

August 10, 2023: 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
[¹²⁵I]-AB-MECA	A ₃ adenosine agonist radioligand	ACSPT (2022) 5(8):625 MP (1994) 45:978
ADAC	selective A ₁ adenosine agonist	BP (1987) 36:1697
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
BTH₄	non-N-containing adenosine antagonist (7)	JMC (1996) 39:398
CI-IB-MECA	selective A ₃ adenosine agonist (13)	JMC (1994) 37:3614 BP (2020) 117:113934
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
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
FE@SUPPLY (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
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
ICBM (MRS1163)	selective A ₃ adenosine agonist affinity label (4)	BBRC (1994) 203:570
I-ZM241,385	selective A _{2A} adenosine antagonist radioligand	MP (1996) 48:970
LC260	selective A ₃ adenosine agonist, 2-triazole (15)	JMC (2006) 49:7373
LJ529	selective A ₃ agonist (4'-S-Cl-IB-MECA, 3) (39a) (6)	JMC (2003) 46:3775 JMC (2006) 49:273 JMC (2007) 50:3159

LJ1258 (MRS3884)	selective A ₃ agonist (4'-S-IB-MECA, 5h)	BMC (2009) 17:8003
LJ1351 (MRS3973)	hA ₃ receptor antagonist (3-Br-Bn, <i>N,N</i> -diMe, 6c)	BMCL (2008) 18:1612
LJ1888 (LJ1251, MRS3820)	selective A ₃ adenosine antagonist (6e)	JMC (2008) 51:6609
	(9d)	JMC (2007) 50:3159
	(3c)	JMC (2017) 60:7459
LJ2126 (MRS5292)	hA ₃ receptor antagonist/A _{2A} agonist (4a)	JMC (2012) 55:342
LJ2163 (MRS5450)	hA ₃ receptor antagonist (6a)	JMC (2021) 64:12525
LJ2521 (MRS5584)	hA ₃ receptor antagonist (6c)	JMC (2021) 64:12525
LJ2698 (MRS5014, FM101)	hA ₃ receptor antagonist (9b)	JMC (2007) 50:3159
	(3c)	JMC (2017) 60:7459
LJ3429 (MRS7002)	selective A ₃ seleno-adenosine agonist (3p)	JMC (2017) 60:3422
LJ4378 (MRS5281)	hA ₃ receptor antagonist/A _{2A} agonist (4g)	JMC (2012) 55:342
LJ4517 (MRS7049)	hA _{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	JMC (2006) 49:3354
	(4)	ACSPT (2022) 5(8):625
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)	JMC (2002) 45:4471
	(7a)	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 hA ₃ adenosine antagonist (10)	JMC (1996) 39:4142
MRS1178	A _{2B} adenosine antagonist (39)	JMC (1998) 41:2835
MRS1186	selective hA ₃ adenosine antagonist (3)	JMC (1996) 39:4142
MRS1191	selective hA ₃ adenosine antagonist (DHP, 2)	JMC (1997) 40:2596
		NP (2017) 114:101
MRS1220	selective hA ₃ adenosine antagonist (12)	JMC (1996) 39:4142
		PS (2021) 17:737
MRS1292	selective A ₃ adenosine antagonist (14)	JMC (2002) 45:4471
MRS1334	selective hA ₃ adenosine antagonist (DHP, 24g)	JMC (1997) 40:2596
		PS (2021) 17:737
MRS1458	irreversible (sulfonyl-F) A ₃ antagonist (19)	BC (1999) 10:667
MRS1477	allosteric enhancer of TRPV1 channels (DHP)	JPET (2012) 340:152
MRS1523	selective A ₃ adenosine antagonist (4)	JMC (1999) 42:706
		PS (2021) 17:737
		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	(<i>N</i>)-methanocarba-adenosine (5c), A ₃ agonist	JMC (2000) 43:2196
MRS1656	(<i>S</i>)-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)	JMC (2002) 45:4471
	(7c)	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)	JMC (2002) 45:4471
	(9c)	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)	JMC (2005) 48:1745
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
MRS2055	P2Y ₁₂ agonist (17b)	JMC (2002) 45:4057
MRS2154	P2X ₂ antagonist, dihydropyridine deriv. (5a)	JANS (2000) 81:152
MRS2159	selective P2X ₁ antagonist, pyridoxal deriv.	JMC (2001) 44:340
MRS2160	P2X ₁ and P2X ₂ 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 P2X ₂ 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	P2X ₁ allosteric enhancer (2)	JMC (1998) 41:2201
MRS2220	P2X ₁ 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	P2X ₁ , P2X ₂ , P2X ₄ 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
