February 16, 2024: Compounds introduced or investigated in Kenneth A. Jacobson's lab (kennethj@niddk.nih.gov) at NIDDK (Molecular Recognition Section, MRS) or through collaborations. Orange compounds are or will soon be available commercially as research tools:

| Abbreviation | Action | Reference (year, vol:page) ** |
|---|---|---|
| **AB-MECA** | selective $A_3$ adenosine agonist, to radioiodinate | JMC (1994) 37:636 |
| **ADAC (MRS998)** | selective $A_1$ adenosine agonist | BP (1987) 36:1697 |
| | **(46)** | JMC (2012) 55:8075 |
| **Alexa488-APEC** | fluorescent $A_{2A}$ adenosine receptor agonist | EJP (2008) 590:36 |
| **APEC** | selective $A_{2A}$ adenosine agonist **(6)*** | JMC (1994) 37:3614 |
| **3′-Benzylamino-3′-deoxy-ATP** | | |
| | Potent P2X agonist **(25)** | DDR (1994) 31:206 |
| **Benzyl-NECA** | potent $A_3$ adenosine agonist | MP (1994) 45:1101 |
| **Biotin-ADAC** | $A_1$ adenosine receptor agonist biotin conjugate | BP (1987) 36:1697 |
| **Biotin-TAC** | $M_2$ muscarinic antagonist (**9**) | BC (1992) 3:234 |
| **$BTH_4$** | non-N-containing adenosine antagonist **(7)** | JMC (1996) 39:398 |
| **Cl-IB-MECA** | selective $A_3$ adenosine agonist **(13)** | JMC (1994) 37:3614 |
| **(namodenoson, CF102)** | | BP (2020) 117:113934 |
| | | NP (2017) 114:101 |
| **CMB6446** | selective $A_{2B}$ adenosine antagonist | BMC (2003) 11:77 |
| **CSC** | selective $A_{2A}$ adenosine antagonist | JMC (1993) 36:1333 |
| **DBXR** | xanthine riboside as adenosine antagonist | JMC (1994) 37:4020 |
| **DBXRM** | selective $A_3$ adenosine agonist | JMC (1994) 37:4020 |
| **m-DITC-ADAC** | selective $A_1$ adenosine agonist affinity label **(46)** | JMC (1989) 32:1043 |
| **p-DITC-ADAC** | selective $A_1$ adenosine agonist affinity label **(45)** | JMC (1989) 32:1043 |
| **m-DITC-APEC** | selective $A_{2A}$ adenosine agonist affinity label **(11)** | JMR (1989) 32:1043 |
| **p-DITC-APEC** | selective $A_{2A}$ adenosine agonist affinity label **(12)** | JMR (1989) 32:1043 |
| **m-DITC-XAC** | selective $A_1$ adenosine antagonist affinity label **(10)** | JMC (1989) 32:1043 |
| **p-DITC-XAC** | selective $A_1$ adenosine antagonist affinity label **(9)** | JMC (1989) 32:1043 |
| **DPCPX** (John Daly) | selective $A_1$ adenosine antagonist **(1)** | BP (1988) 37:3653 |
| | **(15)** | JMC (1988) 31:613 |
| **DU124182** | selective $A_3$ adenosine PAM (2-cPent-4-O-Ph) | MP (2002) 62:81 |
| **DU124183** | selective $A_3$ adenosine PAM (2-cPent-4-NH-Ph) | MP (2002) 62:81 |
| | | MP (2003) 63:1021 |
| **DU124184** | selective $A_3$ adenosine PAM (2-cPent-4-NH-cPent) | MP (2002) 62:81 |
| **DU124482** | selective $A_3$ adenosine PAM (2-Ph-4-NH-cPent) | MP (2002) 62:81 |
| **FE@SUPPY** | | |
| **(MRS1532)** | selective $A_3$ adenosine antagonist **(7)** | JMC (1999) 42:706 |
| **FITC-ADAC** | fluorescent $A_1$ adenosine receptor agonist | BP (1987) 36:1697 |
| **FITC-APEC** | fluorescent $A_{2A}$ adenosine receptor agonist* | JF (1992) 2:217 |
| **I-AB-MECA** | $A_3$ adenosine agonist **(26)** | JMC (1994) 37:636 |
| | | MP (1994) 45:978 |
| **IB-MECA** | selective $A_3$ adenosine agonist **(16)** | JMC (1994) 37:636 |
| **(piclidenoson, CF101)** | | NP (2017) 114:101 |
| **IB-MECA prodrug** | selective $A_3$ adenosine agonist diester **(38)** | JMC (1995) 38:1720 |
| **IB-MECA prodrugs** | selective $A_3$ adenosine agonist diesters **(5-7)** | CCC (2006) 71:912 |

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| **ICBM (MRS1163)** | selective $A_3$ adenosine agonist affinity label **(4)** | BBRC (1994) 203:570<br>PS (2023) in press |
| **[$^{125}$I]I-ZM241,385** | selective $A_{2A}$ adenosine antagonist radioligand | MP (1996) 48:970 |
| **[$^{125}$I]I-AB-MECA** | $A_3$ adenosine agonist radioligand | ACSPT (2022) 5(8):625<br>MP (1994) 45:978 |
| **[$^{125}$I]I-azido-PAPA-APEC** | $A_{2A}$ adenosine agonist photoaffinity radioligand | MP (1991) 39:130 |
| **LC260** | selective $A_3$ adenosine agonist, 2-triazole **(15)** | JMC (2006) 49:7373 |
| **LJ529** CHEMBL200732 | selective $A_3$ agonist **(**4′-S-Cl-IB-MECA, **3)**<br>**(39a)**<br>**(6)** | JMC (2003) 46:3775<br>JMC (2006) 49:273<br>JMC (2007) 50:3159 |
| **LJ1258 (MRS3884)** | selective $A_3$ agonist **(**4′-S-IB-MECA, **5h)** CHEMBL522152 | BMC (2009) 17:8003 |
| **LJ1351 (MRS3973)** | h$A_3$ receptor antagonist **(**3-Br-Bn, *N*,*N*-diMe, **6c)** | BMCL (2008) 18:1612 |
| **LJ1888 (LJ1251, MRS3820)** | selective $A_3$ adenosine antagonist **(6e)**<br>**(9d)**<br>**(3c)** | JMC (2008) 51:6609<br>JMC (2007) 50:3159<br>JMC (2017) 60:7459 |
| **LJ2126 (MRS5292)** | h$A_3$ receptor antagonist/$A_{2A}$ agonist **(4a)** | JMC (2012) 55:342 |
| **LJ2163 (MRS5450)** | h$A_3$ receptor antagonist **(6a)** | JMC (2021) 64:12525 |
| **LJ2521 (MRS5584)** | h$A_3$ receptor antagonist **(6c)** | JMC (2021) 64:12525 |
| **LJ2698 (MRS5014, FM101)** | h$A_3$ receptor antagonist **(9b)**<br>**(3c)** | JMC (2007) 50:3159<br>JMC (2017) 60:7459 |
| **LJ3429 (MRS7002)** | selective $A_3$ seleno-adenosine agonist **(3p)** | JMC (2017) 60:3422 |
| **LJ3440 (MRS5742)** CHEMBL4088081 | selective $A_3$ agonist **(**4′-Se-IB-MECA, **3d)** | JMC (2017) 60:3422 |
| **LJ4378 (MRS5281)** | h$A_3$ receptor antagonist/$A_{2A}$ agonist **(4g)** | JMC (2012) 55:342 |
| **LJ4517 (MRS7049)** | h$A_{2A}$ receptor nucleoside antagonist **(2)** | JMC (2022) 65(8):6325 |
| **cLNA-adenosine** | first carbocyclic “locked” nucleoside **(23)** | OL (2003) 5:1665 |
| **LUF5999** | weak $A_3$ adenosine allosteric modulator | BP (2011) 82:658 |
| **LUF6000** | selective $A_3$ adenosine allosteric enhancer<br>**(4)** | JMC (2006) 49:3354<br>ACSPT (2022) 5(8):625 |
| **metrifudil** | mixed $A_1$/$A_3$ adenosine agonist, 2-Me-Bn **(11)** | JMC (2005) 48:1745 |
| **MG325** | selective $A_1$ adenosine agonist, nonnucleoside **(27)** | ACSCN (2021) 12:3410 |
| **MMPD** | $A_1$ adenosine partial agonist PET ligand **(22b)** | JMC (2018) 61:9966 |
| **MRS512** | $A_1$/$A_3$ adenosine antagonist (xanthine, **21**) | JMC (1994) 37: 3373 |
| **MRS541** | IB-Ado, $A_3$ low efficacy agonist **(4)**<br>**(7a)** | JMC (2002) 45:4471<br>JMC (2000) 43:2196 |
| **MRS542** | $A_3$ adenosine low efficacy agonist/antagonist (**5**) | JMC (2002) 45:4471 |
| **MRS582** | carbocyclic IB-MECA, $A_3$ adenosine agonist **(3)** | JMC (2000) 43:2196 |
| **MRS1067** | selective flavonoid $A_3$ adenosine antagonist (**11e**) | JMC (1996) 39:2293 |
| **MRS1177** | selective h$A_3$ adenosine antagonist (**10**) | JMC (1996) 39:4142 |
| **MRS1178** | $A_{2B}$ adenosine antagonist (**39**) | JMC (1998) 41:2835 |
| **MRS1186** | selective h$A_3$ adenosine antagonist (**3**) | JMC (1996) 39:4142 |
| **MRS1191** | selective h$A_3$ adenosine antagonist (DHP, **2**) | JMC (1997) 40:2596<br>NP (2017) 114:101 |

