Supporting Information

REVIEW

Recent developments in multimodality fluorescence imaging probes

Jianhong Zhao[a], Junwei Chen[a], Shengnan Ma[a], Qianqian Liu[a], Lixian Huang[a], Xiani Chen[a], Kaiyan Lou[a,*], Wei Wang[a,b,*]

[a]*Shanghai Key Laboratory of Chemical Biology, School of Pharmacy, and State Key Laboratory of Bioengineering Reactor, East China University of Science and Technology, Shanghai 200237, China*

[b]*Department of Chemistry and Chemical Biology, University of New Mexico, Albuquerque, NM 87131-0001, USA*

*Corresponding authors. Tel./fax: +86 21 64253299 (Kaiyan Lou); Tel.: +1 505 2770756; fax: +1 505 2772609 (Wei Wang).

E-mail addresses: kylou@ecust.edu.cn (Kaiyan Lou); wwang@unm.edu (Wei Wang).

Table S1 Comparison of optical fluorescence imaging with other imaging modalities (adapted from reference[1] with modifications).

Modalities	Spatial Resolution	Depth of Penetration	Imaging time	Sensitivity (mol/L)	Multiplexing Capability	Safety	Cost	Clinical Availability	Imaging/Contrast Agent	Information Provided
OFI	Highest in vitro cell imaging Low in vivo tissue imaging (2-3 mm)	< 1 cm	s–min	High (10^{-9}-10^{-12})	Yes	Relatively safe	Low	Optical guided surgery	Organic fluorophores Quantum dots Polymer dots Upconversion materials, etc.	Functional information: biomarker, physiological information, receptor, and etc.
CT	High (0.5–1 mm)	Unlimited	min	Low for soft tissues (ND)	No	Ionizing radiation	Relatively high	Yes	Iodinated molecules Gold nanoparticles Bi_2S_3, TaO_x, etc.	Mainly 3D anatomy
MRI	High (~1 mm)	Unlimited	(min)	Very Low, Better than CT for soft	No	No ionizing radiation	High	Yes	$Gd^{3+}$and Mn^{2+} complexes, Superparamagnetic iron oxide nanoparticles, ^{19}F	3D anatomy Physiological information

				tissues (10^{-3}-10^{-5})					enriched materials, etc.	
PET	low 5–7 mm	Unlimited	s–min	Very High (10^{-11}-10^{-12})	No	Ionizing radiation	High	Yes	Radioisotopes: ^{18}F, ^{64}Cu, ^{68}Ga, ^{89}Zr, etc.	3D distributions of PET nuclides
SPECT	low 8–10 mm	Unlimited	min	High (10^{-10}-10^{-11})	Yes	Ionizing radiation	Relatively high	Yes	Radioisotopes: ^{99m}Tc, ^{111}In, ^{177}Lu, etc.	3D distributions of SPECT nuclides
PAI	Very high 0.15–1 mm	Deep Up to 7 cm	s–min	Relatively low compared with OFI	Yes	Relatively safe	Low	Emerging	High NIR absorbance material: NIRF dyes, gold nanorods, carbon nanotubes, etc.	Both functional and anatomical information

Table S2 Representative OFI/CT dual-modality imaging probes.

Category	Fluorophore	CT Contrast Agent	Imaging Agents	Fluorescence Imaging Conditions	Imaging Modalities	Targeting Moiety	Biological Targets	Combined Therapy	Disease	Reference
Nanoprobe	Cu-doped CdS Quantum dots (QDs)	Ba^{2+}	Ba^{2+}-doped HAp-Cu:CdS QDs-HA	λ_{ex} = 488 nm λ_{em} = 700 nm	NIRF/CT	Hyaluronic acid (HA)	HA receptors	N/A	Cancer	Microchem. J. 2017, 134, 41-48[2]
Nanoprobe	Persistent luminescence nanoparticles ZGGO:Cr,Pr	TaO_x	NGR-ZGGO:Cr,Pr@TaO_x@SiO_2	(λ_{ex} = 254 nm) λ_{em} = 695 nm	NIRF/CT	the cyclic CNGRCGG peptide	CD 13 enzyme	N/A	Cancer	Nanoscale 2015, 7, 17929-17937[3]
Nanoprobe	CdSe/ZnS QDs	Bi_2S_3	Core-shell Bi_2S_3-CdSe/ZnS QD@SiO_2-PEG NPs	λ_{ex} = 488 nm λ_{em} = 633 nm	OFI/CT	N/A	N/A	N/A	N/A	Chem. Commun. 2013, 49, 11800-11802[4]
Nanoprobe	Ag_2S QDs	Iodinated oil	Ag_2S-I@DSPE-PEG_{2000}-FA	λ_{ex} = 868 nm λ_{em} = 1170 nm	OTN-NIR/CT	Folic acid	FA receptors	N/A	Cancer	Nanoscale 2015, 7, 19484-19492[5]
Nanoprobe	Quantum dots (QDs)	Iodinated oil	Core-shell CdSe/ZnS QDs-iodinated oil nanoemulsion	λ_{ex} = 488 nm λ_{em} = 620 nm	NIRF/CT	N/A	Macrophages in atherosclerotic plaques	N/A	Cardiovascular disease	Biomaterial 2013, 34, 209-216[6]
Nanoprobe	Cy5.5	Iodinated oil	Iodinated oil @ Cy5.5-DSPE liposomes	λ_{ex} = 650 nm λ_{ex} = 700 nm	NIRF/CT	N/A	N/A	N/A	Cancer	Mol. Imaging 2013, 12, 148-160[7]
Nanoprobe	Gold nanoclusters (Au NCs)	Au NCs	lysozyme-capped gold nanoclusters (FA-Lys-Au NCs)	λ_{ex} = 550 nm λ_{ex} = 690 nm	NIRF/CT	Folic acid	FA receptors	N/A	Cancer	J. Mater. Chem. B 2016, 4, 1276-1283[8]

Nanoprobe	CdSe/ZnS QDs	Au nanorods (GNRs)	GNR@SiO_2@QDs-FA	λ_{ex} = 488 nm λ_{em} = 620 nm	OFI/CT	Folic acid	FA receptors	PTT	Cancer	J. Mater. Chem. B 2014, 2, 1945-1953[9]
Naoprobe	AIE dye NPAPF	Au NPs	M-NPAPF-Au@DSPE-PEG_{2000} micelles	λ_{ex} = 488 nm λ_{em} = 600-850 nm	NIRF/CT	N/A	N/A	N/A	N/A	Biomaterials 2015, 42, 103-111[10]

Table S3 Representative dual-modality OFI/MRI imaging probes.

Category	Fluorophore	MRI Contrast Agents	Imaging Agents	Fluorescence Imaging Conditions	Imaging Modalities	Targeting Moiety	Biological Targets	Combined Therapy	Disease	Reference
Nanoprobe	IR-808	Gd-DTPA	IR-808-Gd-MSNs (mesoporous silica NPs)	λ_{ex} = 778 nm λ_{em} = 808 nm	NIRF/MRI	N/A	N/A	N/A	Cancer	J. Nanomater. 2016, 6502127[11]
Nanoprobe	Cy5	Gd^{3+}	Gd–Al@MSNs-Cy5	λ_{ex} = 625 nm λ_{ex} = 690 nm	NIRF/MRI	N/A	N/A	N/A	N/A	Anal. Methods 2016, 8, 214-221[12]
Nanoprobe	$Ru(bpy)_3^{2+}$	Gd^{3+}	Ru/Gd–Al@MSNs	λ_{ex} = 480 nm λ_{em} = 700 nm	NIRF/MRI	N/A	N/A	N/A	cancer	Analyst 2014, 139, 4613-4619[13]
Nanoprobe	Persistent luminescence nanoparticles	Gd-DTPA	Gd(III)-PLNPs	λ_{ex} = 254 nm λ_{em} = 700 nm	NIRF/MRI	N/A	N/A	N/A	cancer	Anal. Chem. 2014, 86, 4096-4101[14]
Nanoprobe	Lanthanide nanocrystals (upconversion NCs)	$NaGdF_4$/NaDy F_4 (dual T_1/T_2 mode)	$NaDyF_4$:Yb^{3+}/$NaGdF_4$: Yb^{3+},Er^{3+} NCs-Ce6	λ_{ex} = 980 nm (NIRF/PDT) λ_{em} = 523, 546, 660 nm	NIRF/MRI	N/A	N/A	PDT (chlorin e6)	cancer	Nanoscale, 2014, 6, 12609-12617[15]
Nanoprobe	Carbon QDs (CQDs)	Gd^{3+}	Gd-encapsulated CQDs	λ_{ex} = 354 nm λ_{em} = ~ 445 nm	OFI/MRI	N/A	N/A	N/A	Cardiovascular disease	J. Mater. Chem. B, 2017, 5, 92-101[16]
Nanoprobe	CQDs	Gd-DTPA	CQD–DTPA–Gd	λ_{ex} = 350-500 nm λ_{em} = 460-580 nm	OFI/MRI	N/A	N/A	N/A	N/A	Carbon 2015, 93, 742-750[17]
Nanoprobe	Tb^{3+}-doped	Gd_2O_3	Gd_2O_3:Tb	λ_{ex} = 285 nm λ_{em} = 543.5 nm	OFI/MRI	N/A	N/A	N/A	N/A	Phys. Chem. Chem. Phys. 2015, 17, 1189-1196[18]
Star-like polymer	Porphyrin	Gd-DTPA	PEG-PP-DPTA-Gd^{3+}	λ_{ex} = 600 nm λ_{em} = 710 nm	NIRF/MRI	N/A	N/A	N/A	cancer	Polymer 2016, 88, 94-101[19]
Dendrimer	Fluorescent POSS	Gd^{3+}	POSS–HPG–Gd	λ_{em}= 570 nm	OFI/MRI	N/A	N/A	N/A	cancer	Polym. Chem. 2013, 4, 1517-1524[20]
Dendrimer (two-step)	Rhodamine Green	Gd-DTPA	Gd(III)-1B4M-DTPA-PAMAM-Biotin/ Rodamine Green	N/A	OFI/MRI	N/A	N/A	N/A	Ovarian cancer	Bioconjugate Chem. 2007, 18, 1474–1482[21]

