One-pot Synthesis and Conformational Features of *N,N'*-disubstituted Ketene Aminals

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Supporting Information

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General procedure for Method A.

To a solution of an isothiocyanate **1** (1.0 mmol) in dry DMF (2 mL) was added an amine **2** (1.0 mmol). After stirring for 20 min, sodium hydride (95%, 38 mg, 1.5 mmol) or DBU (1.5 mmol) was added under nitrogen. The mixture was stirred for 5 min, and an activated methylene compound **4** (1.5 mmol) and EDCI (288 mg, 1.5 mmol) were added in that order. The reaction was heated to 80 °C for a period of 1-12 h. After cooling to room temperature, the reaction was quenched with water and extracted with ethyl acetate (3 x 5 mL). The organic phase was washed with saturated sodium chloride aqueous solution and dried over magnesium sulfate. The solvent was removed to give a crude product. Purification of the crude product on a silica gel column with 20-50% EtOAc in hexanes provided pure **5**.

When mercury (II) chloride (1 eq) was used as the thiocarbonyl activating agent, the reaction was conducted at room temperature for 1 h and followed with same work up procedure to afford **5**.

General procedure for Method B.

To a solution of an activated methylene compound **4** (1.5 mmol) in dry DMF (2 mL) was added sodium hydride (95%, 38 mg, 1.5 mmol) under nitrogen. After stirring for 5 min, an isothiocyanate **1** (1.0 mmol) was added. The mixture was stirred for 30 min at 60 °C. An amine **2** (1.5 mmol) and EDCI (288 mg, 1.5 mmol) were added in that order. The reaction was heated to 80 °C for a period of 1-12 h. After cooling to room temperature, the reaction was quenched with water and extracted with ethyl acetate (3 x 5 mL). The organic phase was washed with saturated aqueous sodium chloride solution and dried over magnesium sulfate. The solvent was removed to give a crude product. Purification of the crude product on a silica gel column with 20-50% EtOAc in hexanes provided pure **5**.

When mercury (II) chloride (1 eq) was used as the thiocarbonyl-activating agent, the reaction was conducted at room temperature for 1 h and followed with same work up procedure to afford **5**.

When or 2-chloro-1-methylpyridinium iodide (1 eq) was used as the thiocarbonyl activating agent, the reaction was conducted at 80 °C for 12 h and followed with same work up as above procedure to afford **5**.

The following are the reaction times (at 80 °C), spectral data and elemental analyses for compounds **5a-5f**.

3-Butylamino-2-cyano-3-(phenylamino)acrylic acid methyl ester (5a).

Compound **5a** shows two sets of signals in CDCl₃ for both N-H and N-CH₂ protons in CDCl₃. ¹H COSY NMR experiments indicate the **5a-Z** to **5a-E** ratio is 44:56 in CDCl₃ by integration of N-CH₂ protons. It shows only one set of signals in CD₃CN.

Reaction time: 1 h; mp 64-79 °C; ¹H NMR (CDCl₃) δ 10.54 (s, 0.44H, Ph-N-H--O for **5a-Z**), 9.05 (s, 0.56H, *n*-Bu-N-H--O for **5a-E**), 6.93-7.40 (m, 5H), 6.65 (s, 0.56H, Ph-N-H for **5a-E**), 4.95 (s, 0.44H, *n*-Bu-N-H for **5a-Z**), 3.69 (s, 3H), 2.96 (br s, 0.88 H, N-CH₂ for **5a-Z**), 2.78 (br s, 1.12H, N-CH₂ for **5a-E**), 1.38 (m, 2H), 1.19 (m, 2H), 0.76 (t, 3H, J = 7.4 Hz) ppm; ¹H NMR (CD₃CN, N-H protons not located) δ 7.38 (t, 2H, J = 7.9 Hz), 7.21 (t, 1H, J = 7.7 Hz), 7.16 (d, 2H, J = 7.7 Hz), 3.69 (s, 3H), 3.08 (m, 2H), 1.51 (quintet, 2H, J = 7.4 Hz), 1.29 (sextet, 2H, J = 7.4 Hz), 0.86 (t, 3H, J = 7.4 Hz) ppm; ¹³C NMR (CD₃CN) δ 169.8, 161.9, 138.3, 129.0, 124.9, 122.7, 118.5, 58.2, 50.3, 43.3, 30.8, 19.0, 12.5

ppm; IR (KBr) 3252, 2932, 2195, 1652, 1624, 1531 cm^{-1} ; HRMS for $\text{C}_{15}\text{H}_{19}\text{N}_3\text{O}_2$, calcd for $(\text{M}+\text{H})^+$: 274.1556, measured: 274.1566; Anal. Calcd for $\text{C}_{15}\text{H}_{19}\text{N}_3\text{O}_2$: C 65.91; H 7.00; N 15.37. Found: C 65.79; H 6.93; N 15.40.