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| **MRS1220** | selective $hA_3$ adenosine antagonist (**12**) | JMC (1996) 39:4142<br>PS (2021) 17:737<br>ACSPT (2023) 6:1266 |
| **MRS1292** | selective $A_3$ adenosine antagonist (**14**) | JMC (2002) 45:4471 |
| **MRS1334** | selective $hA_3$ adenosine antagonist (DHP, **24g**) | JMC (1997) 40:2596<br>PS (2021) 17:737 |
| **MRS1458** | irreversible (sulfonyl-F) $A_3$ antagonist **(19)** | BC (1999) 10:667 |
| **MRS1476** | selective $hA_3$ adenosine antagonist (**6**)<br>**(38)** | JMC (1999) 42:706<br>JMC (1998) 41:3186 |
| **MRS1477** | allosteric enhancer of TRPV1 channels (DHP) | JPET (2012) 340:152 |
| **MRS1486** | selective $A_3$ adenosine antagonist (**45**) | JMC (1998) 41:3186 |
| **MRS1505** | selective $A_3$ adenosine antagonist (**44**) | JMC (1998) 41:3186 |
| **MRS1523** | selective $A_3$ adenosine antagonist (**4**)<br>**(39b)** | JMC (1999) 42:706<br>JMC (1998) 41:3186<br>PS (2021) 17:737<br>NP (2017) 114:101 |
| **MRS1595** | selective $A_{2B}$ adenosine antagonist **(14)** | DDR (1999) 47:178 |
| **MRS1649** | permanently charged $A_3$ antagonist (**11**) | JMC (1999) 42:4232 |
| **aristeromycin** | carbocyclic-adenosine **(5b)**, $A_{2A}$ agonist | JMC (2000) 43:2196 |
| **MRS1655** | (N)-methanocarba-adenosine **(5c)**, $A_3$ agonist | JMC (2000) 43:2196 |
| **MRS1656** | (S)-methanocarba-adenosine **(5d)**, racemic | JMC (2000) 43:2196 |
| **MRS1667** | prodrug (**24**) of permanently charged $A_3$ antagonist | JMC (1999) 42:4232 |
| **MRS1706** | selective $A_{2B}$ adenosine antagonist **(20)** | JMC (2000) 43:1165 |
| **MRS1740** | $A_3$ adenosine low efficacy agonist/antagonist | JMC (2002) 45:4471 |
| **MRS1743** | $A_3$ adenosine low efficacy agonist (**17**)<br>**(7c)** | JMC (2002) 45:4471<br>JMC (2000) 43:2196 |
| **MRS1748** | $A_{2B}$ adenosine antagonist, long residence time (**17**) | BP (2022) 200:115027 |
| **MRS1754** | selective $A_{2B}$ adenosine antagonist **(27)** | JMC (2000) 43:1165 |
| **[$^3$H]MRS1754** | selective $A_{2B}$ adenosine antagonist radioligand | BP (2001) 61:657 |
| **MRS1758** | $A_{2B}$ adenosine antagonist **(18)** | BP (2022) 200:115027 |
| **MRS1760** | $A_3$ adenosine low efficacy agonist/antagonist (**18**)<br>**(9c)** | JMC (2002) 45:4471<br>JMC (2000) 43:2196 |
| **MRS1761** | 2-Cl-(N)-methanocarba-$N^6$-cyclopentyl-Ado **(8c)** | JMC (2000) 43:2196 |
| **MRS1765** | selective $A_{2B}$ adenosine antagonist **(33)** | JMC (2000) 43:1165 |
| **MRS1781** | (N)-methanocarba-$N^6$-cyclopentyl-Ado **(6c)** | JMC (2000) 43:2196 |
| **MRS1845** | inhibitor of store-operated calcium channels | BP (2003) 65:329 |
| **MRS1873** | mixed $A_{1/3}$ adenosine agonist **(21)** | JMC (2019) 62:1502 |
| **MRS1878** | mixed $A_{2A/2B}$ adenosine antagonist (**22**) | BP (2022) 200:115027 |
| **MRS1898** | selective $A_3$ adenosine agonist (**5**)<br>[$^{125}$I]MRS1898 | JMC (2005) 48:1745<br>PS (2009) 5:31 |
| **MRS1940** | (N)-methanocarba-NECA **(5)**, potent AR agonist | BMCL (2001) 11:1333 |
| **MRS1941** | (N)-methanocarba-guanosine **(8)**, weak $A_3$ ligand | BMCL (2001) 11:2295 |
| **MRS1942** | (N)-methanocarba-NBTI, ENT1 inhibitor | OL (2001) 3:597 |
| **MRS1947** | $N^6$-Me-(N)-methanocarba-inosine **(13)** weak at $A_3$ | JMC (2016) 59:11006 |
| **MRS1957** | (N)-methanocarba-inosine **(5)**, weak at $A_3$ | BMCL (2001) 11:2295 |
| **MRS1997** | (N)-methanocarba-MECI **(6)**, weak $A_3$ agonist | BMCL (2001) 11: 2295 |