			labelled avidin							
Nanoprobe	PFVBT	iron oxide	IOs@PLGA-PEG-FOL	λ_{ex}= 518 nm λ_{em}= 636 nm	NIRF/MRI	Folic acid	Folate receptor	N/A	cancer	Adv. Funct. Mater. 2012, 22, 3107–3115[22]
Nanoprobe	Sulforhodam-ine101 (SR101)	Fe_3O_4	Fe_3O_4-PEG-PAE-SR101	λ_{ex} = 592 nm λ_{em} = 612 nm	OFI/MRI	PAE	Cancer microenviroment	N/A	Cancer	J. Mater. Chem. 2010, 20, 5454-5461[23]
Nanoprobe (core-shell)	Cy5.5	USPIOs	Cy5.5-APTES-USPIOs-silica(SCION)	λ_{ex} = 675 nm λ_{em} = 694 nm	NIRF/MRI	N/A	N/A	N/A	N/A	Nanotechnology 2010, 21, 175704[24]
Nanoprobe	Cy7	iron oxide nanocrystals	FeO-PAV-RGD-DSPC-PEG-DSPE-Cy7	λ_{ex} = 710-760 nm λ_{em} = 810-875 nm	NIRF/MRI	RGD	$\alpha_v\beta_3$ integrin	Chemothe rapy (PAV)	Cancer	ACS Nano 2011, 5, 4422-4433[25]
Nanoprobe (core-shell)	NIR797	SPIO	NIR797-PLL-SPIO-PAA	λ_{ex}=684-729 nm λ_{em}=745 nm	NIRF/MRI	N/A	dendritic cells in the draining lymph nodes	N/A	Cancer metastasis	Cytotherapy 2014, 16, 699-710[26]
Nanoprobe (core-shell)	CdSe-CdS QDs	Fe_3O_4	mPEG-silica-CdSe-Cds-Fe_3O_4	N/A	NIRF/MRI	N/A	N/A	N/A	cancer	Nat. Commun. 2014, 5, 5093[27]
Nanoprobe (core-shell)	NIR-830	Hydrophobic iron oxide nanocrystals	IONP-NIR830	λ_{ex} = 684-729 nm λ_{em}= 745 nm (long pass filter)	NIRF/MRI	N/A	sentinel lymph node	N/A	Cancer metastasis	J. Biomater. Appl. 2013, 28, 100-111[7]
Nanoprobe (core-shell, liposome)	CdSe QDs	Fe_3O_4	cRGD-MF-liposomes	λ_{ex} = 468 nm λ_{em} = 532 nm	OFI/MRI	cRGDyk	$\alpha_v\beta_3$ integrin	N/A	Cancer metastasis	J. Liposome Res. 2015, 25, 89-100[28]
Nanoprobe	Oligo(*p*-phenyleneethynyl ene)	Fe_3O_4	MNPs@OPE-PEG-FA	λ_{ex} = 720 nm (two-photon) λ_{em} = ~ 460 nm	OFI/MRI	Folic acid	Folate receptor	N/A	cancer	Nanoscale 2015, 7, 8907-8919[29]
Nanoprobe	Cy5.5	Superparamagn etic iron oxide NPs (SPIONs)	RMNs-HSA-Cy5.5	N/A	NIRF/MRI	S-S	GSH-triggered protein release	Protein drug delivery	cancer	ACS Appl. Mater. Interfaces 2017, 9, 19184-19192[30]
Nanoprobe	Cy5.5	Nano-Fe_3O_4	Cy5.5-GX1-nanoFe_3O_4	N/A	NIRF/MRI	GX1 (peptide)	New vessels of gastric cancer	N/A	gastric cancer	Artif. Cells, Nanomed., Biotechnol. 2017, 45, 399-403[31]
Nanoprobe (antibody)	Cy5.5	Fe_3O_4	Cy5.5-OPN-DMSA-MNPs (COD-MNPs),	N/A	OFI/MRI	OPN antibody	Osteopontin (OPN)	N/A	atherosclero sis	Biomaterials 2017, 112, 336-345[32]
Nanoprobe (core-shell)	ICG	SPIO	SPIO@Liposome-ICG-RGD	N/A	NIRF/MRI	RGD	$\alpha_v\beta_3$ integrin	N/A	Liver cancer	Oncotarget 2017, 8, 32741-32751[33]
Nanoprobe (core-shell)	Cy3	Iron NPs	Cy3-S6 aptamer-conjugated magentic core-gold shell NPs	λ_{ex} = 1064 nm (PTT)	OFI/MRI	S6 aptamer	Circulating tumor cells (CTC)s	PTT	cancer	Mol. Pharm. 2013, 10, 857-866[34]
Nanoprobe (core-shell)	$CuInS_2$ (QDs)	Mn^{2+}	PEGylated $CuInS_2$@ZnS:Mn	λ_{ex} =503-548 nm λ_{em} = 560 nm (long-pass filter)	OFI/MRI	N/A	N/A	N/A	cancer	Biomaterials 2014, 35,1608-1617[35]
Nanoprobe (core-shell)	ETTA	^{19}F	ETTA@PSI_{OAm}–PDTES-RGD	λ_{ex} = 362 nm λ_{em} = around 490	OFI/MRI	RGD	$\alpha_v\beta_3$ integrin	N/A	cancer	Nanoscale 2017, 9, 7163-7168[36]

				nm						
Nanoprobe (core-shell)	Cy5	^{19}F	Folate-mFLAME-DOX	N/A	OFI/MRI	Folic acid	Folate receptor	Chemothr apy (DOX)	cancer	Chem. Sci. 2015, 6, 1986-1990[37]
closomers	sulforhodamine-B	^{19}F	^{19}F-B_{12}-FL (double-labelled isosahedral B_{12} ion)	λ_{em} = 570 nm	OFI/MRS	N/A	N/A	N/A	N/A	Chem. Commun. 2014, 50, 5793-5795[38]
Enzyme	Cy5.5	Gd-DOTA	Gd^{3+}-bCD-PLL--Cy5.5-rhodamine (dual-labelled bacterial cytosine deaminase)	N/A	NIRF/MRI	N/A	endothelial progenitor cells (EPCs)	N/A	cancer	PLoS One. 2012, 7, e50575[39] Mol. Imaging 2011, 10, 359-369[40]
Small molecule	IR-783	Gd-DOTA	Gd^{3+}-IR-783-PEG	λ_{ex} = 745 nm λ_{em} = 810 nm	NIRF/MRI	IR-783	Enhanced cell uptake through organic-anion transporting polypeptides (OATPs)	N/A	cancer	JACS 2015, 137, 9108-9116[41]
Small molecules	Cy7, BODIPY, Fluorescein, Rhodamine	Gd-DOTA	Cy7-Gd, FL-Gd, BDP-Gd, Rhoda-Gd	Depending on the dye used	OFI/MRI	Cy7	Enhanced cell uptake	N/A	N/A	Bioconjugate Chem. 2011, 22, 2227-2236[42]
Small molecule	Cy7	Gd-DTPA	LS-479-Gd^{3+}	N/A	NIRF/MFI	Cy7 dye	Serum albumin	N/A	N/A	Chem. Commun. 2010, 46, 3705-3707[43]
Small molecule (two-step)	Alexa Fluor 488	Gd-DOTA	Biotin-Gd-DOTA-mGluR5-antagonist/Alexa Fluor 488 labelled avidin	N/A	OFI/MRI	$mGluR_5$-antagonis ts	metabotropic Glu receptor subtype 5 ($mGluR_5$)	N/A	CNS disorders	ACS Chem. Neurosci. 2014, 5, 128-137[44]
Small Molecule	Zinpyr-1	Mn-ZP1	ZP1-Mn^{2+}	N/A	OFI/MRI	N/A	Zn^{2+}	N/A	N/A	Chem. Commun. 2010, 46, 4139-4141[45]
Small molecule	Zpy	Gd-Zpy	Gd-Zpy	λ_{ex} = 488 nm λ_{em} = 528 nm	OFI/MRI	N/A	Zn^{2+}	N/A	N/A	Tetrahedron 2012, 68, 306-310[46]
Small molecule	CA (a coumarin dye)	Gd-DO3A	DO3A-Gd-CA	λ_{ex} = 408 nm λ_{em} = 460 nm	OFI/MRI	N/A	F^-	N/A	N/A	Sensors 2016, 16, 2165[47]
Small molecule	DPPZ	Gd^{3+}	$Gd(TTA)_3$-DPPZ	λ_{ex} = 340 nm	OFI/MRI	N/A	F^-	N/A	N/A	Dalton Trans. 2016, 45, 17616-17623[48]

Table S4 Representative OFI/MRI/CT tri-modality imaging probes.

Category	Fluorophore	MRI Contrast Agents	Imaging Agents	Fluorescence Imaging Conditions	Imaging Modalities	Targeting Moiety	Biological Targets	Combined Therapy	Disease	Reference
MOF	ZnO	Fe_3O_4	Fe^{2+}-adsorbed ZIF-8	λ_{ex} = 440 nm λ_{em} = 535 nm	FL/MRI/CT	N/A	N/A	N/A	Cancer	Adv. Funct. Mater. 2017, 27, 1603926[49]
Nanoprobe	Nitrogen-doped Carbon Quantum Dots	Superpara magnetic Fe_3O_4 NPs	C-Fe_3O_4 QDs	λ_{ex} = 420, 440 nm λ_{em} = 520, 570 nm	OFI/MRI/CT	N/A	N/A	N/A	Cancer	Adv. Funct. Mater. 2016, 26, 8694-8706[50]
Nanoprobe	Rhodamine B	Superpara magnetic Fe_3O_4 NPs	Fe_3O_4 @dye-hybrid@ Au-PEG nanocomposites (Au NPs as CT contrast agent)	λ_{ex} = 555 nm λ_{em} = 580 nm	OFI/MRI/CT	N/A	N/A	PTT	Cancer	Small 2013, 9, 2500-2508[51]
Nanoprobe	Cy5	Superpara magnetic Fe_3O_4 NPs	I-fmSiO4@SPIONs (iodinated oil as CT contrast agent)	N/A	OFI/MRI/CT	N/A	N/A	N/A	N/A	Int. J. Nanomed. 2014, 9, 2527-2538[52]
Nanoprobe	DOX Cy5.5	Iron-oxide NPs	Cy5.5-WS_2-IO@MS-PEG/DOX (WS_2 as CT contrast agent)	DOX Cy5.5	NIRF /MRI/CT	N/A	N/A	PTT chemothe rapy	Cancer	Biomaterials 2015, 60, 62-71[53]
Nanoprobe	IR820	Gd-DOTA	Gd-DOTA, Iohexol, IR-820 loaded liposomes	λ_{ex} = 785 nm λ_{em} = 830 nm	NIRF/MRI/CT	N/A	N/A	PTT	Cancer	Int. J. Nanomed. 2017, 12, 4467-4478[54]
Nanoprobe	ICG	Gd_2O_3	Gd_2O_3–AuNCs–ICG (AuNCs and Gd_2O_3 as CT contrast agent)	λ_{ex} = 635 nm	NIRF/MRI/CT	N/A	N/A	PDT	Cancer	ACS Appl. Mater. Interfaces 2017, 9, 6941-6949[55]
Nanoprobe	Gold nanoclusters (AuNCs)	Gd^{3+}	Gd^{3+}-A-AuNCs@SiO_2 NPs	λ_{ex} = 445-490 nm λ_{em} >515 nm	OFI/MRI/CT	N/A	N/A	N/A	Cancer	Chem. Eur. J. 2014, 20, 8876-8882[56]
Nanoprobe (Albumin)	Albumin entrapped gold nanoclusters (CT-active)	Gd-DTPA	Hybrid gold–gadolinium NCs	λ_{em} = 660 nm	NIRF/MRI/CT	N/A	N/A	N/A	Cancer	Nanoscale 2013, 5, 1624–1628[57]
Nanoprobe	Eu^{3+} doped $GdVO_4$ nanocastings	$GdVO_4$	amino acids-capped $GdVO_4$:Eu^{3+} nanocastings	λ_{ex} = 330 nm λ_{em} = 620 nm	OFI/MRI/CT	N/A	N/A	N/A	Cancer	Nanoscale 2014, 6, 12042–12049[58]
Nanoprobe	CaF_2:Yb^{3+}/Er^{3+}/Mn^{2+} (UPNPs)	Mn^{2+}, Yb^{3+}	UCHNs-PAMA-Pt(IV)	λ_{ex} = 980 nm λ_{em} = 655 nm	OFI/MRI/CT	N/A	N/A	Chemoth erapy	Cancer	Biomaterials 2015, 50, 154-163[59]
Nanoprobe	$NaGdF_4$:Yb^{3+}/Er^{3+}	$NaGdF_4$	$NaGdF_4$:Yb^{3+}/Er^{3+}@NaGdF	λ_{ex} = 793, 980	OFI/MRI/CT	N/A	N/A	N/A	Cancer	ACS Appl. Mater. Interfaces 2015,

