

Compounds introduced or investigated in Ken Jacobson's lab (kennethj@niddk.nih.gov) at NIDDK or through collaborations. Orange compounds are or will soon be available commercially as research tools:

<u>Abbreviation</u>	<u>Action</u>	<u>Reference (year, vol:page) **</u>
AB-MECA	selective A ₃ adenosine agonist, to radioiodinate	JMC (1994) 37:636
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*	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	JMC (1994) 37:3614
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
DU124183	selective A ₃ adenosine allosteric enhancer	MP (2003) 63:1021
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	MP (1994) 45:978
IB-MECA	selective A ₃ adenosine agonist	JMC (1994) 37:636
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
LJ529	selective A ₃ thio-adenosine agonist (39a)	JMC (2006) 49:273
LJ1251	selective A ₃ adenosine antagonist (6e)	JMC (2008) 51:6609
LJ3429	selective A ₃ seleno-adenosine agonist (3p)	JMC (2017) 60:3422
cLNA-adenosine	first carbocyclic "locked" nucleoside (23)	OL (2003) 5:1665
LUF6000	selective A ₃ adenosine allosteric enhancer	JMC (2006) 49:3354
MMPD	A ₁ adenosine partial agonist PET ligand (22b)	JMC (2018) 61:9966
MRS541	A ₃ adenosine low efficacy agonist	JMC (2002) 45:4471
MRS542	A ₃ adenosine low efficacy agonist/antagonist	JMC (2002) 45:4471
MRS1067	selective A ₃ adenosine antagonist	JMC (1996) 39:2293
MRS1191	selective A ₃ adenosine antagonist (DHP, 2)	JMC (1997) 40:2596
MRS1220	selective A ₃ adenosine antagonist	JMC (1996) 39:4142
MRS1292	selective A ₃ adenosine antagonist	JMC (2002) 45:4471
MRS1334	selective A ₃ adenosine antagonist (DHP, 24g)	JMC (1997) 40:2596
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	JMC (1999) 42:706
MRS1595	selective A _{2B} adenosine antagonist (14)	DDR (1999) 47:178
MRS1706	selective A _{2B} adenosine antagonist (20)	JMC (2000) 43:1165
MRS1740	A ₃ adenosine low efficacy agonist/antagonist	JMC (2002) 45:4471
MRS1754	selective A _{2B} adenosine antagonist (27)	JMC (2000) 43:1165
MRS1765	selective A _{2B} adenosine antagonist (33)	JMC (2000) 43:1165
MRS1845	inhibitor of store-operated calcium channels	BP (2003) 65:329
MRS1898	selective A ₃ adenosine agonist	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
MRS1957	(N)-methanocarba-inosine (5), weak at A ₃	BMCL (2001) 11:2295
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
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 P2X7 antagonist (2)	BMCL (2008) 18:571
MRS2339	cardiac P2X4 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
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
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
MRS2670	selective P2Y ₁₄ agonist (4-thio)	JMC (2007) 50:2030
MRS2690	selective P2Y ₁₄ agonist (2-thio)	JMC (2007) 50:2030
MRS2693	selective P2Y ₆ agonist	JMC (2006) 49:5532
MRS2698	selective P2Y ₂ agonist	JMC (2007) 50:1166
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
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	JMC (2005) 48:1745
MRS3581	selective Br-76 A ₃ adenosine agonist	NMB (2009) 36:3
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 P2Y ₆ receptor agonist	MCC (2013) 4:1156
MRS4149	alkyne-functionalized P2Y ₁₄ antagonist (22)	ACSCB (2014) 9:2833
MRS4160	clickable P2Y _{2/4/6} receptor agonist (26)	JMC (2014) 57:3874
MRS4162	fluorescent P2Y _{2/4/6} receptor agonist	JMC (2014) 57:3874
MRS4174	fluorescent P2Y ₁₄ receptor antagonist	ACSCB (2014) 9:2833
MRS4183	fluorescent 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
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
MRS4552	Nucleotide CD73 inhibitor (9h)	JMC (2019) 62:3677
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	BMCL (2008) 18:2813
MRS5206	selective fluorescent A _{2A} agonist (AF488)	NI (2013) 63:42
MRS5216	dendrimeric A ₃ adenosine agonist	PR (2012) 65:338
MRS5218	selective fluorescent 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 A _{2A} adenosine antagonist	BP (2010) 80:506
MRS5347	fluorescent 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 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 A ₃ adenosine antagonist	BP (2012) 83:1552
MRS5474	selective A ₁ adenosine agonist	JMC (2012) 123:373
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	JMC (2012) 55:4847
MRS5701	selective water soluble A ₁ /A ₃ adenosine agonist	JMC (2013) 56:5949
MRS5728	gold-immobil. A ₁ /A _{2A} adenosine antagonist (26b)	PS (2013) 9:183
MRS5776	selective A ₃ adenosine antagonist	JMC (2013) 56:5949
MRS5841	selective water soluble A ₃ adenosine agonist	JMC (2013) 56:5949
MRS5842	fluorescent (Alexa647) A _{2A} receptor antagonist	JCR (2018) 283:135
MRS5854	A _{2A} adenosine receptor affinity label	ACSMCL (2014) 5:1043
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)	JMC (2014) 57: 9901
	(10)	ACSMCL (2015) 6:804
MRS7116	selective A ₃ adenosine agonist	MCC (2015) 6:555
MRS7126	selective A ₃ adenosine agonist	MCC (2015) 6:555
MRS7134	5HT 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	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	5HT _{2B} methanocarba antagonist (23)	JMC (2016) 59:11006
MRS7220	selective A ₃ adenosine agonist, lacking 6-NH (21)	JMC (2016) 59:3249
MRS7221	5HT ₂ methanocarba antagonist (26)	JMC (2016) 59:11006
MRS7232	dopamine transporter allosteric modulator (10)	JMC (2017) 60:3109
MRS7292	dopamine transporter allosteric modulator (9)	JMC (2017) 60:3109
MRS7299	opioid antagonist (nucleoside) (28)	ACSO (2018) 3:12658
MRS7323	P-gp inhibitor (8)	MP (2019) 96:180
MRS7352	sulfonated A _{2A} receptor antagonist (13)	MCC (2017) 8:1659
MRS7396	fluorescent A _{2A} receptor antagonist (11)	MCC (2017) 8:1659
MRS7416	fluorescent A _{2A} receptor antagonist (12)	MCC (2017) 8:1659
MRS7469	A ₁ receptor agonist (9)	JMC (2019) 62:1502
MRS7497	human A ₃ receptor antagonist (adenine deriv.)	MCC (2018) 9:1920
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
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
WS98	fluorescent A _{2A} receptor 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: 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.; 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; ACS Omega, ACSO; PR, Pharmacol. Res.; PS, Purinergic Signalling; PONE, PLoS ONE; TIPS, Trends Pharmacol. Sci.; JCR, J. Controlled Release; ; AC, Analytical Chemistry.