MRS2306	selective P2X ₇ antagonist (2)	BMCL (2008) 18:571
MRS2339	cardiac P2X ₄ agonist	JMC (2010) 53:2562
MRS2340	(N)-methanocarba-ATP, P2X, P2Y agonist	DDR (2004) 61:227
MRS2343	2-Cl-N ⁶ -Me-(N)-methanocarba-ATP, P2Y ₁ agonist (14a)	JMC (2002) 45:2090
MRS2352	β,γ-me-(N)-methanocarba-ATP, P2Y ₁ agonist (17a)	JMC (2002) 45:2090
MRS2365	selective P2Y ₁ agonist	JMC (2002) 45:2090
MRS2367	2-Cl-(N)-methanocarba-ATP, P2Y ₁ agonist (12a)	JMC (2002) 45:2090
MRS2395	P2Y ₁₂ antagonist (moderate potency)	JMC (2002) 45:5694
MRS2427	selective P2X ₇ 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
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 P2X ₇ antagonist	EER (2010) 91:425
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
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
MRS2693	selective P2Y ₆ agonist	JMC (2006) 49:5532
MRS2698	selective P2Y ₂ agonist	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
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 P2X ₄ agonist	JMC (2010) 53:2562
MRS2950	nonnucleotide P2Y ₁ receptor antagonist (2a)	BMC (2012) 20:5254
MRS2957	Potent and selective P2Y ₆ agonist (23)	JMC (2010) 53:4488
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 P2X ₄ agonist	JMC (2013) 56:902
		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
MRS3481 (LJ1254)	orthogonal A ₃ adenosine agonist for neoceptor	JMC (2006) 49:2689
MRS3558	selective A ₃ adenosine agonist (18)	JMC (2005) 48:1745
MRS3581	selective Br-76 A ₃ adenosine agonist	NMB (2009) 36:3
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	JMC (2005) 48:8103
MRS3642 (LJ1256)	selective A ₃ adenosine antagonist	BMCL (2006) 16:596
MRS3771	selective A ₃ adenosine antagonist	BMCL (2006) 16:596
MRS3777	selective A ₃ adenosine antagonist	JMC (2005) 48:4910
MRS3997	A _{2B} adenosine agonist (28)	JMC (2007) 50:1810
MRS4062	selective P2Y ₄ agonist	JMC (2011) 54:4018
MRS4063	clickable P2Y ₆ receptor agonist (15)	MCC (2013) 4:1156
MRS4074	in vivo, cardiac P2X ₄ agonist	JMC (2013) 56:902
MRS4084	in vivo, cardiac P2X ₄ 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
		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	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
		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
MRS4590	(N)-methanocarba-GTP (4d)	BIOM (2022) 12:584
MRS4591	(S)-methanocarba-GMP-PCP (4b)	BIOM (2022) 12:584
MRS4596	P2X ₄ 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) (8)	ACSML (2020) 11:1281 JMC (2020) 63:9563
MRS4654	P2Y ₁₄ receptor antagonist (32)	JMC (2021) 64:5099
MRS4656	P2Y ₆ receptor antagonist (16)	BMCL (2021) 41:128008
MRS4695	P2Y ₆ receptor antagonist (7)	BMCL (2021) 41:128008
MRS4706	P2Y ₆ receptor antagonist (14)	BMCL (2021) 41:128008
MRS4719	P2X ₄ receptor antagonist (21u)	JMC (2022) 5:13967
MRS4738	P2Y ₁₄ receptor antagonist (15)	JMC (2022) 65:3434
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
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) (63)	JMC (2022) 65:3434 JMC (2023), 66(13):9076
MRS4815	P2Y ₁₄ receptor antagonist double prodrug (143) (64)	JMC (2022) 65:3434 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
MRS4833	P2Y ₁₄ receptor antagonist (15)	JMC (2023), 66(13):9076
MRS4839	P2Y ₆ receptor antagonist (27)	BMCL (2022) 75:128981
MRS4841	P2Y ₆ receptor antagonist (25)	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
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
MRS4911	P2Y ₁₄ R antag. carbamate prodrug (51) of MRS4833	JMC (2023), 66(13):9076
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
MRS5147	selective Br-76 A ₃ adenosine antagonist	NMB (2009) 23:232
MRS5151	selective A ₃ adenosine agonist (18a)	BMCL (2008) 18:2813

