



## Supporting Information

for

### **Synthesis of substituted triazole–pyrazole hybrids using triazenylpyrazole precursors**

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### **Information on the availability of the data and the physical material of the target compounds**

General information: The following list includes the materials produced in this study which were made available through the Molecule Archive at KIT (<https://compound-platform.eu/>). The archive stores the materials for further reuse and review – interested academic scientists can order materials for different scientific collaborations or as reference compounds. The materials can be found via the DOI link given below or can be accessed through the Molecule Archive list in the Chemotion repository: <https://chemotion-repository.net/home/moleculeArchive>

Compound	Smiles Code	Sample DOI
19g	<chem>[N-]=[N+]=Nc1nn(c(c1)C)c1ccc(cc1)C#N</chem>	<a href="https://dx.doi.org/10.14272/KIQBPEXSAZKVRR-UHFFFAOYSA-N.3">https://dx.doi.org/10.14272/KIQBPEXSAZKVRR-UHFFFAOYSA-N.3</a>
17e	<chem>N#Cc1ccc(cc1)n1nc(cc1C)/N=N/N(C(C)C)C(C)C</chem>	<a href="https://dx.doi.org/10.14272/RSDVJJOPRTZAOO-XUTLUUPIISA-N.1">https://dx.doi.org/10.14272/RSDVJJOPRTZAOO-XUTLUUPIISA-N.1</a>
18e	<chem>N#Cc1ccc(cc1)n1nc(cc1/N=N/N(C(C)C)C(C)C)C</chem>	<a href="https://dx.doi.org/10.14272/WPXPVVIOPAJXSL-XUTLUUPIISA-N.1">https://dx.doi.org/10.14272/WPXPVVIOPAJXSL-XUTLUUPIISA-N.1</a>
17f	<chem>CC(N(C(C)C)/N=N/c1nn(c(c1)C)c1ccc(cc1)[N+](=O)[O-])C</chem>	<a href="https://dx.doi.org/10.14272/LQZXCDPUXUEILJ-HTXNQAPBSA-N.1">https://dx.doi.org/10.14272/LQZXCDPUXUEILJ-HTXNQAPBSA-N.1</a>
18f	<chem>CC(N(C(C)C)/N=N/c1cc(nn1c1ccc(cc1)[N+](=O)[O-])C)C</chem>	<a href="https://dx.doi.org/10.14272/VRKHTXPHTAWWEY-HTXNQAPBSA-N.1">https://dx.doi.org/10.14272/VRKHTXPHTAWWEY-HTXNQAPBSA-N.1</a>

17k	CCOC(=O)c1cn(nc1/N=N/N(C(C)C)C(C)C)Cc1ccc(cc1)Br	<a href="https://dx.doi.org/10.14272/ZYMNXIBCZDWSHX-XTQSDGFTSA-N.1">https://dx.doi.org/10.14272/ZYMNXIBCZDWSHX-XTQSDGFTSA-N.1</a>
18k	CCOC(=O)c1cnn(c1/N=N/N(C(C)C)C(C)C)Cc1ccc(cc1)Br	<a href="https://dx.doi.org/10.14272/FFWКУULMXDRWPI-GHVJWSGMSA-N.1">https://dx.doi.org/10.14272/FFWКУULMXDRWPI-GHVJWSGMSA-N.1</a>
17d	CC(N(C(C)C)/N=N/c1nn(c(c1)C)Cc1ccc(cc1)C	<a href="https://dx.doi.org/10.14272/FEHNUWIZIPJQLZ-CZIZESTLSA-N.1">https://dx.doi.org/10.14272/FEHNUWIZIPJQLZ-CZIZESTLSA-N.1</a>
18d	CC(N(C(C)C)/N=N/c1cc(nn1Cc1cccc1)C)C	<a href="https://dx.doi.org/10.14272/OSZGZNAJFDDFLV-CZIZESTLSA-N.1">https://dx.doi.org/10.14272/OSZGZNAJFDDFLV-CZIZESTLSA-N.1</a>
17r	N#Cc1cn(nc1/N=N/N(C(C)C)C(C)C)Cc1ccc(cc1)F	<a href="https://dx.doi.org/10.14272/ADGUCVKMBUJWJM-LSDHQDQOSA-N.1">https://dx.doi.org/10.14272/ADGUCVKMBUJWJM-LSDHQDQOSA-N.1</a>
18r	N#Cc1cnn(c1/N=N/N(C(C)C)C(C)C)Cc1ccc(cc1)F	<a href="https://dx.doi.org/10.14272/HEZWXNUXEKJBQT-QURGRASLSA-N.1">https://dx.doi.org/10.14272/HEZWXNUXEKJBQT-QURGRASLSA-N.1</a>