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| **MRS2055** | $P2Y_{12}$ agonist **(17b)** | JMC (2002) 45:4057 |
| **MRS2154** | P2X2 antagonist, dihydropyridine deriv. **(5a)** | JANS (2000) 81:152 |
| **MRS2159** | selective P2X1 antagonist, pyridoxal deriv. | JMC (2001) 44:340 |
| **MRS2160** | P2X1 and P2X2 antagonist, pyridoxal deriv. **(38)** | JMC (2002) 45:4057 |
| **MRS2179** | selective $P2Y_1$ deoxyribose antagonist **(9)** | JMC (1998) 41:183 |
| | **(2)** | JMC (1999) 42:1625 |
| **MRS2191** | $P2Y_1$ and P2X2 antagonist, pyridoxal deriv. **(42)** | JMC (2002) 45:4057 |
| **MRS2210** | nonnucleotide $P2Y_1$ antagonist, related to PPADS | DDR (2002) 57:173 |
| **MRS2211** | selective, nonnucleotide $P2Y_{13}$ antagonist | BP (2005) 70:266 |
| **MRS2216** | selective $P2Y_1$ deoxyribose antagonist **(6)** | JMC (1999) 42:1625 |
| **MRS2219** | P2X1 allosteric enhancer **(2)** | JMC (1998) 41:2201 |
| **MRS2220** | P2X1 antagonist **(3)** | JMC (1998) 41:2201 |
| **MRS2231** | weak $P2Y_1$ deoxyribose antagonist **(6)** | JCIM (2017) 57:3104 |
| **MRS2239** | selective $P2Y_1$ deoxyribose antagonist **(15)** | JCIM (2017) 57:3104 |
| **MRS2242** | selective $P2Y_1$ deoxyribose partial agonist **(13)** | JMC (1999) 42:1625 |
| **MRS2255** | $P2Y_1$ bisphosphate anhydrohexitol agonist **(36)** | JMC (1999) 42:1625 |
| **MRS2257** | P2X1, P2X2, P2X4 antagonist, pyridoxal deriv. **(9)** | JMC (2001) 44:340 |
| **MRS2268** | $P2Y_1$ methanocarba bisphosphate agonist **(4a)** | JMC (2000) 43:829 |
| **MRS2275** | selective $P2Y_1$ methanocarba antagonist **(19)** | JCIM (2017) 57:3104 |
| **MRS2277** | $P2Y_1$ acyclic bisphosphate antagonist **(37)** | JCIM (2017) 57:3104 |
| **MRS2279** | selective $P2Y_1$ methanocarba antagonist **(5)** | JMC (2003) 46:4974 |
| **MRS2283** | $P2Y_1$ anhydrohexitol antagonist **(32)** | JCIM (2017) 57:3104 |
| | **(12)** | BMC (2004) 12:5619 |
| **MRS2286** | selective $P2Y_1$ acyclic bisphosphate antagonist (**12**) | JMC (2002) 45:5694 |
| **MRS2297** | selective $P2Y_1$ antagonist (**13**) | JMC (2002) 45:5694 |
| **MRS2298** | selective $P2Y_1$ acyclic bisphosphate antagonist | BP (2004) 68:1995 |
| **MRS2303** | $P2Y_1$ acyclic bisphosphate antagonist **(35)** | JCIM (2017) 57:3104 |
| **MRS2304** | (N)-methanocarba-AMP, no effect at $P2Y_1$ **(4a)** | JMC (2002) 45:208 |
| **MRS2306** | selective P2X7 antagonist **(2)** | BMCL (2008) 18:571 |
| **MRS2312** | (S)-methanocarba-ATP, weak $P2Y_1$/$P2Y_2$ ag. **(8a)** | JMC (2002) 45:208 |
| **MRS2339** | cardiac P2X4 agonist | JMC (2010) 53:2562 |
| | 2-Cl-(N)-methanocarba-AMP, weak $P2Y_1$ ag. **(13a)** | JMC (2002) 45:2090 |
| **MRS2340** | (N)-methanocarba-ATP, P2X, P2Y agonist | DDR (2004) 61:227 |
| | **(6a)** | JMC (2002) 45:2090 |
| **MRS2341** | (N)-methanocarba-UTP, $P2Y_2$/$P2Y_4$ agonist **(5a)** | JMC (2002) 45:208 |
| **MRS2343** | 2-Cl-$N^6$-Me-(N)-methanocarba-ATP, | |
| | $P2Y_1$ agonist **(15a)** | JMC (2002) 45:2090 |
| **MRS2347** | 2-MeS-(N)-methanocarba-AMP, weak $P2Y_1$ ag. **(10a)** | JMC (2002) 45:2090 |
| **MRS2352** | β,γ-me-(N)-methanocarba-ATP, $P2Y_1$ agonist **(17a)** | JMC (2002) 45:2090 |
| **MRS2365** | selective $P2Y_1$ agonist (2-MeS-ADP analogue, **9a**) | JMC (2002) 45:2090 |
| **MRS2367** | 2-Cl-(N)-methanocarba-ATP, $P2Y_1$ agonist **(12a)** | JMC (2002) 45:2090 |
| **MRS2371** | $N^6$-Me-methanocarba-ATP, $P2Y_1$ ag. **(14a)** | JMC (2002) 45:2090 |
| **MRS2395** | $P2Y_{12}$ antagonist (moderate potency) | JMC (2002) 45:5694 |
| **MRS2427** | selective P2X7 antagonist **(16)** | BMCL (2008) 18:571 |
| **MRS2457** | TNA-bisphosphate, $P2Y_1$ antagonist **(9)** | BMC (2004) 12:5619 |
| **MRS2488** | TNA-triphosphate, $P2Y_2$ agonist **(13)** | BMC (2004) 12:5619 |

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| **MRS2496** | selective $P2Y_1$ antagonist | BP (2004) 68:1995 |
| **MRS2481** | blocker of $Ca^{2+}$ channel formed by amyloid pept. | PNAS (2009) 106:3348 |
| **MRS2500** | selective $P2Y_1$ methanocarba antagonist | JMC (2003) 46:4974 |
| **MRS2503** | selective $P2Y_1$ methanocarba antagonist **(26)** | JCIM (2017) 57:3104 |
| **MRS2519** | selective $P2Y_1$ methanocarba antagonist **(22)** | JCIM (2017) 57:3104 |
| **MRS2520** | selective $P2Y_1$ methanocarba antagonist **(20)** | JCIM (2017) 57:3104 |
| **MRS2540** | selective P2X7 antagonist | EER (2010) 91:425 |
| **MRS2567** | Selective $P2Y_6$ antagonist | BP (2004) 67:1763 |
| **MRS2576** | nonselective, irrev. P2Y receptor antagonist | BP (2004) 67:1763 |
| **MRS2577** | irrev. $P2Y_4$/$P2Y_6$ receptor antagonist | BP(2004) 67:1763 |
| **MRS2578** | selective $P2Y_6$ antagonist (irreversible, insurmountable) | BP (2004) 67:1763 |
| | inactive at $P2Y_{14}R$ | BMCL (2015) 25:4733 |
| **MRS2584** | $P2Y_1$ carbocyclic-LNA antagonist **(21)** | BMC (2004) 12:5619 |
| **MRS2603** | $P2Y_1$/$P2Y_{13}$ antagonist, nonnucleotide | BP (2005) 70:266 |
| **MRS2608** | precursor of radiolabeled $P2Y_1$ antagonist **(14)** | JMC (2007) 50:3229 |
| **MRS2611** | selective $P2Y_1$ methanocarba antagonist **(27)** | JCIM (2017) 57:3104 |
| **MRS2633** | $P2Y_6$ (S)-methanocarba 2′-d agonist **(10)** | JMC (2005) 48:8108 |
| **MRS2666** | $P2Y_6$ 2-OBH agonist **(19)** | JMC (2006) 49:5532 |
| **MRS2670** | selective $P2Y_{14}$ agonist (4-thio) **(13)** | JMC (2007) 50:2030 |
| **MRS2690** | selective $P2Y_{14}$ agonist (2-thio) **(15)** | JMC (2007) 50:2030 |
| | **(3)** | BMCL (2015) 25:4733 |
| **MRS2693** | selective $P2Y_6$ agonist **(32)** | JMC (2006) 49:5532 |
| **MRS2698** | selective $P2Y_2$ agonist **(8)** | JMC (2007) 50:1166 |
| **MRS2703** | caged $P2Y_{1/12/13}$ agonist **(4)** | BP (2008) 75:1341 |
| **MRS2768** | selective $P2Y_2$ agonist **(30)** | BMC (2008) 16:6319 |
| **MRS2782** | potent and selective $P2Y_6$ agonist, α,β-me-UDP **(9)** | BMC (2008) 16:6319 |
| **MRS2801** | putative allosteric $P2Y_2$ receptor partial agonist (**7**) | BMCL (2009) 19:3002 |
| **MRS2802** | selective $P2Y_{14}$ agonist **(12)** | JMC (2010) 53:471 |
| **MRS2815** | mixed $P2Y_6$ and $P2Y_{14}$ agonist **(11)** | JMC (2010) 53:4488 |
| **MRS2816** | carboxylic $P2Y_1$ antagonist **(8)** | BC (2010) 21:1190 |
| **MRS2829** | precursor of radioiodinated $P2Y_1$ antagonist **(6)** | PR (2010) 62:344 |
| **MRS2892** | amine-functionalized $P2Y_{14}$ agonist **(3a)** | BC (2009) 20:1650 |
| **MRS2900** | selective $P2Y_1$ methanocarba antagonist **(29)** | JCIM (2017) 57:3104 |
| **MRS2905** | selective $P2Y_{14}$ agonist **(11)** | JMC (2010) 53:471 |
| **MRS2907** | selective $P2Y_{14}$ agonist **(18)** | JMC (2010) 53:471 |
| **MRS2925** | cardiac P2X4 agonist | JMC (2010) 53:2562 |
| **MRS2927** | slightly selective $P2Y_4$ agonist **(34)** | JMC (2011) 54:4018 |
| **MRS2???** | slightly selective $P2Y_4$ agonist **(15)** | JMC (2011) 54:4018 |
| **MRS2950** | nonnucleotide $P2Y_1$ receptor antagonist **(2a)** | BMC (2012) 20:5254 |
| **MRS2957** | Potent and selective $P2Y_6$ agonist **(23)** | JMC (2010) 53:4488 |
| | **(12)** | BMCL (2015) 25:4733 |
| **MRS2964** | Potent and selective $P2Y_6$ agonist **(15)** | JMC (2010) 53:4488 |
| **MRS2973** | pan-agonist of $P2Y_2$, $P2Y_4$ and $P2Y_6$ | JMC (2011) 54:4018 |
| **MRS2978** | in vivo, cardiac P2X4 agonist | JMC (2013) 56:902 |