(core-shell)	(UCNPs)		$_4$:Nd^{3+}@Sodium-Gluconate	nm λ_{em} = 525, 540, 656 nm						7, 16257-16265[60]
Nanoprobe	Gd_2O_3:Yb^{3+}, Er^{3+} nanorods (up-conversion luminescence material)	Gd_2O_3	PEGylated Gd_2O_3:Yb^{3+}, Er^{3+} nanorods (Gd and Yb as CT contrast agent)	λ_{ex} = 980 nm	OFI/MRI/CT	N/A	N/A	N/A	N/A	Biomaterials 2013, 34, 1712-1721[6]
Nanoprobe	BaGdF5:Yb/Er NPs (UCNPs)	$BaGdF_5$	PEGylated $BaGdF_5$:Yb/Er nanoprobes (Ba, Gd, Yb as CT contrast agent)	λ_{ex} = 980 nm λ_{em} = 500-600 nm 600-700 nm	OFI/MRI/CT	N/A	N/A	N/A	Splenic disease	Biomaterials 2012, 33, 9232-9238[61]
Nanoprobe (core-shell)	$NaLuF_4$-based upconversion nanophosphors	Gd-DTPA	$NaLuF_4$:Yb^{3+},Tm^{3+}@SiO_2-GdDTPA (Yb, Tm as CT contrast agent)	λ_{ex} = 980 nm λ_{em} = 450-500 nm	OFI/MRI/CT	N/A	N/A	N/A	N/A	Biomaterials 2012, 33, 5394-5405[62]
Nanoprobe	Upconversion nanoparticles (UCNPs)	$NaGdF_4$	NaY/GdF_4: Yb, Er, Tm@SiO_2-Au@PEG_{5000}	λ_{ex} = 980 nm λ_{em} = 500-560 nm & 620-680 nm	OFI/MRI/CT	N/A	N/A	N/A	Cancer	Biomaterials 2012, 33, 1079-1089[63]

Table S5 Representative OFI/PET dual-modality imaging probes.

Category	Fluorophore	Radioisotope /Chelator	Imaging Agents	Fluorescence Imaging Conditions	Imaging Modalities	Targeting Moiety	Biological Targets	Combined Therapy	Disease	Reference
Antibody	IRDye 800CW	^{89}Zr-DFO	^{89}Zr-*N*-sucDf-mAb-IRDye800CW	ICG filter	NIRF/PET	Cetuximab / bevacizumab	EGFR/VEGF	N/A	Cancer	Nat. Protoc. 2013, 8, 1010-1018[64]
Antibody	IRDye 800CW(/Fluorescein/CF790)	^{64}Cu/^{68}Ga-DOTA	mAb7-^{64}Cu-DOTA-IRDye 800	N/A	NIRF/PET	mAb7 (anti-EpCAM mAb)	Epithelial cell adhesion molecules (EpCAM)	N/A	Prostate cancer	J. Med. Chem. 2013, 56, 406-416[65]
Antibody	IRDye 800CW	^{64}Cu-DOTA	^{64}Cu-(DOTA)$_n$-anti-EpCAM-(IRDye 800)$_m$	λ_{ex} = 785 nm λ_{em} = 830 nm	NIRF/PET	Anti-EpCAM mAbs	EpCAM	N/A	Cancer	Prostate 2012, 72, 129-146[66]
Antibody	IRDye 800CW	^{64}Cu-DOTA	^{64}Cu-(DOTA)$_n$-anti-EpCAM-(IRDye 800)$_m$	λ_{ex} = 768 nm λ_{em} = 830 ± 5 nm	NIRF/PET/CT	Anti-EpCAM mAbs	EpCAM (Metastatic lymph node)	N/A	Prostate cancer	J. Nucl. Med. 2012, 53, 1427-1437[67]
Antibody	IRDye 800CW	^{64}Cu-NOTA	^{64}Cu-NOTA-TRC105-800CW ^{64}Cu-NOTA-cetuximab-800CW (as control)	λ_{ex} = 778 nm λ_{em} = 806 nm	NIRF/PET	TRC105/cetuximab	CD105/EGFR	N/A	Breast cancer	Mol. Pharmaceutics 2012, 9, 645-653[68]
Antibody	IRDye 800CW	^{89}Zr-DFO	^{89}Zr-Df-TRC105-800CW	λ_{ex} = 778 nm λ_{em} = 806 nm	NIRF/PET	TRC105/cetuximab	CD105/EGFR	N/A	Breast cancer	Mol. Pharmaceutics 2012, 9, 2339-2349[69]
Antibody	IRDye 800	^{64}Cu-DOTA	^{64}Cu-(DOTA)$_n$-Trastuzumab-(IRDye800)$_m$	λ_{ex} = 785 nm	NIRF/PET	Trastuzumab	HER-2	N/A	Breast cancer	Transl. Oncol. 2010, 3, 307-317[70]
Antibody	Alexa Fluor 750	^{64}Cu-DOTA	^{64}Cu-DOTA-NuB2-Alexa Fluor 750	Tunable filter 650 to 850 nm	NIRF/PET	NuB2	CD20	N/A	Lymphoma cancer	Oncol. Rep. 2009, 22, 115-119[71]
Antibody	Cy7	^{18}F (labelled via boron trap)	mAb-^{18}F-labelled Cy7	λ_{ex} = 730 nm λ_{em} = 810 nm	NIRF/PET	EpCAM/ Cetuximab-1	Prostate tumor/EGFR	N/A	Cancer	Bioconjugate Chem. 2016, 27, 1390-1399[72]
Antibody	^{18}F-BODIPY	^{18}F (labelled via DMAP activation)	mAb-^{18}F-labelled BODIPY	N/A	OFI/PET	Trastuzumab	HER-2	N/A	Her2 positive breast cancer	Angew. Chem. Int. Ed. 2012, 51, 4603-4606[73]
Peptide	^{18}F-BODIPY	^{18}F (labelled via Lewis acid activation and click	Bombesin-^{18}F-labelled BODIPY	N/A	OFI/PET/CT	Bombesin	Bombesin receptor	N/A	Prostate cancer	EJNMMI Res. 2015, 5, 43[74]

		chemistry)								
Peptide	^{18}F-BODIPY	^{18}F (labelled via Lewis acid activation)	RGD-^{18}F-labelled BODIPY	N/A	OFI/PET	RGD	$\alpha_v\beta_3$integrin	N/A	Cancer	Theranostics 2013, 3, 181-189[75]
Peptide	Sulfo-Cy7	^{68}Ga-FSC	Sulfo-Cy7-FSC-MG Sulfo-Cy7-FSC-RGD	λ_{ex} = 730 nm λ_{em} = 790 nm	NIRF/PET	Minigastrin analog (MG)/RGD	cholecystokinin-2 (CCK-2) receptor / $\alpha_v\beta_3$integrin	N/A	Cancer	Bioconjugate Chem. 2017, 28, 1722-1733[76]
Peptide (site-specific labeling via click chemistry)	Sulfo-Cy5	^{64}Cu-sarcophagine	^{64}Cu-E4-Fl	N/A	NIRF/PET	Exendin-4	Glucagon-like peptide 1 receptor (GLP-1R)	N/A	Cancer	Bioconjugate Chem. 2014, 25, 1323-1330[77]
Peptide	Cy5.5	^{64}Cu-BaAnSar (sarcophagin e derivative)	^{64}Cu-BaAnSar-RGD$_2$-Cy5.5	Cy5.5 filter	NIRF/PET	(RGD)$_2$	$\alpha_v\beta_3$ integrin	N/A	Cancer	Mol. Imaging Biol. 2012, 14, 718-724[78]
Peptide, Photo-click chemistry	Parazoline	^{68}Ga-NOTA	^{68}Ga-NOTA-Parazoline-AE105	λ_{ex} = 365 nm λ_{em} = 570 nm (605 ± 35 nm)	OFI/PET	AE105	urokinase-type plasminogen activator receptor (uPAR)	N/A	Cancer	Bioconjugate Chem. 2016, 27, 1200-1204[79]
Peptide, BCN-based MSAP platform	Cy5.5	^{64}Cu-NOTA	(^{64}Cu-NOTA)-Cy5.5-BCN-AE105 (^{64}Cu-CHS1)	Cy5.5 filter	NIRF/PET	AE105	uPAR	N/A	Cancer	Angew. Chem. Int. Ed. 2015, 54, 5981-5984[80]
Peptide, Cysteine-based MSAP platform	Cy5.5	^{64}Cu-DOTA	^{64}Cu-DOTA-NT-Cy5.5	Cy5.5 filter	NIRF/PET/CT	Neurotensin (NT)	G-protein-coupled neurotensin receptor (NTR)	N/A	Cancer	Mol. Pharmaceutics 2015, 12, 3054-3061[81]
Peptide, Cysteine-based MSAP platform	ZW-1	^{64}Cu-DOTA	^{64}Cu-RGD-C(DOTA)-ZW-1	λ_{ex} = 775 nm λ_{em} = 790 nm	NIRF/PET	c(RGDyK)	$\alpha_v\beta_3$ integrin	N/A	Cancer	Theranostics 2012, 2, 746-756[82]
Peptide, Lysine-based MSAP platform	IRDye 650	^{68}Ga-DOTA	^{68}Ga-HZ220	λ_{ex} = 640 nm λ_{ex} = 680-780 nm	NIRF/PET	RM2 (nonapeptide)	Gastrin-releasing peptide receptor (GRPR)	N/A	Prostate cancer	J. Nucl. Med. 2017, 58, 29-35[83]
Peptide,	IRDye	^{68}Ga-DOTA	^{68}Ga-MMC (IRDye	N/A	NIRF/PET	TOC	Somatostatin	N/A	Cancer	ACS Med. Chem. Lett. 2017, 8, 720-