21sd	N#Cc1cn(nc1n1nnc(c1)c1cccc1)Cc1c(c(F)cc(c1)F	<a href="https://dx.doi.org/10.14272/LBYPTGDZZSOCSK-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/LBYPTGDZZSOCSK-UHFFFAOYSA-N.1</a>
21ud	COC(=O)c1ccc(cc1)Cn1cc(c(n1)n1nnc(c1)c1cccc1)C#N	<a href="https://dx.doi.org/10.14272/YZSLXIHSIJQQMB-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/YZSLXIHSIJQQMB-UHFFFAOYSA-N.1</a>
21ga	CCCC1nnn(c1)c1nn(c(c1)C)c1ccc(cc1)C#N	<a href="https://dx.doi.org/10.14272/WZTARLNNZGQBDW-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/WZTARLNNZGQBDW-UHFFFAOYSA-N.1</a>
21rd	N#Cc1cn(nc1n1nnc(c1)c1cccc1)Cc1cccc1	<a href="https://dx.doi.org/10.14272/DGWASOOTEXXJBK-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/DGWASOOTEXXJBK-UHFFFAOYSA-N.1</a>
21fa	CCCC1nnn(c1)c1cc(n(n1)Cc1cccc1)C	<a href="https://dx.doi.org/10.14272/PKNOMBYAWYDCG-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/PKNOMBYAWYDCG-UHFFFAOYSA-N.1</a>
21gd	N#Cc1ccc(cc1)n1nc(cc1C)n1nnc(c1)c1cccc1	<a href="https://dx.doi.org/10.14272/QJHTUPAVPUUSNY-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/QJHTUPAVPUUSNY-UHFFFAOYSA-N.1</a> <a href="https://dx.doi.org/10.14272/QJHTUPAVPUUSNY-UHFFFAOYSA-N.2">https://dx.doi.org/10.14272/QJHTUPAVPUUSNY-UHFFFAOYSA-N.2</a>
17q	COC(=O)c1ccc(cc1)Cn1nc(c(c1)C#N)/N=N/N(C(C)C)C(C)C	<a href="https://dx.doi.org/10.14272/FZUUXBMFWLBSAE-XTQSDGFTSA-N.1">https://dx.doi.org/10.14272/FZUUXBMFWLBSAE-XTQSDGFTSA-N.1</a>
18q	COC(=O)c1ccc(cc1)Cn1ncc(c1/N=N/N(C(C)C)C(C)C)C#N	<a href="https://dx.doi.org/10.14272/HQEHAWORIRDNAT-GHVJWSGMSA-N.1">https://dx.doi.org/10.14272/HQEHAWORIRDNAT-GHVJWSGMSA-N.1</a>
21ce	COC1ccc(cc1)c1nnn(c1)c1ccn(n1)Cc1cccc1	<a href="https://dx.doi.org/10.14272/JMPSOWDQCFVJPL-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/JMPSOWDQCFVJPL-UHFFFAOYSA-N.1</a>
19q	CCOC(=O)Cn1nc(c(c1)C#N)N=[N+]=[N-]	<a href="https://dx.doi.org/10.14272/HEIIGJFYWAHNFX-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/HEIIGJFYWAHNFX-UHFFFAOYSA-N.1</a>
17a	CC(N(C(C)C)/N=N/c1ccn(n1)Cc1cccc1)C	<a href="https://dx.doi.org/10.14272/MGAVNYXVFXWSSZ-HTXNQAPBSA-N.1">https://dx.doi.org/10.14272/MGAVNYXVFXWSSZ-HTXNQAPBSA-N.1</a>
18a	CC(N(C(C)C)/N=N/c1ccnn1Cc1cccc1)C	<a href="https://dx.doi.org/10.14272/ZIDRUQYCDSSWJM-VHEBQXMUSA-N.1">https://dx.doi.org/10.14272/ZIDRUQYCDSSWJM-VHEBQXMUSA-N.1</a>
21ic	CC(=O)OCc1nnn(c1)c1nn(c(c1)C)c1cc(c(cc1Cl)[N+](=O)[O-]	<a href="https://dx.doi.org/10.14272/QIRBWRVTFHDFHS-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/QIRBWRVTFHDFHS-UHFFFAOYSA-N.1</a>
17h	CCOC(=O)c1cn(nc1/N=N/N(C(C)C)C(C)C)Cc1cccc1	<a href="https://dx.doi.org/10.14272/GKODORMDVGUGHL-LSDHQDQOSA-N.1">https://dx.doi.org/10.14272/GKODORMDVGUGHL-LSDHQDQOSA-N.1</a>
18h	CCOC(=O)c1cnn(c1/N=N/N(C(C)C)C(C)C)Cc1cccc1	<a href="https://dx.doi.org/10.14272/UBBFWZTUXPGXCP-QURGRASLSA-N.1">https://dx.doi.org/10.14272/UBBFWZTUXPGXCP-QURGRASLSA-N.1</a>
