

Supporting Information

Complexity of $\alpha\beta6$ -Integrin Targeting RGD Peptide Trimers: Emergence of Non-Specific Binding by Synergistic Interaction

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1. Analytical data for cyclic peptide alkyne building blocks

cyclo[FR(Pbf)GD(tBu)LAYp(NMe)K(pentynoic amide)] (FY)

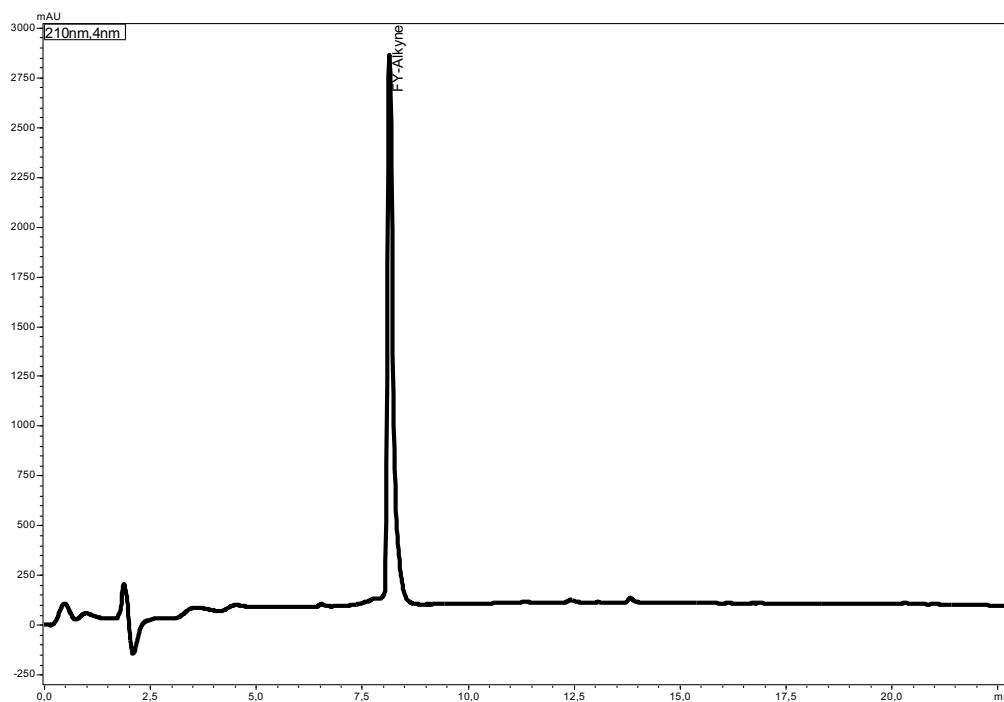


Figure S1: Analytical HPLC (UV 210 nm) of **FY**. HPLC analysis was performed using analytical column C1, 0.5 mL/min; gradient: 10–90% MeCN in H₂O containing 0.1% TFA in 20 min. $t_R = 8.2$ min.

