

SUPPORTING INFORMATION

Near-infrared (NIR) fluorescence-based small organic molecules for cancer imaging and therapy

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Table S1. Summary of NIR fluorescence-based organic molecules for cancer imaging and therapy (abbreviation: FL = Fluorescence; PET = Positron emission tomography; PA = Photoacoustic; PDT = Photodynamic therapy; PIT = Photoimmunotherapy; PTT = Photothermal therapy).

Substance No	Target	Absorption/emission wavelength (nm)	Tumor cells	Tumor xenograft animal model	Imaging	Therapeutic	Ref.
1	Receptor (GRPR)	808/1100	-	PC3 (prostate)	FL	-	56
2	Receptor (GRPR)	749/775	PC3 (prostate)	PC3 (prostate)	FL	-	57
3	Receptor (GRPR)	673/691	PC3 (prostate) LnCAP (prostate)	PC3 (prostate)	FL	-	58
4b	Receptor (GRPR)	651/668	PC3 (prostate)	PC3 (prostate)	FL PET	-	59
5b	Receptor (GRPR)	780/825	CFPAC-1 (pancreas)	CFPAC-1 (pancreas)	FL	-	60
6	Receptor (SSTR2)	778/832	HCT-116 (colon)	-	FL	-	63
7	Receptor (SSTR2)	690/716	HeLa (cervix) A549 (lung)	-	FL	-	67
8	Receptor (Integrin)	710/820	-	4T1 (breast)	FL	-	70
9	Receptor (Integrin)	808/1055	-	U87MG (glioblastoma)	FL PET	-	71
10	Receptor (Integrin)	808/1000	U87MG (glioblastoma) 143B (bone)	U87MG (glioblastoma) 143B (bone)	FL	-	78
11	Receptor (CB2R)	760/781	Jurkat T leukemia cells	-	FL	-	84
12b	Receptor (CB2R)	725/785	DBT (brain)	DBT (brain)	FL	-	85
13	Receptor (CB2R)	778/832	DMS-53 (lung)	DMS-53 (lung)	FL	-	88
14	Receptor (CD133)	742/1047	HT-29 (colon) U87MG (glioblastoma)	HT-29 (colon)	FL	-	90
15b	Receptor (NK1R)	770/785	HEK293 (kidney)	HEK293 (kidney)	FL	-	92
16b	Receptor (CCK2R)	-/-	HEK293 (kidney)	HEK293 (kidney)	FL	-	94
17b	Receptor (ER)	-/-	-	MCF-7 (breast)	FL	-	96
18b	Receptor (EGFR)	670/700	Gli36Δ5 (glioblastoma)	Gli36Δ5 (glioblastoma)	FL	-	98
19	Receptor (FR)	745/-	-	L1210A (leukemia)	FL	-	100
20	Receptor (FR)	776/793	KB (cervix)	KB (cervix)	FL	-	101
21	Receptor (FR)	670/700	-	MCF-7 (breast)	FL	-	102
22a 22b	Receptor (FR)	652/674 (22a) 656/676 (22b)	KB (cervix)	KB (cervix)	FL	-	103
23	Receptor (FR)	610/680	SKOV-3 (ovary)	SKOV-3 (ovary)	FL	-	104

