Appendix: Chemical and physical properties

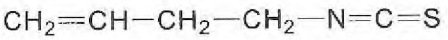
Isothiocyanates

2-Propenyl (allyl) isothiocyanate

Chemical name: 3-isothiocyanato-1-propene

CAS: 57-06-7

Structure:



Composition: C_4H_5NS

Relative molecular mass: 99.2

Boiling-point: 148–154 °C

Partition coefficient: 2.3 (Jiao *et al.*, 1994; Zhang, 2001)

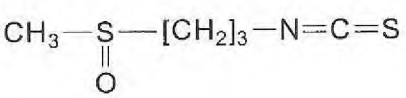
Comments: Lipophillic, highly volatile and very pungent

3-Methylsulfinylpropyl isothiocyanate (iberin)

Chemical name: 1-isothiocyanato-3 (methylsulfinyl)propane

CAS: 505-44-2

Structure:



Composition: $C_5H_9NOS_2$

Relative molecular mass: 163.3

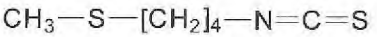
Comments: Water-soluble, non-volatile

4-Methylthiobutyl isothiocyanate (erucin)

Chemical name: 1-isothiocyanato-4-(methylthio)butane

CAS: 4430-36-8

Structure:



Composition: $C_6H_{11}NS_2$

Relative molecular mass: 161.3

Boiling-point: 136 °C

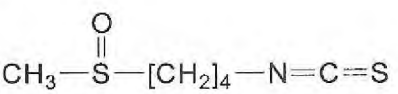
Comments: Volatile

4-Methylsulfinylbutyl isothiocyanate (sulforaphane)

Chemical name: 1-isothiocyanato-4-(methylsulfinyl)butane

CAS: 4478-93-7

Structure:



Composition: $C_6H_{11}NOS_2$

Relative molecular mass: 177.3

Boiling-point: 125–135 °C

Partition coefficient: 0.45 (Zhang, 2001)

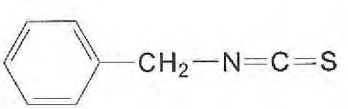
Comments: Water-soluble, non-volatile

Benzyl isothiocyanate

Chemical name: benzyl isothiocyanate

CAS: 622-78-6

Structure:



Composition: C_8H_7NS

Relative molecular mass: 149.2

Boiling-point: 242 °C

Partition coefficient: 3.0 (Jiao *et al.*, 1994; Zhang, 2001)

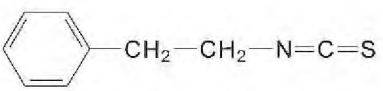
Comments: Lipophillic, partially volatile

2-Phenethyl isothiocyanate

Chemical name: 2-isothiocyanato-ethylbenzene

CAS: 2257-09-2

Structure:



Composition: C_9H_9NS

Relative molecular mass: 163.2

Boiling-point: 140 °C

Partition coefficient: 3.1 (Jiao *et al.*, 1994; Zhang, 2001)

Comments: Lipophillic, highly volatile

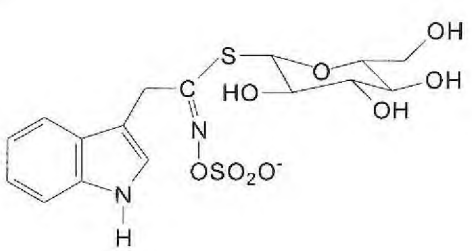
Indoles

Glucobrassicin

Chemical names: Indole-3-ylcarbinol glucosinolate; 3-indolylacet-thio-(*S*-β-glucopyranosido)hydroximyl-*O*-sulfate

CAS: 4356-52-9

Structure:



Composition: $C_{16}H_{20}N_2O_9S_2$

Relative molecular mass: 448.5

Melting-point: 148–150 °C (Gmelin & Virtanen, 1961; Hanley *et al.*, 1990)