Lysine-based MSAP platform	800CW		800CW)-TOC			(octapeptide)	receptor (SSTR)			725[84]
Lysine-based MSAP platform	MHI-148 (Cy7)	^{64}Cu-DOTA	^{64}Cu-DOTA-Lys-MHI-148	λ_{ex} = 740 nm λ_{em} = 820 nm	NIRF/PET	MHI-148	tumor	N/A	Cancer	Nucl. Med. Biol. 2013, 40, 351-360[85]
Nanoprobe (peptides as targeting groups)	QD705	2-^{18}F-fluoropropionate	^{18}F-FP-QD-RGD-BBN	λ_{ex} = 420 nm λ_{em} = 705 nm	NIRF/PET	RGD-bombesin (BBN)	$\alpha_v\beta_3$ integrin/GRPR	N/A	Prostate cancer	J. Nucl. Med. 2015, 56, 1278-1284[86]
Nanoprobe	NIR797	^{68}Ga-NOTA	^{68}Ga-MNP-SiO_2(NIR797)	λ_{ex} = 710-760 nm λ_{em} = 780-950nm	NIRF/PET/MRI	N/A	Sentinel lymph node	N/A	Cancer	Nanomedicine 2012, 7, 219-229[87]
Small Biomolecules	BODIPY	^{18}F-BODIPY	^{18}F-Bodipy-C_{16}/triglyceride	λ_{ex} = 460-490 nm λ_{em} = 510-550 nm	OFI/PET	triglyceride	Human primary adipocyte cells (Brown adipose tissue)	N/A	Obesity	PLoS One 2017, 12, e0182297[88]
Small Biomolecule	Cy7	^{18}F (labelled *via* boron trap)	^{18}F-BOMB Lymphoseek	λ_{ex} = 755 nm λ_{em} = 772 nm	NIRF/PET	Lymphoseek	Sentinel lymph node	N/A	Cancer	Bioconjugate Chem. 2010, 21, 1811-1819[89]
Small Molecule	Cy5	^{18}F	^{18}F-labeled Cy5	λ_{ex} = 640 nm λ_{em} = 700 nm	NIRF/PET	N/A	N/A	N/A	Cancer	Int. J. Mol. Sci. 2017, 18, 1214[90]
Small Molecule	Fluorescein	^{18}F	^{18}F-labeled fluorescein	λ_{ex} = 450 nm λ_{em} = 535 nm	OFI/PET	N/A	Spontaneous cerebrospinal fluid leaks	N/A	Trauma (Brain and Spine Damage)	Theranostics 2017, 7, 2377-2391[91]
Small Molecule	BODIPY	^{18}F-BODIPY	^{18}F-labeled ammonium BODIPY	λ_{ex} = 488 nm λ_{em} = 518 nm	OFI/PET/CT	N/A	N/A	N/A	Myocardial perfusion	Chem. Eur. J. 2016, 22, 12122-12129[92]
Small Molecule	Rodamine	^{18}F	^{18}F-labeled Rodamine	N/A	OFI/PET	N/A	N/A	N/A	Myocardial perfusion	Nucl. Med. Biol. 2015, 42, 796-803[93]
Small Molecule	BODIPY	^{18}F-BODIPY	^{18}F-labeled BODIPY	N/A	OFI/PET	N/A	N/A	N/A	Myocardial perfusion	Nucl. Med. Biol. 2014, 41, 120-126[94]

Table S6 Representative OFI/SPECT dual-modality imaging probes.

Category	Fluorophore	Radioisotope/ Chelator	Imaging Agents	Fluorescence Imaging Conditions	Imaging Modalities	Targeting Moiety	Biological Targets of Interest	Combined Therapy	Disease	Reference
Antibody	IRDye800CW	^{111}In-DTPA	^{111}In-DTPA-labetuzumab-IRDye800CW	λ_{ex} = 745 nm λ_{em} = 810-885 nm (ICG filter)	NIRF/SPECT	Labetuzumab (mAb)	carcinoembryonic antigen (CEA) expressing micrometastases	N/A	Colorectal cancer	J. Nucl. Med. 2017, 58, 706-710[95]
Antibody	IRDye800CW	^{111}In-DTPA	^{111}In-DTPA-MN-14-IRDye800CW	λ_{ex} = 745 nm λ_{em} = 810-885 nm (ICG)	NIRF/SPECT	MN-14 (mAb)	carcinoembryonic antigen (CEA)	N/A	Colorectal cancer	J. Nucl. Med. 2014, 55, 1519-1524[96]
Antibody	IRDye800CW	^{111}In-DTPA	^{111}In-DTPA-D2B-IRDye800CW	N/A	NIRF/SPECT	D2B (mAb)	Prostate-specific membrane antigen (PSMA)	N/A	Prostate cancer	J. Nucl. Med. 2014, 55, 995-1001[97]
Antibody	IRDye800CW	^{111}In-DTPA	^{111}In-DTPA-G250-IRDye800CW	N/A	NIRF/SPECT	G250 (mAb)	CAIX expressing tumor	N/A	Renal tumor	J. Urol. 2015, 194, 532-538[98]
Antibody	ZW800-1	^{111}In-DTPA	^{111}In-DTPA-Lys(ZW800)-Cys-ATN-658	λ_{ex} = 773 nm λ_{em} = 790 nm (ZW800-1)	NIRF/SPECT	ATN-658 (mAb)	Urokinase-type plasminogen activator receptor (uPAR)	N/A	cancer	Oncotarget 2014, 6, 14260-14273[99]
Antibody, Lysine-based MSAP platform	Cy5.5 / Cy7	^{111}In-SMCC	trastuzumab-Cy5.5-SMCC cetuximab-Cy7-SMCC	N/A	NIRF/PET	Trastuzumab / cetuximab	HER-2/EGFR	N/A	cancer	Bioorg. Med. Chem. 2009, 17, 5176-5181[100]
Lysine-based MSAP platform	IRDye800CW	^{99m}Tc/Re-MAS$_3$	Pam-Tc/Re-800 (lysine as linker)	N/A	NIRF/SPECT/CT	Bisphosphonates	Breast cancer microcalcification	N/A	Breast cancer	J. Am. Chem. Soc. 2008, 130, 17648-17649[101]
Lysine-based MSAP platform	Cy5.5	^{111}In-DTPA	^{111}In-MSAP-RGD	λ_{ex} = 615-665 nm λ_{em} = 695-770 nm	NIRF/SPECT	RGD (peptide)	$\alpha_v\beta_3$ integrin expressing cancer	N/A	Cancer	ChemBioChem 2012, 13, 1039-1045[102]
Lysine-based MSAP platform	Cy5.5	^{111}In-DOPA	^{111}In-DOPA-Cy5.5-PEG$_{5000}$-RGD (lysine as linker)	N/A	NIRF/SPECT	RGD (peptide)	$\alpha_v\beta_3$ integrin expressing cancer	N/A	Cancer	PLoS One 2013, 8, e58290[103]
Lysine-based MSAP platform	Cy7	^{99m}Tc-nicotinic acid and tricine	^{99m}Tc-PC-1007 (lysine as linker)	λ_{ex} = 745 nm λ_{em} = 820 nm	NIRF/SPECT	Cy7	Cancer	N/A	Cancer	Bioorg. Med. Chem. Lett. 2013, 23, 6350-6354[104]
Lysine-based MSAP platform	IR783	^{111}In-DOTA	^{111}In-DOTA-Lys(PEG)-Cys-IR783	λ_{ex} = 561nm λ_{em} = mCherry filter	NIRF/SPECT	N/A	N/A	N/A	Cancer	PLoS One 2014, 9, e95406[105]
Lysine-based MSAP platform	Cy5.5	^{99m}Tc-HYNIC	Avidin preinjection ^{99m}Tc-HYNIC-lysine(Cy5.5)-PEG$_4$-biotin	N/A	NIRF/SPECT	biotin	Avidin pretargeted cancer cells	N/A	Cancer	Sci. Rep. 2016, 6, 18905[106]
nanoprobe	ICG	^{99m}Tc-albumin colloid	ICG-^{99m}Tc-nanocolloid	Handheld NIRF fluorescence camera	NIRF/SPECT	N/A	Sentinel lymph node	N/A	Cancer	Eur. J. Nucl. Med. Mol. Imaging 2016, 43, 1857-1867[107] Eur. J. Nucl. Med. Mol. Imaging 2015, 42, 1631-1638[108]

nanoprobe	ICG	^{177}Lu-DOTA	ICG@DPDCs-^{177}Lu (cerasome nanoparticles)	λ_{ex} = 745 nm λ_{em} = 820 nm	NIRF/SPECT/CT	N/A	(Lewis lung carcinoma)	PTT	Cancer	J. Nucl. Med. 2012, 53, 1034-1040[109] ACS Appl. Mater. Interfaces 2015, 7, 22095-22105[110]
nanoprobe	Alexa 647	^{111}In/Gd-DOTA	^{111}In/Gd-DOTA @HPG (polymer nanoparticles)	N/A	OFI/SPECT/MRI	N/A	Tumor vascular structure	N/A	Cancer	Bioconjugate Chem. 2012, 23, 372-381[111]
nanoprobe	Fluorescein	^{111}In/Gd-DOTA	Multimodal liposomes	N/A	OFI/SPECT/MRI	N/A	(biodistribution)	N/A	N/A	Biomaterials 2013, 34, 1179-1192[112]
nanoprobe	Cy7	^{111}In-DTPA	Annexin A5-CCPM polymeric micelles	N/A	NIRF/SPECT/CT	Annexin A5 (protein)	Phosphatidylserine on dying cells (apoptosis)	N/A	Cancer/ Hepatic apoptosis	J. Nucl. Med. 2011, 52, 958-964[113] Mol. Imaging 2013, 12, 182-190[114]
nanoprobe	YPO_4 NPs	$^{111}InCl_3$	PEG-^{111}In-YPO_4 NPs	λ_{ex} = 980 nm λ_{em} = 1000-1350 nm	OTN-NIR/SPECT/CT	N/A	N/A	N/A	N/A	J. Photopolym. Sci. Technol. 2016, 29, 525-532[115]
Small biomolecules (RNA)	Alexa Fluor 633	^{99m}Tc-MAG3	^{99m}Tc and Alexa Fluor 633 labelled 28S fungal rRNA-targeted MORF	N/A	OFI/SPECT/CT	Sequence-specific MORF	28S rRNA gene of Aspergillus	N/A	Fungal infection	Nucl. Med. Biol. 2013, 40, 89-96[116]
Small biomolecules (LPS)	BODIPY	^{111}In-DOTA	^{111}In-DOTA-Bodipy-LPS	λ_{ex} = 514 nm λ_{em} = 537-600 nm	OFI/SPECT/CT	LPS	Hepatocytes and Kuppfer cells in liver	N/A	Gram-negative bacteria infection	ACS Chem. Biol. 2014, 9, 656-662[117]
Small biomolecules (RGD)	CdTe QDs	$^{188}Re(His)(CO)_3$	^{188}Re-HGRGD(D)F-CdTe QDs	N/A	NIRF/SPECT	RGD (peptide)	$\alpha_v\beta_3$ integrin expressing cancer	N/A	Cancer	Talanta 2011, 85, 936-942[118]
Small molecule	$Re(pyta)(CO)_3$	$^{99m}Tc(IDA)(CO)_3$	$Re(pyta)(CO)_3$-$^{99m}Tc(IDA)(CO)_3$	λ_{ex} = 321 nm λ_{em} = 496 nm	OFI/SPECT	N/A	N/A	N/A	N/A	Dalton Trans. 2014, 43, 439-450[119]

Table S7 Representative OFI/PAI dual-modality imaging probes.

