | 15.214 | 769338 | 0.83 | 189619 | 0.83 | Phenol, 2-methyl-4-(1,1,3,3-tetramethylbutyl)- |
| 44 | 15.343 | 1613034 | 1.75 | 475671 | 2.07 | Psicofuranine |
| 45 | 15.410 | 896182 | 0.97 | 196814 | 0.86 | Phenol, 2-methyl-4-(1,1,3,3-tetramethylbutyl)- |
| 46 | 15.510 | 174144 | 0.19 | 78477 | 0.34 | Pentadec-7-ene, 7-bromomethyl- |
| 47 | 15.577 | 2188129 | 2.37 | 1099135 | 4.79 | 1-Octadecene |
| 48 | 15.650 | 265908 | 0.29 | 121604 | 0.53 | Decane, 2,3,5,8-tetramethyl- |
| 49 | 15.952 | 508714 | 0.55 | 185490 | 0.81 | Isopropyl myristate |
| 50 | 16.134 | 102837 | 0.11 | 54362 | 0.24 | 9,9-Dimethoxybicyclo[3.3.1]nona-2,4-dione |
| 51 | 16.237 | 427694 | 0.46 | 200054 | 0.87 | 2-Pentadecanone, 6,10,14-trimethyl- |
| 52 | 16.577 | 90503 | 0.10 | 51769 | 0.23 | 1,2-Benzenedicarboxylic acid, bis(2-methylpro |
| 53 | 16.792 | 426637 | 0.46 | 112113 | 0.49 | Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3 |
| 54 | 16.965 | 495206 | 0.54 | 63850 | 0.28 | Bromoacetic acid, tridecyl ester |
| 55 | 17.366 | 1893030 | 2.05 | 733144 | 3.19 | 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene |
| 56 | 17.519 | 724160 | 0.78 | 193773 | 0.84 | Hexadecanoic acid, methyl ester |
| 57 | 17.675 | 1600267 | 1.73 | 546368 | 2.38 | Benzenepropanoic acid, 3,5-bis(1,1-dimethylet |
| 58 | 17.779 | 338430 | 0.37 | 76462 | 0.33 | 2-Dodecen-1-yl(-)succinic anhydride |
| 59 | 17.981 | 338870 | 0.37 | 86571 | 0.38 | Glutaric acid, dodecyl 2-methoxyphenyl ester |