Substance No	Target	Absorption/emission wavelength (nm)	Tumor cells	Tumor xenograft animal model	Imaging	Therapeutic	Ref.
24	Receptor (PSMA)	745/-	-	22Rv1 (prostate)	FL	-	100
25	Receptor (PSMA)	743/767	-	PC3 PIP (prostate)	FL	-	107
26	Receptor (PSMA)	760/781	22Rv1 (prostate)	22Rv1 (prostate)	FL	-	108
27	Receptor (EGFR)	640/690	HCC70 (breast)	-	FL	PDT	109
28b	Receptor (EGFR)	689/700	A431 (epidermoid)	A431 (epidermoid)	FL	PIT	110
29	Receptor (Glut)	770/808	-	HT-29 (colon)	FL	PTT	113
30	Enzyme (Cathepsin S)	670/695	4T1 (breast)	4T1 (breast)	FL	-	120
31	Enzyme (Cathepsin B)	675/695	SCC7 (squamous cells)	SCC7 (squamous cells)	FL	-	122
32	Enzyme (MMP)	675/695	SCC7 (squamous cells)	SCC7 (squamous cells)	FL	-	122
33	Enzyme (Neutrophil elastase)	700/725	RBL-2H3 (leukemia)	A549 (lung)	FL PA	-	127
34	Enzyme (Tyrosinase)	610/740	B16F10 (melanoma)	B16F10 (melanoma)	FL	-	129
35	Enzyme (hNQO1)	606/755	SHIN3 (ovary)	SHIN3 (ovary)	FL	-	131
36	Enzyme (GGT)	680/720	OVCAR5 (ovary)	HCT-116 (colon)	FL	-	134
37	Enzyme (GGT)	680/720	U87MG (glioblastoma)	U87MG (glioblastoma)	FL	-	135
38	Enzyme (ALP)	575/685	HepG2 (liver)	HepG2 (liver)	FL	-	139
39	Enzyme (ALP)	685/730	HeLa (cervix)	HeLa (cervix)	FL	-	140
40	Enzyme (ACP)	700/765	HeLa (cervix) PC3 (prostate)	-	FL	-	144
41	Enzyme (β -Galactosidase)	660/730	SKOV-3 (ovary)	A549 (lung)	FL	-	146
42a	Enzyme (β -Galactosidase)	633/715 (42a)	SKOV-3 (ovary)	SKOV-3 (ovary)	FL	-	147
42b	Enzyme (β -Galactosidase)	723/853 (42b)	(42a)				
43	Enzyme (β -Galactosidase)	690/725	SKOV-3 (ovary)	-	FL	-	148
44	Enzyme (APN)	665/705	HepG2 (liver)	HepG2 (liver)	FL	-	152
45	Enzyme (LAP)	670/705	HepG2 (liver)	HepG2 (liver)	FL	-	155
46	Enzyme (LAP)	650/710	HepG2 (liver)	HepG2 (liver)	FL	-	156
47a	Enzyme (carboxylesterase)	540/685	HepG2 (liver)	HepG2 (liver)	FL	-	157
48	Enzyme (APN)	685/720	HepG2 (liver) 4T1 (breast)	4T1 (breast)	FL	PDT	158
49	Enzyme (GGT)	688/720	HepG2 (liver)	4T1 (breast)	FL	PDT	159
50	Enzyme (LAP)	693/720	HCT-116 (colon)	HCT-116 (colon)	FL	PDT	160

Substance No	Target	Absorption/emission wavelength (nm)	Tumor cells	Tumor xenograft animal model	Imaging	Therapeutic	Ref.
51	Enzyme (PC-PLC)	670/720	MDA-MB-231 (breast)	-	FL	PDT	163
52	Enzyme (Cathepsin B)	650/720	HeLa (cervix)	H640 (lung)	FL	PDT	164
53	Enzyme (Tyrosinase)	640/706	B16F10 (melanoma)	-	FL	PDT	165
54	Enzyme (β -Galactosidase)	688/720	SKOV-3 (ovary)	SKOV-3 (ovary)	FL	PTT	166
55	Enzyme (ALP)	710/735	PC3 (prostate)	PC3 (prostate)	FL	PTT	167
56a	GSH	600/810	HeLa (cervix)	-	FL	-	170
57a 57b	GSH	780/805	HeLa (cervix)	SCC7 (squamous cells)	FL	-	171
58a	GSH	710/812	HeLa (cervix)	-	FL	-	172
59a	GSH	700/810	U87 (glioblastoma)	EAC (ascites tumor)	FL	-	173
60a	GSH	720/810	U87 (glioblastoma)	EAC (ascites tumor)	FL	-	174
61a	GSH	698/735	HeLa (cervix)	-	FL	-	175
62a	GSH	730/736	HeLa (cervix)	-	FL	-	176
63a	GSH	700/795	HeLa (cervix)	-	FL	-	177
64a	GSH	670/719	MCF-7 (breast)	-	FL	-	179
65a	GSH	808/928	-	4T1 (breast)	FL	-	181
66a	GSH	760/810	U87 (glioblastoma)	MDA-MB-231 (breast)	FL	-	182
67a	GSH, Hcy, Cys	669/708	Peritoneal carcinoma	HGC-27 (stomach)	FL	-	183
68	GSH	465/665	MCF-7 (breast)	Bcap-37 (breast)	FL	Anticancer drug (CPT)	184
69	GSH	660/702	HepG2 (liver)	-	FL	Anticancer drug (CPT)	187
70	GSH	750/850	Bcap-37 (breast)	Bcap-37 (breast)	FL	Anticancer drug (CPT)	188
71	GSH	465/674	HeLa (cervix)	HeLa (cervix)	FL	Anticancer drug (CPT)	189
72	GSH	680/-	A549 (lung)	A549 (lung)	FL PA	Anticancer drug (Gemcitabine)	190
73	H ₂ S	730/830	MCF-7 (breast)	MCF-7 (breast)	FL	-	193
74	H ₂ S	527/716	HCT-116 (colon)	-	FL	-	194
75a	H ₂ S	640/725	HCT-116 (colon)	HCT-116 (colon)	FL	-	195