Category	Fluorophore	Photoacoustic contrast agent	Imaging Agents	Imaging Conditions	Imaging Modalities	Targeting Moiety	Biological Targets	Combined Therapy	Disease	Reference
Nanoprobe (core-shell)	ICG	Au Nanorods	Au@liposome–ICG	λ_{ex} = 745 nm λ_{em} = 840 nm λ_{ex} = 780 nm (MSOT)	NIRF/MSOT	(EPR effect)	cancer	PTT	Liver cancer	Bioconjugate Chem. 2017, 28, 1221-1228[120]
Nanoprobe (core-shell)	ICG	Au Nanorods	ICG-loaded Au@SiO_2	λ_{ex} = 745 nm λ_{em} = 800 nm λ_{ex} = 680-960 nm (MSOT)	NIRF/MSOT	N/A	N/A	N/A	Cancer, Leg ischemia of diabetic disease	Nanoscale 2016, 8, 14480-14488[121]
Nanoprobe (core-shell)	NIR-797	Au Nanorods	double-labeled NIR-liposome–AuNR hybrids	λ_{ex} = 700-900 nm (MSOT)	NIRF/MSOT	N/A	N/A	N/A	Cancer	J. Am. Chem. Soc. 2012, 134, 13256-13258[122]
Nanoprobe (core-shell)	QDs	Au Nanorods	Au NRs@SiO_2-QDs-Ad/CD-PGEA (Au NRs as CT contrast agent)	λ_{em} ≈ 690 nm	NIRF/PAI/CT	N/A	N/A	PTT Chemotherapy Genetherapy	Cancer	Small 2017, 13, 1603133[123]
Nanoprobe (core-shell)	ICG	Ag NPs	ICG-Ag@PANI	λ_{ex} = 704 nm λ_{em} = 735 nm	NIRF/PAI	(EPR effect)	cancer	PTT PDT	Cancer	ACS Appl. Mater. Interfaces 2016, 8, 34991-35003[124]
Nanoprobe (core-shell)	Cy5.5	IR825	PFOB@IR825-HA-Cy5.5 (PFOB as X-ray contrast agent)	λ_{ex} = 640 nm λ_{em} = 650-800 nm	OFI/PAI/CT	Hyaluronic acid (HA)	Hyaluronidases in the tumor	PTT	Cancer	Biomaterial 2017, 132, 72-84[125]
Nanoprobe	NIR-830	Iron oxide nanoparticles (IONP)	NIR-830-$Z_{HER2:342}$-IONP NIR-830-BSA-IONP	λ_{ex} = 797 nm λ_{em} = 830 nm	OFI/PAI	$Z_{HER2:342}$ (a 58 amino acid scaffold protein)	HER-2	N/A	Cancer	Nanomedicine 2014, 10, 669-677[126]
Nanoprobe (core-shell)	Cypat-C18 or PPCy-C8	Cypat-C18 or PPCy-C8	Dye-liposome@perfluorocarbon	λ_{ex} = 700 nm λ_{em} = 775 nm	NIRF/PAI	N/A	Sentinel lymph node	PTT	Cancer metathesis	ACS Nano 2011, 5, 173-182[127]
Nanoprobe	Chlorin e6	SWCNT	Ce6@Albumin-EB@SWCNT	λ_{ex} = 670 nm (NIRF) λ_{ex} = 808 nm (PA&PTT) λ_{ex} = 630 nm (PDT)	NIRF/PAI	N/A	N/A	PTT PDT	Cancer	Biomaterial 2016, 103, 219-228[128]
Nanoprobe	Dox	Hollow gold nanoshells (HAuNS)	Dox@PEG-HAuNS	λ_{ex} = 500 nm (OFI) λ_{em} = 600 nm λ_{ex} = 800 nm (PAI)	OFI/PAI	N/A	N/A	PTT	Cancer	J. Controlled Release 2013, 172, 152-158[129]
Nanoprobe (PEGlyated NIR dye)	CR780 (croconaine dye)	CR780	CR780-PEG5K	λ_{ex} = 633 nm (NIRF) λ_{ex} = 808 nm (PTT)	NIRF/PAI	N/A	N/A	PTT	Cancer	Biomaterial 2017, 129, 28-36[130]
Nanoprobe (PEGlyated NIR dye)	TBD (a BODIPY dimer)	TBD	PEGylated TBD	λ_{ex} = 740 nm (NIRF) λ_{em} = 820 nm λ_{ex} = 790 nm (PAI)	NIRF/PAI	N/A	N/A	N/A	Cancer	Biomacromolecules 2017, 18, 249-256[131]
Nanoprobe	ICG	ICG	rNGO-PEG/ICG	λ_{ex} = 633 nm (NIRF) λ_{ex} = 780 nm (PAI)	NIRF/PAI	N/A	N/A	N/A	Cancer	Nanoscale Res. Lett. 2016, 11, 85[132]

Nanoprobe	ICG	ICG	Liposomal ICG	λ_{em} = 800 nm λ_{ex} = 720-860 nm (MSOT)	NIRF/MSOT	N/A	N/A	N/A	Breast cancer	Eur. Radiol. 2016, 26, 1843-1851[133]
Nanoprobe	ICG	ICG	PEGylated liposomal ICG	λ_{ex} = 745 nm (NIRF) λ_{em} = 810-875 nm λ_{ex} = 680-900 nm (MSOT)	NIRF/MSOT	N/A	N/A	N/A	Cancer	Biomaterial 2015, 37, 415-424[134]
Antibody	ICG	ICG	Targeted PEGylated liposome-ICG-DOX	λ_{ex} = 780 nm (NIRF) λ_{em} = 810 nm λ_{ex} = 680-900 nm (MSOT)	NIRF/MSOT	hCTM01 (antibody)	MUC-1	Chemotherapy (DOX)	Cancer	Int. J. Pharm. 2015, 482, 2-10[135]
Antibody	Fluorescein	BHQ3	BHQ3-Fluorescein Trastuzumab	λ_{ex} = 700 nm (PAI) λ_{ex} = 445-490 nm λ_{em} > 515 nm	OFT/PAI	trastuzumab	Her2	N/A	Cancer	Mol. Imaging 2014, 13, 1-9[136]
Small molecule	ICG	ICG	ICG	λ_{ex} = 784 nm (NIRF) λ_{em} = 830 nm λ_{em}=618, 668 nm	NIRF/MOST	N/A	Sentinel lymph nodes	N/A	Cancer metathesis	Radiology 2010, 255, 442-450[137]
Small molecule	CDnir7	CDnir7	CDnir7	λ_{ex} = 900 nm (PA)	NIRF/MSOT	CDnir7	microphages	N/A	Inflammation	Chem. Commun. 2014, 50, 6589-6591[138]
Small molecule	Cy7-derived dye	Cy7-derived dye	Cy7-NMDAR targeting group	λ_{ex} = 750 nm (NIRF) λ_{em} = 780 nm λ_{ex} = 700-900 nm (MSOT)	NIRF/MSOT	Competitive or noncompetitive antagonists of NMDAR	*N*-methyl-D-aspartate receptors (NMDARs)	N/A	Neuropsychiatric pathologies	Chem. Commun. 2015, 51, 15149-15152[139]
Small molecule	Usq (a squaraine dye)	Usq	Usq	λ_{ex} = 675 ± 15 nm (NIRF) λ_{em} = 700 ± 10 nm λ_{ex} = 680 nm (MSOT)	NIRF/MSOT	Squaraine dye as Michael acceptor	Blood aminothiols	N/A	N/A	Chem. Sci. 2016, 7, 4110-4116[140]

References:

[1] James ML, Gambhir SS. A molecular imaging primer: modalities, imaging agents, and applications[J]. Physiol. Rev., 2012, 92:897-965.

[2] Chen YL, Wang SY, Liu RS, et al. Remnant living cells that escape cell loss in late-stage tumors exhibit cancer stem cell-like characteristics[J]. Cell Death & Disease, 2012, 3

[3] Lu Y-C, Yang C-X, Yan X-P. Radiopaque tantalum oxide coated persistent luminescent nanoparticles as multimodal probes for in vivo near-infrared luminescence and computed tomography bioimaging[J]. Nanoscale, 2015, 7:17929-17937.

[4] Chen J, Yang X-Q, Meng Y-Z, et al. Reverse microemulsion-mediated synthesis of Bi2S3-QD@SiO2-PEG for dual modal CT-fluorescence imaging in vitro and in vivo[J]. Chem. Commun., 2013, 49:11800-11802.

[5] Qin M-Y, Yang X-Q, Wang K, et al. In vivo cancer targeting and fluorescence-CT dual-mode imaging with nanoprobes based on silver sulfide quantum dots and iodinated oil[J]. Nanoscale, 2015, 7:19484-19492.

[6] Liu Z, Pu F, Huang S, et al. Long-circulating Gd2O3:Yb3+, Er3+ up-conversion nanoprobes as high-performance contrast agents for multi-modality imaging[J]. Biomaterials, 2013, 34:1712-1721.

[7] Zhou Z, Chen H, Lipowska M, et al. A dual-modal magnetic nanoparticle probe for preoperative and intraoperative mapping of sentinel lymph nodes by magnetic resonance and near infrared fluorescence imaging[J]. J. Biomater. Appl., 2013, 28:100-111, 112.

[8] Liu Y, Tian G-F, He X-W, et al. Microwave-assisted one-step rapid synthesis of near-infrared gold nanoclusters for NIRF/CT dual-modal bioimaging[J]. J. Mater. Chem. B, 2016, 4:1276-1283.

[9] Xia H-X, Yang X-Q, Song J-T, et al. Folic acid-conjugated silica-coated gold nanorods and quantum dots for dual-modality CT and fluorescence imaging and photothermal therapy[J]. J. Mater. Chem. B, 2014, 2:1945-1953.

[10] Zhang J, Li C, Zhang X, et al. In vivo tumor-targeted dual-modal fluorescence/CT imaging using a nanoprobe co-loaded with an aggregation-induced emission dye and gold nanoparticles[J]. Biomaterials, 2015, 42:103-111.