Ultraviolet absorption spectra: (Gmelin & Virtanen, 1961; Agerbirk *et al.*, 1998)

Nuclear magnetic resonance spectra: (Hanley *et al.*, 1990; Agerbirk *et al.*, 1998)

Infrared absorption spectra: (Gmelin & Virtanen, 1961; Hanley *et al.*, 1990)

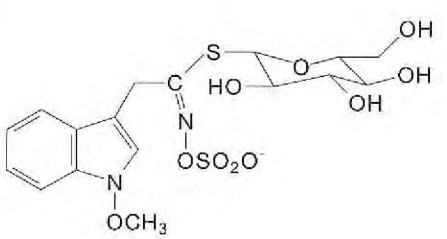
Mass spectrometry (m/z): (Hanley *et al.*, 1990)

Neoglucobrassicin

Chemical names: 1-methoxyindole-3-ylcarbinol glucosinolate; β-D-glucopyranose, 1-thio-,1-[1-methoxy-*N*-(sulfoxy)-1*H*-indole-3-ethanimidate]

CAS: 5187-84-8

Structure:



Composition: $C_{17}H_{22}N_2O_{10}S_2$

Relative molecular mass: 478.5

Melting-point: 158–162 °C (Hanley *et al.*, 1990)

Ultravioletabsorption spectra: (Agerbirk *et al.*, 1998)

Nuclear magnetic resonance spectra: (Hanley *et al.*, 1990; Agerbirk *et al.*, 1998)

Infrared absorption spectra: (Hanley *et al.*, 1990)

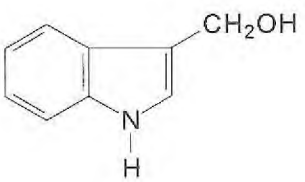
Mass spectrometry (m/z): (Hanley *et al.*, 1990)

Indole-3-carbinol

Chemical names: 1*H*-indole-3-methanol; 3-hydroxymethylindole; indol-3-ylmethanol

CAS: 700-06-1

Structure:



Composition: C_9H_9NO

Relative molecular mass: 147.2

Description: White crystals (Leete & Marion, 1953), colourless crystals (Styngach *et al.*, 1973)

Melting-point: 99–100 °C (Leete & Marion, 1953; Thesing, 1954; Silverstein *et al.*, 1954; Ames *et al.*, 1956; Henry & Leete, 1957; Styngach *et al.*, 1973; Le Borgne *et al.*, 1997)

Ultraviolet absorption spectra: (Leete & Marion, 1953; (Mendez, 1970; Goyal *et al.*, 2001)

Nuclear magnetic resonance spectra: (Hinman & Lang, 1965; Burton *et al.*, 1986; Hwu *et al.*, 1996; Le Borgne *et al.*, 1997)

Infrared absorption spectra: (Leete & Marion, 1953; Styngach *et al.*, 1973; Hwu *et al.*, 1996; Le Borgne *et al.*, 1997)

Mass spectrometry: (*m/z):* (Hwu *et al.*, 1996; Prinsen *et al.*, 1997; Delonga *et al.*, 2001)

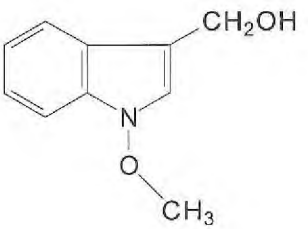
Stability: Unstable in hot alkali and sensitive to acids (Leete & Marion, 1953)

N-Methoxyindole-3-carbinol

Chemical names: 1-methoxyindole-3-methanol; 1*H*-indole-3-methanol

CAS: 110139-35-0

Structure:



Composition: $C_{10}H_{11}NO_2$

Relative molecular mass: 177.2

Melting-point: 92–94 °C (0.1 Torr) (Hanley *et al.*, 1990)

Solubility: Sparingly soluble

Nuclear magnetic resonance spectra: (Hanley *et al.*, 1990; Stephensen *et al.*, 2000)