17l	N#Cc1cn(nc1/N=N/N(C(C)C)C(C)C)C(C)C	<a href="https://dx.doi.org/10.14272/XUZXRALOPOUFGP-BMRADRMJSA-N.1">https://dx.doi.org/10.14272/XUZXRALOPOUFGP-BMRADRMJSA-N.1</a>
18l	N#Cc1cnn(c1/N=N/N(C(C)C)C(C)C)C(C)C	<a href="https://dx.doi.org/10.14272/IJEPRRMQECALCS-WUKNDPDISA-N.1">https://dx.doi.org/10.14272/IJEPRRMQECALCS-WUKNDPDISA-N.1</a>
21fe	COC1ccc(cc1)c1nnn(c1)c1nn(c(c1)C)C1cccc1	<a href="https://dx.doi.org/10.14272/HKYHACNKJZVDCN-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/HKYHACNKJZVDCN-UHFFFAOYSA-N.1</a>

17n	<chem>N#Cc1cn(nc1/N=N/N(C(C)C)C(C)C)Cc1cccc1</chem>	<a href="https://dx.doi.org/10.14272/AONLLYWVGOMLR-XUTLUUPISA-N.2">https://dx.doi.org/10.14272/AONLLYWVGOMLR-XUTLUUPISA-N.2</a>
18n	<chem>CC(N(C(C)C)/N=N/c1n(ncc1C#N)Cc1cccc1)C</chem>	<a href="https://dx.doi.org/10.14272/AQYSAXXLCHFEGV-QZQOTICOSA-N.2">https://dx.doi.org/10.14272/AQYSAXXLCHFEGV-QZQOTICOSA-N.2</a>
15b	<chem>CC(N(C(C)C)/N=N/c1n[nH]c(c1)C)C</chem>	<a href="https://dx.doi.org/10.14272/SSAXAAXODLOITE-BUHFOSPRSA-N.1">https://dx.doi.org/10.14272/SSAXAAXODLOITE-BUHFOSPRSA-N.1</a>
19c	<chem>[N-]=[N+]=Nc1ccn(n1)Cc1cccc1</chem>	<a href="https://dx.doi.org/10.14272/VYAIIDYJDVIYCE-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/VYAIIDYJDVIYCE-UHFFFAOYSA-N.1</a>
19m	<chem>CCOC(=O)c1cn(nc1N=[N+]=[N-])Cc1cccc(c1)C#N</chem>	<a href="https://dx.doi.org/10.14272/OZCFNQRRYBYULQ-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/OZCFNQRRYBYULQ-UHFFFAOYSA-N.1</a>
21hd	<chem>[O-][N+](=O)c1ccc(cc1)n1nc(cc1C)n1nnc(c1)c1cccc1</chem>	<a href="https://dx.doi.org/10.14272/UFCSIROIFJMCPW-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/UFCSIROIFJMCPW-UHFFFAOYSA-N.1</a>
21vb	<chem>COC(=O)c1nnn(c1)c1nn(cc1C#N)Cc1ccc(cc1)F</chem>	<a href="https://dx.doi.org/10.14272/UUNQVGVZWMJXOZ-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/UUNQVGVZWMJXOZ-UHFFFAOYSA-N.1</a>
19i	<chem>[N-]=[N+]=Nc1nn(c(c1)C)c1ccc(cc1Cl)[N+](=O)[O-]</chem>	<a href="https://dx.doi.org/10.14272/GQMYHPXVWUDUZCD-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/GQMYHPXVWUDUZCD-UHFFFAOYSA-N.1</a>
21tf	<chem>COC(=O)c1ccc(cc1)c1nnn(c1)c1nn(cc1C#N)Cc1ccc(cc1)C</chem>	<a href="https://dx.doi.org/10.14272/DMRAVMAMSLYEBQ-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/DMRAVMAMSLYEBQ-UHFFFAOYSA-N.1</a>
21ed	<chem>Cc1[nH]nc(c1)n1nnc(c1)c1cccc1</chem>	<a href="https://dx.doi.org/10.14272/BTYPCTNIHDBBSH-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/BTYPCTNIHDBBSH-UHFFFAOYSA-N.1</a>
21id	<chem>Clc1cc(ccc1n1nc(cc1C)n1nnc(c1)c1cccc1)[N+](=O)[O-]</chem>	<a href="https://dx.doi.org/10.14272/NASFABBFATRIZ-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/NASFABBFATRIZ-UHFFFAOYSA-N.1</a>
21nd	<chem>CCOC(=O)c1cn(nc1n1nnc(c1)c1cccc1)Cc1ccc(cc1)Br</chem>	<a href="https://dx.doi.org/10.14272/VTYPYIREEKHMKL-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/VTYPYIREEKHMKL-UHFFFAOYSA-N.1</a>
