

Table 2b. List of nitrogen-containing heterocyclic volatile organic compounds (VOCs) in human body.

CAS-number	Compound name	Formula	Faeces	Urine	Breath	Skin	Milk	Blood	Saliva	Semen
<i>Azirine/ aziridine [C2N ring]</i>										
4025-37-0	2-(aziridin-1-yl) ethanamine	C4H10N2	[223]							
5628-99-9	1-Vinyl-aziridine	C4H7N								[241]
<i>Azete / azetidine [C3N ring]</i>										
5961-33-1	3-methyl-3-phenylazetidine	C10H13N							[110]	
15216-10-1	Azetidine, 1-nitroso-	C3H6N2O								[241]
<i>Pyrrolidines, pyrroline/dihydropyrroles [C4N ring]</i>										
79286-79-6	3-Aminopyrrolidine	C4H10N2								[241]
616-45-5	2-oxopyrrolidine / 2-pyrrolidone	C4H7NO			[408]			[125]		
123-75-1	pyrrolidine	C4H9N			[408]	[409]			[117]	
40499-83-0	3-Pyrrolidinol	C4H9NO								[241]
3760-54-1	Pyrrolidinecarboxaldehyde	C5H9NO			[272]					
257-04-6	Proline	C5H9NO2	[249]		[41]					
51-35-4	Hydroxyproline	C5H9NO3			[41]					
10552-94-0	1H-Pyrrole, 2,5-dihydro-1-nitroso / 3-Pyrroline, N-nitroso	C4H6N2O								[241]
54-11-5	nicotine	C10H14N2			[398]	[178, 182]				
5724-81-2	1-pyrroline	C4H7N			[399]					
109-96-6	1H-Pyrrole, 2,5-dihydro / 3-Pyrroline	C4H7N								[241]
85213-22-5	2-acetyl-1-pyrroline	C6H9NO		[208]						
<i>Pyrrole [C4N ring]</i>										
109-97-7 / 16199-06-7	pyrrole / 1H-pyrrole	C4H5N	[9]	[193, 194, 196, 198, 255, 256, 258]	[6, 106, 275, 364]		[156]	[106, 125]	[110, 117]	[241]

96-54-8	1-methylpyrrole	C5H7N	[9]	[194, 255]	[6, 364]		[106]
636-41-9	2-methyl-(1H)-pyrrole	C5H7N		[194, 196, 255]	[408]	[178]	
616-43-3	3-methyl-(1H)-pyrrole	C5H7N	[222]	[193]	[408]	[178]	[125]
1192-58-1	1-methyl-(1H)-pyrrole-2-carbaldehyde / 2-formyl-1-methylpyrrole	C6H7NO			[408]		
1072-83-9	Ethanone, 1-(1H-pyrrol-2-yl)- / 2-acetylpyrrole	C6H7NO			[341, 400]		
600-28-2	2,3-dimethyl-(1H)-pyrrole	C6H9N			[408]		
625-82-1	2,4-dimethyl-(1H)-pyrrole	C6H9N			[408]		
625-84-3	2,5-dimethylpyrrole ui	C6H9N		[255, 256, 258]	[6]		
617-92-5	1-ethyl-(1H)-pyrrole	C6H9N		[194]	[408]		
1551-06-0	2-ethylpyrrole	C6H9N			[408]		
1551-16-2	3-ethyl-(1H)-pyrrole	C6H9N			[408]		
930-87-0	1,2,5-trimethyl-(1H)-pyrrole	C7H11N			[383, 408]		
3855-78-5	2,3,4-trimethyl-(1H)-pyrrole	C7H11N			[408]		
2199-41-9	2,3,5-trimethyl-(1H)-pyrrole	C7H11N			[6]		
5690-96-0	Pyrrole 4-ethyl-2-methyl	C7H11N		[196]			
589-33-3	1-butylpyrrole	C8H13N		[255, 256, 258]			
1551-12-8	2-pentylpyrrole	C9H15N				[182]	
1438-94-4	N-Furfurylpyrrole	C9H9NO					[111]
<i>Pyrazoles and imadazoles and other diazoles [C3N2 ring]</i>							
na	aminopyrazole u.i	C3H5N3			[400]		
1453-58-3	3-methyl-(1H)-pyrazole	C4H6N2	[222]		[383, 408]		
60-27-5	creatinine	C4H7N3O			[339]		
534-26-9	4,5-dihydro-2-methyl-(1H)-imidazole	C4H8N2				[178]	
3718-04-5	4-vinyl imidazole	C5H6N2				[176]	