2-Benzenesulfonyl-3-(4-methoxy-phenylamino-3-propylamino-acrylonitrile (5b).

Compound **5b** shows only one set of signals both in CDCl_3 and in DMSO-d_6 .

Reaction time: 1 h; mp 73-78 $^{\circ}\text{C}$; ^1H NMR (CDCl_3 , N-H protons not located) δ 7.85 (d, 2H, $J = 7.5$ Hz), 7.57 (t, 1H, $J = 7.3$ Hz), 7.48 (t, 2H, $J = 7.3$ Hz), 6.91 (d, 2H, $J = 8.9$ Hz), 6.84 (d, 2H, $J = 8.9$ Hz), 3.78 (s, 3H), 2.87 (m, 2H), 1.42 (sextet, 2H, $J = 7.2$ Hz), 0.78 (t, 3H, $J = 7.4$ Hz) ppm; ^1H NMR (DMSO-d_6) δ 9.07 (s, 1H, Ar-N-H), 7.76 (d, 2H, $J = 7.1$ Hz), 7.62-7.68 (m, 3H), 7.59 (t, 1H, $n\text{-Pr-N-H}$, $J = 5.5$ Hz), 6.78 (d, 2H, $J = 8.8$ Hz), 6.69 (d, 2H, $J = 8.8$ Hz), 3.69 (s, 3H), 3.03 (m, 2H), 1.41 (sextet, 2H, $J = 7.2$ Hz), 0.74 (t, 3H, $J = 7.2$ Hz) ppm; ^{13}C NMR (CDCl_3) δ 159.8, 158.4, 144.5, 133.0, 130.2, 129.6, 126.3, 125.6, 118.2, 115.3, 68.5, 55.9, 47.0, 23.2, 11.4 ppm; ^{13}C NMR (DMSO-d_6) δ 158.3, 156.8, 144.5, 132.8, 131.8, 129.7, 125.7, 124.1, 117.7, 114.6, 66.8, 55.5, 45.5, 22.6, 11.3 ppm; IR (KBr) 3341, 3242, 2961, 2173, 1605, 1532, 1511, 1358, 1300, 1242, 1143 cm^{-1} ; HRMS for $\text{C}_{19}\text{H}_{21}\text{N}_3\text{O}_3\text{S}$, calcd for $(\text{M}+\text{H})^+$: 372.1398, measured: 372.1382; Anal. Calcd for $\text{C}_{19}\text{H}_{21}\text{N}_3\text{O}_3\text{S}$: C 61.43; H 5.69; N 11.31. Found: C 61.52; H 5.54; N 11.27.

3-Butylamino-2-cyano-3-(4-methoxy-phenylamino)-N,N-dimethyl-acrylamide (5c).

Compound 5c shows two sets of signals in CDCl_3 for both N-H and N-CH₂ protons in CDCl_3 . ^1H COZY NMR experiments indicate the **5c-Z** to **5c-E** ratio is 60:40 in CDCl_3 by integration of N-CH₂ protons. It shows only one set of signals in CD_3CN .