**Table S1** continued

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Peak# | R.Time | Area | Area% | Height | Height% | Name |
| 60 | 18.196 | 1281602 | 1.39 | 423387 | 1.84 | Dibutyl phthalate |
| 61 | 18.399 | 5411656 | 5.86 | 1144550 | 4.98 | Pentadecanoic acid |
| 62 | 18.745 | 693785 | 0.75 | 170359 | 0.74 | 5-Eicosene, (E)- |
| 63 | 18.861 | 8517166 | 9.22 | 2610749 | 11.37 | 1-Octadecene |
| 64 | 18.985 | 559030 | 0.60 | 165914 | 0.72 | Hexadecane, 4-methyl- |
| 65 | 19.151 | 266106 | 0.29 | 63250 | 0.28 | 1H-1,2,4-Triazole, 1-octadecanoyl- |
| 66 | 19.450 | 451454 | 0.49 | 155868 | 0.68 | 2H-2,4a-Ethanonaphthalen-8(5H)-one, hexahyd |
| 67 | 19.495 | 888029 | 0.96 | 223424 | 0.97 | Isopropyl palmitate |
| 68 | 19.997 | 237839 | 0.26 | 74242 | 0.32 | Eicosanoic acid |
| 69 | 20.352 | 296490 | 0.32 | 63663 | 0.28 | Pentadecanoic acid |
| 70 | 20.774 | 210326 | 0.23 | 50097 | 0.22 | 18,19-Secoyohimban-19-oic acid, 16,17,20,21- |
| 71 | 21.450 | 480308 | 0.52 | 92181 | 0.40 | trans-2-Dodecen-1-ol, pentafluoropropionate |
| 72 | 21.475 | 100914 | 0.11 | 73016 | 0.32 | 2-(2-Carbamoylethyl)-2,3-dihydro-6-hydroxy-3 |
| 73 | 21.647 | 690627 | 0.75 | 126637 | 0.55 | 10-Octadecenoic acid, methyl ester |
| 74 | 22.096 | 823511 | 0.89 | 138658 | 0.60 | Phytol, acetate |
| 75 | 23.398 | 19351394 | 20.94 | 2126400 | 9.26 | 6-Octadecenoic acid, (Z)- |
| 76 | 24.182 | 1642259 | 1.78 | 282620 | 1.23 | Octadecanoic acid, 2-(2-hydroxyethoxy)ethyl e |
| 77 | 24.780 | 1049722 | 1.14 | 181487 | 0.79 | Tetradecanamide |
| 78 | 24.875 | 96115 | 0.10 | 86818 | 0.38 | Cyclohexanol, 2-methyl-, cis- |
| 79 | 24.909 | 643379 | 0.70 | 108932 | 0.47 | Decane, 4-cyclohexyl- |
| 80 | 25.151 | 7228918 | 7.82 | 1165658 | 5.08 | Trifluoroacetoxy hexadecane |
| 81 | 25.376 | 626731 | 0.68 | 110530 | 0.48 | 2-methyltetracosane |
| 82 | 25.796 | 597973 | 0.65 | 92932 | 0.40 | Tetracosyl acetate |
| 83 | 27.959 | 1366662 | 1.48 | 209523 | 0.91 | N,N-Dimethyldodecanamide |
| 84 | 30.513 | 2474954 | 2.68 | 316980 | 1.38 | 2-Propenoic acid, pentadecyl ester |
| 85 | 30.645 | 47976 | 0.05 | 53719 | 0.23 | 2-Oxepanone, 7-butyl- |

Ciprofloxacin

**A close-up of a molecule

Description automatically generated with low confidence**

**Figure S1.** 2D and 3D binding interactions of ciprofloxacin against dihydrofolate reductase (PDB ID: 1DIS), respectively. The 3D interactions show the ligand in a binding pocket of the enzyme. Dashed lines indicate the interactions between the ligands and the amino acids of the enzyme.