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| | | PS (2020) 16:61 |
| **MRS3210** | carbocyclic-LNA adenosine **(23)** | OL (2003) 5:1665 |
| **MRS3342** | 2-I-$N^6$-Me LNA adenosine **(19)** | BMC (2004) 12:5619 |
| **MRS3366** | orthogonal $A_{2A}$ adenosine agonist for neoceptor | TIPS (2007) 28:111 |
| **MRS3474** | putative allosteric $P2Y_1$ receptor NAM (**20**) | OBC(2005) 3:2016 |
| **MRS3481 (LJ1254)** | orthogonal $A_3$ adenosine agonist for neoceptor | JMC (2006) 49:2689 |
| **MRS3489** | selective $A_3$ adenosine agonist, 2,2-di-Ph-Et **(34)** | JMC (2005) 48:1745 |
| **MRS3554** | selective $A_3$ adenosine agonist, 2,5-di-Cl-Bn **(20)** | JMC (2005) 48:1745 |
| **MRS3558 (CF502)** | selective $A_3$ adenosine agonist, 3-Cl-Bn **(18)** | JMC (2005) 48:1745 |
| **MRS3581** | selective Br-76 $A_3$ adenosine agonist | NMB (2009) 36:3 |
| **MRS3602** | selective $A_3$ adenosine agonist, 2,5-di-MeO-Bn **(26)** | JMC (2005) 48:1745 |
| **MRS3609** | selective $A_3$ adenosine agonist **(35)** | JMC (2005) 48:1745 |
| **MRS3611** | selective $A_3$ adenosine agonist **(36)** | JMC (2005) 48:1745 |
| **MRS3630** | mixed $A_1$ and $A_3$ adenosine agonist **(2)** | JMC (2005) 48:8103 |
| **MRS3638** | mixed $A_1$ and $A_3$ adenosine agonist **(3)** | JMC (2005) 48:8103 |
| **MRS3642 (LJ1256)** | selective $A_3$ adenosine antagonist **(7)** | BMCL (2006) 16:596 |
| **MRS3706** | mixed $A_1$ and $A_3$ adenosine agonist **(1)** | JMC (2005) 48:8103 |
| **MRS3771** | selective $A_3$ adenosine antagonist **(6)** | BMCL (2006) 16:596 |
| **MRS3775** | selective $A_3$ adenosine antagonist **(21,** CAY 10498**)** | JMC (2005) 48:4910 |
| **MRS3777** | selective $A_3$ adenosine antagonist **(22)** | JMC (2005) 48:4910 |
| **MRS3997** | $A_{2B}$ adenosine agonist **(28)** | JMC (2007) 50:1810 |
| **MRS4062** | selective $P2Y_4$ agonist **(16)** | JMC (2011) 54:4018 |
| **MRS4063** | clickable $P2Y_6$ receptor agonist **(15)** | MCC (2013) 4:1156 |
| **MRS4074** | in vivo, cardiac P2X4 agonist | JMC (2013) 56:902 |
| **MRS4084** | in vivo, cardiac P2X4 agonist | JMC (2013) 56:902 |
| **MRS4129** | selective fluorescent (AF488) $P2Y_6$R agonist | MCC (2013) 4:1156 |
| **MRS4149** | alkyne-functionalized $P2Y_{14}$ antagonist **(22)** | ACSCB (2014) 9:2833<br>ACSML (2020) 11:1281 |
| **MRS4160** | clickable $P2Y_{2/4/6}$ receptor agonist **(26)** | JMC (2014) 57:3874 |
| **MRS4162** | fluorescent (Bodipy) $P2Y_{2/4/6}$ receptor agonist | JMC (2014) 57:3874 |
| **MRS4174** | fluorescent (AF488) $P2Y_{14}$ receptor antagonist **(30)** | ACSCB (2014) 9:2833 |
| **MRS4183** | fluorescent (Bodipy) $P2Y_{14}$ receptor agonist **(11)** | BMCL (2015) 25:4733 |
| **MRS4202** | adenosine kinase inhibitor **(34)** | JMC (2016) 59:6860 |
| **MRS4203** | adenosine kinase inhibitor **(38a)** | JMC (2016) 59:6860 |
| **MRS4217** | selective $P2Y_{14}$ antagonist **(65)** | JMC (2016) 59:6149 |
| **MRS4322** | mixed $A_{1/3}$ adenosine agonist **(8a)** | RSCA (2021) 11:27369<br>PS (2020) 16:543 |
| **MRS4380** | adenosine kinase inhibitor **(55)** | JMC (2016) 59:6860 |
| **MRS4383** | $P2Y_6$ receptor (S)-methanocarba agonist **(18)** | MCC (2017) 8:1897 |
| **MRS4387** | $P2Y_6$ receptor dinucleotide agonist **(24)** | MCC (2017) 8:1897 |
| **MRS4458** | selective $P2Y_{14}$ antagonist **(20)** | JMC (2018) 61:4860 |
| **MRS4478** | selective $P2Y_{14}$ antagonist **(30)** | JMC (2018) 61:4860 |
| **MRS4519** | $P2Y_{14}$ receptor antagonist **(**minimal deriv., **2)** | ACSML (2020) 11:1281 |
| **MRS4552** | Nucleotide CD73 inhibitor **(9h)** | JMC (2019) 62:3677 |
| **MRS4554** | $P2Y_6$ receptor agonist **(28)** | BMCL (2021) 45:128137 |
| **MRS4589** | (S)-methanocarba-GTP **(4a)** | BIOM (2022) 12:584 |