21na	<chem>CCCCc1nnn(c1)c1nn(cc1C(=O)OCC)Cc1ccc(cc1)Br</chem>	<a href="https://dx.doi.org/10.14272/YERIOOVHZOGENU-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/YERIOOVHZOGENU-UHFFFAOYSA-N.1</a>
21nc	<chem>CCOC(=O)c1cn(nc1n1nnc(c1)COC(=O)C)Cc1ccc(cc1)Br</chem>	<a href="https://dx.doi.org/10.14272/JINGCLNWAMKPG-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/JINGCLNWAMKPG-UHFFFAOYSA-N.1</a>
21me	<chem>CCOC(=O)c1cn(nc1n1nnc(c1)c1ccc(cc1)OC)Cc1cccc(c1)C#N</chem>	<a href="https://dx.doi.org/10.14272/KJMWCYALHNEPDX-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/KJMWCYALHNEPDX-UHFFFAOYSA-N.1</a>
21mh	<chem>CCOC(=O)c1cn(nc1n1nnc(c1)CN1C(=O)c2c(C1=O)cccc2)Cc1cccc(c1)C#N</chem>	<a href="https://dx.doi.org/10.14272/RJXQILXRDFYRBG-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/RJXQILXRDFYRBG-UHFFFAOYSA-N.1</a>
21lc	<chem>CCOC(=O)c1cn(nc1n1nnc(c1)COC(=O)C)Cc1cc(F)cc(c1)F</chem>	<a href="https://dx.doi.org/10.14272/OEMVMGJIOKDNBC-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/OEMVMGJIOKDNBC-UHFFFAOYSA-N.1</a>
19t	<chem>[N-]=[N+]=Nc1nn(cc1C#N)Cc1ccc(cc1)C</chem>	<a href="https://dx.doi.org/10.14272/NMQYIKIIUJYZLGH-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/NMQYIKIIUJYZLGH-UHFFFAOYSA-N.1</a>
19n	<chem>CCOC(=O)c1cn(nc1N=[N+]=[N-])Cc1ccc(cc1)Br</chem>	<a href="https://dx.doi.org/10.14272/XWYLZJSXZASHCL-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/XWYLZJSXZASHCL-UHFFFAOYSA-N.1</a>
21hc	<chem>CC(=O)OCc1nnn(c1)c1nn(c(c1)C)c1ccc(cc1)[N+](=O)[O-]</chem>	<a href="https://dx.doi.org/10.14272/GFUNAXVZSJSISA-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/GFUNAXVZSJSISA-UHFFFAOYSA-N.1</a>
21ia	<chem>CCCCc1nnn(c1)c1nn(c(c1)C)c1ccc(cc1Cl)[N+](=O)[O-]</chem>	<a href="https://dx.doi.org/10.14272/JCVTZTZCOPFHML-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/JCVTZTZCOPFHML-UHFFFAOYSA-N.1</a>
21ta	<chem>CCCCc1nnn(c1)c1nn(cc1C#N)Cc1ccc(cc1)C</chem>	<a href="https://dx.doi.org/10.14272/FGLOKNGZLSDWMZ-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/FGLOKNGZLSDWMZ-UHFFFAOYSA-N.1</a>
21tg	<chem>N#Cc1cn(nc1n1nnc(c1)c1ccc(cc1)N(C)C)Cc1ccc(cc1)C</chem>	<a href="https://dx.doi.org/10.14272/PIHYCVSEWQEZE-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/PIHYCVSEWQEZE-UHFFFAOYSA-N.1</a>
21pd	<chem>N#Cc1cn(nc1n1nnc(c1)c1cccc1)C(C)C</chem>	<a href="https://dx.doi.org/10.14272/OYRDJONMMXESTQ-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/OYRDJONMMXESTQ-UHFFFAOYSA-N.1</a>

21pa	<chem>CCCCc1nnn(c1)c1nn(cc1C#N)C(C)C</chem>	<a href="https://dx.doi.org/10.14272/NOJZURFWHMPYCF-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/NOJZURFWHMPYCF-UHFFFAOYSA-N.1</a>
17j	<chem>CCOC(=O)c1cn(nc1/N=N/N(C(C)C)C(C)C)Cc1cccc(c1)C#N</chem>	<a href="https://dx.doi.org/10.14272/NUENLEYWZUNRJJ-ZNTNEXAZSA-N.1">https://dx.doi.org/10.14272/NUENLEYWZUNRJJ-ZNTNEXAZSA-N.1</a>
18j	<chem>CCOC(=O)c1cnn(c1/N=N/N(C(C)C)C(C)C)Cc1cccc(c1)C#N</chem>	<a href="https://dx.doi.org/10.14272/WTPBPRNMORPMPY-WCWDXBQESA-N.1">https://dx.doi.org/10.14272/WTPBPRNMORPMPY-WCWDXBQESA-N.1</a>