Infrared absorption spectra: (Hanley *et al.*, 1990)

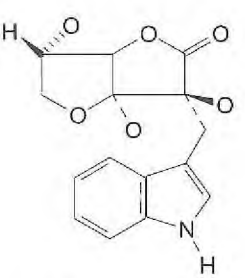
Mass spectrometry (m/z): (Hanley *et al.*, 1990)

Ascorbigen

Chemical name: 2-*C*-(1*H*-indol-3-ylmethyl)-β-L-lyxo-3-hexulofuranosonic acid g-lactone

CAS: 8075-98-7

Structure:



Composition: $C_{15}H_{15}NO_6$

Relative molecular mass: 305.3

Nuclear magnetic resonance spectra: (Agerbirk *et al.*, 1998)

Infrared absorption spectra: (Gmelin & Virtanen, 1961)

Mass spectrometry (m/z): (Agerbirk *et al.*, 1998)

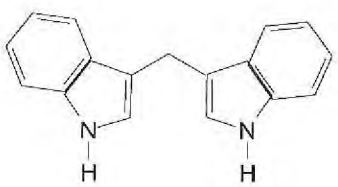
Stability: 90% present in acidic medium (pH < 1, 37 °C) after 3 h, whereas only 15% present after 3 days (Yudina *et al.*, 2000a)

3,3´-Diindolylmethane

Chemical name: 3,3´-diindolylmethane

CAS: 1968-05-4

Structure:



Composition: $C_{17}H_{14}N_2$

Relative molecular mass: 246.3

Description: White to off-white crystal

Melting-point: 164–165 °C (Leete & Marion, 1953; Thesing, 1954)

Ultraviolet absorption spectra: (Leete & Marion, 1953)

Nuclear magnetic resonance spectra: (Grose & Bjeldanes, 1992)

Infrared absorption spectra: (Leete & Marion, 1953)

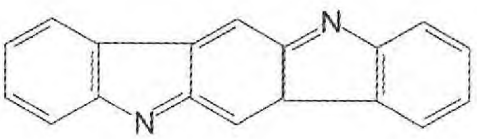
Mass spectrometry (m/z): (Grose & Bjeldanes, 1992)

Indolo[3,2-*b*]carbazole

Chemical name: 6,12-diaza-indeno[1,2-*b*]fluorene

CAS: 241-55-4

Structure:



Composition: $C_{18}H_{10}N_2$

Relative molecular mass: 254.3

Ultraviolet absorption spectra: (Robinson, 1963; Hünig & Steinmetzer, 1976)

Nuclear magnetic resonance spectra: (Hünig & Steinmetzer, 1976; Yudina *et al.*, 2000b)

Mass spectrometry (m/z): (Gardner *et al.*, 1957; Hünig & Steinmetzer, 1976)