25016-16-4	1-(1H)-pyrazol-4-yl)-ethanone	C5H6N2O	[194]		
1072-68-0	1,4-dimethylpyrazole	C5H8N2		[408]	
694-31-5	1,5-dimethyl-(1H)-pyrazole	C5H8N2		[408]	[178]
67-51-6	(1H)-3,5-dimethylpyrazole	C5H8N2		[408]	
105-20-4	(1H)-pyrazole-3-ethanamine / betazole	c5H9N3	[222]		
59-98-3	1H-Imidazole, 4,5-dihydro-2- (phenylmethyl)- / Tolazoline	C10H12N2		[374]	
<i>Triazoles [C2N3 rings]</i>					
288-88-0	1H-1,2,4-Triazole	C2H3N3			[241]
4923-01-7	1H-1,2,4-Triazol-3-amine, 5- methyl	C3H6N4			[241]
<i>Tetraazoles [C1N4 rings]</i>					
51410-11-8	1-tetrazol-2-ylethanone	C3H4N4O	[222]		
<i>Piperidines [C5Nring]</i>					
110-89-4	piperidine	C5H11N	[193, 196]		
2591-86-8	1-Piperidinecarboxyaldehyde	C6H11NO	[196]		
931-20-4	1-methyl-2-piperidinone	C6H11NO	[193, 196]		
39546-32-2	4-Piperidinecarboxamide / Isonipecotamide	C6H12N2O			[241]
62985-38-0	1-piperidinemethanamine	C6H14N2			[178]
1484-80-6	2-ethylpiperidine	C7H15N			[178]
35794-11-7	Piperidine, 3,5-dimethyl-	C7H15N			[241]
3040-44-6	1-piperidineethanol	C7H15NO			[178]
94-62-2	piperine	C17H19NO 3		[400]	
7031-93-8	2,2,6,6-Tetramethyl-piperidinol	C9H19NO		[400]	
4620-54-6	1-phenyl-3-(1-piperidiny)-2- buten-1-one	C15H19NO			[178]

694-05-3	1,2,3,6-Tetrahydropyridine	C5H9N				[409]			
<i>Pyridines [C5N ring]</i>									
110-86-1	pyridine	C5H5N	[9]	[193, 194, 196, 258]	[6, 43, 275, 341, 348, 364, 407]	[176, 178, 185, 192]	[125]	[111]	[241]
108-48-5	2,6-dimethylpyridine	C7H9N	[9]	[196]	[408]				
536-78-7	3-ethylpyridine	C7H9N			[408]				
85665-88-9	2-isobutyl-4-methylpyridine	C10H15N			[408]		[125]		
109-06-8	2-methylpyridine / picoline	C6H7N			[364]	[178]	[125]	[110]	
108-99-6	3-methylpyridine	C6H7N		[193, 194]	[364, 408]		[125]	[110, 111]	
108-89-4	p-picoline / 4-methylpyridine	C6H7N			[408]				
n/a	picoline ui	C6H7N		[256, 258]					
1121-55-7	3-Ethenylpyridine / 3-vinylpyridine	C7H7N						[111]	
ui	ethenylpyridine	C7H7N						[117]	
583-61-9	2,3-dimethylpyridine	C7H9N					[125]		
589-93-5	2,5-dimethylpyridine	C7H9N					[125]		
108-75-8	2,4,6-Trimethyl pyridine	C8H11N		[196]					
2294-76-0	2-pentylpyridine	C10H15N					[125]		
462-08-8	3-pyridinamine	C5H6N2				[178]			
504-24-5	4-pyridinamine	C5H6N2				[178]			
695-34-1	4-methylpyridinamine	C6H8N2				[178]			
54-11-5	nicotine	C10H14N2			398,	[178, 182]			
108-96-3	4(1H)-pyridinone	C5H5NO				[178]			
100-54-9	3-pyridinecarbonitrile	C6H4N2	[9]						
100-55-0	Nicotinyl alcohol / 3-pyridinemethanol	C6H7NO			[341]				
36357-38-7	5-acetyl-2-methylpyridine	C8H9NO	[9]						
<i>Piperazines [C4N2 ring]</i>									

