

Table 10d. Table showing all the unsaturated ketones reported in the literature that have been detected in faeces, urine, breath, skin secretions, milk, blood and saliva from healthy humans

CAS-number	Compound name	Faeces	Urine	Breath	Skin	Milk	Blood	Saliva
78-94-4	3-buten-2-one / methyl vinyl ketone			Br		M		Sa
814-78-8	3-methyl-3-buten-2-one		U	Br				Sa
625-33-2	3-penten-2-one	F	U	Br		M		Sa
1629-58-9	1-penten-3-one			Br				Sa
141-79-7	4-methyl-3-penten-2-one	F	U	Br				
25044-01-3	2-methyl-1-penten-3-one	F						
565-62-8	3-methyl-2-penten-4-one			Br				
109-49-9	1-hexen-5-one			Br				
1629-60-3	1-hexene-3-one					M		
2497-21-4	4-hexen-3-one	F		Br				
763-93-9	3-hexen-2-one			Br				
10575-41-4	4-hexyn-3-one			Br				
1604-28-0	6-methyl-3,5-heptadien-2-one	F			Sk			
110-93-0	6-methyl-5-hepten-2-one	F	U	Br	Sk			Sa
38284-27-4	3,5-octadien-2-one					M		
65767-22-8	(Z)-1,5-Octadien-3-one					M		
4312-99-6	1-octen-3-one		U			M		Sa
1669-44-9	3-octen-2-one	F				M		
14129-48-7	4-octen-3-one					M		
32064-72-5	2-nonen-4-one				Sk			
24415-26-7	1-nonen-3-one					M		
689-67-8	6,10-dimethyl-5,9-undecadien-2-one				Sk			
3796-70-1	geranylacetone					M		
	unsaturated aromatic							
122-00-9	p-acetyltoluene			Br				
98-86-2	acetophenone	F	U	Br	Sk	M		Sa
645-13-6	isopropylacetophenone				Sk			
119-61-9	benzophenone	F			Sk			Sa
103-79-7	1-phenyl-2-propanone	F						
93-55-0	1-phenyl-1-propanone	F						
613-89-8	2-aminoacetophenone					M		
577-16-2	1-(2-methylphenyl)-ethanone	F		Br				
2040-14-4	1-(2-methylphenyl)-1-propanone			Br				
88-29-9	7-acetyl-6-ethyl-1,1,4,4-tetramethyltetralin / musk 36A				Sk			
21145-77-7	2-acetyl-3,5,5,6,8,8-hexamethyl-5,6,7,8-tetrahydronaphthalene				Sk			Sa
	unsaturated cyclic							
1192-62-7	2-acetylfuran	F	U	Br		M		
1193-79-9	2-acetyl-5-methylfuran	F		Br				Sa
3194-15-8	1-(2-furyl)-1-propanone			Br				
932-66-1	1-acetylcyclohexene			Br				
70286-20-3	DL-4-acetyl-1-methylcyclohexene ui			Br				

CAS-number	Compound name	Faeces	Urine	Breath	Skin	Milk	Blood	Saliva
1203-08-3	4-(2,6,6-trimethylcyclohexa-1,3-dienyl)but-3-en-2-one		U					
3168-90-9	1-acetyl-2-methylcyclopentene / 1-(2-methyl-1-cyclopenten-1-yl)-ethanone	F						Sa
1767-84-6	1-(2-methyl-2-cyclopenten-1-yl)ethanone			Br				
125-12-2	ionone (beta)		U		Sk	M		Sa
127-41-3	ionone (alpha)		U		Sk			Sa
ui	1-ethyl-3-methyl- β -ionone				Sk			
23726-93-4	beta-damascenone		U					
79-69-6	Z-alpha-irone				Sk			
79-68-5	gamma-irone				Sk			
	unsaturated cyclic (ketone in ring)							
930-30-3	2-cyclopenten-1-one			Br				
1120-73-6	2-methyl-2-cyclopentene-1-one		U	Br				
2758-18-1	1-methyl-1-cyclopenten-3-one			Br				
55683-21-1	3,4,5-trimethyl-2-cyclopenten-1-one			Br				
930-68-7	1-cyclohexen-3-one			Br				
1193-18-6	3-methyl-2-cyclohexen-1-one		U	Br				
5113-66-6	2-cyclohexen-1-one, 5-methyl-2-(1-methylethyl)-			Br				
89-81-6	3-methyl-6-(1-methylethyl)-2-cyclohexen-1-one		U	Br				Sa
99-49-0	carvone			Br				
5524-05-0	(+)-dihydrocarvone							Sa
5948-04-9	trans-dihydrocarvone							Sa
2244-16-8	(S)-carvone / (+)-carvone / (S)-2-methyl-5-(1-methylethenyl)-2-cyclohexen-1-one		U	Br				Sa
503-93-5	eucarvone / 2,6,6-trimethyl-2,4-cycloheptadien-1-one		U					
28226-49-5	car-2-en-4-one		U					
78-59-1	isophorone / 3,5,5-trimethylcyclohex-2-en-1-one		U					
488-10-8	jasmone				Sk			
13215-88-8	megastigmatrienone							Sa
89-82-7	pulegone		U					Sa
499126-76-0	6,6-dimethyl-2-methylenebicyclo[2.2.1]heptan-3-one		U					
82304-66-3	7,9-di-tert-butyl-1-oxaspiro(4.5)deca-6,9-diene-2,8-dione	F						
4075-07-4	androsta-4,16-dien-3-one		U					
18339-16-7	5alpha-androst-16-en-3-one		U			M		
3658-77-3	4-hydroxy-2,5-dimethyl-3(2H)furanone					M		

NOTES

ui unidentified isomer