17g	<chem>CC(N(C(C)C)/N=N/c1nn(c(c1)C)c1ccc(cc1Cl)[N+](=O)[O-])C</chem>	<a href="https://dx.doi.org/10.14272/TYZBFJHLBYOAAUCZIZESTLSA-N.1">https://dx.doi.org/10.14272/TYZBFJHLBYOAAUCZIZESTLSA-N.1</a>
18g	<chem>CC(N(C(C)C)/N=N/c1cc(nn1c1ccc(cc1Cl)[N+](=O)[O-])C)C</chem>	<a href="https://dx.doi.org/10.14272/ACQCSRYTLZFICQCZIZESTLSA-N.1">https://dx.doi.org/10.14272/ACQCSRYTLZFICQCZIZESTLSA-N.1</a>
21ea	<chem>CCCCc1nnn(c1)c1n[nH]c(c1)C</chem>	<a href="https://dx.doi.org/10.14272/QKYKTOGQTOIHKO-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/QKYKTOGQTOIHKO-UHFFFAOYSA-N.1</a>
21eb	<chem>COC(=O)c1nnn(c1)c1n[nH]c(c1)C</chem>	<a href="https://dx.doi.org/10.14272/AXYCMAQNQSYSIG-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/AXYCMAQNQSYSIG-UHFFFAOYSA-N.1</a>
21vg	<chem>N#Cc1cn(nc1n1nnc(c1)c1ccc(cc1)N(C)C)Cc1ccc(cc1)F</chem>	<a href="https://dx.doi.org/10.14272/UIXMTYDHDCHVFR-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/UIXMTYDHDCHVFR-UHFFFAOYSA-N.1</a>
19f	<chem>[N-]=[N+]=Nc1nn(c(c1)C)Cc1cccc1</chem>	<a href="https://dx.doi.org/10.14272/CUZSOFWTCLMWBL-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/CUZSOFWTCLMWBL-UHFFFAOYSA-N.1</a>
17m	<chem>CCOC(=O)Cn1nc(c(c1)C#N)/N=N/N(C(C)C)C(C)C</chem>	<a href="https://dx.doi.org/10.14272/GMSYXQOQYOUAHU-FBMGVBCBSA-N.2">https://dx.doi.org/10.14272/GMSYXQOQYOUAHU-FBMGVBCBSA-N.2</a>
18m	<chem>CCOC(=O)Cn1ncc(c1/N=N/N(C(C)C)C(C)C)C#N</chem>	<a href="https://dx.doi.org/10.14272/UVXRQPKXJULFTRISLYRVAYSAN.2">https://dx.doi.org/10.14272/UVXRQPKXJULFTRISLYRVAYSAN.2</a>
17b	<chem>CC(N(C(C)C)/N=N/c1ccn(n1)Cc1ccc(c(c1)Br)C</chem>	<a href="https://dx.doi.org/10.14272/OJEKMYNEGYNUPP-CZIZESTLSA-N.1">https://dx.doi.org/10.14272/OJEKMYNEGYNUPP-CZIZESTLSA-N.1</a>
18b	<chem>Brc1ccc(cc1)Cn1nccc1/N=N/N(C(C)C)C(C)C</chem>	<a href="https://dx.doi.org/10.14272/PLVZHOAUEJAYPSFMQUCEESA-N.1">https://dx.doi.org/10.14272/PLVZHOAUEJAYPSFMQUCEESA-N.1</a>
17i	<chem>CCOC(=O)c1cn(nc1/N=N/N(C(C)C)C(C)C)Cc1cc(F)cc(c1)F</chem>	<a href="https://dx.doi.org/10.14272/HJNVDSRILWJTQVZNTNEXAZSA-N.1">https://dx.doi.org/10.14272/HJNVDSRILWJTQVZNTNEXAZSA-N.1</a>
18i	<chem>CCOC(=O)c1cnn(c1/N=N/N(C(C)C)C(C)C)Cc1cc(F)cc(c1)F</chem>	<a href="https://dx.doi.org/10.14272/XCKSGKZXEXJBOYWCWDXBQESA-N.1">https://dx.doi.org/10.14272/XCKSGKZXEXJBOYWCWDXBQESA-N.1</a>
17o	<chem>N#Cc1cn(nc1/N=N/N(C(C)C)C(C)C)Cc1cc(F)cc(c1)F</chem>	<a href="https://dx.doi.org/10.14272/WSQPCVJPBSUDNZ-XTQSDGFTSA-N.2">https://dx.doi.org/10.14272/WSQPCVJPBSUDNZ-XTQSDGFTSA-N.2</a>
18o	<chem>CC(N(C(C)C)/N=N/c1n(ncc1C#N)Cc1cc(F)cc(c1)F)C</chem>	<a href="https://dx.doi.org/10.14272/ZFEWCQZPKGQXCJ-GHVJWSGMSA-N.2">https://dx.doi.org/10.14272/ZFEWCQZPKGQXCJ-GHVJWSGMSA-N.2</a>
21jh	<chem>CCOC(=O)c1c[nH]nc1n1nnc(c1)CN1C(=O)c2c(C1=O)cccc2</chem>	<a href="https://dx.doi.org/10.14272/GMOYQWJQIYZFIE-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/GMOYQWJQIYZFIE-UHFFFAOYSA-N.1</a>