MRS5158	(6) selective A ₃ adenosine allosteric enhancer (11) (12a)	JMC (2009) 15:3994 ACSPT (2022) 5(8):625 JMC (2022) 65(22):15238
MRS5190	selective A ₃ adenosine allosteric enhancer (12) (12b)	ACSPT (2022) 5(8):625 JMC (2022) 65(22):15238
MRS5202	<i>N</i> 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	JMC (2012) 55:4847
MRS5676	mixed A ₃ agonist+dopamine transporter modulator	JPET (2016) 357:24
MRS5679	highly selective A ₃ adenosine agonist	JMC (2012) 55:4847
MRS5698	highly selective A ₃ adenosine agonist (31)	JMC (2012) 55:4847
MRS5701	selective water soluble A ₁ /A ₃ adenosine agonist (6)	JMC (2013) 56:5949
MRS5728	gold-immobil. A ₁ /A _{2A} adenosine antagonist (26a)	PS (2013) 9:183
MRS5763	selective fluorescent (AF488) A ₃ AR antagonist (23)	EJMC (2020) 186:111886
MRS5776	selective A ₃ adenosine antagonist	JMC (2013) 56:5949
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 hA ₃ adenosine antagonist (16)	JMC (2013) 56:5949
MRS5923	selective A ₃ adenosine antagonist (8)	PONE (2014) 9: e97858
MRS5942	novel A ₁ /A _{2A} /A ₃ adenosine antagonist (23)	JCIM (2015) 55:550
MRS5979	ferrocene-containing A ₃ adenosine agonist	JMC (2014) 57: 9901

MRS5980	highly selective A ₃ adenosine agonist (33) (10)	JMC (2014) 57: 9901 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
MRS7154	selective A ₃ adenosine agonist (12)	ACSMCL (2015) 6:804
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
MRS7240	mixed A _{2A/3} adenosine antagonist (36)	SR (2017) 7:6398
MRS7249	N ⁶ -cPr ₂ Me-2-Cl-(N)-methanocarb-A-5'-Pr-ester (27)	JMC (2016) 59:11006
MRS7292	dopamine transporter allosteric modulator (9)	JMC (2017) 60:3109
MRS7293	N ⁶ -cPr ₂ Me-2-Cl-(N)-methanocarb-A-5'-Me-ester (25)	JMC (2016) 59:11006
MRS7299	opioid antagonist (nucleoside) (28)	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) (17)	MP (2019) 96:180 EJMC (2022) 231:114103
MRS7331	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	opioid antagonist (nucleoside) (40)	ACSO (2018) 3:12658
MRS7343	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	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) (1)	JMC (2022) 65(22):15238 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) Toti et al., in press
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
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
MRS7774	Fluorescent (JF646) A _{2A} antagonist (12)	PS (2023) Toti et al., in press
MRS7788	selective A ₃ adenosine allosteric enhancer (18)	JMC (2022) 65(22):15238
MRS7799	A ₃ adenosine antagonist, DPTN	PS (2021) 17:737
	A ₃ adenosine antagonist, DPTN (9)	ACMCL (2022) 13:623
[³H]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
MRS7925	5-HT _{2B} methanocarba antagonist (43)	EJMC (2023) 259:115691
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
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
PAPA-XAC	A ₁ adenosine antagonist, to radioiodinate	MP (1987) 32:184
PAPET-ATP	potent P2Y ₁ , P2X ₁ and P2X ₃ agonist (16)	JMC (2002) 45:4057
PPTN	selective P2Y ₁₄ receptor antagonist	MP (2013) 84:41
SPA	water-soluble, selective A ₁ adenosine agonist*	JMC (1992) 35:4143
		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-CI-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

XAC	potent, nonselective adenosine antagonist	PNAS (1985) 28:1334
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

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** journal abbreviation: EJMC, European Journal of Medicinal Chemistry; 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.; NMB, Nucl. Med. Biol.; NP, Neuropharmacology; 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; ACSN, 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.

Many other compounds not listed here are available from MedKoo, <https://medkoo.com/>; Glxxx Labs, Inc., <http://www.glixlabs.com>

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CI-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		

[³ H]XAC	5697		
XAC-BY630	73755041		
XCC	126079		
MRS923	631105		
MRS1041	10247549		
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