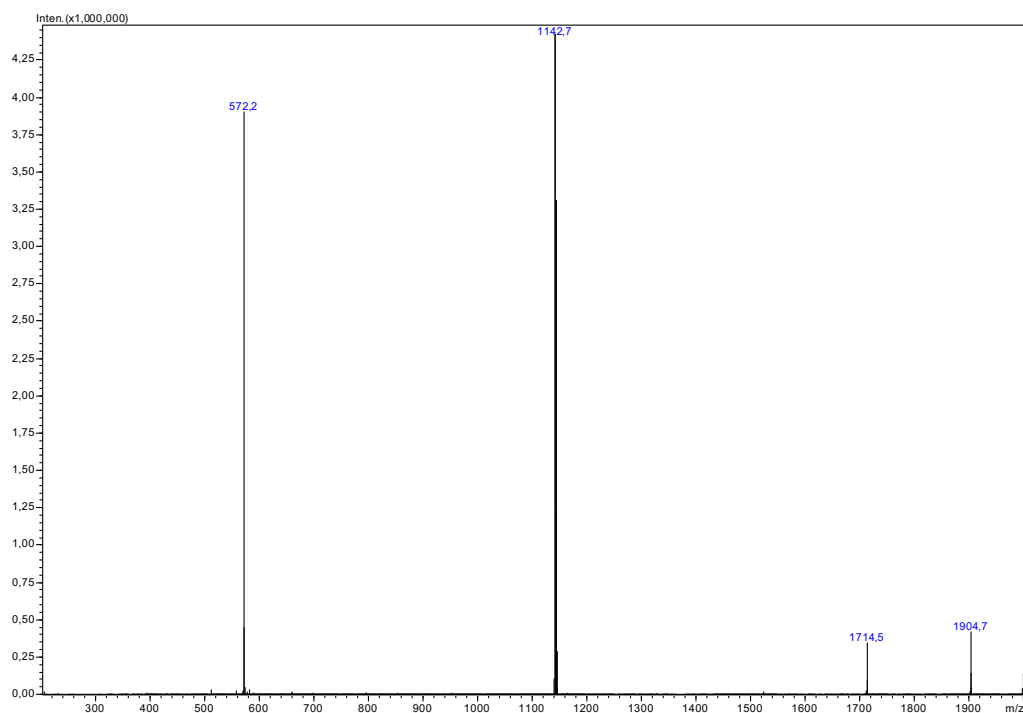


Figure S2: ESI-MS (positive mode) of **FY**. m/z corresponds to molecular composition as follows: 1904.7 $[5M+3H]^{3+}$, 1714.5 $[3M+2H]^{2+}$, 1142.7 $[M+H]^+$, 572.2 $[M+2H]^{2+}$.

cyclo[YR(Pbf)GD(tBu)LAFp(NMe)K(pentynoic amide)] (YF)

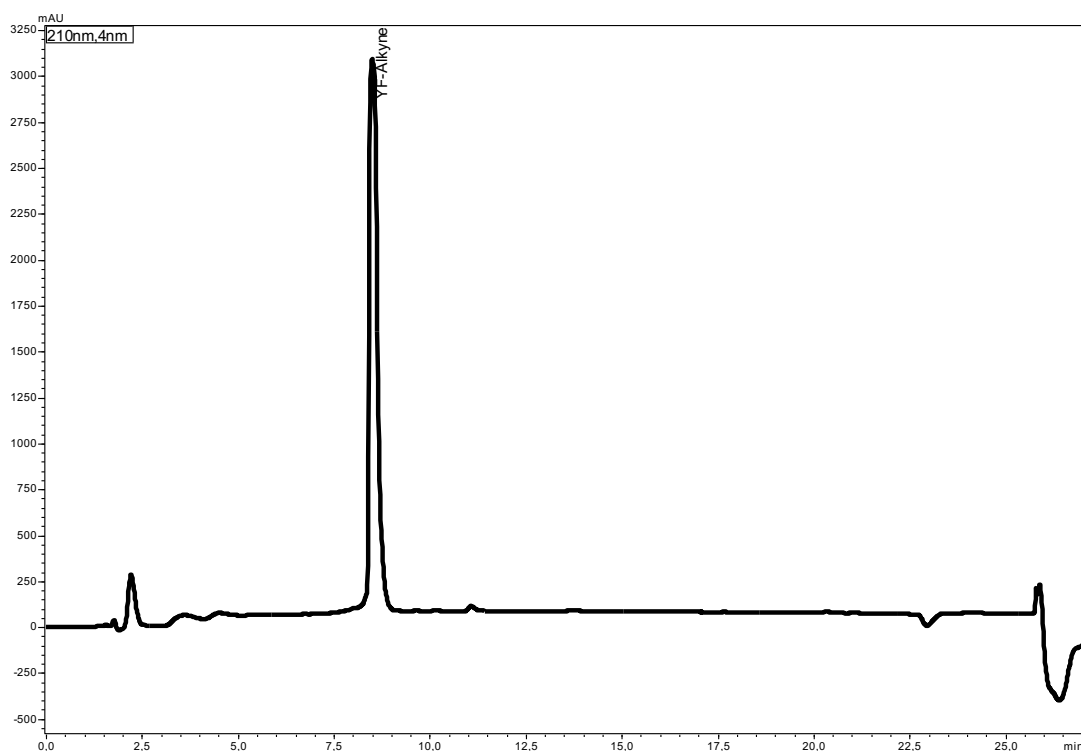


Figure S3: Analytical HPLC (UV 210 nm) of YF. HPLC analysis was performed using analytical column C1, 0.5 mL/min; gradient: 10–90% MeCN in H₂O containing 0.1% TFA in 20 min. $t_R = 8.2$ min.