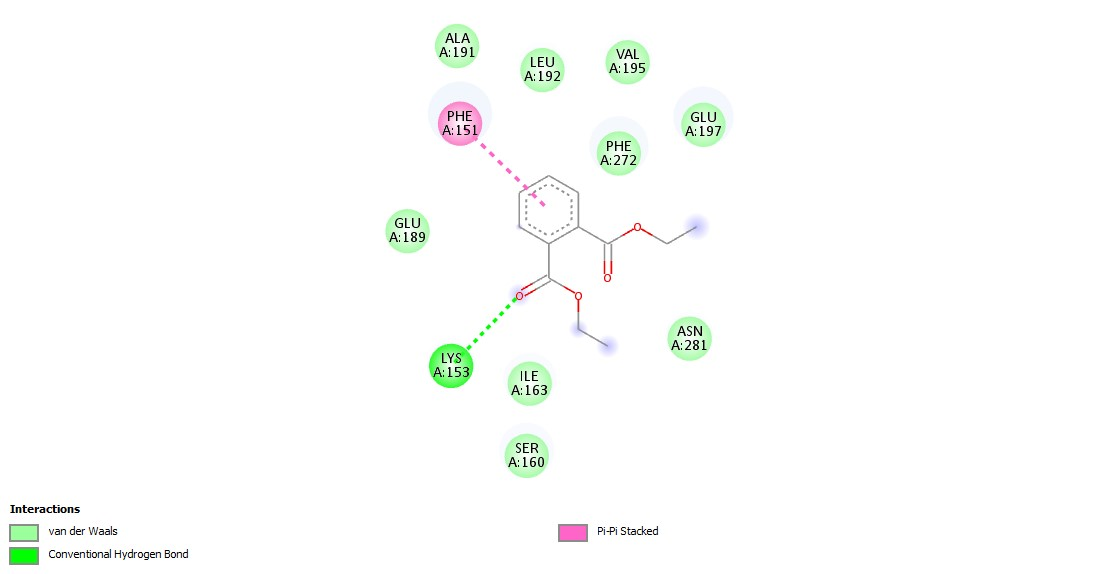
Pentadecanoic acid

A close-up of a molecule

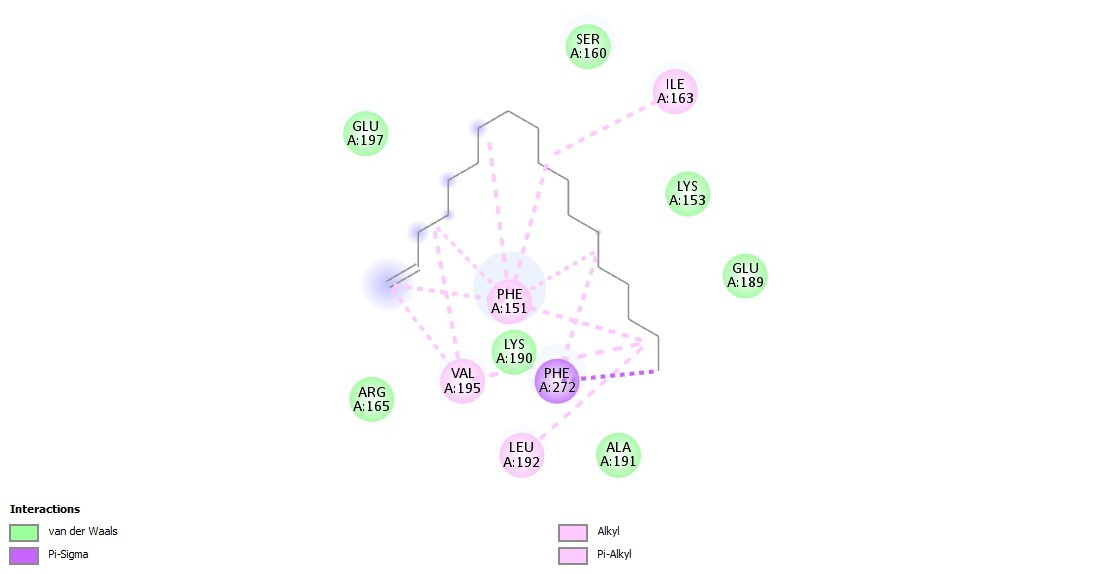
Description automatically generated with low confidence

Diethyl phthalate

A picture containing graphic design, cartoon, screenshot, art

Description automatically generated

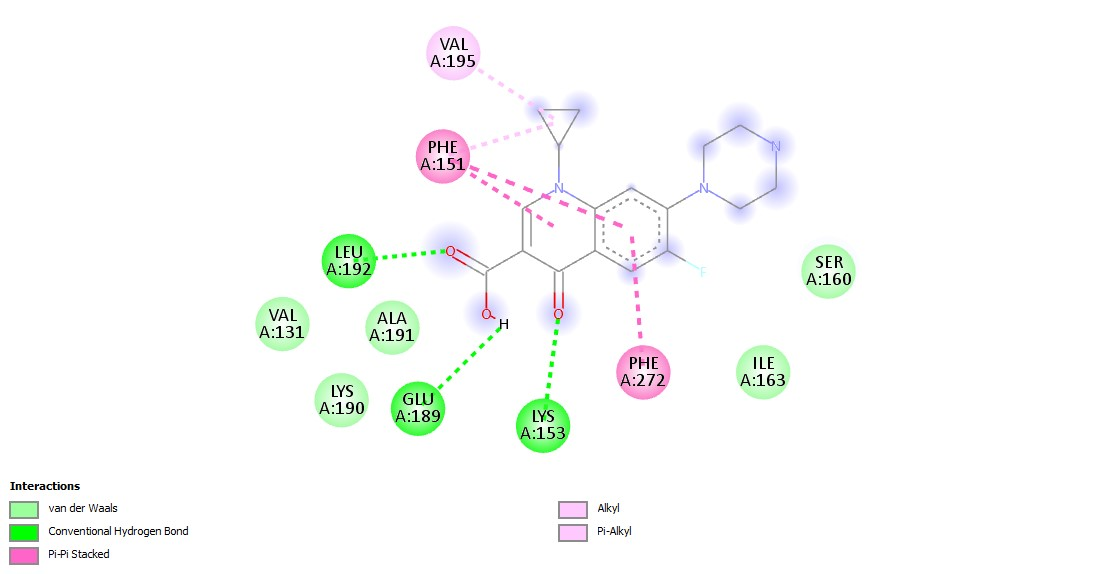
A picture containing cartoon, clipart, graphics, graphic design