[11] Zhu F-P, Chen G-T, Wang S-J, et al. Dual-modality imaging probes with high magnetic relaxivity and near-infrared fluorescence based highly aminated mesoporous silica nanoparticles[J]. J. Nanomater., 2016:6502127.

[12] Gao A, Zhang D, Yin X-B. Near infrared fluorescence-magnetic resonance dual-modal imaging with Cy5-labeled, Gd-Al co-doped mesoporous silica nanoparticles[J]. Anal. Methods, 2016, 8:214-221.

[13] Zhang D, Gao A, Xu Y, et al. Gd-Al co-doped mesoporous silica nanoparticles loaded with Ru(bpy)32+ as a dual-modality probe for fluorescence and magnetic resonance imaging[J]. Analyst (Cambridge, U. K.), 2014, 139:4613-4619.

[14] Abdukayum A, Yang C-X, Zhao Q, et al. Gadolinium Complexes Functionalized Persistent Luminescent Nanoparticles as a Multimodal Probe for Near-Infrared Luminescence and Magnetic Resonance Imaging in Vivo[J]. Anal. Chem., 2014, 86:4096-4101.

[15] Zhang Y, Das GK, Vijayaragavan V, et al. "Smart" theranostic lanthanide nanoprobes with simultaneous up-conversion fluorescence and tunable T1-T2 magnetic resonance imaging contrast and near-infrared activated photodynamic therapy[J]. Nanoscale, 2014, 6:12609-12617.

[16] Pan Y, Yang J, Fang Y, et al. One-pot synthesis of gadolinium-doped carbon quantum dots for high-performance multimodal bioimaging[J]. J. Mater. Chem. B, 2017, 5:92-101.

[17] Shi Y, Pan Y, Zhong J, et al. Facile synthesis of gadolinium (III) chelates functionalized carbon quantum dots for fluorescence and magnetic resonance dual-modal bioimaging[J]. Carbon, 2015, 93:742-750.

[18] Chen F, Chen M, Yang C, et al. Terbium-doped gadolinium oxide nanoparticles prepared by laser ablation in liquid for use as a fluorescence and magnetic resonance imaging dual-modal contrast agent[J]. Phys. Chem. Chem. Phys., 2015, 17:1189-1196.

[19] Hu H, Sheng Y, Ye M, et al. A porphyrin-based magnetic and fluorescent dual-modal nanoprobe for tumor imaging[J]. Polymer, 2016, 88:94-101.

[20] Liu J, Li K, Geng J, et al. Single molecular hyperbranched nanoprobes for fluorescence and magnetic resonance dual modal imaging[J]. Polym. Chem., 2013, 4:1517-1524.

[21] Xu H, Regino CAS, Koyama Y, et al. Preparation and Preliminary Evaluation of a Biotin-Targeted, Lectin-Targeted Dendrimer-Based Probe for Dual-Modality Magnetic Resonance and Fluorescence Imaging[J]. Bioconjugate Chem., 2007, 18:1474-1482.

[22] Li K, Ding D, Huo D, et al. Conjugated Polymer Based Nanoparticles as Dual-Modal Probes for Targeted In Vivo Fluorescence and Magnetic Resonance Imaging[J]. Adv. Funct. Mater., 2012, 22:3107-3115, S3107/3101-S3107/3107.

[23] Gao GH, Heo H, Lee JH, et al. An acidic pH-triggered polymeric micelle for dual-modality MR and optical imaging[J]. J. Mater. Chem., 2010, 20:5454-5461.

[24] Bumb A, Regino CAS, Perkins MR, et al. Preparation and characterization of a magnetic and optical dual-modality molecular probe[J]. Nanotechnology, 2010, 21:175704/175701-175704/175709.

[25] Gianella A, Jarzyna PA, Mani V, et al. Multifunctional nanoemulsion platform for imaging guided therapy evaluated in experimental cancer[J]. ACS Nano, 2011, 5:4422-4433.

[26] Chen Y-C, Wen S, Shang S-A, et al. Magnetic resonance and near-infrared imaging using a novel dual-modality nano-probe for dendritic cell tracking in vivo[J]. Cytotherapy, 2014, 16:699-710.

[27] Chen O, Riedemann L, Etoc F, et al. Magneto-fluorescent core-shell supernanoparticles[J]. Nat. Commun., 2014, 5:5093.

[28] Wang F, Chen Z, Zhu L. cRGD-conjugated magnetic-fluorescent liposomes for targeted dual-modality imaging of bone metastasis from prostate cancer[J]. J. Liposome Res., 2015, 25:89-100.

[29] Yin C, Hong B, Gong Z, et al. Fluorescent oligo(p-phenyleneethynylene) contained amphiphiles-encapsulated magnetic nanoparticles for targeted magnetic resonance and two-photon optical imaging in vitro and in vivo[J]. Nanoscale, 2015, 7:8907-8919.

[30] Yang HY, Jang M-S, Li Y, et al. Multifunctional and Redox-Responsive Self-Assembled Magnetic Nanovectors for Protein Delivery and Dual-Modal Imaging[J]. ACS Appl. Mater. Interfaces, 2017, 9:19184-19192.

[31] Yan XJ, Song XY, Wang ZB. Construction of specific magnetic resonance imaging/optical dual-modality molecular probe used for imaging angiogenesis of gastric cancer[J]. Artificial Cells Nanomedicine and Biotechnology, 2017, 45:399-403.

[32] Qiao H, Wang Y, Zhang R, et al. MRI/optical dual-modality imaging of vulnerable atherosclerotic plaque with an osteopontin-targeted probe based on Fe3O4 nanoparticles[J]. Biomaterials, 2017, 112:336-345.

[33] Chen Q, Shang W, Zeng C, et al. Theranostic imaging of liver cancer using targeted optical/MRI dual-modal probes[J]. Oncotarget, 2017, 8:32741-32751.

[34] Fan Z, Senapati D, Singh AK, et al. Theranostic magnetic core-plasmonic shell star shape nanoparticle for the isolation of targeted rare tumor cells from whole blood, fluorescence imaging, and photothermal destruction of cancer[J]. Mol. Pharm., 2013, 10:857-866.

[35] Ding K, Liu C, Hou Y, et al. Magnetically engineered Cd-free quantum dots as dual-modality probes for fluorescence/magnetic resonance imaging of tumors[J]. Biomaterials, 2014, 35:1608-1617.

[36] Guo C, Xu M, Xu S, et al. Multifunctional nanoprobes for both fluorescence and 19F magnetic resonance imaging[J]. Nanoscale, 2017, 9:7163-7168.

[37] Nakamura T, Sugihara F, Matsushita H, et al. Mesoporous silica nanoparticles for 19F magnetic resonance imaging, fluorescence imaging, and drug delivery[J]. Chem. Sci., 2015, 6:1986-1990.
[38] Goswami LN, Khan AA, Jalisatgi SS, et al. Synthesis and in vitro assessment of a bifunctional closomer probe for fluorine (19F) magnetic resonance and optical bimodal cellular imaging[J]. Chem. Commun., 2014, 50:5793-5795.
[39] Wang X-Y, Ju S, Li C, et al. Non-invasive imaging of endothelial progenitor cells in tumor neovascularization using a novel dual-modality paramagnetic/near-infrared fluorescence probe[J]. PLoS One, 2012, 7:e50575.
[40] Ju S, Qiu Y, Li C, et al. Multimodality Imaging of Endothelial Progenitor Cells with a Novel Multifunctional Probe Featuring Positive Magnetic Resonance Contrast and Near-Infrared Fluorescence[J]. Mol. Imaging, 2011, 10:359-369.
[41] Harrison VSR, Carney CE, MacRenaris KW, et al. Multimeric near IR–MR contrast agent for multimodal in vivo imaging[J]. J. Am. Chem. Soc., 2015, 137:9108-9116.
[42] Yamane T, Hanaoka K, Muramatsu Y, et al. Method for enhancing cell penetration of Gd3+-based MRI contrast agents by conjugation with hydrophobic fluorescent dyes[J]. Bioconjugate Chem., 2011, 22:2227-2236.
[43] Guo K, Berezin MY, Zheng J, et al. Near infrared-fluorescent and magnetic resonance imaging molecular probe with high T1 relaxivity for in vivo multimodal imaging[J]. Chemical Communications, 2010, 46:3705-3707.
[44] Mishra A, Mishra R, Gottschalk S, et al. Microscopic Visualization of Metabotropic Glutamate Receptors on the Surface of Living Cells Using Bifunctional Magnetic Resonance Imaging Probes[J]. Acs Chem. Neurosci., 2014, 5:128-137.
[45] You Y, Tomat E, Hwang K, et al. Manganese displacement from Zinpyr-1 allows zinc detection by fluorescence microscopy and magnetic resonance imaging[J]. Chem. Commun. (Cambridge, U. K.), 2010, 46:4139-4141.
[46] Dong D, Jing X, Zhang X, et al. Gadolinium(III)-fluorescein complex as a dual modal probe for MRI and fluorescence zinc sensing[J]. Tetrahedron, 2012, 68:306-310.
[47] Wang Y, Song R, Feng H, et al. Visualization of Fluoride Ions In Vivo Using a Gadolinium(III)-Coumarin Complex-Based Fluorescence/MRI Dual-Modal Probe[J]. Sensors, 2016, 16
[48] Wang Y, Song R, Guo K, et al. A gadolinium(III) complex based dual-modal probe for MRI and fluorescence sensing of fluoride ions in aqueous medium and in vivo[J]. Dalton Trans., 2016, 45:17616-17623.
[49] Du T, Zhao C, Rehman FU, et al. In Situ Multimodality Imaging of Cancerous Cells Based on a Selective Performance of Fe2+-Adsorbed Zeolitic Imidazolate Framework-8[J]. Advanced Functional Materials, 2017, 27
[50] Liu X, Jiang H, Ye J, et al. Nitrogen-doped carbon quantum dot stabilized magnetic iron oxide nanoprobe for fluorescence, magnetic resonance, and computed tomography triple-modal in vivo bioimaging[J]. Adv. Funct. Mater., 2016, 26:8694-8706.
[51] Dong WJ, Li YS, Niu DC, et al. A simple route to prepare monodisperse Au NP-decorated, dye-doped, superparamagnetic nanocomposites for optical, MR, and CT trimodal imaging[J]. Small, 2013, 9:2500-2508.
[52] Xue S, Wang Y, Wang M, et al. Iodinated oil-loaded, fluorescent mesoporous silica-coated iron oxide nanoparticles for magnetic resonance imaging/computed tomography/fluorescence trimodal imaging[J]. Int. J. Nanomed., 2014, 9:2527-2538.
[53] Yang G, Gong H, Liu T, et al. Two-dimensional magnetic WS2@Fe3O4 nanocomposite with mesoporous silica coating for drug delivery and imaging-guided therapy of cancer[J]. Biomaterials, 2015, 60:62-71.
[54] Wu B, Wan B, Lu S-T, et al. Near-infrared light-triggered theranostics for tumor-specific enhanced multimodal imaging and photothermal therapy[J]. Int. J. Nanomed., 2017, 12:4467-4478.
[55] Han L, Xia J-M, Hai X, et al. Protein-stabilized gadolinium oxide-gold nanoclusters hybrid for multimodal imaging and drug delivery[J]. ACS Appl. Mater. Interfaces, 2017, 9:6941-6949.
[56] Wu X, Li C, Liao S, et al. Silica-Encapsulated Gd3+-Aggregated Gold Nanoclusters for In Vitro and In Vivo Multimodal Cancer Imaging[J]. Chemistry-a European Journal, 2014, 20:8876-8882.
[57] Hu DH, Sheng ZH, Zhang PF, et al. Hybrid gold-gadolinium nanoclusters for tumor-targeted NIRF/CT/MRI triple-modal imaging in vivo[J]. Nanoscale, 2013, 5:1624-1628.
[58] Dong K, Ju E, Liu J, et al. Ultrasmall biomolecule-anchored hybrid GdVO4 nanophosphors as a metabolizable multimodal bioimaging contrast agent[J]. Nanoscale, 2014, 6:12042-12049.
[59] Deng X, Dai Y, Liu J, et al. Multifunctional hollow CaF2:Yb3+/Er3+/Mn2+-poly(2-aminoethyl methacrylate) microspheres for Pt(IV) pro-drug delivery and tri-modal imaging[J]. Biomaterials, 2015, 50:154-163.
[60] Ma D, Meng L, Chen Y, et al. NaGdF4:Yb3+/Er3+@NaGdF4:Nd3+@Sodium-Gluconate: Multifunctional and Biocompatible Ultrasmall Core-Shell Nanohybrids for UCL/MR/CT Multimodal Imaging[J]. Acs Applied Materials & Interfaces, 2015, 7:16257-16265.