21th	<chem>N#Cc1cn(nc1n1nnc(c1)CN1C(=O)c2c(C1=O)cccc2)Cc1ccc(cc1)C</chem>	<a href="https://dx.doi.org/10.14272/FODYZQGXSSTMHJ-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/FODYZQGXSSTMHJ-UHFFFAOYSA-N.1</a>
21oa	<chem>CCCCc1nnn(c1)c1n[nH]cc1C#N</chem>	<a href="https://dx.doi.org/10.14272/USLFBJCHBNQGGJB-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/USLFBJCHBNQGGJB-UHFFFAOYSA-N.1</a>
21he	<chem>COc1ccc(cc1)c1nnn(c1)c1cc(n(n1)c1ccc(cc1)[N+](=O)[O-])C</chem>	<a href="https://dx.doi.org/10.14272/IZEQOYLPBRFYRC-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/IZEQOYLPBRFYRC-UHFFFAOYSA-N.1</a>
21jc	<chem>CCOC(=O)c1c[nH]nc1n1nnc(c1)COC(=O)C</chem>	<a href="https://dx.doi.org/10.14272/RJHHGQMRVYAAGU-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/RJHHGQMRVYAAGU-UHFFFAOYSA-N.1</a>
21of	<chem>COC(=O)c1ccc(cc1)c1nnn(c1)c1n[nH]cc1C#N</chem>	<a href="https://dx.doi.org/10.14272/FXIYGLHLKLOXQB-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/FXIYGLHLKLOXQB-UHFFFAOYSA-N.1</a>
19s	<chem>[N-]=[N+]=Nc1nn(cc1C#N)Cc1cc(F)cc(c1)F</chem>	<a href="https://dx.doi.org/10.14272/WBMURKUEYYRUPK-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/WBMURKUEYYRUPK-UHFFFAOYSA-N.1</a>
19l	<chem>CCOC(=O)c1cn(nc1N=[N+]=[N-])Cc1cc(F)cc(c1)F</chem>	<a href="https://dx.doi.org/10.14272/BZRWHBSLSABJOL-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/BZRWHBSLSABJOL-UHFFFAOYSA-N.1</a>

21jd	<chem>CCOC(=O)c1c[nH]nc1n1nnc(c1)c1ccc cc1</chem>	<a href="https://dx.doi.org/10.14272/JZSBUPSAIWVYFE-UHFFFAOYSA-N.2">https://dx.doi.org/10.14272/JZSBUPSAIWVYFE-UHFFFAOYSA-N.2</a>
19e	<chem>[N-]=[N+]=Nc1cc([nH]n1)C</chem>	<a href="https://dx.doi.org/10.14272/ASYITVIZQLPDSI-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/ASYITVIZQLPDSI-UHFFFAOYSA-N.1</a>
21ab	<chem>COC(=O)c1nnn(c1)c1n[nH]cc1</chem>	<a href="https://dx.doi.org/10.14272/PWKBPBPHBEDIORH-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/PWKBPBPHBEDIORH-UHFFFAOYSA-N.1</a>
21bb	<chem>COC(=O)c1nnn(c1)c1ccn(n1)C1CCCC 1</chem>	<a href="https://dx.doi.org/10.14272/RZTMDUAYRSTLAQ-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/RZTMDUAYRSTLAQ-UHFFFAOYSA-N.1</a>
21ae	<chem>COc1ccc(cc1)c1nnn(c1)c1n[nH]cc1</chem>	<a href="https://dx.doi.org/10.14272/PQOYNAQPLQYWL-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/PQOYNAQPLQYWL-UHFFFAOYSA-N.1</a>
21aa	<chem>CCCCc1cn(nn1)c1cc[nH]n1</chem>	<a href="https://dx.doi.org/10.14272/NLSVJZHXBPIQPM-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/NLSVJZHXBPIQPM-UHFFFAOYSA-N.1</a>
21ef	<chem>COC(=O)c1ccc(cc1)c1nnn(c1)c1n[nH] c(c1)C</chem>	<a href="https://dx.doi.org/10.14272/ICPVQAYXOPZIKF-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/ICPVQAYXOPZIKF-UHFFFAOYSA-N.1</a>
19b	<chem>[N-]=[N+]=Nc1ccn(n1)C1CCCC1</chem>	<a href="https://dx.doi.org/10.14272/CEJMUQXTWWQJBT-UHFFFAOYSA-N.2">https://dx.doi.org/10.14272/CEJMUQXTWWQJBT-UHFFFAOYSA-N.2</a>