109-01-3	1-methylpiperazine	C5H12N2				[178]		
13961-37-0	2-ethylpiperazine	C6H14N2				[178]		
106-55-8	2,5-dimethylpiperazine	C6H14N2				[178]		
Diazines (pyrazines and pyrimidenes) [C4N2 rings aromatic]								
<i>Pyrazines [1,4]</i>								
290-37-9	pyrazine	C4H4N2		[194, 256, 258]	[6]	[178]	[106, 125]	[241]
20744-39-2	4-Pyridazinamine	C4H5N3			[369]			
109-08-0	2-methylpyrazine	C5H6N2	[9]	[194, 196, 251, 255, 256, 258]	[408]			[241]
4177-16-6	2-vinylpyrazine	C6H6N2		[193, 256, 258]				
5910-89-4	2,3-dimethylpyrazine	C6H8N2		[196, 255, 256, 258]			[125]	[111] [241]
123-32-0	2,5-dimethylpyrazine	C6H8N2		[196, 255, 258]	[331]		[125]	[241]
108-50-9	2,6-dimethylpyrazine	C6H8N2		[193, 196, 256, 258]		[178]		[111] [241]
13925-00-3	Ethyl pyrazine	C6H8N2		[196]				
ui	trimethylpyrazine	C7H10N2				[178]	[125]	
14667-55-1	2,3,5-trimethylpyrazine	C7H10N2		[196, 255, 256],				
13925-03-6	2-methyl-6-ethyl-pyrazine / 2-ethyl-6-methyl-pyrazine	C7H10N2		[196, 255]				
13360-64-0	2-ethyl-5-methylpyrazine	C7H10N2					[125]	
29460-90-0	2-isopropylpyrazine	C7H10N2					[125]	
13925-09-2	2-methyl-6-vinylpyrazine	C7H8N2		[256]				
13360-65-1	3-ethyl-2,5-dimethylpyrazine	C8H12N2				[178]		[241]
29461-03-8	2-methyl-5-propyl-pyrazine	C8H12N2					[125]	

15986-81-9	2-methyl-3-isopropylpyrazine	C8H12N2					[125]	
13925-06-9	2-isobutyl-3-methylpyrazine	C9H14N2					[125]	
24683-00-9	3-isobutyl-2-methoxypyrazine	C9H14N2O				[162]		
	<i>Pyrimidines [1,3]</i>							
289-95-2	pyrimidine / 1,3-diazine	C4H4N2			[6]			[241]
873-83-6	6-aminouracil / 4-Amino-2,6-dihydroxypyrimidine	C4H5N3O2			[383]			
65-86-1	orotic acid	C5H4N2O4			[400]			
5053-43-0	2-methyl-1,3-diazine	C5H6N2			[408]			
1558-17-4	Pyrimidine, 4,6-dimethyl-	C6H8N2						[241]
874-14-6	1,3-dimethyl-2,4(1H,3H)-pyrimidinedione	C6H8N2O2			[408]			
20651-30-3	5-methyl-2-methylthio-4(1H)-pyrimidinone	C6H8N2OS				[178]		
951-77-9	Cytidine, 2'-deoxy-	C9H13N3O4						[241]
	INDOLES							
120-72-9	indole	C8H7N	[9, 216, 222, 223, 247, 248]	[194, 202, 250, 253]	[29, 57, 267, 281, 308, 337, 355, 378, 379, 383, 389, 399]	[190, 178]	[127]	[110, 111, 116, 117, 418]
95-20-5	2-methyl indole	C9H9N			[408]			
83-34-1	3-methylindole / skatole	C9H9N	[9, 216, 222, 248]	[208]	[378]	[162]		418,421,116,
614-96-0	5-methyl indole	C9H9N			[408]			
933-67-5	7-methyl indole	C9H9N			[408]			
16096-32-5	4-methyl-1H-indole	C9H9N						[111]
na	Methyl indole u.i	C9H9N	[223]	[256]				
61-54-1	Tryptamine	C10H12N2			[45]			