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| **MRS4590** | (N)-methanocarba-GTP **(4d)** | BIOM (2022) 12:584 |
| **MRS4591** | (S)-methanocarba-GMP-PCP **(4b)** | BIOM (2022) 12:584 |
| **MRS4596** | P2X4 receptor antagonist **(22c)** | JMC (2022) 5:13967 |
| **MRS4598** | Nucleotide CD73 inhibitor **(16)** | JMC (2022) 65:2409 |
| **MRS4602** | Nucleotide CD73 inhibitor **(21)** | JMC (2022) 65:2409 |
| **MRS4608** | $P2Y_{14}$ receptor antagonist **(**quinuclidine, **17)** | JMC (2020) 63:9563 |
| **MRS4616** | $P2Y_{14}$ receptor antagonist **(**quaternary N, **21)** | JMC (2020) 63:9563 |
| **MRS4620** | Nucleotide CD73 inhibitor **(18)** | JMC (2022) 65:2409 |
| **MRS4622** | Nucleotide CD73 inhibitor **(20)** | JMC (2022) 65:2409 |
| **MRS4625** | $P2Y_{14}$ receptor antagonist **(4)** | ACSML (2020) 11:1281 |
| | **(8)** | JMC (2020) 63:9563 |
| **MRS4654** | $P2Y_{14}$ receptor antagonist **(32)** | JMC (2021) 64:5099 |
| **MRS4656** | $P2Y_6$ receptor antagonist **(16)** | BMCL (2021) 41:128008 |
| | **(6)** | BMCL (2022) 75:128981 |
| **MRS4695** | $P2Y_6$ receptor antagonist **(7)** | BMCL (2021) 41:128008 |
| | **(4)** | BMCL (2022) 75:128981 |
| **MRS4706** | $P2Y_6$ receptor antagonist **(14)** | BMCL (2021) 41:128008 |
| **MRS4719** | P2X4 receptor antagonist **(21u)** | JMC (2022) 5:13967 |
| **MRS4738** | $P2Y_{14}$ receptor antagonist **(15)** | JMC (2022) 65:3434 |
| | **(2b)** | JMC (2023) 66:9076 |
| **MRS4741** | $P2Y_{14}$ receptor antagonist prodrug **(37c)** | JMC (2021) 64:5099 |
| **MRS4745** | $P2Y_{14}$ receptor antagonist **(22)** | JMC (2022) 65:3434 |
| **MRS4746** | $P2Y_{14}$ receptor antagonist **(23)** | JMC (2022) 65:3434 |
| **MRS4748** | $P2Y_{14}$ receptor antagonist **(38)** | JMC (2022) 65:3434 |
| **MRS4757** | $P2Y_{14}$ receptor antagonist ester prodrug **(144)** | JMC (2022) 65:3434 |
| **MRS4758** | $P2Y_{14}$ receptor antagonist ester prodrug **(145)** | JMC (2022) 65:3434 |
| **MRS4759** | mixed $A_3$ agonist/$P2Y_{14}$ receptor antagonist | ACSPT (2022), 5:973 |
| **MRS4774** | $P2Y_6$ receptor antagonist **(8)** | BMCL (2021) 41:128008 |
| **MRS4773** | $P2Y_6$ receptor antagonist **(9)** | BMCL (2021) 41:128008 |
| **MRS4779** | $P2Y_{14}$ receptor antagonist prodrug **(141)** | JMC (2022) 65:3434 |
| | **(63)** | JMC (2023), 66(13):9076 |
| **MRS4806** | $P2Y_{14}$ receptor antagonist ester prodrug **(146)** | JMC (2022) 65:3434 |
| **MRS4815** | $P2Y_{14}$ receptor antagonist double prodrug **(143)** | JMC (2022) 65:3434 |
| | **(64)** | JMC (2023), 66(13):9076 |
| **MRS4817** | $P2Y_6$ receptor antagonist **(24)** | BMCL (2022) 75:128981 |
| **MRS4820** | $P2Y_{14}$ receptor antagonist **(8)** | JMC (2023), 66(13):9076 |
| **MRS4830** | $P2Y_6$ receptor antagonist **(11)** | BMCL (2022) 75:128981 |
| **MRS4833** | $P2Y_{14}$ receptor antagonist **(15)** | JMC (2023), 66(13):9076 |
| **MRS4839** | $P2Y_6$ receptor antagonist **(25)** | BMCL (2022) 75:128981 |
| **MRS4841** | $P2Y_6$ receptor antagonist **(27)** | BMCL (2022) 75:128981 |
| **MRS4842** | $P2Y_6$ receptor antagonist **(28)** | BMCL (2022) 75:128981 |
| **MRS4845** | $P2Y_{14}$ receptor antag. double prodrug **(62)** of PPTN | JMC (2023), 66(13):9076 |
| **MRS4849** | $P2Y_{14}$R antag. carbamate prodrug **(61)** of PPTN | JMC (2023), 66(13):9076 |
| **MRS4853** | $P2Y_6$ receptor antagonist **(26)** | BMCL (2022) 75:128981 |
| **MRS4855** | $P2Y_{14}$ receptor antag. prodrug **(50)** of MRS4833 | JMC (2023), 66(13):9076 |
| **MRS4910** | $P2Y_{14}$R antag. ester prodrug **(49)** of MRS4833 | JMC (2023), 66(13):9076 |

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| **MRS4911** | $P2Y_{14}R$ antag. carbamate prodrug **(51)** of MRS4833 | JMC (2023), 66(13):9076 |
| **MRS4917** | $P2Y_{14}R$ antag. | unpublished |
| **MRS5024 (LJ1915)** | selective $A_3$ adenosine antagonist **(5d)** | BMCL (2009) 17:3733 |
| **MRS5025 (LJ1916)** | selective $A_3$ adenosine antagonist **(5e)** | BMCL (2009) 17:3733 |
| **MRS5127** | selective $A_3$ adenosine antagonist **(8)** | JMC (2012) 36:3 |
| | $[^{125}I]$MRS5127 | BP (2010) 79:967 |
| **MRS5147** | selective Br-76 $A_3$ adenosine antagonist | NMB (2009) 23:232 |
| **MRS5151** | selective $A_3$ adenosine agonist **(18a)** | BMCL (2008) 18:2813 |
| | **(6)** | JMC (2009) 15:3994 |
| **MRS5219** | biotin-conjugated selective $A_3$ adenosine ag. **(17a)** | JMC (2009) 15:3994 |
| **MRS5158** | selective $A_3$ adenosine allosteric enhancer **(11)** | ACSPT (2022) 5(8):625 |
| | **(12a)** | JMC (2022) 65(22):15238 |
| **MRS5190** | selective $A_3$ adenosine allosteric enhancer **(12)** | ACSPT (2022) 5(8):625 |
| | **(12b)** | JMC (2022) 65(22):15238 |
| **MRS5202** | $N^6$-(3-I-Bn)-2-Cl-(N)-methanocarba-A-4′-trunc. **(3)** | JMC (2016) 59:11006 |
| **MRS5206** | selective fluorescent $A_{2A}$ agonist (AF488) | NI (2013) 63:42 |
| **MRS5216** | dendrimeric $A_3$ adenosine agonist | PR (2012) 65:338 |
| **MRS5218** | selective fluorescent (Cy5) $A_3$ adenosine agonist | BP (2013) 85:1171 |
| **MRS5221** | clickable $A_3$ adenosine agonist **(5)** | BMCP (2011) 11:11 |
| **MRS5233** | triazole-model $A_3$ adenosine agonist **(3)** | BMCP (2011) 11:11 |
| **MRS5246** | dendrimeric $A_3$ adenosine agonist **(6)** | BMCP (2011) 11:11 |
| **MRS5303** | quantum dot-immobil. $A_{2A}$ adenosine agonist **(13)** | JNB (2010) 8:11 |
| **MRS5318** | amine-functionalized $A_{2A}$ adenosine antagonist **(7)** | BMCL (2011) 21:2740 |
| **MRS5342** | clickable $A_3$ adenosine agonist **(9)** | BC (2012) 23:232 |
| **MRS5346** | selective fluorescent (AF488) $A_{2A}$AR antagonist | BP (2010) 80:506 |
| **MRS5347** | fluorescent (TAMRA) $A_{2A}$ adenosine antagonist | BMCL (2013) 23:26 |
| **MRS5383** | dendrimeric selective $A_{2A}$ adenosine antagonist **(17)** | BMCL (2011) 21:2740 |
| **MRS5398** | clickable adenosine receptor antagonist **(4)** | BC (2011) 22:1115 |
| **MRS5415** | selective $A_3$ adenosine agonist **(32)** | JMC (2012) 36:3 |
| **MRS5418** | fluorescent (Bodipy) $A_{2A}$ adenosine antagonist | BMCL (2013) 23:26 |
| **MRS5424** | fluorescent $A_{2A}$ receptor agonist (AF532) | JN (2008) 590:36 |
| **MRS5425** | selective F-18 $A_{2A}$ adenosine antagonist | NMB (2011) 38:897 |
| **MRS5449** | selective fluorescent (AF488) $A_3$AR antagonist | BP (2012) 83:1552 |
| **MRS5474** | selective $A_1$ adenosine agonist **(10)** | JMC (2012) 55:8075 |
| | | NP (2017) 114:101 |
| **MRS5474** | Enterovirus A71 antiviral **(31)** | BMCL (2020) 30:127599 |
| **MRS5543** | light switchable adenosine agonist | BC (2014) 25:1847 |
| **MRS5621** | $A_{2A}$ adenosine agonist, D-His conjugate **(42)** | JMC (2012) 55:538 |
| **MRS5630** | gold-immobil. $A_3$ adenosine agonist **(21b)** | PS (2013) 9:183 |
| **MRS5655** | highly selective $A_3$ adenosine agonist **(27)** | JMC (2012) 55:4847 |
| **MRS5657** | highly selective $A_3$ adenosine ag. (p-F, $N^6$-Me, **13)** | JMC (2012) 55:4847 |
| **MRS5661** | highly selective $A_3$ adenosine ag. (2-pyridyl, **19)** | JMC (2014) 57: 9901 |
| | **(10)** | JMC (2012) 55:4847 |
| **MRS5663** | highly selective $A_3$ adenosine ag. (o-Cl, $N^6$-Me, **14)** | JMC (2012) 55:4847 |
| | **(11)** | JMC (2014) 57: 9901 |
| **MRS5676** | mixed $A_3$ agonist+dopamine transporter modulator | JPET (2016) 357:24 |