19d	<chem>[N-]=[N+]=Nc1ccn(n1)Cc1ccc(cc1)Br</chem>	<a href="https://dx.doi.org/10.14272/MPLVWOQSFNIWDU-UHFFFAOYSA-N.2">https://dx.doi.org/10.14272/MPLVWOQSFNIWDU-UHFFFAOYSA-N.2</a>
15a	<chem>CC(N(C(C)C)/N=N/c1n[nH]cc1)C</chem>	<a href="https://dx.doi.org/10.14272/LKGAYQXGDXKVD-A-OUKQBFOZSA-N.1">https://dx.doi.org/10.14272/LKGAYQXGDXKVD-A-OUKQBFOZSA-N.1</a>
21sa	<chem>CCCCc1nnn(c1)c1nn(cc1C#N)Cc1cc(F) cc(c1)F</chem>	<a href="https://dx.doi.org/10.14272/APGSEIDPRRFBQ-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/APGSEIDPRRFBQ-UHFFFAOYSA-N.1</a>
21ec	<chem>CC(=O)OCc1nnn(c1)c1n[nH]c(c1)C</chem>	<a href="https://dx.doi.org/10.14272/LUTGSYAMTQUJGA-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/LUTGSYAMTQUJGA-UHFFFAOYSA-N.1</a>
21od	<chem>N#Cc1c[nH]nc1n1nnc(c1)c1cccc1</chem>	<a href="https://dx.doi.org/10.14272/VSYUPFQKDFVQCM-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/VSYUPFQKDFVQCM-UHFFFAOYSA-N.1</a>
21be	<chem>COc1ccc(cc1)c1nnn(c1)c1ccn(n1)C1C CCC1</chem>	<a href="https://dx.doi.org/10.14272/SYHGOJNCDVCRGL-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/SYHGOJNCDVCRGL-UHFFFAOYSA-N.1</a>
21qa	<chem>CCCCc1nnn(c1)c1nn(cc1C#N)CC(=O) OCC</chem>	<a href="https://dx.doi.org/10.14272/ZOQWDAUGOCUFLP-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/ZOQWDAUGOCUFLP-UHFFFAOYSA-N.1</a>
21ja	<chem>CCCCc1nnn(c1)c1n[nH]cc1C(=O)OCC</chem>	<a href="https://dx.doi.org/10.14272/CDDXWUAJGLDUKH-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/CDDXWUAJGLDUKH-UHFFFAOYSA-N.1</a>
21de	<chem>COc1ccc(cc1)c1nnn(c1)c1ccn(n1)Cc1 ccc(cc1)Br</chem>	<a href="https://dx.doi.org/10.14272/QXNOXRDOZJZFO-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/QXNOXRDOZJZFO-UHFFFAOYSA-N.1</a>
21db	<chem>COC(=O)c1nnn(c1)c1ccn(n1)Cc1ccc(c c1)Br</chem>	<a href="https://dx.doi.org/10.14272/CNHRLRYEDLASIW-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/CNHRLRYEDLASIW-UHFFFAOYSA-N.1</a>
21lf	<chem>CCOC(=O)c1cn(nc1n1nnc(c1)c1ccc(cc 1)C(=O)OC)Cc1cc(F)cc(c1)F</chem>	<a href="https://dx.doi.org/10.14272/WJPCYFBJDHGFTN-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/WJPCYFBJDHGFTN-UHFFFAOYSA-N.1</a>
21oc	<chem>N#Cc1c[nH]nc1n1nnc(c1)COC(=O)C</chem>	<a href="https://dx.doi.org/10.14272/QROBBVJEUOFHFJ-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/QROBBVJEUOFHFJ-UHFFFAOYSA-N.1</a>
17c	<chem>CC(N(C(C)C)/N=N/c1ccn(n1)C1CCCC1 )C</chem>	<a href="https://dx.doi.org/10.14272/JJSUJDRUQGTCCKX-BMRADRMJSA-N.1">https://dx.doi.org/10.14272/JJSUJDRUQGTCCKX-BMRADRMJSA-N.1</a>
18c	<chem>CC(N(C(C)C)/N=N/c1ccnn1C1CCCC1) C</chem>	<a href="https://dx.doi.org/10.14272/BWAGQJOINMBVOL-WUKNDPDISA-N.1">https://dx.doi.org/10.14272/BWAGQJOINMBVOL-WUKNDPDISA-N.1</a>
21kd	<chem>CCOC(=O)c1cn(nc1n1nnc(c1)c1cccc 1)Cc1cccc1</chem>	<a href="https://dx.doi.org/10.14272/BFHMQUIVAONQIIQ-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/BFHMQUIVAONQIIQ-UHFFFAOYSA-N.1</a>