948-65-2	2-phenylindole	C14H11N						[130]	
n/a	indole, substituted	unknown			[178]				
59-48-3	1,3-dihydro-(2H)-indol-2-one	C8H7NO	[223]						[110]
3040-34-4	3-Methyldioxyindole	C9H9NO2			[45]				
87-51-4	Indole-3-acetate / Indoleaceic acid	C10H8NO2			[45]				
608-07-1	5-Methoxyindoleacetate	C11H11NO3			[45]				
20696-57-5	tryptophan amide	C11H13N3O			[383]				
1210-83-9	N-Acetylserotonin	C12H14N2O2			[45]				
2208-41-5	6-Hydroxymelatonin	C13H16N2O3			[45]				
<i>Quinoline and hydroquinolines</i>									
2051-28-7	Quinoline, decahydro-	C9H17N			[282]				
635-46-1	1,2,3,4-tetrahydroquinoline	C9H11NO2				[178]			
101187-81-7	4,8-Dihydroxyquinoline	C9H7NO2			[45]				
3517-61-1	4,6-Dihydroxyquinoline	C9H7NO2			[45]				
7661-55-4	5-methylquinoline	C10H9N						[126]	
93-37-8	2,7-Dimethyl-quinoline	C11H11N		[250]					
2437-72-1	2,3,4-trimethylquinoline	C12H13N				[178]			
<i>Cyclic amide / lactam</i>									
675-20-7	2-piperidinone / δ -Valerolactam / piperidone	C5H9NO	[9, 247]	[258]	[399, 408]	[180]		[125]	[116]
105-60-2	caprolactam / 1-aza-2-cycloheptanone	C6H11NO			[399, 408]				
4030-22-2	3,4-dimethyl-1,5-dihydro-(2H)-pyrrol-2-one	C6H9NO			[408]				
59-48-3	1,3-dihydro-(2H)-indol-2-one	C8H7NO	[223]						[110]

20651-30-3	5-methyl-2-methylthio-4(1H)-pyrimidinone	C6H8N2OS		[178]	
874-14-6	1,3-dimethyl-2,4(1H,3H)-pyrimidinedione	C6H8N2O2	[408]		
486-56-6	coctinine / (5S)-1-methyl-5-(3-pyridinyl)-2-pyrrolidinone	C10H12N2O	[398]		
951-77-9	Cytidine, 2'-deoxy-	C9H13N3O4			[241]
<i>Other multicyclic CN heterocyclics</i>					
58-08-2	caffeine	C8H10N4O2			[114]
274-40-8	Indolizine	C8H7N			[111]
62989-33-7	Tetrahydrobiopterin	C9H15N5O3	[400]		
2440-22-4	2-(2H-benzotriazol-2-yl)-4-methylphenol	C13H11N3O		[178]	
611-64-3	9-Methyl-acridine	C14H11N	[300]		
CNO heterocyclics					
<i>Oxazoles, (&oxaline, oxazolidine, isoxazole, isoxazline, isoxazolidine) [C3NO]</i>					
na	2-Acetylisoxazolidine / N-Acetylisoxazolidine	C5H9NO2	[377]		
1772-43-6	Oxazole, 4,5-dihydro-2,4,4-trimethyl	C6H11NO			[241]
288-14-2	Isoxazole	C3H3NO	[196]		[241]
288-42-6	oxazole / 1,3-oxazole	C3H3NO	[408]	[178]	
20662-83-3	Oxazole, 4,5-dimethyl-	C5H7NO			[241]
20662-84-4	Oxazole, trimethyl-	C6H9NO			[241]
40953-15-9	Oxazole, 2,5-diethyl-4-methyl-	C8H13NO			[241]
77311-04-7	5-butyl-2-ethyl-1,3-oxazole	C9H15NO	[383]		
26131-91-9	4,5-Dimethyl-2-isobutyloxazole	C9H15NO			[241]
273-53-0	benzoxazole	C7H5NO		[125]	

<i>Other CNO hetereocyclics</i>					
17220-38-1	Furazandiamine	C2H4N4O	[248]		
5807-02-3	2-(N-morpholino)-acetonitrile	C6H10N2O		[408]	
100-74-3	4-ethylmorpholine	C6H13NO			[176]
2832-99-7	N-Thio-valero-morpholine	C9H17NOS			[241]
4225-26-7	2-(4-morpholinyl)- benzothiazole	C11H12N2 OS	[47]		