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| | **(36)** | JMC (2016) 59:11006 |
| **MRS5678** | highly selective $A_3$ adenosine ag. (p-F, **28)** | JMC (2012) 55:4847 |
| **MRS5679** | highly selective $A_3$ adenosine ag. (biphenyl, **35)** | JMC (2012) 55:4847 |
| **MRS5698** | highly selective $A_3$ adenosine agonist **(**3,4-$F_2$, **31)** | JMC (2012) 55:4847 |
| | | PS (2015) 11:371 |
| **MRS5699** | highly selective $A_3$ adenosine ag. (p-$NH_2$, **32)** | JMC (2012) 55:4847 |
| **MRS5700** | highly selective $A_3$ adenosine ag. (m-COOH, **33)** | JMC (2012) 55:4847 |
| **MRS5701** | selective water soluble $A_1/A_3$ adenosine agonist **(6)** | JMC (2013) 56:5949 |
| | **(34)** | JMC (2012) 55:4847 |
| **MRS5728** | gold-immobil. $A_1/A_{2A}$ adenosine antagonist **(26a)** | PS (2013) 9:183 |
| **MRS5761-MRS5762** | $A_3$ adenosine antagonists | US 9,227,979 B2 |
| | | MCC (2019) 10:1094 |
| **MRS5763** | selective fluorescent (AF488) $A_3$AR antagonist **(23)** | EJMC (2020) 186:111886 |
| **MRS5776** | selective $A_3$ adenosine antagonist | JMC (2013) 56:5949 |
| **MRS5811-MRS5840** | $A_3$ adenosine antagonists | US 9,227,979 B2 |
| | | MCC (2019) 10:1094 |
| **MRS5841** | selective water-soluble $A_3$ adenosine agonist **(7)** | JMC (2013) 56:5949 |
| | | NP (2017) 114:101 |
| **MRS5842** | fluorescent (Alexa647) $A_{2A}$ receptor antagonist | JCR (2018) 283:135 |
| **MRS5854** | $A_{2A}$ adenosine receptor affinity label | ACSML (2014) 5:1043 |
| **MRS5861** | selective sulfonate h$A_3$ adenosine antagonist **(16)** | JMC (2013) 56:5949 |
| **MRS5911** | $A_{2B}$ adenosine agonist | BP (2018) 151:201 |
| | (originally from IJzerman lab) | DDR (2000) 49:85 |
| **MRS5923** | selective $A_3$ adenosine antagonist **(8)** | PONE (2014) 9:e97858 |
| **MRS5930** | $A_3$ antagonist, an adenine deriv. **(1)** | JMC (2016) 59:11006 |
| | $A_3$ antagonist, $\alpha_{2B}$ adrenergic receptor ligand **(9)** | PONE (2014) 9:e97858 |
| **MRS5942** | novel $A_1/A_{2A}/A_3$ adenosine antagonist **(23)** | JCIM (2015) 55:550 |
| **MRS5969** | furan-2-yl-ethynyl selective $A_3$ adenosine ag. **(27)** | JMC (2014) 57: 9901 |
| **MRS5975** | c-hexylethynyl selective $A_3$ adenosine agonist **(38)** | JMC (2014) 57: 9901 |
| **MRS5976** | c-propylethynyl selective $A_3$ adenosine agonist **(37)** | JMC (2014) 57: 9901 |
| **MRS5979** | ferrocene-containing $A_3$ adenosine agonist **(36)** | JMC (2014) 57: 9901 |
| **MRS5980** | highly selective $A_3$ adenosine agonist **(33)** | JMC (2014) 57: 9901 |
| | **(10)** | ACSMCL (2015) 6:804 |
| **MRS7111** | selective $A_3$ adenosine agonist (2-triazole) **(23)** | ACSMCL (2015) 6:804 |
| **MRS7116** | selective $A_3$ adenosine agonist **(9)** | MCC (2015) 6:555 |
| **MRS7126** | selective $A_3$ adenosine agonist **(15)** | MCC (2015) 6:555 |
| **MRS7134** | 5-$HT_2$ methanocarba antagonist and $A_1$ agonist **(14)** | JMC (2016) 59:11006 |
| **MRS7135** | selective $A_3$ adenosine agonist **(11)** | ACSMCL (2015) 6:804 |
| **MRS7138** | selective $A_3$ adenosine agonist **(17)** | MCC (2015) 6:555 |
| **MRS7140** | selective $A_3$ adenosine agonist **(19)** | ACSMCL (2015) 6:804 |
| **MRS7144** | selective $A_3$ adenosine agonist **(20)** | ACSMCL (2015) 6:804 |
| **MRS7145** | photoactivatable $A_{2A}$ receptor antagonist | JCR (2018) 283:135 |
| **MRS7146** | selective $A_3$ adenosine agonist, cPr-me **(17)** | ACSMCL (2015) 6:804 |
| **MRS7151** CHEMBL4079448 | | |
| | selective $A_3$ agonist **(**4′-Se-Cl-IB-MECA, **3p)** | JMC (2017) 60:3422 |
| **MRS7154** | selective $A_3$ adenosine agonist **(12)** | ACSMCL (2015) 6:804 |