Description automatically generated

1-Octadecene

**Figure S2.** 2D and 3D binding interactions of compounds against D-alanine:D-alanine ligase (DDl) (PDB ID: 2Zdg), respectively. The 3D interactions show the ligand in a binding pocket of the enzyme. Dashed lines indicate the interactions between the ligands and the amino acids of the enzyme.

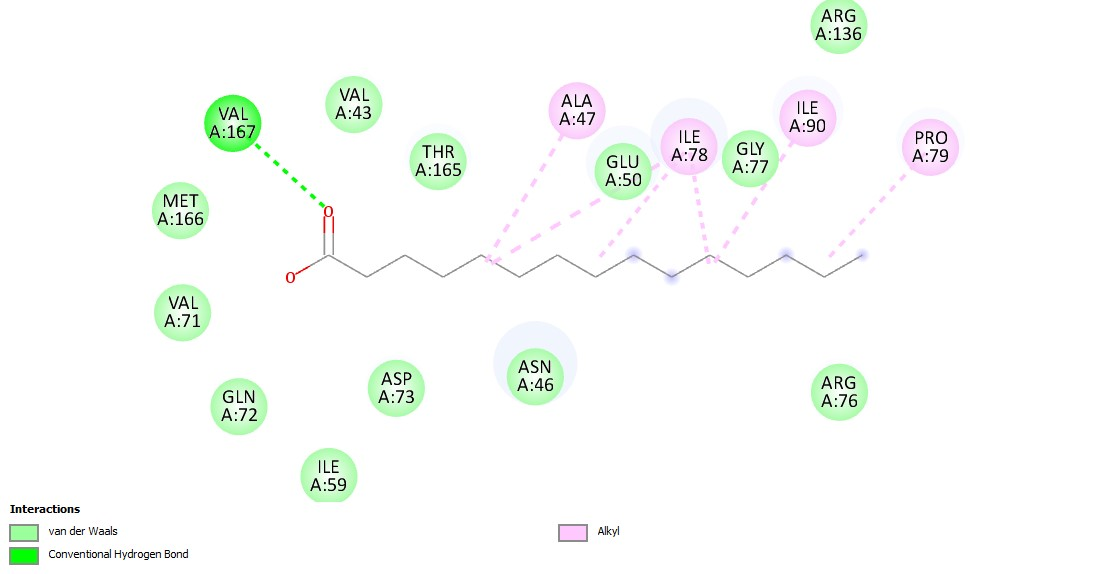
A close-up of a molecule

Description automatically generated with low confidence

Ciprofloxacin

**Figure S3.** 2D and 3D binding interactions of ciprofloxacin against DDl (PDB ID: 2Zdg), respectively. The 3D interactions show the ligand in a binding pocket of the enzyme. Dashed lines indicate the interactions between the ligand and the amino acids of the enzyme.