Reaction time: 12 h; Colorless oil; ^1H NMR (CDCl_3) δ 11.36 (s, 0.6H, Ar-N-H-O for **5b-Z**), 9.89 (s, 0.4H, *n*-Bu-N-H-O for **5b-E**), 7.04 (d, 2H, $J = 8.8$ Hz), 6.86 (d, 2H, $J = 8.8$ Hz), 6.70 (s, 0.4H, Ar-N-H for **5b-E**), 4.75 (s, 0.6H, *n*-Bu-N-H for **5b-Z**), 3.80 (s, 3H), 3.07 (s, 6H), 2.80-3.0 (m, 2H, N-CH₂), 1.50-1.40 (m, 2H), 1.20-1.30 (m, 2H), 0.83 (t, 3H, $J = 7.3$ Hz) ppm; ^1H NMR (CD_3CN , N-H protons not located) δ 7.09 (d, 2H, $J = 8.9$ Hz), 6.92 (d, 2H, $J = 8.9$ Hz), 3.79 (s, 3H), 3.08 (m, 2H), 2.98 (s, 6H), 1.48 (quintet, 2H, $J = 7.2$ Hz), 1.29 (sextet, 2H, $J = 7.3$ Hz), 0.88 (t, 3H, $J = 7.3$ Hz) ppm; ^{13}C NMR (CD_3CN) δ 170.8, 162.8, 156.6, 131.0, 124.1, 120.6, 114.1, 57.2, 54.8, 43.0 (2C), 37.1, 31.0, 19.2, 12.5 ppm; IR (KBr) 3269, 2957, 2932, 2178, 1608, 1591, 1511 cm^{-1} ; HRMS for $\text{C}_{17}\text{H}_{24}\text{N}_4\text{O}_2$, calcd for (M-H)⁺: 315.1821, measured: 315.1837; Anal. Calcd for $\text{C}_{17}\text{H}_{24}\text{N}_4\text{O}_2$: C 64.53; H 7.64; N 17.70. Found: C 63.93; H 7.73; N 17.32.

***E*-[2-Benzoyl-3-tert-butylamino-3-(4-chlorophenylamino)acrylonitrile] (5d).**

Compound **5d** shows only one set of signals both in CDCl₃ and in CD₃CN. ¹⁵N-HMBC and HMQC NMR experiments correlate the non-hydrogen bonded N-H (s, 6.97 ppm) and the 2'-H (7.27 ppm) of 4'-chlorophenyl group to the same nitrogen (95.0 ppm), while the hydrogen bonded N-H (s, 11.15 ppm) and *t*-butyl group to the other nitrogen (129.7 ppm). The NOE observed between N-H proton (6.97 ppm) of aniline and *t*-butyl group protons indicates it is the *E* stereoisomer.

Reaction time: 12 h; mp 174-180 °C; ¹H NMR (CDCl₃) δ 11.15 (s, H, *t*-Bu-N-H--O), 7.67 (d, 2H, J = 8.6 Hz), 7.33-7.45 (m, 6H), 7.09 (d, 2H, J = 8.6 Hz), 7.00 (s, 1H, Ar-N-H), 1.42 (s, 9H) ppm; ¹H NMR (CD₃CN) δ 11.51 (s, H, *t*-Bu-N-H--O), 7.62 (dd, 2H, J = 8.0, 1.4 Hz), 7.37-7.46 (m, 6H), 7.27 (d, 2H, J = 8.3 Hz), 6.97 (s, 1H, Ar-N-H), 1.50 (s, 9H) ppm; ¹⁵N NMR (CD₃CN) δ 129.7 (*t*-Bu-N), 95.0 (Ar-N) ppm; ¹³C NMR (CD₃CN) δ 191.6, 161.6, 139.9, 137.8, 130.4, 129.4, 128.8, 127.7, 127.5, 124.8, 120.4, 71.6, 53.1, 28.1 ppm; IR (KBr) 3294, 2979, 2200, 1617, 1568, 1491 cm⁻¹; HRMS for C₂₀H₂₀ClN₃O, calcd for (M-H)⁺: 352.1217; Found: 352.1227; Anal. Calcd for C₂₀H₂₀ClN₃O: C 67.88; H 5.69; N 11.87; Cl 10.01. Found: C 67.70; H 5.68; N 11.84; Cl 10.35.

(2-Cyano-3-oxo-3-phenyl-1-phenylamino-propenylamino)acetic acid *tert*-butyl ester (5e**).**

Compound **5e** shows two sets of signals in CDCl₃ for both N-H and N-CH₂ protons in CDCl₃. ¹H COSY NMR experiments indicate the **5e-Z** to **5e-E** ratio is 70:30 in CDCl₃ by integration of N-CH₂ protons. It shows only one set of signals in CD₃CN.

