

Appendix: Chemical and physical properties

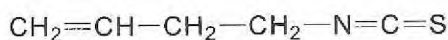
Isothiocyanates

2-Propenyl (allyl) isothiocyanate

Chemical name: 3-isothiocyanato-1-propene

CAS: 57-06-7

Structure:



Composition: $\text{C}_4\text{H}_5\text{NS}$

Relative molecular mass: 99.2

Boiling-point: 148–154 °C

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

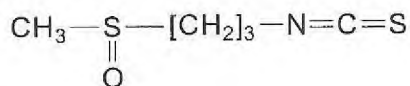
Comments: Lipophilic, highly volatile and very pungent

3-Methylsulfinylpropyl isothiocyanate (iberin)

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

CAS: 505-44-2

Structure:



Composition: $\text{C}_5\text{H}_9\text{NOS}_2$

Relative molecular mass: 163.3

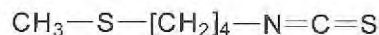
Comments: Water-soluble, non-volatile

4-Methylthiobutyl isothiocyanate (erucin)

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

CAS: 4430-36-8

Structure:



Composition: $\text{C}_6\text{H}_{11}\text{NS}_2$

Relative molecular mass: 161.3

Boiling-point: 136 °C

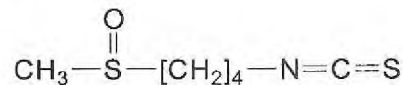
Comments: Volatile

4-Methylsulfinylbutyl isothiocyanate (sulforaphane)

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

CAS: 4478-93-7

Structure:



Composition: $\text{C}_6\text{H}_{11}\text{NOS}_2$

Relative molecular mass: 177.3

Boiling-point: 125–135 °C

Partition coefficient: 0.45 (Zhang, 2001)

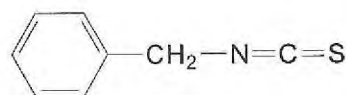
Comments: Water-soluble, non-volatile

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)

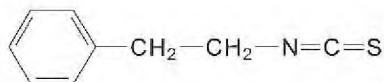
Comments: Lipophilic, partially volatile

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: Lipophilic, highly volatile

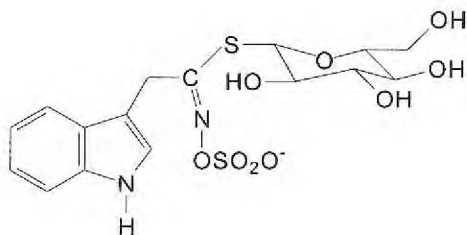
Indoles

Glucobrassicin

Chemical names: Indole-3-ylcarbinol glucosinolate; 3-indolylacet-thio-(S - β -glucopyranosido)hydroxymyl- 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)

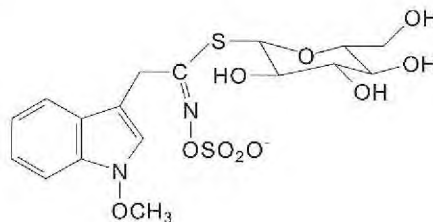
Mass spectrometry (m/z): (Hanley *et al.*, 1990)

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)

Ultraviolet absorption spectra: (Agerbirk *et al.*, 1998)

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

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

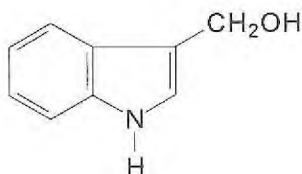
Mass spectrometry (m/z): (Hanley *et al.*, 1990)

Indole-3-carbinol

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

CAS: 700-06-1

Structure:



Composition: C₉H₉NO

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)

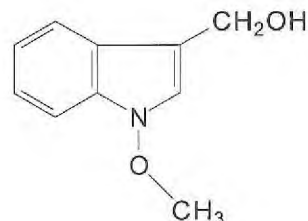
Stability: Unstable in hot alkali and sensitive to acids (Leete & Marion, 1953)

N-Methoxyindole-3-carbinol

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

CAS: 110139-35-0

Structure:



Composition: C₁₀H₁₁NO₂

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)

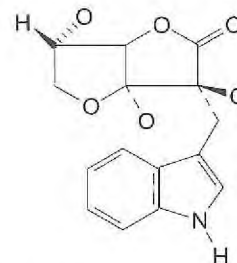
Mass spectrometry (m/z): (Hanley *et al.*, 1990)

Ascorbigen

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

CAS: 8075-98-7

Structure:



Composition: C₁₅H₁₅NO₆

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: C₁₇H₁₄N₂

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)

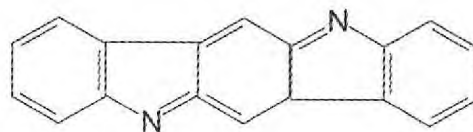
Mass spectrometry (m/z): (Grose & Bjeldanes, 1992)

Indolo[3,2-b]carbazole

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

CAS: 241-55-4

Structure:



Composition: C₁₈H₁₀N₂

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

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