[61] Zeng S, Tsang M-K, Chan C-F, et al. PEG modified BaGdF5:Yb/Er nanoprobes for multi-modal upconversion fluorescent, in vivo X-ray computed tomography and biomagnetic imaging[J]. Biomaterials, 2012, 33:9232-9238.
[62] Xia A, Chen M, Gao Y, et al. Gd3+ complex-modified NaLuF4-based upconversion nanophosphors for trimodality imaging of NIR-to-NIR upconversion luminescence, X-Ray computed tomography and magnetic resonance[J]. Biomaterials, 2012, 33:5394-5405.
[63] Xing H, Bu W, Zhang S, et al. Multifunctional nanoprobes for upconversion fluorescence, MR and CT trimodal imaging[J]. Biomaterials, 2012, 33:1079-1089.
[64] Cohen R, Vugts DJ, Stigter-van Walsum M, et al. Inert coupling of IRDye800CW and zirconium-89 to monoclonal antibodies for single- or dual-mode fluorescence and PET imaging[J]. Nature Protocols, 2013, 8:1010-1018.
[65] Ghosh SC, Ghosh P, Wilganowski N, et al. Multimodal chelation platform for near-infrared fluorescence/nuclear imaging[J]. J. Med. Chem., 2013, 56:406-416.
[66] Hall MA, Kwon S, Robinson H, et al. Imaging prostate cancer lymph node metastases with a multimodality contrast agent[J]. Prostate, 2012, 72:129-146.
[67] Hall MA, Pinkston KL, Wilganowski N, et al. Comparison of mAbs Targeting Epithelial Cell Adhesion Molecule for the Detection of Prostate Cancer Lymph Node Metastases with Multimodal Contrast Agents: Quantitative Small-Animal PET/CT and NIRF[J]. Journal of Nuclear Medicine, 2012, 53:1427-1437.
[68] Zhang Y, Hong H, Engle JW, et al. Positron Emission Tomography and Optical Imaging of Tumor CD105 Expression with a Dual-Labeled Monoclonal Antibody[J]. Molecular Pharmaceutics, 2012, 9:645-653.
[69] Hong H, Zhang Y, Severin GW, et al. Multimodality Imaging of Breast Cancer Experimental Lung Metastasis with Bioluminescence and a Monoclonal Antibody Dual-Labeled with Zr-89 and IRDye 800CW[J]. Molecular Pharmaceutics, 2012, 9:2339-2349.
[70] Sampath L, Kwon S, Hall MA, et al. Detection of cancer metastases with a dual-labeled near-infrared/positron emission tomography imaging agent[J]. Transl. Oncol., 2010, 3:307-317.
[71] Paudyal P, Paudyal B, Iida Y, et al. Dual functional molecular imaging probe targeting CD20 with PET and optical imaging[J]. Oncology Reports, 2009, 22:115-119.
[72] Rodriguez EA, Wang Y, Crisp JL, et al. New dioxaborolane chemistry enables F-18 -positron-emitting, fluorescent F-18 -multimodality biomolecule generation from the solid phase[J]. Bioconjugate Chem., 2016, 27:1390-1399.
[73] Hendricks JA, Keliher EJ, Wan D, et al. Synthesis of F-18 BODIPY: bifunctional reporter for hybrid optical/positron emission tomography imaging[J]. Angew. Chem. Int. Ed., 2012, 51:4603-4606.
[74] Paulus A, Desai P, Carney B, et al. Development of a clickable bimodal fluorescent/PET probe for in vivo imaging[J]. EJNMMI Res., 2015, 5:1-9.
[75] Liu S, Lin T-P, Li D, et al. Lewis Acid-Assisted Isotopic F-18-F-19 Exchange in BODIPY Dyes: Facile Generation of Positron Emission Tomography/Fluorescence Dual Modality Agents for Tumor Imaging[J]. Theranostics, 2013, 3:181-189.
[76] Summer D, Grossrubatscher L, Petrik M, et al. Developing targeted hybrid imaging probes by chelator scaffolding[J]. Bioconjugate Chem., 2017, 28:1722-1733.
[77] Brand C, Abdel-Atti D, Zhang Y, et al. In Vivo Imaging of GLP-1R with a Targeted Bimodal PET/Fluorescence Imaging Agent[J]. Bioconjugate Chemistry, 2014, 25:1323-1330.
[78] Liu SL, Li D, Huang CW, et al. Efficient construction of PET/fluorescence probe based on sarcophagine cage: An opportunity to integrate diagnosis with treatment[J]. Mol. Imaging Biol., 2012, 14:718-724.
[79] Sun L, Ding J, Xing W, et al. Novel strategy for preparing dual-modality optical/PET imaging probes via photo-click chemistry[J]. Bioconjugate Chem., 2016, 27:1200-1204.
[80] Sun Y, Ma X, Cheng K, et al. Strained cyclooctyne as a molecular platform for construction of multimodal imaging probes[J]. Angew. Chem. Int. Ed., 2015, 54:5981-5984.
[81] Deng H, Wang H, Wang M, et al. Synthesis and Evaluation of 64Cu-DOTA-NT-Cy5.5 as a Dual-Modality PET/Fluorescence Probe to Image Neurotensin Receptor-Positive Tumor[J]. Mol. Pharmaceutics, 2015, 12:3054-3061.
[82] Zhu L, Guo N, Li Q, et al. Dynamic PET and Optical Imaging and Compartment Modeling using a Dual-labeled Cyclic RGD Peptide Probe[J]. Theranostics, 2012, 2:746-756.
[83] Zhang H, Desai P, Koike Y, et al. Dual-modality imaging of prostate cancer with a fluorescent and radiogallium-labeled gastrin-releasing peptide receptor antagonist[J]. J. Nucl. Med., 2017, 58:29-35.
[84] Ghosh SC, Vargas SH, Rodriguez M, et al. Synthesis of a Fluorescently Labeled Ga-68-DOTA-TOC Analog for Somatostatin Receptor Targeting[J]. Acs Med. Chem. Lett., 2017, 8:720-725.
[85] Xiao L, Zhang Y, Yue W, et al. Heptamethine cyanine based Cu-64-PET probe PC-1001 for cancer imaging: Synthesis and in vivo evaluation[J]. Nucl. Med. Biol., 2013, 40:351-360.
[86] Hu K, Wang H, Tang G, et al. In vivo cancer dual-targeting and dual-modality imaging with functionalized quantum dots[J]. J. Nucl. Med., 2015, 56:1278-1284.
[87] Kim JS, Kim YH, Kim JH, et al. Development and in vivo imaging of a PET/MRI nanoprobe with enhanced NIR fluorescence by dye encapsulation[J]. Nanomedicine, 2012, 7:219-229.
[88] Paulus A, Maenen M, Drude N, et al. Synthesis, radiosynthesis and in vitro evaluation of F-18-Bodipy-C-16/triglyceride as a dual modal imaging agent for brown adipose tissue[J]. PLoS One, 2017, 12:0182297.
[89] Ting R, Aguilera TA, Crisp JL, et al. Fast F-18 Labeling of a Near-Infrared Fluorophore Enables Positron Emission Tomography and Optical Imaging of Sentinel Lymph Nodes[J]. Bioconjugate Chemistry, 2010, 21:1811-1819.