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Abbreviations

AC	aberrant crypts
ACF	aberrant crypt foci
Akt	serine–threonine protein kinase
AFAR	aflatoxin B_1 aldehyde reductase
AFB_1	aflatoxin B_1
Ah	aryl hydrocarbon
AKR	aldo–keto reductase
AOM	azoxymethane
ARE	antioxidant response element
AT	*N*-acetyltransferase
ATF	activating transcription factor
AUC	area under the time–plasma concentration curve
B[a]P	benzo[*a*]pyrene
BBN	*N*-butyl-*N*-(4-hydroxybutyl)nitrosamine
BOP	*N*-nitrosobis(2-oxopropyl)amine
BPDE	7,8-dihydroxy-9,10-epoxy-7,8,9,10-tetrahydrobenzo[*a*]pyrene
BROD	benzyloxyresorufin-*O*-dealkylase
bw	body weight
bZIP	cap 'n' collar basic region leucine zipper [transcription factor]
CARET	β-carotene and retinol efficacy trial
CAT	chloramphenicol acetyltransferase
CC	case–control study
CDK	cyclin-dependent kinase
CG	cysteinylglycinase
CI	confidence interval
COX	cyclo-oxygenase
CT	5,6,11,12,17,18-hexahydrocyclononal-[1,2-*b*:4,5-*b*′:7,8-*b*′′]triindole
CYP	cytochrome P450
DHPN	dihydroxydi-*N*-propylnitrosamine
DIM	3,3′-diindolylmethane
DMABP	3′,2′-dimethyl-4-aminobiphenyl
DMBA	7,12-dimethylbenz[*a*]anthracene
DMH	1,2-dimethylhydrazine
EROD	ethoxyresorufin *O*-dealkylase
EGF	epithelial growth factor
EGFR	epithelial growth factor receptor
EMSA	electrophoretic mobility-shift analysis
EPIC	European Prospective Investigation into Cancer and Nutrition
ER	estrogen receptor
ERE	estrogen response element
ETS	environmental tobacco smoke
F	female
F_1	first filial generation
FAA	*N*-2-fluorenylacetamide
FFQ	food frequency questionnaire
FMO	flavin-related monooxygenase
GADD	growth arrest in response to DNA damage
GCL	glutamate cysteine ligase
GCLC	glutamate cysteine ligase catalytic
GCS	γ-glutamylcysteine synthetase
GGT	γ-glutamyl transferase
GSH	glutathione
GSSG	reduced glutathione
GST	glutathione *S*-transferase
GST-P	glutathione *S*-transferase placental form
HPLC	high-performance liquid chromatography
HPV	human papillomavirus
I3C	indole-3-carbinol
i.p.	intraperitoneally
IQ	2-amino-3-methylimidazo[4,5-*f*]quinoline
ITC	isothiocyanate
i.v.	intravenously
LD_{50}	median lethal dose
LTr1	2-(indol-3-ylmethyl)-3,3′-diindolyl methane
M	men or male
MAM	methylalkylthiomalate
MAP	M-associated protein
MeIQx	2-amino-3,8-dimethylimidazo[4,5-*f*]quinoxaline
Min	multiple intestinal neoplasia
MNNG	*N*-methyl-*N*′-nitro-*N*-nitrosoguanidine
MNU	*N*-methyl-*N*-nitrosourea
MROD	methoxyresorufin-*O*-dealkylase

MRP	multidrug-resistance-associated protein
NAC	*N*-acetylcysteine
NDEA	*N*-nitrosodiethylamine
NDMA	*N*-nitrosodimethylamine
NF-IL6	nuclear factor–interleukin 6
NIFOX	nifedipine oxidation
NMBA	*N*-nitrosomethylbenzylamine
NNAL	4-(methylnitrosamino)-1-(3-pyridyl)-1-butanol
NNK	4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone
NQO1	NAD(P)H:quinone oxidoreductase
NR	not reported
Nrf2	nuclear factor–erythroid 2 p45-related factor 2
NSAID	non-steroidal anti-inflammatory drug
ODC	ornithine decarboxylase
OR	odds ratio
8-oxodG	8-oxo-7,8-dihydro-2′-deoxyguanosine
PCNA	proliferating cell nuclear antigen
PhIP	2-amino-1-methyl-6-phenylimidazo[4,5-*b*]pyridine
PI3K	phosphatidyl inositol 3-kinase
PROD	pentoxyresorufin *O*-dealkylase
PSA	prostate-specific antigen
PTEN	phosphatase and tensin homologue deleted on chromosome 10
Rb	retinoblastoma
RR	relative risk
S9 mix	9000 × *g* supernatant of rodent liver
s.c.	subcutaneously
TBRM	total binding of radioactive material
TCDD	2,3,7,8-tetrachloro-*para*-dibenzodioxin
TGF	transforming growth factor
TPA	12-*O*-tetradecanoylphorbol 13-acetate
TRAIL	tumour necrosis factor-related apoptosis-inducing ligand
UGT	UDP-glucuronosyl transferase
v/v	volume per volume
W	women
w/w	weight per weight
XRE	xenobiotic response element