19g	<chem>[N-] ]=[N+]=Nc1nn(c(c1)C)c1ccc(cc1)C#N</chem>	<a href="https://dx.doi.org/10.14272/KIQBPEXSAZKVRU-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/KIQBPEXSAZKVRU-UHFFFAOYSA-N.1</a>
21td	<chem>N#Cc1cn(nc1n1nnc(c1)c1cccc1)Cc1c cc(cc1)C</chem>	<a href="https://dx.doi.org/10.14272/ZHUFVXOCSYMTKK-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/ZHUFVXOCSYMTKK-UHFFFAOYSA-N.1</a>

<b>21gh</b>	<chem>N#Cc1ccc(cc1)n1nc(cc1C)n1nnc(c1)C N1C(=O)c2c(C1=O)cccc2</chem>	<a href="https://dx.doi.org/10.14272/DWYBPGPEFGKM&lt;br/&gt;QS-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/DWYBPGPEFGKM QS-UHFFFAOYSA-N.1</a>
<b>21ee</b>	<chem>COc1ccc(cc1)c1nnn(c1)c1n[nH]c(c1)C</chem>	<a href="https://dx.doi.org/10.14272/WNRIJNCEJHFAPB-&lt;br/&gt;UHFFFAOYSA-N.2">https://dx.doi.org/10.14272/WNRIJNCEJHFAPB- UHFFFAOYSA-N.2</a>
<b>19o</b>	<chem>[N-]=[N+]=Nc1n[nH]cc1C#N</chem>	<a href="https://dx.doi.org/10.14272/FMLLTFUXLLAWN-&lt;br/&gt;UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/FMLLTFUXLLAWN- UHFFFAOYSA-N.1</a>
<b>19a</b>	<chem>[N-]=[N+]=Nc1cc[nH]n1</chem>	<a href="https://dx.doi.org/10.14272/KKKGXLRKPKJON-&lt;br/&gt;UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/KKKGXLRKPKJON- UHFFFAOYSA-N.1</a>
<b>19p</b>	<chem>[N-]=[N+]=Nc1nn(cc1C#N)C(C)C</chem>	<a href="https://dx.doi.org/10.14272/XHQDUCMTSCUCR&lt;br/&gt;X-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/XHQDUCMTSCUCR X-UHFFFAOYSA-N.1</a>
<b>19r</b>	<chem>[N-]=[N+]=Nc1nn(cc1C#N)Cc1cccc1</chem>	<a href="https://dx.doi.org/10.14272/BZGHBVIXEDKDEK-&lt;br/&gt;UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/BZGHBVIXEDKDEK- UHFFFAOYSA-N.1</a>
<b>19k</b>	<chem>CCOC(=O)c1cn(nc1N=[N+]=[N- ])Cc1cccc1</chem>	<a href="https://dx.doi.org/10.14272/KCAXRYJMUFAPLD-&lt;br/&gt;UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/KCAXRYJMUFAPLD- UHFFFAOYSA-N.1</a>
<b>19v</b>	<chem>[N- ]=[N+]=Nc1nn(cc1C#N)Cc1ccc(cc1)F</chem>	<a href="https://dx.doi.org/10.14272/KJPMFOGUNJZON&lt;br/&gt;N-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/KJPMFOGUNJZON N-UHFFFAOYSA-N.1</a>
<b>19h</b>	<chem>[N- ]=[N+]=Nc1nn(c(c1)C)c1ccc(cc1)[N+]( =O)[O-]</chem>	<a href="https://dx.doi.org/10.14272/HISYWPICEGTOTQ-&lt;br/&gt;UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/HISYWPICEGTOTQ- UHFFFAOYSA-N.1</a>
<b>19d</b>	<chem>[N-]=[N+]=Nc1ccn(n1)Cc1ccc(cc1)Br</chem>	<a href="https://dx.doi.org/10.14272/MPLVWOQSFNIW&lt;br/&gt;DU-UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/MPLVWOQSFNIW DU-UHFFFAOYSA-N.1</a>
<b>19j</b>	<chem>[N-]=[N+]=Nc1n[nH]cc1C(=O)OCC</chem>	<a href="https://dx.doi.org/10.14272/FSJHWJVEYJIYBP-&lt;br/&gt;UHFFFAOYSA-N.1">https://dx.doi.org/10.14272/FSJHWJVEYJIYBP- UHFFFAOYSA-N.1</a>
<b>15c</b>	<chem>CCOC(=O)c1c[nH]nc1/N=N/N(C(C)C) C(C)C</chem>	<a href="https://dx.doi.org/10.14272/XLGLVRGMYSDF&lt;br/&gt;W-FOCLMDBBSA-N.1">https://dx.doi.org/10.14272/XLGLVRGMYSDF W-FOCLMDBBSA-N.1</a>