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| **MRS7158** | $N^6$-diMe-(N)-methanocarba **(42),** inactive $A_3$ | JMC (2016) 59:11006 |
| **MRS7168** | novel mixed $A_1/A_3$ adenosine agonist **(14)** | ACSCB (2016) 11:2763 |
| **MRS7185** | 5-$HT_{2B}$ methanocarba antagonist **(23)** | JMC (2016) 59:11006 |
| **MRS7216** | tethered $A_{2A}$ adenosine agonist for bone (**8a**) | ART (2022) 24:265 |
| **MRS7220** | selective $A_3$ adenosine agonist, lacking 6-NH **(21)** | JMC (2016) 59:3249 |
| **MRS7221** | 5-$HT_2$ methanocarba antagonist **(26)** | JMC (2016) 59:11006 |
| **MRS7232** | dopamine transporter allosteric modulator **(10)** | JMC (2017) 60:3109 |
| | **(24)** | ACSO (2018) 3:12658 |
| **MRS7235** | $N^6$-diMe-(N)-methanocarba ester **(29),** inactive $A_3$ | JMC (2016) 59:11006 |
| **MRS7240** | mixed $A_{2A/3}$ adenosine antagonist (**36**) | SR (2017) 7:6398 |
| **MRS7249** | $N^6$-c$Pr_2$Me-2-Cl-(N)-methanocarb-A-5′-Pr-ester **(27)** | JMC (2016) 59:11006 |
| **MRS7251** | dopamine transporter allosteric modulator **(14)** | JMC (2017) 60:3109 |
| | **(30)** | ACSO (2018) 3:12658 |
| **MRS7292** | dopamine transporter allosteric modulator **(9)** | JMC (2017) 60:3109 |
| **MRS7293** | $N^6$-c$Pr_2$Me-2-Cl-(N)-methanocarb-A-5′-Me-ester **(25)** | JMC (2016) 59:11006 |
| **MRS7296** | dopamine transporter allosteric modulator, rib. **(29)** | JMC (2017) 60:3109 |
| **MRS7299** | κ-opioid antagonist (nucleoside) **(28)** | ACSO (2018) 3:12658 |
| **MRS7304** | dopamine transporter allosteric modulator **(16)** | JMC (2017) 60:3109 |
| | **(32)** | ACSO (2018) 3:12658 |
| **MRS7322** | fluorescent (Cy5) $A_{2A}$ receptor antagonist **(9)** | MCC (2017) 8:1659 |
| | | Cells (2020) 9:1200 |
| **MRS7323** | P-gp and ABCG2 inhibitor **(8)** | MP (2019) 96:180 |
| | **(17)** | EJMC (2022) 231:114103 |
| **MRS7331** | κ-opioid antagonist (nucleoside) **(39)** | ACSO (2018) 3:12658 |
| **MRS7334** | $A_3$ adenosine receptor agonist, $K_i$ 0.28 nM **(16)** | ACSML (2020) 11:1935 |
| **MRS7335** | κ-opioid antagonist (nucleoside) **(40)** | ACSO (2018) 3:12658 |
| **MRS7343** | κ-opioid partial agonist (nucleoside) **(43)** | ACSO (2018) 3:12658 |
| **MRS7344** | photocleavable $A_3$ adenosine agonist | PR (2021) 170:105731 |
| **MRS7352** | sulfonated $A_{2A}$ receptor antagonist **(13)** | MCC (2017) 8:1659 |
| **MRS7358** | κ-opioid antagonist (truncated nucleoside) **(54)** | ACSO (2018) 3:12658 |
| **MRS7395** | fluorescent (AF647) $A_{2A}$ receptor antagonist **(10)** | MCC (2017) 8:1659 |
| | | Cells (2020) 9:1200 |
| **MRS7396** | fluorescent (Bodipy) $A_{2A}$ receptor antagonist **(11)** | MCC (2017) 8:1659 |
| **MRS7416** | fluorescent (AF488) $A_{2A}$ receptor antagonist **(12)** | MCC (2017) 8:1659 |
| **MRS7422** | $A_3$ adenosine agonist (Cl-IB-MECA) prodrug **(5)** | PS (2020) 16:367 |
| **MRS7431** | $A_3$ adenosine antagonist in PAM series **(17)** | JMC (2022) 65(22):15238 |
| | **(1)** | ACSPT (2022) 5(8):625 |
| **MRS7469** | $A_1$ receptor agonist **(9)** | JMC (2019) 62:1502 |
| **MRS7476** | $A_3$ adenosine agonist (MRS5698) prodrug **(6)** | PS (2020) 16:367 |
| **MRS7489** | $A_{2A}$ adenosine agonist **(4)** | CS (2021) 12:960 |
| **MRS7497** | human $A_3$ receptor antagonist **(**adenine deriv., **17)** | MCC (2018) 9:1920 |
| **MRS7535** | fluorescent (Cy7) $A_3$ antagonist **(19)** | PS (2023) 19, 565 |
| **MRS7551** | selective $A_3$ adenosine allosteric enhancer **(13)** | ACSPT (2022) 5(8):625 |
| | **(14)** | JMC (2022) 65(22):15238 |
| **MRS7591** | human and mouse $A_3$ receptor partial agonist **(15)** | JMC (2020) 63:4334 |
| **MRS7608** | ABCG2 inhibitor **(37c)** | EJMC (2022) 231:114103 |

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| **MRS7618** | $A_3$ adenosine agonist **(11)** | EJMC (2022) 228:113983 |
| **MRS7663** | $A_{2B}$ adenosine antagonist, irreversible (**29**) | BP (2022) 200:115027 |
| **MRS7704** | Enterovirus A71 antiviral **(48)** | BMCL (2020) 30:127599 |
| **MRS7734** | macrocyclic precursor $A_3$ adenosine agonist **(11)** | ACSPT (2023) 6:1288 |
| **MRS7735** | macrocyclic $A_3$ adenosine agonist **(12)** | ACSPT (2023) 6:1288 |
| **MRS7774** | Fluorescent (JF646) $A_{2A}$ antagonist **(12)** | PS (2023) 19, 565 |
| **MRS7788** | selective $A_3$ adenosine allosteric enhancer **(18)** | JMC (2022) 65(22):15238 |
| **MRS7792** | $A_3$ partial agonist, ester, $N^6$-2-Ph-Et **(27)** | EJMC (2022) 228:113983 |
| **MRS7799** | $A_3$ adenosine antagonist, DPTN | PS (2021) 17:737 |
| | $A_3$ adenosine antagonist, DPTN (**9**) | ACMCL (2022) 13:623 |
| | | ACSPT (2023) 6:1266 |
| **[$^3$H]MRS7799** | $A_3$ adenosine antagonist radioligand | ACMCL (2022) 13:623 |
| **MRS7800** | ABCG2 inhibitor **(64)** | EJMC (2022) 231:114103 |
| **MRS7816** | selective $A_1$ adenosine antagonist **(22)** | CC (2021) 57:12305 |
| **MRS7827** | selective $A_3$ adenosine allosteric enhancer **(7)** | ACSPT (2022) 5(8):625 |
| | **(20)** | JMC (2022) 65(22):15238 |
| **MRS7907** | $A_3$ adenosine antagonist (**16d**) | ACMCL (2022) 13:623 |
| | | ACSPT (2023) 6:1266 |
| **MRS7925** | 5-$HT_{2B}$ methanocarba antagonist **(43)** | EJMC (2023) 259:115691 |
| **MRS7932** | selective $A_1$ adenosine allosteric enhancer **(21)** | ACMCL (2023) 14(12):1640 |
| **MRS7935** | selective $A_1$ adenosine allosteric enhancer **(15)** | ACMCL (2023) 14(12):1640 |
| **MRS7944** | selective $A_1$ adenosine allosteric enhancer **(12)** | ACMCL (2023) 14(12):1640 |
| **MRS8033** | macrocyclic $A_3$ adenosine agonist **(19)** | ACSPT (2023) 6:1288 |
| **MRS8035** | macrocyclic precursor $A_3$ adenosine agonist **(18)** | ACSPT (2023) 6:1288 |
| **MRS8054** | selective $A_3$ adenosine allosteric enhancer **(39)** | JMC (2022) 65(22):15238 |
| **MRS8074** | $A_3$ adenosine antagonist (**19**) | ACMCL (2022) 13:623 |
| **MRS8099** | 5-$HT_{2B}$ methanocarba antagonist **(45)** | EJMC (2023) 259:115691 |
| **MRS8134** | 5-$HT_{2B}$ methanocarba antagonist **(48)** | EJMC (2023) 259:115691 |
| **MRS8247** | selective $A_3$ adenosine allosteric enhancer (C8) | unpublished |
| **MRS8308** | selective $A_3$ adenosine allosteric enhancer (C9) | unpublished |
| **MRS8339** | selective $A_3$ adenosine allosteric enhancer (piperid.) | unpublished |
| **MRS8340** | selective $A_3$ adenosine allosteric enhancer (piperaz.) | unpublished |
| **NCK33** | polo-box domain, Polo-like kinase1 inhibitor **(79)** | JMC (2020) 63:14087 |
| **NCK100** | polo-box domain, Polo-like kinase1 inhibitor **(143)** | JMC (2020) 63:14087 |
| **NCK106** | polo-box domain, Polo-like kinase1 inhibitor **(145)** | JMC (2020) 63:14087 |
| **NCK103** | PBD, Polo-like kinase1 inhibitor **(15)** | ACSPT (2023) 6(3):422 |
| **NCK149** | PBD, Polo-like kinase1 inhibitor **(43)** | ACSPT (2023) 6(3):422 |
| **NCK167** | PBD, Polo-like kinase1 inhibitor prodrug **(78)** | ACSPT (2023) 6(3):422 |
| **NCK173** | PBD, Polo-like kinase1 inhibitor prodrug **(80)** | ACSPT (2023) 6(3):422 |
| **NCK189** | PBD, Polo-like kinase1 inhibitor, Allopole-A **(3)** | PNAS (2023) Park et al. |
| **NCK190** | PBD, Plk1 inhibitor prodrug, Allopole **(4)** | PNAS (2023) Park et al. |
| **NCK195** | PBD, Polo-like kinase1 inhibitor, biotin conj. **(22)** | PNAS (2023) Park et al. |
| **NECA N1-oxide** | potent, nonselective adenosine agonist **(29)** | MP (1994) 45:1101 |
| **NECI** | inosine-related $A_3$ adenosine **(53)** | MP (1994) 45:1101 |
| **PAPA-APEC** | selective $A_{2A}$ adenosine agonist, to radioiodinate* | PNAS (1989) 86:6572 |
| | | MP (1991) 40:639 |

