

Frag Xtal Screen

Fragment Screen for Crystallographic Screening

Cat.# X-FS-101



| Plate ID | Fragment | Scifinder Name | CAS ID | MW |
|----------|----------|--|--------------|--------|
| A1 | | Benzoic acid, 3-methyl-, hydrazide | 13050-47-0 | 150,18 |
| A2 | | 1H-Isoindol-3-amine | 76644-74-1 | 168,62 |
| A3 | | Thiourea, N-(4-bromo-2-chlorophenyl)-N'-methyl- | 838813-44-8 | 279,58 |
| A4 | | 1H-Azepine, hexahydro-1-(6-methyl-4-pyrimidinyl)- | 1055196-50-3 | 227,74 |
| A5 | | 4-Morpholineethanamine, β-ethyl-β-methyl- | 914206-26-1 | 172,30 |
| A6 | | 1,3-Benzodioxole-5-methanamine, N-cyclopentyl- | 114413-77-3 | 219,30 |
| A7 | | 1-Piperidineacetamide, N-1,3-benzodioxol-5-yl- | 487006-82-6 | 262,30 |
| A8 | | 1,3,5-Cycloheptatrien-1-amine, N-(1-methylethyl)-7-[(1-methylethyl)imino]- | 3337-06-2 | 204,32 |

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| A9 | | 2H -Benzimidazol-2-one, 1,3-dihydro-5-[(2-pyridinylmethyl)amino]- | 876898-01-0 | 240,26 |
| A10 | | Ethanone, 2-amino-1-(4-bromophenyl)-, hydrochloride (1:1) | 5467-72-1 | 250,52 |
| A11 | | Imidazo[2,1-c][1,2,4]triazine, 3-(3,4-difluorophenyl)-1,4,6,7-tetrahydro- | 219929-40-5 | 236,22 |
| A12 | | Benzeneacetic acid, 3-chloro-alpha-hydroxy- | 61008-98-8 | 186,59 |
| B1 | | 1H -Pyrazole-5-methanamine, 1,3-dimethyl- | 499770-63-7 | 125,20 |
| B2 | | 2-Furanmethanamine, N-methyl-5-(3-pyridinyloxy)- | 859850-77-4 | 204,23 |
| B3 | | Benzoic acid, 2-hydroxy-, compd. with N,N-diethylethanimidamide (1:1) | 301843-27-6 | 252,30 |
| B4 | | Acetamide, 2-[(cyanomethyl)methylamino]-N-(6-methyl-2-pyridinyl)- | 1311649-76-9 | 218,25 |

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| B5 | | Benzoic acid, 3-(dimethylamino)-, hydrazide | 205927-64-6 | 179,22 |
| B6 | | Benzeneacetic acid, 4-fluoro-, hydrazide | 34547-28-9 | 168,17 |
| B7 | | Pyrrolidine, 2-(2,3-dihydro-1,4-benzodioxin-6-yl)- | 524674-08-6 | 205,25 |
| B8 | | 1H-Pyrazole-4-carbonitrile, 5-amino-3-(1-pyrrolidinyl)- | 1119391-48-8 | 177,20 |
| B9 | | 1-Piperidinecarboximidamide, hydriodide (1:1) | 102392-91-6 | 255,10 |
| B10 | | 3-Isoxazolecarboxamide, 5-methyl-N-(2,2,2-trifluoroethyl)- | 878595-52-9 | 208,13 |
| B11 | | 1-Piperidineacetamide, 4-methyl-N-[3-(1-methylethyl)-5-isoxazolyl]- | 923192-35-2 | 265,35 |
| B12 | | 2-Thiophenebutanamide, gamma-oxo-N-[1-(3-pyridinyl)ethyl]- | 923810-83-7 | 288,36 |

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| C1 | | 3-Pyridinecarbonitrile, 4,6-dimethyl-2-[[3-(4-morpholinyl)propyl]amino]- | 831183-48-3 | 274,36 |
| C2 | | 2-Thiazolamine, 4-methyl-5-(1-methyl-1H-imidazol-2-yl)- | 929975-79-1 | 194,26 |
| C3 | | 1,3,5-Triazine-2,4-diamine, 6-[1-(hexahydro-1H-azepin-1-yl)ethyl]-N2,N2-dimethyl- | 923208-22-4 | 264,37 |
| C4 | | 3-Pyridineethanamine | 20173-24-4 | 122,17 |
| C5 | | 3-Thiophenecarboximidamide, hydrochloride (1:1) | 51528-02-0 | 162,64 |
| C6 | | 2-Furanmethanamine, 5-(trifluoromethyl)- | 868755-68-4 | 165,11 |
| C7 | | Methanone, 1-piperidinyl-3-piperidinyl- | 845885-83-8 | 232,75 |
| C8 | | Benzoic acid, 4-(aminomethyl)-, methyl ester, hydrochloride (1:1) | 6232-11-7 | 201,65 |