[90] An F-F, Kommidi H, Chen N, et al. A conjugate of pentamethine cyanine and F-18 as a positron emission tomography/near-infrared fluorescence probe for multimodality tumor imaging[J]. Int. J. Mol. Sci., 2017, 18:1214.
[91] Kommidi H, Guo H, Chen N, et al. An F-18 -positron-emitting, fluorescent, cerebrospinal fluid probe for imaging damage to the brain and spine[J]. Theranostics, 2017, 7:2377-2391.
[92] Chansaenpak K, Wang H, Wang M, et al. Synthesis and evaluation of F-18 -ammonium BODIPY dyes as potential positron emission tomography agents for myocardial perfusion imaging[J]. Chem. Eur. J. , 2016, 22:12122-12129.
[93] Bartholoma MD, Zhang SH, Akurathi V, et al. F-18-labeled rhodamines as potential myocardial perfusion agents: comparison of pharmacokinetic properties of several rhodamines[J]. Nucl. Med. Biol., 2015, 42:796-803.
[94] Liu S, Li D, Shan H, et al. Evaluation of F-18-labeled BODIPY dye as potential PET agents for myocardial perfusion imaging[J]. Nucl. Med. Biol., 2014, 41:120-126.
[95] Hekman MCH, Rijpkema M, Bos DL, et al. Detection of micrometastases using SPECT/fluorescence dual-modality imaging in a CEA-expressing tumor model[J]. J. Nucl. Med., 2017, 58:706-710.
[96] Rijpkema M, Oyen WJ, Bos D, et al. SPECT- and fluorescence image-guided surgery using a dual-labeled carcinoembryonic antigen-targeting antibody[J]. J. Nucl. Med., 2014, 55:1519-1524.
[97] Lutje S, Rijpkema M, Franssen GM, et al. Dual-modality image-guided surgery of prostate cancer with a radiolabeled fluorescent anti-PSMA monoclonal antibody[J]. J. Nucl. Med., 2014, 55:995-1001.
[98] Muselaers CHJ, Rijpkema M, Bos DL, et al. Radionuclide and fluorescence imaging of clear cell renal cell carcinoma using dual labeled anti-carbonic anhydrase IX antibody G250[J]. J. Urol., 2015, 194:532-538.
[99] Boonstra MC, van Driel PBAA, van Willigen DM, et al. uPAR-targeted multimodal tracer for pre- and intraoperative imaging in cancer surgery[J]. Oncotarget, 2015, 6:14260-14273.
[100] Xu H, Eck PK, Baidoo KE, et al. Toward preparation of antibody-based imaging probe libraries for dual-modality positron emission tomography and fluorescence imaging[J]. Bioorg. Med. Chem., 2009, 17:5176-5181.
[101] Bhushan KR, Misra P, Liu F, et al. Detection of breast cancer microcalcifications using a dual-modality SPECT/NIR fuorescent probe[J]. J. Am. Chem. Soc., 2008, 130:17648-17649.
[102] Bunschoten A, Buckle T, Visser NL, et al. Multimodal interventional molecular imaging of tumor margins and distant metastases by targeting alpha v beta 3 Integrin[J]. ChemBioChem, 2012, 13:1039-1045.
[103] Guo Y, Yuan H, Cho H, et al. High efficiency diffusion molecular retention tumor targeting[J]. PLoS One, 2013, 8:e58290.
[104] Zhang Y, Xiao L, Popovic K, et al. Novel cancer-targeting SPECT/NIRF dual-modality imaging probe Tc-99m-PC-1007: Synthesis and biological evaluation[J]. Bioorganic & Medicinal Chemistry Letters, 2013, 23:6350-6354.
[105] Guo Y, Yuan H, Claudio NM, et al. PEG-Like Nanoprobes: Multimodal, Pharmacokinetically and Optically Tunable Nanomaterials[J]. Plos One, 2014, 9
[106] Dong C, Yang S, Shi J, et al. SPECT/NIRF dual modality imaging for detection of intraperitoneal colon tumor with an avidin/biotin pretargeting system[J]. Sci. Rep., 2016, 6:18905.
[107] KleinJan GH, Bunschoten A, van den Berg NS, et al. Fluorescence guided surgery and tracer-dose, fact or fiction?[J]. Eur. J. Nucl. Med. Mol. Imaging, 2016, 43:1857-1867.
[108] Stoffels I, Leyh J, Poppel T, et al. Evaluation of a radioactive and fluorescent hybrid tracer for sentinel lymph node biopsy in head and neck malignancies: prospective randomized clinical trial to compare ICG-(99m)Tc-nanocolloid hybrid tracer versus (99m)Tc-nanocolloid[J]. Eur J Nucl Med Mol Imaging, 2015, 42:1631-1638.
[109] Brouwer OR, Buckle T, Vermeeren L, et al. Comparing the Hybrid Fluorescent-Radioactive Tracer Indocyanine Green-Tc-99m-Nanocolloid with Tc-99m-Nanocolloid for Sentinel Node Identification: A Validation Study Using Lymphoscintigraphy and SPECT/CT[J]. Journal of Nuclear Medicine, 2012, 53:1034-1040.
[110] Jing L, Shi J, Fan D, et al. Lu-177-labeled cerasomes encapsulating Indocyanine Green for cancer theranostics[J]. ACS Appl. Mater. Interfaces, 2015, 7:22095-22105.
[111] Saatchi K, Soema P, Gelder N, et al. Hyperbranched polyglycerols as trimodal imaging agents: design, biocompatibility, and tumor uptake[J]. Bioconjugate Chem., 2012, 23:372-381.
[112] Mitchell N, Kalber TL, Cooper MS, et al. Incorporation of paramagnetic, fluorescent and PET/SPECT contrast agents into liposomes for multimodal imaging[J]. Biomaterials, 2013, 34:1179-1192.
[113] Zhang R, Lu W, Wen X, et al. Annexin A5-Conjugated Polymeric Micelles for Dual SPECT and Optical Detection of Apoptosis[J]. Journal of Nuclear Medicine, 2011, 52:958-964.
[114] Zhang R, Huang M, Zhou M, et al. Annexin A5-functionalized nanoparticle for multimodal imaging of cell death[J]. Mol. Imaging, 2013, 12:182-190.
[115] Kamimura M, Saito R, Hyodo H, et al. Over-1000 nm near-infrared fluorescence and SPECT/CT dual-modal in vivo imaging based on rare-earth doped ceramic nanophosphors[J]. J. Photopolym. Sci. Technol., 2016, 29:525-532.
[116] Wang Y, Chen L, Liu X, et al. Detection of Aspergillus fumigatus pulmonary fungal infections in mice with Tc-99m-labeled MORF oligomers targeting ribosomal RNA[J]. Nucl. Med. Biol., 2013, 40:89-96.
[117] Duheron V, Moreau M, Collin B, et al. Dual labeling of lipopolysaccharides for SPECT-CT imaging and fluorescence microscopy[J]. ACS Chem. Biol., 2014, 9:656-662.
[118] Li Z, Zhang G, Shen H, et al. Synthesis and cell uptake of a novel dual modality 188Re-HGRGD (D) F-CdTe QDs probe[J]. Talanta, 2011, 85:936-942.

[119] Francois A, Auzanneau C, Le Morvan V, et al. A functionalized heterobimetallic 99mTc/Re complex as a potential dual-modality imaging probe: synthesis, photophysical properties, cytotoxicity and cellular imaging investigations[J]. Dalton Trans., 2014, 43:439-450.
[120] Guan T, Shang W, Li H, et al. From detection to resection: photoacoustic tomography and surgery guidance with Indocyanine Green loaded gold nanorod@liposome core-shell nanoparticles in liver cancer[J]. Bioconjugate Chem., 2017, 28:1221-1228.
[121] Peng D, Du Y, Shi Y, et al. Precise diagnosis in different scenarios using photoacoustic and fluorescence imaging with dual-modality nanoparticles[J]. Nanoscale, 2016, 8:14480-14488.
[122] Lozano N, Al-Jamal WT, Taruttis A, et al. Liposome-Gold Nanorod Hybrids for High-Resolution Visualization Deep in Tissues[J]. J. Am. Chem. Soc., 2012, 134:13256-13258.
[123] Duan S, Yang YJ, Zhang CL, et al. NIR-responsive polycationic gatekeeper-cloaked hetero-nanoparticles for multimodal imaging-guided triple-combination therapy of cancer[J]. Small, 2017, 13:1603133.
[124] Tan X, Wang J, Pang X, et al. Indocyanine green-loaded silver nanoparticle@polyaniline core/shell theranostic nanocomposites for photoacoustic/near-infrared fluorescence imaging-guided and single-light-triggered photothermal and photodynamic therapy[J]. ACS Appl. Mater. Interfaces, 2016, 8:34991-35003.
[125] Liang X, Fang L, Li X, et al. Activatable near infrared dye conjugated hyaluronic acid based nanoparticles as a targeted theranostic agent for enhanced fluorescence/CT/photoacoustic imaging guided photothermal therapy[J]. Biomaterials, 2017, 132:72-84.
[126] Xi L, Satpathy M, Zhao Q, et al. HER-2/neu targeted delivery of a nanoprobe enables dual photoacoustic and fluorescence tomography of ovarian cancer[J]. Nanomedicine (N. Y., NY, U. S.), 2014, 10:669-677.
[127] Akers WJ, Kim C, Berezin M, et al. Noninvasive Photoacoustic and Fluorescence Sentinel Lymph Node Identification using Dye-Loaded Perfluorocarbon Nanoparticles[J]. Acs Nano, 2011, 5:173-182.
[128] Xie LS, Wang GH, Zhou H, et al. Functional long circulating single walled carbon nanotubes for fluorescent/photoacoustic imaging-guided enhanced phototherapy[J]. Biomaterials, 2016, 103:219-228.
[129] Lee HJ, Liu Y, Zhao J, et al. In vitro and in vivo mapping of drug release after laser ablation thermal therapy with doxorubicin-loaded hollow gold nanoshells using fluorescence and photoacoustic imaging[J]. J. Control. Release, 2013, 172:152-158.
[130] Tang L, Zhang F, Yu F, et al. Croconaine nanoparticles with enhanced tumor accumulation for multimodality cancer theranostics[J]. Biomaterials, 2017, 129:28-36.
[131] Miki K, Enomoto A, Inoue T, et al. Polymeric Self-Assemblies with Boron-Containing Near-Infrared Dye Dimers for Photoacoustic Imaging Probes[J]. Biomacromolecules, 2017, 18:249-256.
[132] Chen J, Liu C, Zeng G, et al. Indocyanine green loaded reduced graphene oxide for in vivo photoacoustic/fluorescence dual-modality tumor imaging[J]. Nanoscale Res. Lett., 2016, 11:85.
[133] Ermolayev V, Dean-Ben XL, Mandal S, et al. Simultaneous visualization of tumour oxygenation, neovascularization and contrast agent perfusion by real-time three-dimensional optoacoustic tomography[J]. Eur. Radiol., 2016, 26:1843-1851.
[134] Beziere N, Lozano N, Nunes A, et al. Dynamic imaging of PEGylated indocyanine green (ICG) liposomes within the tumor microenvironment using multi-spectral optoacoustic tomography (MSOT)[J]. Biomaterials, 2015, 37:415-424.
[135] Lozano N, Al-Ahmady ZS, Beziere NS, et al. Monoclonal antibody-targeted PEGylated liposome-ICG encapsulating doxorubicin as a potential theranostic agent[J]. International Journal of Pharmaceutics, 2015, 482:2-10.
[136] Maeda A, Bu JC, Chen J, et al. Dual in vivo photoacoustic and fluorescence imaging of HER2 expression in breast tumors for diagnosis, margin assessment, and surgical guidance[J]. Mol. Imaging, 2014, 13:1-9.
[137] Kim C, Song KH, Gao F, et al. Sentinel lymph nodes and lymphatic vessels: noninvasive dual-modality in vivo mapping by using indocyanine green in rats-volumetric spectroscopic photoacoustic imaging and planar fluorescence imaging[J]. Radiology, 2010, 255:442-450.
[138] Kang N-Y, Park S-J, Ang XWE, et al. A macrophage uptaking near-infrared chemical probe CDnir7 for in vivo imaging of inflammation[J]. Chem. Commun., 2014, 50:6589-6591.
[139] Sim N, Gottschalk S, Pal R, et al. Wavelength-dependent optoacoustic imaging probes for NMDA receptor visualisation[J]. Chem. Commun., 2015, 51:15149-15152.
[140] Anees P, Joseph J, Sreejith S, et al. Real time monitoring of aminothiol level in blood using a near-infrared dye assisted deep tissue fluorescence and photoacoustic bimodal imaging[J]. Chem. Sci., 2016, 7:4110-4116.