

## Supplemental Tables

### Supplemental Table S1.

#### Physicochemical characteristics of Iodine-Based Contrast Media

Name	Structure	Ionicity	Application	Concentration (mg/ml)	Molecular Weight (Dalton)	Osmolality 37°C (mOsm/kg)	Viscosity 37°C (mPa·s)	1-Butanol/Water Partition Coefficient 37°C P (log P)
Iohexol	Monomeric	Nonionic	IV	300	821	690	6.2	0.082 (-1.086)
Iopromide	Monomeric	Nonionic	IV	300	791	586	4.6	0.149 (-0.827)
Iopamidol	Monomeric	Nonionic	IV	300	777	616	4.7	0.089 (-1.050)
Iomeprol	Monomeric	Nonionic	IV	300	777	521	4.5	0.105 (-0.979)
Ioversol	Monomeric	Nonionic	IV	300	807	645	5.5	0.031 (-1.509)
Iobitridol	Monomeric	Nonionic	IV	300	835	695	6.0	NA
Iodixanol	Dimeric	Nonionic	IV	320	1550	290	11.4	0.028 (-1.552)
Diatrizoate*	Monomeric	Ionic	Oral	370	614	2150	8.9	0.044 (-1.356)
Ioxitalamate*	Monomeric	Ionic	Oral	300	644	1710	5.3	NA

NA = not available

## Supplemental Table S2.

### Physicochemical characteristics and stability constants of Gadolinium-Based Contrast Agents

Name	Ligand	Structure	Ionicity	Molecular Weight ( <i>Dalton</i> )	Osmolality ( <i>mOsm/kg</i> )	Viscosity 37°C ( <i>mPa·s</i> )	T1 relaxivity in blood, 1.5T ( <i>L/mmol·s</i> )	T2 relaxivity in blood, 1.5T ( <i>L/mmol·s</i> )
Gadopentetate	DTPA	Linear	Ionic	939.0	1960	2.9	4.3	4.4
Gadodiamide	DTPA-BMA	Linear	Nonionic	537.6	789	1.4	4.6	6.9
Gadobenate	BOPTA	Linear	Ionic	1058.2	1970	5.4	6.7	8.9
Gadoxetate	EOB-DTPA	Linear	Ionic	682.0	688	1.2	7.3	9.1
Gadoteridol	HP-DO3A	Macrocyclic	Nonionic	558.7	630	1.3	4.4	5.5
Gadobutrol	BT-DO3A	Macrocyclic	Nonionic	604.7	1603	4.9	5.3	5.4
Gadoterate	DOTA	Macrocyclic	Ionic	558.6	1350	2.0	4.2	6.7
Gadopiclenol	NA	Macrocyclic	Nonionic	970.1	843	7.6	12.8	15.1

Name	Ligand	Thermodynamic Stability (pH 14) (Log K <sub>therm</sub> )	Conditional Stability (pH 7.4) (Log K <sub>cond</sub> )	Kinetic Stability (37°C, pH 1) (T <sub>1/2</sub> ; hours)	Dissociation Constant K <sub>obs</sub> (s <sup>-1</sup> )	Excess Ligand (mmol/l)	Stability Classification EMA
Gadopentetate	DTPA	22.5	18.4	0.16	0.58	1	Low
Gadodiamide	DTPA-BMA	16.9	14.9	0.01	12.7	25	Low
Gadobenate	BOPTA	22.6	18.4	NA	0.41	0	Intermediate
Gadoxetate	EOB-DTPA	23.5	18.7	NA	0.16		Intermediate
Gadoteridol	HP-DO3A	23.8	17.1	2.0	0.00026	0.5	High
Gadobutrol	BT-DO3A	21.8	15.5	7.9	0.000028	1	High
Gadoterate	DOTA	25.6	19.3	26.4	0.000008	0	High
Gadopiclesol	NA	18.7	15.5	120.0	0.000002	NA	NA

NA = not available

Sources S2: *van der Molen, Eur J Radiol 2008; Port, Biometals 2008; Rohrer, Invest Radiol 2005; Robic, Invest Radiol 2019; Szomolanyi, Invest Radiol 2019; Personal communication with medical departments of Bayer Healthcare, Bracco Imaging, GE Healthcare, Guerbet.*