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| C9 | | Benzenecarboximidamide, 4-(trifluoromethyl)- | 38980-96-0 | 224,61 |
| C10 | | Guanidine, N-(4-ethoxy-8-methyl-2-quinazolinyl)- | 923803-92-3 | 270,37 |
| C11 | | 1H-Indole-3-ethanamine, N-[(1-methyl-1H-pyrrol-2-yl)methyl]- | 289487-79-2 | 253,34 |
| C12 | | Benzenemethanamine, 2-chloro-N-methyl-5-nitro- | 1177318-36-3 | 237,08 |
| D1 | | 1H-Imidazole-2-methanamine, N,1-dimethyl- | 1049717-38-5 | 198,09 |
| D2 | | Imidazo[1,2-a]pyridine-2-acetamide, N-phenyl- | 1090352-33-2 | 251,28 |
| D3 | | Cyclohexanecarboxamide, N-[(tetrahydro-2-furanyl)methyl]- | 401597-32-8 | 211,30 |
| D4 | | 4(3H)-Quinazolinone, 2-[[[(1-cyclopropylethyl)methylamino]methyl]- | 1090518-66-3 | 257,33 |

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| D5 | | 3-Pyridinecarboxylic acid, 6-(dimethylamino)- | 82846-28-4 | 166,18 |
| D6 | | 3-Furancarboxamide, 2,5-dimethyl-N-4-pyridinyl- | 501442-73-5 | 216,24 |
| D7 | | 1H-Pyrazole-4-acetamide, 1,3,5-trimethyl-N-2-pyridinyl- | 1171575-61-3 | 244,29 |
| D8 | | 1-Isoquinolineacetamide, 2-acetyl-1,2-dihydro-N,N-dimethyl- | 1090496-96-0 | 258,32 |
| D9 | | Benzenemethanol, α-(aminomethyl)-4-fluoro- | 456-05-3 | 155,17 |
| D10 | | Acetamide, N-[3-(aminomethyl)phenyl]- | 96783-68-5 | 164,20 |
| D11 | | Phenol, 5-(aminomethyl)-2-methoxy-, hydrochloride (1:1) | 89702-89-6 | 153,18 |
| D12 | | 4-Pyridinemethanamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)- | 774553-49-0 | 242,27 |

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| Plate ID | Fragment | Scifinder Name | CAS ID | MW |
|----------|----------|---|--------------|--------|
| E1 | | Carbamimidothioic acid, (2-chlorophenyl)methyl ester | 14122-38-4 | 200,69 |
| E2 | | 6H-Purin-6-one, 1,9-dihydro-8-(1-piperidinyl)- | 312923-57-2 | 219,25 |
| E3 | | Furo[2,3-d]pyrimidine-3(4H)-propanamine, 4-imino-N,N,5,6-tetramethyl- | 929868-45-1 | 248,33 |
| E4 | | 1H-Imidazole-1-acetamide, N-(4-methylcyclohexyl)- | 1118862-09-1 | 221,30 |
| E5 | | INDEX NAME NOT YET ASSIGNED | 1212574-75-8 | 253,32 |
| E6 | | 3-Oxetanamine, 3-[[5-(1,1-dimethylethyl)-3-isoxazolyl]methyl]- | 1371533-72-0 | 210,28 |
| E7 | | 1,2-Cyclopentanediol, 3-amino-4-(3-methylphenyl)-(1R,2S,3R)- | 1421058-66-3 | 243,74 |
| E8 | | 1,4-Oxazepin-6-ol, hexahydro-, (6R)- | 1022915-33-8 | 153,65 |