Substance No	Target	Absorption/emission wavelength (nm)	Tumor cells	Tumor xenograft animal model	Imaging	Therapeutic	Ref.
76a	H ₂ S	760/920	HCT-116 (colon)	HCT-116 (colon)	FL	-	196
77a	H ₂ S	575/680 980/1140	HCT-116 (colon)	HCT-116 (colon)	FL	-	197
78a	H ₂ O ₂	560/704	HepG2 (liver)	HepG2 (liver)	FL	-	205
79a	H ₂ O ₂	665/684	A375 (melanoma)	A375 (melanoma)	FL	-	206
80a	ClO ⁻ /HClO	633/680	A549 (lung) HepG2 (liver) T98G (glioblastoma)	A549 (lung) HepG2 (liver) MCF-7 (breast)	FL	-	207
81	ClO ⁻ /HClO	620/700	HepG2 (liver) HeLa (cervix) A549 (lung)	-	FL	-	208
82a	O ₂ ^{•-}	675/704	HepG2 (liver)	-	FL	-	209
83a	ClO ⁻ /ONOO ⁻ /HO [•]	620/680	A549 (lung) HepG2 (liver) MCF-7 (breast)	A549 (lung)	FL	-	210
84a	•OH/O ₂ ^{•-}	768/794	PC3 (prostate)	-	FL PET	-	211
85	H ₂ O ₂	605/720	U87MG (glioblastoma)	U87MG (glioblastoma)	FL	Anticancer drug (CPT)	212
86	H ₂ O ₂	680/710	HeLa (cervix) HepG2 (liver)	-	FL	Anticancer drug (5'-DFUR) PDT	213
87a	Nitroreductase	730/782	A549 (lung)	A549 (lung)	FL	-	218
88a	Nitroreductase	670/706	4T1 (breast) HepG2 (liver)	4T1 (breast)	FL	-	219
89a	Nitroreductase	550/705	U251 (glioblastoma)	-	FL	-	220
90a	Nitroreductase	680/780 808/922	-	4T1 (breast)	FL PA	-	221
91a	Nitroreductase	868/921	-	A549 (lung)	FL	-	222
92a	Azoreductase	650/705	MCF-7 (breast)	MCF-7 (breast)	FL	-	223
93	Nitroreductase	980/1046	-	A549 (lung)	FL	PTT	224
94	Nitroreductase	660/716	4T1 (breast)	4T1 (breast)	FL	PDT	225
95	Nitroreductase	635/775	HeLa (cervix)	-	FL	PDT	226
96	Acidic pH	750/768	A431 (epidermoid)	A431 (epidermoid)	FL	-	229
97	Acidic pH	745/778	-	HepG2 (liver)	FL	-	230
98	Acidic pH	637/750	MCF-7 (breast)	MCF-7 (breast)	FL PA	PTT	231

Substance No	Target	Absorption/emission wavelength (nm)	Tumor cells	Tumor xenograft animal model	Imaging	Therapeutic	Ref.
99	Acidic pH	690/742	MDA-MB-231 (breast)	MDA-MB-231 (breast)	FL	PDT	232
100	High viscosity	520/696	-	4T1 (breast)	FL	-	241
101	High viscosity	570/730	HepG2 (liver)	-	FL	-	242
102	Low polarity	650/780	HepG2 (liver)	4T1 (breast)	FL	-	246
103	Low polarity	635/724	HeLa (cervix)	-	FL	-	247
104	Low polarity	594/686	Hep3B (liver) HepG2 (liver) A549 (lung)	-	FL	-	248
105	High viscosity	565/720	HeLa (cervix) A549 (lung) HepG2 (liver)	HeLa (cervix)	FL	PDT	249
106a	NO	1080/-	-	4T1 (breast) A549 (lung)	PA	-	255
107	Passive-targeting	480/721	HeLa (cervix)	U87MG (glioblastoma)	FL	-	257