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|---|---|---|
| **PAPA-TAC** | $M_1$ muscarinic antagonist (**6**) | BC (1992) 3:234 |
| **PAPA-XAC** | $A_1$ adenosine antagonist, to radioiodinate | MP (1987) 32:184 |
| **PAPA-XAC-SANPAH** | $A_1$ radioiodinated photoaffinity label | FL (1989) 257:292 |
| **PAPET-ATP** | potent $P2Y_1$, P2X1 and P2X3 agonist **(16)** | JMC (2002) 45:4057 |
| **PPTN** | selective $P2Y_{14}$ receptor antagonist **(5)** | MP (2013) 84:41<br>BMCL (2015) 25:4733 |
| **SPA** | water-soluble, selective $A_1$ adenosine agonist* | JMC (1992) 35:4143<br>NP (2017) 114:101 |
| **SVP333** | selective $P2Y_2$ allosteric partial agonist **(7c)** | BMC (2012) 20:2304 |
| **TAC** | amine congener, muscarinic antagonist* | BC (1992) 3:234 |
| **TEMPO-APEC** | spin labeled $A_{2A}$ adenosine agonist **(15)** | JMR (1989) 32:1043 |
| **TEMPO-XAC** | spin labeled $A_1/A_{2A}$ adenosine antagonist | BP (1987) 36:1697 |
| **4′-thio-Cl-IB-MECA (LJ-529)** | selective $A_3$ adenosine agonist | JMC (2006) 49:273 |
| **2-thio-UTP** | selective $P2Y_2$ receptor agonist | BP (2006) 71:540 |
| **α-thiophosphates (*Rp* or *Sp*) of various uracil and adenine nucleotides** | selective $P2Y_6R$ or $P2Y_{14}R$ or other P2R agonists | NC (2023) in press. |
| **XAC** | potent, nonselective adenosine antagonist | PNAS (1985) 28:1334<br>ACSPT (2023) 6:1266 |
| | [$^3$H]XAC | NI (1991) 18:207<br>NL (1988) 86:121<br>PNAS (1986) 83:4089 |
| | XAC on solid support (Affi-gel-10) | FL (1989) 257:292 |
| **XCC** | potent, $A_1$ selective adenosine antagonist | JMC (1985) 28:1334 |
| **VUF5455** | selective $A_3$ adenosine allosteric enhancer | MP (2003) 63:1021 |
| **VUF8504** | selective $A_3$ adenosine allosteric enhancer | MP (2001) 60:1057 |
| **WS98** | fluorescent (fluorescein) $A_{2A}$AR antagonist **(15)** | MCC (2019) 10:1094 |
| **3288** | $A_{2A}$ receptor antagonist from mass spec screen | AC (2019) 91:8162 |
| **3588** | $A_{2A}$ receptor antagonist from mass spec screen | AC (2019) 91:8162 |
| **3676** | $A_{2A}$ receptor antagonist from mass spec screen | AC (2019) 91:8162 |

* Available through the NIMH synthesis program (http://nimh-repository.rti.org/)

** journal abbreviation: EJMC, European Journal of Medicinal Chemistry; FL, FEBS Lett.; JANS, J. Autonom. Nerv. Syst.; JCIM, J. Chem. Inf. Modeling; JF, Journal of Fluorescence; JMC, Journal of Medicinal Chemistry; JMR, Journal of Molecular Recognition; JN, Journal of Neurochemistry; JPET, J. Pharmacol. Exp. Ther.; BP, Biochemical Pharmacology; BC, Bioconjugate Chemistry; DDR, Drug Devel. Res.; EER, Exp. Eye Res.; MCC, Med Chem Comm; MP, Molecular Pharmacology; NI, Neurochem. Int.; NL, Neurosci. Lett.; NMB, Nucl. Med. Biol.; NP, Neuropharmacology; OBC, Org. Biomol. Chem.; OL, Organic Lett.; PNAS, Proceedings of the National Academy of Sciences; BMC, Bioorganic and Medicinal Chemistry; BMCL, Bioorganic and Medicinal Chemistry Letters; BMCP, Biomed Central Pharmacol.; ACSCB, ACS Chemical Biology; ACSML, ACS Medicinal Chemistry Letters; ACSCN, ACS Chemical Neuroscience; ACS Omega, ACSO; CCC, Coll. Czech. Chem. Comm.; PR, Pharmacol. Res.; PR, Pharmacological Research; PS, Purinergic Signalling; PONE, PLoS ONE; RSCA, RSC Advances; SR, Scientific Reports; TIPS, Trends Pharmacol. Sci.; JCR, J. Controlled Release; AC, Analytical Chemistry; CS, Chemical Science; BIOM, Biomolecules; ACSPT, ACS

Pharmacology and Translational Science; ART, Arthritis Research and Therapy; US, US patent; NC, Nature Chemistry.

Many other compounds not listed here are available from MedKoo, https://medkoo.com/; Glixx Labs, Inc., http://www.glixxlabs.com

First 19 pages of PubChem "MRS" listings:

| Name | PubChem IDs | CHEMBL | CAS registry no. |
|---|---|---|---|
| IB-MECA | 123683 | | |
| Cl-IB-MECA | 3035850 | | |
| LUF6000 | 11711282 | | |
| ADAC | 2026, 126054, 23789715 | | |
| TEMPO-ADAC | 131718190 | | |
| ADAC-NCS | 131718368 | | |
| APEC | 3081741 | | |
| PAPA-APEC | 3081715 | | |
| $^{125}$I-AZIDO-PAPA-APEC | 3083135 | | |
| p-DITC-APEC | 3037834 | | |
| FITC-APEC | 23772170 | | |
| m-DITC-XAC | 3082962 | | |
| ED-p-DITC-XAC | 3082963 | | |
| XAC | 5697 | | |
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| XAC-BY630 | 73755041 | | |
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