Reaction time: 12 h; mp 146-156 °C; ^1H NMR (CDCl_3) δ 13.11 (s, 0.70H, Ph-N-H-O for **5e-Z**), 11.98 (s, 0.30H, CH_2 -N-H-O for **5e-E**), 7.81 (d, 2H, $J = 7.4$ Hz), 7.13-7.46 (m, 9.3H), 6.22 (s, 0.70H, CH_2 -N-H for **5e-Z**), 3.85 (br s, 1.4H, N-CH $_2$ for **5e-Z**), 3.59 (br s, 0.60H, N-CH $_2$ for **5e-E**), 1.43 (s, 9H), ppm; ^1H NMR (CD_3CN , N-H protons not located) δ 7.73 (dd, 2H, $J = 8.0, 1.3$ Hz), 7.45-7.51 (m, 5H), 7.28-7.36 (m, 3H), 3.82 (d, 2H, $J = 5.3$ Hz), 1.46 (s, 9H) ppm; ^{13}C NMR (CD_3CN) δ 191.5, 167.2, 162.2, 140.0, 137.2, 130.4, 129.3, 127.6, 127.4, 126.1, 124.1, 120.5, 82.3, 54.0, 45.7, 26.8 ppm; IR (KBr) 3254, 3206, 3060, 2977, 2189, 1739, 1616, 1590, 1566, 1528 cm^{-1} ; HRMS for $\text{C}_{22}\text{H}_{23}\text{N}_3\text{O}_3$, calcd for $(\text{M}+\text{H})^+$: 378.1818, measured: 378.1829; Anal. Calcd for $\text{C}_{22}\text{H}_{23}\text{N}_3\text{O}_3$: C 70.01; H 6.14; N 11.13. Found: C 69.80; H 6.22; N 10.90.

3-Butylamino-1-phenyl-3-phenylamino-propenone (**5f**).

Compound **5f** shows two sets of signals both in CDCl_3 and CD_3CN for most protons. ^1H COSY NMR experiments indicate the **5f-Z** to **5f-E** ratio is 83:17 in CDCl_3 and 55:45 in CD_3CN by integration of N-CH $_2$ protons, respectively.

Reaction time: 12 h; Slightly yellow oil; ^1H NMR (CDCl_3) δ 13.12 (s, 0.83H, Ph-N-H-O for **5f-Z**), 11.63 (s, 0.17H, *n*-Bu-N-H-O for **5f-E**), 7.22-7.89 (m, 10H), 6.38 (s, 0.17H, Ph-N-H for **5f-E**), 5.40 (s, 1H, ethylene H), 4.75 (s, 0.83H, *n*-Bu-N-H for **5f-Z**), 3.32 (m, 0.34H, N-CH $_2$ for **5f-E**), 3.22 (m, 1.66H, N-CH $_2$ for **5f-Z**), 1.75 (quintet, 0.34H, $J = 7.2$ Hz), 1.57 (quintet, 1.66H, $J = 7.4$ Hz), 1.50 (sextet, 0.34H, $J = 7.5$ Hz), 1.40 (sextet, 1.66H, $J = 7.5$ Hz), 0.92-0.98 (m, 3H) ppm; ^1H NMR (CD_3CN) δ 13.30 (s, 0.55H, Ph-N-H-O for **5f-Z**), 11.64 (s, 0.45H, *n*-Bu-N-H-O for **5f-E**), 7.22-7.88 (m, 10.45H),

5.46 (s, 1.1H, ethylene H and *n*-Bu-N-H for **5f-Z**), 5.30 (s, 0.45H, ethylene H for **5f-E**), 3.33 (q, 0.90H, $J = 6.3$ Hz, N-CH₂ for **5f-E**), 3.20 (q, 1.1H, $J = 6.7$ Hz, N-CH₂ for **5f-Z**), 1.66 (quintet, 0.9H, $J = 7.4$ Hz), 1.55 (quintet, 1.1H, $J = 7.4$ Hz), 1.45 (sextet, 0.90H, $J = 7.4$ Hz), 1.34 (sextet, 1.1H, $J = 7.4$ Hz), 0.95 (t, 1.35H, $J = 7.4$ Hz), 0.91 (t, 1.65H, $J = 7.4$ Hz) ppm; ¹³C NMR (CD₃CN, two sets of signals) δ 183.6, 182.8, 160.7, 159.6, 141.6, 141.4, 138.1, 136.6, 129.5, 129.4, 129.1, 128.9, 128.0, 127.8, 126.1, 125.8, 125.4, 125.2, 125.0, 124.4, 76.2, 74.9, 41.3, 40.3, 30.7, 30.7, 19.6, 19.4, 12.8, 12.7 ppm; IR (KBr) 3411, 3249, 3056, 2958, 2929, 2870, 1614, 1589, 1556 cm⁻¹; HRMS for C₁₉H₂₂N₂O, Calcd for (M+H)⁺: 295.1810, measured: 295.1826. Anal. Calcd for C₁₉H₂₂N₂O: C 77.51; H 7.53; N 9.51. Found: C 77.45; H 7.73; N 9.54.