A picture containing drawing, cartoon, sketch, clipart

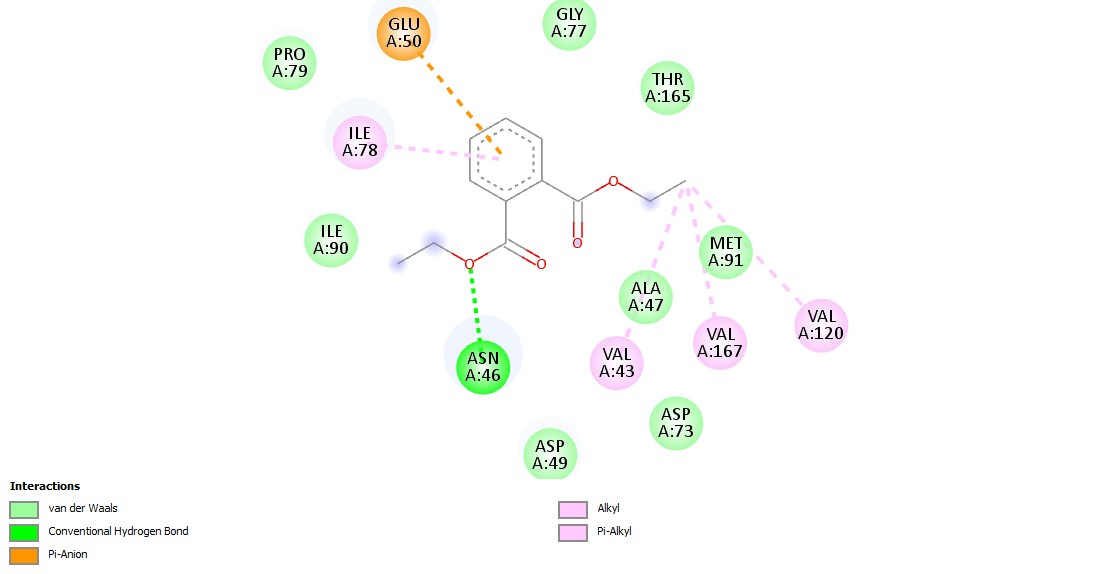
Description automatically generated

Pentadecanoic acid

Diethyl phthalate

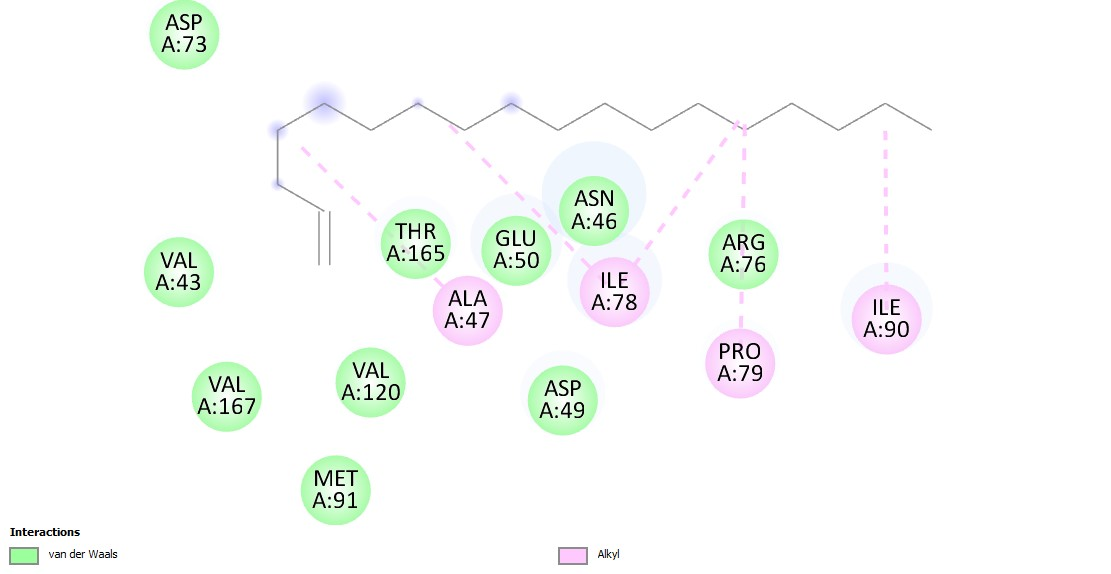
A close-up of a molecule

Description automatically generated with low confidence



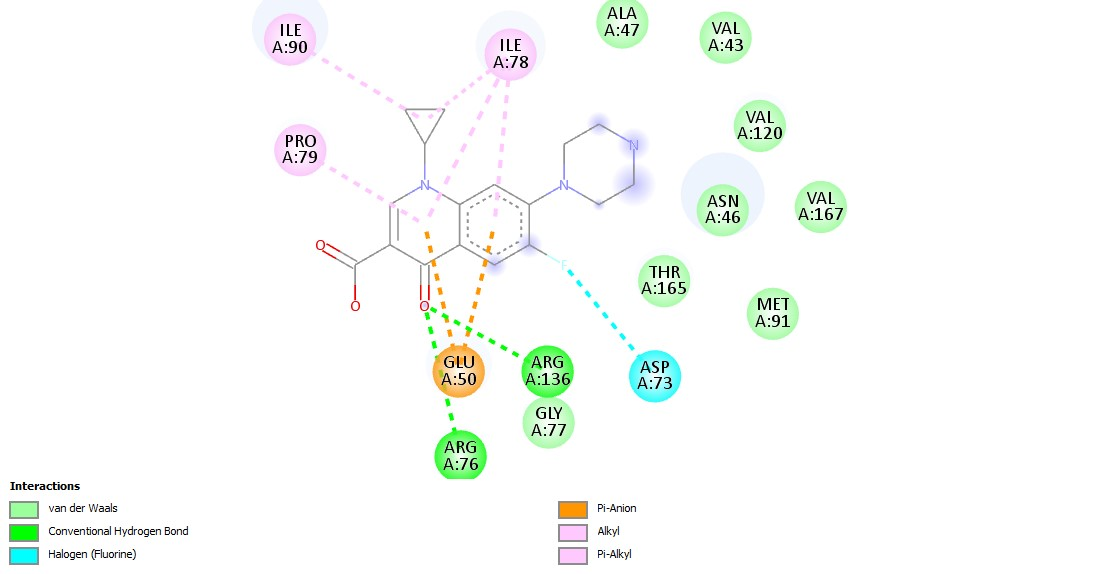
1-Octadecene

A close-up of a structure

Description automatically generated with low confidence

**Figure S4.** 2D and 3D binding interactions of compounds against DNA gyrase B (PDB ID: 1KZN), respectively. The 3D interactions show the ligand in a binding pocket of the enzyme. Dashed lines indicate the interactions between the ligands and the amino acids of the enzyme.

A picture containing diagram, graphic design, screenshot, graphics

Description automatically generated

Ciprofloxacin

**Figure S5.** 2D and 3D binding interactions of ciprofloxacin against DNA gyrase B (PDB ID: 1KZN), respectively. The 3D interactions show the ligand in a binding pocket of the enzyme. Dashed lines indicate the interactions between the ligand and the amino acids of the enzyme.

**Sequence of *Nocardiopsis dassonvillei* strain SOD(B)ST2SA2 that showed activity during secondary screening for antibacterial activity**