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| Plate ID | Fragment | Scifinder Name | CAS ID | MW |
|----------|----------|---|------------------|--------|
| E9 | | NO NAME ASSIGNED IN SCIFINDER | NO CAS AVAILABLE | 354,24 |
| E10 | | 1,2,4-Oxadiazole, 3-(1-methylethyl)-5-(2-pyrrolidinyl)- | 1185170-55-1 | 126,16 |
| E11 | HCl | 3H-Oxazolo[3,4-a]pyrazin-3-one, hexahydro- | 1020349-31-8 | 178,61 |
| E12 | | 1,2-Pyrrolidinedicarboxylic acid, 1-(phenylmethyl) ester, (2S)- | 1148-11-4 | 249,26 |
| F1 | | 3-Pyridinecarboxamide | 98-92-0 | 122,12 |
| F2 | | L-Phenylalanine, methyl ester, hydrochloride (1:1) | 7524-50-7 | 179,22 |
| F3 | | 1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl- | 83-67-0 | 180,16 |
| F4 | | 6H-Purin-6-one, 2-amino-1,9-dihydro- | 73-40-5 | 151,13 |

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|----------|----------|--|-----------|--------|
| F5 | | Benzoic acid, 4-nitro- | 62-23-7 | 167,12 |
| F6 | | 2(3H)-Benzoxazolone, 5-chloro- | 95-25-0 | 169,57 |
| F7 | | Pentanoic acid, 5-amino- | 660-88-8 | 117,15 |
| F8 | | Imidazo[4,5-d]imidazole-2,5(1H,3H)-dione, tetrahydro- | 496-46-8 | 142,12 |
| F9 | | 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- | 7164-43-4 | 171,11 |
| F10 | | L-Histidine, 1-methyl- | 332-80-9 | 169,18 |
| F11 | | 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl- | 58-08-2 | 194,19 |
| F12 | | L-Homoserine, O-[(aminoiminomethyl)amino]- | 543-38-4 | 176,17 |

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|----------|----------|---|------------|--------|
| G1 | | 1H -Thieno[3,4-d]imidazole-6-pentanoic acid, 2-amino-3a,4,6,6a-tetrahydro-, (3aR,6S,6aS)- | 13395-35-2 | 243,33 |
| G2 | | 1,2-Benzenediol, 4-[(1R)-2-amino-1-hydroxyethyl]- | 51-41-2 | 169,18 |
| G3 | | Propanamide, 2-methyl-N-[4-nitro-3-(trifluoromethyl)phenyl]- | 13311-84-7 | 276,21 |
| G4 | | L-Proline, 5-oxo- | 98-79-3 | 129,11 |
| G5 | | D-Arginine | 157-06-2 | 174,20 |
| G6 | | Glycine, glycylglycyl- | 556-33-2 | 189,17 |
| G7 | | 3H-1,2,3-Triazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione | 1468-26-4 | 171,11 |
| G8 | | Benzenesulfonamide, 4-amino-N-(5-methyl-3-isoxazolyl)- | 723-46-6 | 253,28 |

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|----------|----------|--|-------------|--------|
| G9 | | 1-Propanaminium, 3-carboxy-2-hydroxy-N,N,N-trimethyl-, inner salt, (2R)- | 541-15-1 | 161,20 |
| G10 | | 1,2-Benzenediol, 4-nitro- | 3316-09-4 | 155,11 |
| G11 | | Benzenamine, 3-(5-oxazolyl)- | 157837-31-5 | 160,17 |
| G12 | | 1H-Indol-5-ol | 1953-54-4 | 133,15 |
| H1 | | Benzamide, 3-amino- | 3544-24-9 | 136,15 |
| H2 | | Cyclohexanecarboxylic acid, 4-(aminomethyl)-, trans- | 1197-18-8 | 157,21 |
| H3 | | Methionine, N - (aminocarbonyl)- | 30411-84-8 | 192,24 |
| H4 | | Butanedioic acid, 1-(2,2-dimethylhydrazide) | 1596-84-5 | 160,17 |

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|----------|----------|---|-------------|--------|
| H5 | | Benzamide, 4-hydroxy- | 619-57-8 | 137,14 |
| H6 | | 8-Quinolinol, 5-nitro- | 4008-48-4 | 190,16 |
| H7 | | L-Proline, 1-acetyl- | 68-95-1 | 157,17 |
| H8 | | 1,2-Benzenediol, 3,5-dinitro- | 7659-29-2 | 200,11 |
| H9 | | 2,3-Quinoxalinedione, 1,4-dihydro-6,7-dinitro- | 2379-57-9 | 252,14 |
| H10 | | 2-Thiophenesulfonamide, 5-chloro- | 53595-66-7 | 197,66 |
| H11 | | 3-Furancarboxamide, tetrahydro- | 871677-92-8 | 115,13 |
| H12 | | Bicyclo[2.2.1]heptane-1-carboxamide, N-hydroxy- | 256954-29-7 | 155,20 |