Cambridge Structural Database Search Results.

The following is the list of X-ray structures of *N,N'*-disubstituted ketene amins found in Cambridge Structural Database with the following generic structure, where both C-N bonds are acyclic and R₁ and R₂ are not hydrogen. Their chemical structures and literature references are also presented after the list.

N, N'-Disubstituted Amins^a

refcode	R ₁	X	Potential for 2 H-bonds										C=C	geom
			geom	H-bon	ph1	R ₂	Y	geom	H-bon	ph2	twist			
ROHMIK	Ar	thiaz	a	y	-157	Ar	NO2	a	y	-165	5	1.438	aa	
KOVGUX	Ar	NO2	s	n	1	Ar	NO2	s	n	5	71	1.451	ss	
BEGFUO-a	Ar	NO2	s	n	1	Ar	C=S	s	n	-5	101	1.491	ss	
" -b	Ar	NO2	s	n	-1	Ar	C=S	a	n	179	101	1.486	sa	
CAVHUC	CH3	NO2	s	n	2	CH3	C=S	a	n	-179	95	1.490	sa	
PUHCIE	CH3	NO2	s	n	1	CH3	C=S	a	n	179	89	1.490	sa	
HASFAI	CH3	NO2	s	n	0	CH3	C=N-	a	n	-174	69	1.483	sa	
KOVGOR	CH2	NO2	s	n	2	CH2	NO2	a	n	176	87	1.477	sa	
WESNOX-a	CHCC	SO2	s	n	14	CHCC	SO2	a	n	-173	70	1.474	sa	
" -b	CHCC	SO2	s	n	1	CHCC	SO2	a	n	-175	80	1.488	sa	

Potential for 1 H-bond													
refcode	R ₁	X	geom	H-bon	ph1	R ₂	Y	geom	H-bon	ph2	twist	C=C	geom
5e	CH2	C=O	a	y	-157	Ar	CN	a	-	-152	3	1.426	aa
5d	CCCC	C=O	a	y	-176	Ar	CN	s	-	33	10	1.428	as
NOFBEP	CH3	NO2	s	n	3	CH3	CH=C	a	-	-178	66	1.467	sa
BATVEX	CH2	NO2	a	y	-168	CH3	H	s		2	2	1.429	as
BEZCOY	CH3	NO2	a	y	177	CH2	H	s		5	0	1.433	as
CAWXIH	N=C	NO2	a	y	178	CH3	H	s		7	3	1.406	as
GIQRUT	CHCC	NO2	a	y	-173	SO2	H	s		6	6	1.453	as
PUDGEA	CHCC	NO2	a	y	178	CH3	H	s		6	1	1.424	as
RAZDIF-a	CH2	NO2	a	y	178	CH3	H	s		3	0	1.409	as
" -b	CH2	NO2	a	y	177	CH3	H	s		4	-1	1.431	as
TADZAZ01	CH2	NO2	a	y	180	CH3	H	s		-1	4	1.425	as
		TADZAZ								disordered			

^a twist = X-C=C-N1 torsional angle, Ph1 = C=C-N1-R1 torsional angle, Ph2 = C=C-N2-R2 torsional angle.

Detailed structure and references (the intramolecular hydrogen bonds were indicated by dash bonds).

5d

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5e

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BATVEX

(1-(2-(4-Methylimidazol-5-yl)-methylthio)-ethylamino)-1-methylamino-2-nitroethene

P. E. Glover, K. Prout

Cryst. Struct. Commun. **1981**, *10*, 1295.

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BEGFUO

2-Nitro-N-phenyl-3,3-bis(phenylamino)prop-2-enethioamide hydrate at 173 K.

D. M. Argilagos, R. W. Kunz, A. Linden, H. Heimgartner

Helv. Chim. Acta **1998**, *81*, 2388.

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BEZCOY

2-((5-((5-(Dimethylammoniomethyl)-2-furyl)methylthio)ethylamino)-2-methylamino-1-nitroethylene
hydrogen oxalate

B. Kojic-Prodic, Z. Ruzic-Toros, R. Toso

Acta Crystallogr., Sect. B **1982**, *38*, 1837.

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CAVHUC

N-Benzoyl-3,3-bis(methylamino)-2-nitrothioacrylamide at 173 K.