>SOD-B\_907-R

CTCCCCSGGCSGGGGGCGCTTATGCGTTAGCTACGGCGCGGAAACCGTGGAAAGTCCCCACACCTAKYGCCCAACGTTTACGGCATGGACTACCAGGGTATCTAATCCTGTTCGCTCCCCATGCTTTCGCTCCTCAGCGTCAGGTAAGGCCCAGAGACCCGCCTTCGCCACCGGTGTTCCTCCTGATATCTGCGCATTTCACCGCTACACCAGGAATTCCAGTCTCCCCTACCTACCTCTAGCATGCCCGTATCCACTGCAGAACCGGAGTTAAGCCCCGGTCTTTCACAGCAGACGCGACACGCCGCCTACGAGCTCTTTACGCCCAATAATTCCGGACAACGCTCGGACCCTACGTATTACCGCGGCTGCTGGCACGTAGTTAGCCGGTCCTTATTCCCCACCTACCGTCAACCCGAAGAGAACTTCGAGCCTGCGTTGGTGGTAAAAGAGGTTTACAACCCGAAGGCCGTCATCCCCCACGCGGCGTCGCTGCGTCAGGCTTTCGCCCATTGCGCAATATTCCCCACTGCTGCCTCCCGCAGGAGTCTGGGCCGTGTCTCAGTCCCAGTGTGGCCGGTCGCCCTCTCAGGCCGGCTACCCGTAATCGCCTTGGTAGGCCGTTACCCCACCAACAAGCTGATAGGCCGCGAGCCCATCCCTGACCGAAAAACTTTCCACCCTCCACCATGAGGTGGCGGGTCGTATCCGGTATTAGACGGCGTTTCCACCGCTTATCCCGGAGTCAGGGGCAGGTTGCTCACGTGTTACTCACCCGTTCGCCGCTCGTGTACCCCGAAAGGGCCTTACCGCTCGACTTGCATGTGTTAAGCACGCCGCCAGCGTTCGTCCTGAGCCATAWWYWMAAMTYCT

>SOD-B\_1492-R

CMGGCCCCMMCCTTCACTCACTCCCTCCMACAAGGGGTTAGGCCGCAAGTTTCGGGTGTTGCCGACTTTCWTGACGTGACGGGCGGTGTGTACAAGGCCCGGGAACGTATTCACCGCGGCGTTGCTGATCCGCGATTACTAGCGACTCCACCTTCATGGGGTCGAGTTGCAGACCCCAATCCGAACTGAGACCGGCTTTTAGGGATTCGCTCCACCTTACGGTATCGCACGCCCATTGTACCGGCCATTGTAGCATGTTTGCAGCCCAAGACATAAGGGGCATGATGACTTGACGTCATCCCCACCTTCCTCCGAGTTGACCCCGGCAGTCTCCCATGAGTCCCCACCATTACGTGCTGGCAACATGGAACAAGGGTTGCGCTCGTTGCGGGACTTAACCCAACATCTCACGACACGAGCTGACGACAGCCATGCACCACCTGTCACCCGCCAACTAAATGACCTCACATCTCTGCGAGTCCACGGGTGATGTCAAACCTTGGTAAGGTTCTTCGCGTTGCGTCGAATTAAGCAACATGCTCCGCCGCTTGTGCGGGCCCCCGTCAATTCCTTTGAGTTTTAGCCTTGCGGCCGTACTCCCCAGGCGGGGCGCTTAATGCGTTAGCTACGGCGCGGAAACCGTGGAAAGTCCCCACACCTAGCGCCCAACGTTTACGGCATGGACTACCAGGGTATCTAATCCTGTTCGCTCCCCATGCTTTCGCTCCTCAGCGTCAGGTAAGGCCCAGAGACCCGCCTTCGCCACCGGTGTTCCTCCTGATATCTGCGCATTTCACCGCTACACCAGGAATTCCAGTCTCCCCTACCTACCTCTAGCATGCCCGTATCCACTGCAGAACCGGAGTTAAGCCCCGGTCTTTCACAGCAGACGCGACACGCCGCCTACGAGCTCTTTACGCCCATAATTCCGGACAACGCTCGGACCCTACGTATTACCGCGGCTGCTGGCACGTAGTTAGCCGGTCCTTATTCCCCACCTACCGTCAACCCGAAGARAACTTCGAGCCTGCGTTGGTGGTAAAGAGGTTTACAACCGAAGGCGTCATCCCCCACGCGCGTCGCTGCGTCAGCTTCGCATGGCCAAWWTCCATGCTGCTCCGCAGAGCTGACGKGTYYCAGTCAAGKTGACGTCGCCYTCAGCGATACGATGCATGTGCGTACTCACAMAGCKATAGCGCGGACCCATCT