A. Linden, D. Moya Argilagos, H. Heimgartner, M. I. Garcia Trimino, A. Macias Cabrera

Acta Crystallogr., Sect. C (Cr. Str. Comm.) **1999**, 55, 1692.

CAWXIH

1-(5-Dimethylaminomethyl)-furfurylthiopropen-2-one 1-methylamino-2-nitroethenylhydrazone

G. Chiari, D. Viterbo

J. Chem. Soc., Perkin Trans.2 **1983**, 1815.

GIQRUT

1-Cyclohexylamino-1-((4'-cyclo-octylamino)pyrid-3'-ylsulfonamido)-2-nitroethylene

B. Masereel, J. Wouters, L. Pochet, D. Lambert

J. Med. Chem. **1998**, 41, 3239.

HASFAI

N-(3,3-bis(Methylamino)-1-(methylthio)-2-nitroprop-2-enylidene)benzamide at $-100\text{ }^{\circ}\text{C}$; absolute configuration.

M. I. Garcia Trimino, A. Linden, H. Heimgartner, A. Macias Cabrera

Helv. Chim. Acta **1993**, 76, 2817.

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KOVGOR

1,1-bis(n-Propylamino)-2,2-dinitroethylene

K. Baum, S. S. Bigelow, N. V. Nguyen, T. G. Archibald, R. Gilardi, J. L. Flippen-Anderson, C. George

J. Org. Chem. **1992**, 57, 235.

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KOVGUX

1,1-bis(Phenylamino)-2,2-dinitroethylene

K. Baum, S. S. Bigelow, N. V. Nguyen, T. G. Archibald, R. Gilardi, J. L. Flippen-Anderson, C. George

J. Org. Chem. **1992**, 57, 235.

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NOFBEP

2-(2-(N,N'-Dimethylamidinio)-2-nitroethanylidene)-5,5-dimethylcyclohexan-1,3-dione

A. Ya. Strakov, O. Ya. Neiland, T. F. Kozlovskaya, I. A. Strakova, M. V. Petrova, A. A. Kemme, A. F.

Mishnev

Zh. Org. Khim., **1997**, 33, 1044.

PUDGEA

1-(alpha-Methylbenzylamino)-1-methylamino-2-nitroethene

K. Mohanalingam, M. Nethaji, P. K. Das

J. Mol. Struct. **1996**, 378, 177.

PUHCIE

3,3-bis(Methylamino)-N-(3-phenylpropenoyl)-2-nitroprop-2-enethioamide acetone solvate at 173 K.

M. I. Garcia Trimino, A. Macias Cabrera, H. Velez Castro, A. Rosado Perez, D. Moya Argilagos, A.

Linden, H. Heimgartner

Helv. Chim. Acta **1998**, 81, 718.

RAZDIF

N-(2-(((2-((Dimethylamino)methyl)-4-thiazolyl)methyl)thio)ethyl)-N'-methyl-2-nitro-1,1-ethenediamine

G. A. Stephenson, T. J. Wozniak, J. G. Stowell, S. R. Bryn

J. Mol. Struct. **1996**, 380, 93.

ROHMIK

2-(Benzo[1,2-b:4,5-b']dithiazol-2-yl)-2-nitro-N,N'-diphenylethane-1,1-diamine

D. M. Argilagos, M. I. G. Trimino, A. M. Cabrera, A. Linden, H. Heimgartner

Helv. Chim. Acta **1997**, 80, 273.

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TADZAZ

Ranitidine hydrochloride

N-(2-((5-(Dimethylaminomethyl)-2-furanyl)-methylthio) ethyl)-N'-methyl-2-nitro-1,1-ethenediamine
hydrochloride

T. Ishida, Y. In, M. Inoue

Acta Crystallogr., Sect. C (Cr. Str. Comm.) **1990**, 46, 1893.

TADZAZ01

Ranitidine hydrochloride

Z-Dimethyl-((5-(2-(1-methylamino-2-nitroethenylamino)ethylthiomethyl)-2-furyl)methyl)ammonium
chloride at 100 K; polymorph II;

A. Hempel, N. Camerman, D. Mastropaolo, A. Camerman

Acta Crystallogr., Sect. C (Cr. Str. Comm.) **2000**, 56, 1048.

WESNOX

2,2-bis(Isopropylamino)-1,1-bis(trifluoromethanesulfonyl)ethene acetonitrile solvate

M. Hanack, J. Hackenberg, O. Menke, L. R. Subramanian, R. Schlichenmaier

Synthesis **1994**, 249.

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