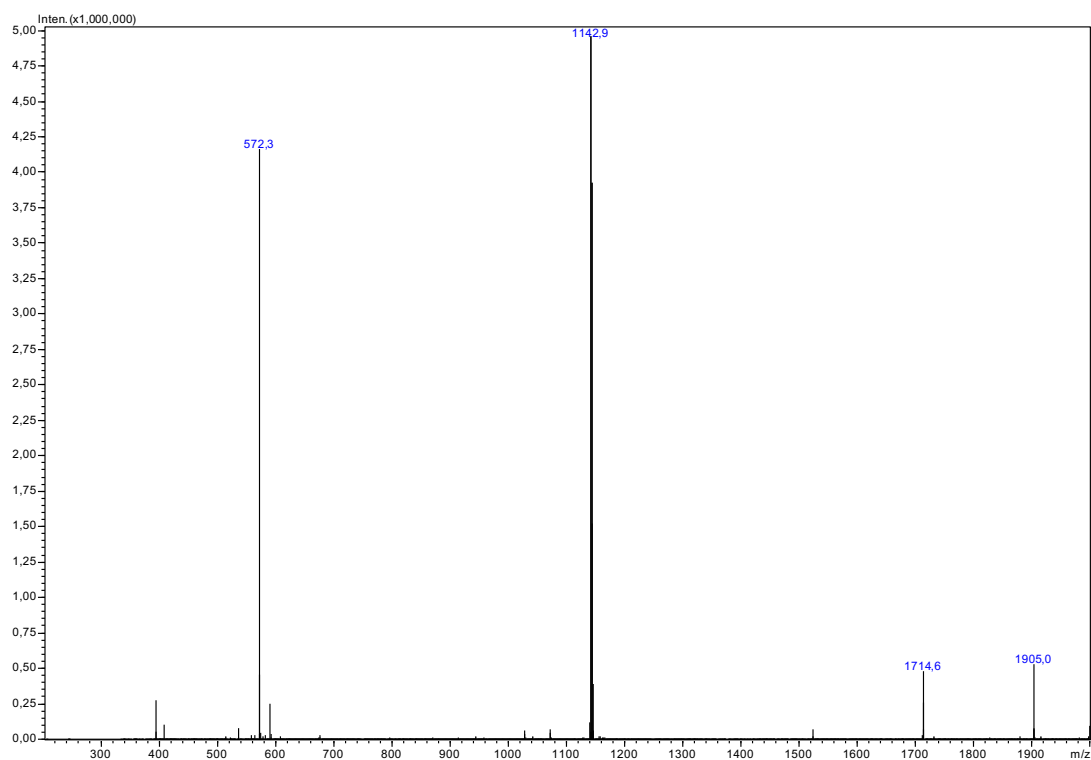


Figure S4: ESI-MS (positive mode) of YF. m/z corresponds to molecular composition as follows: 1905 [5M+3H]³⁺, 1714.6 [3M+2H]²⁺, 1142.9 [M+H]⁺, 572.3 [M+2H]²⁺.

2. ESI-MS data for peptide trimers

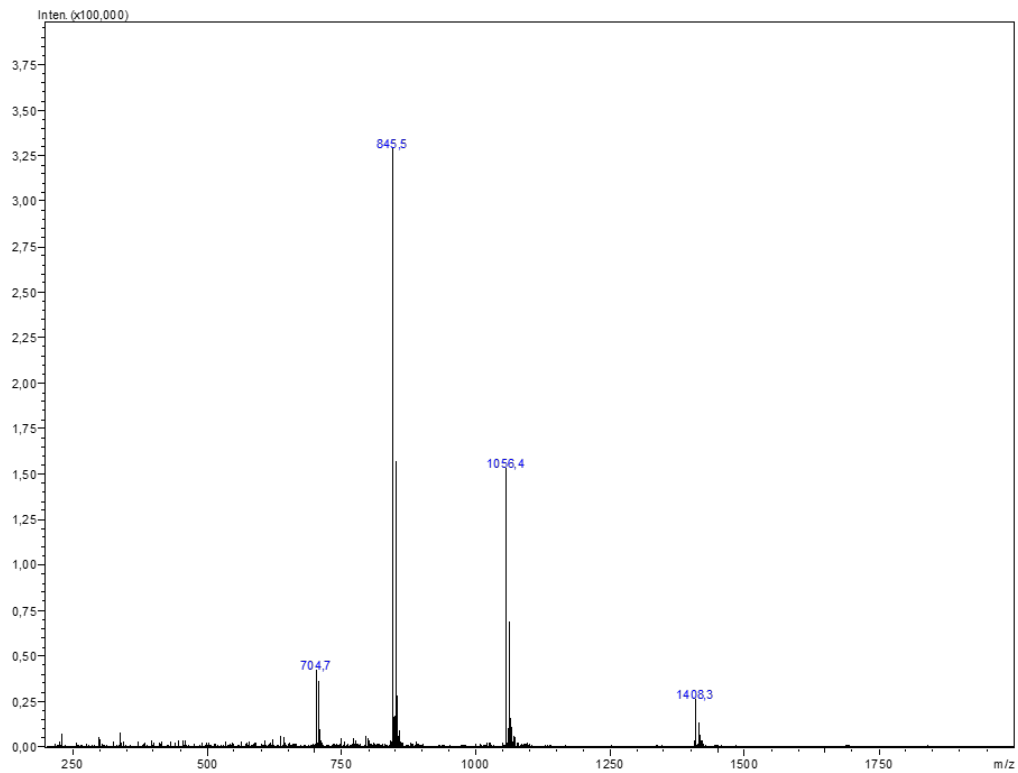


Figure S5: ESI-MS (positive mode) of **Y1Y**. m/z corresponds to molecular composition as follows: 1408.3 $[M+3H]^{3+}$, 1056.4 $[M+4H]^{4+}$, 845.5 $[M+5H]^{5+}$, 704.7 $[M+6H]^{6+}$.

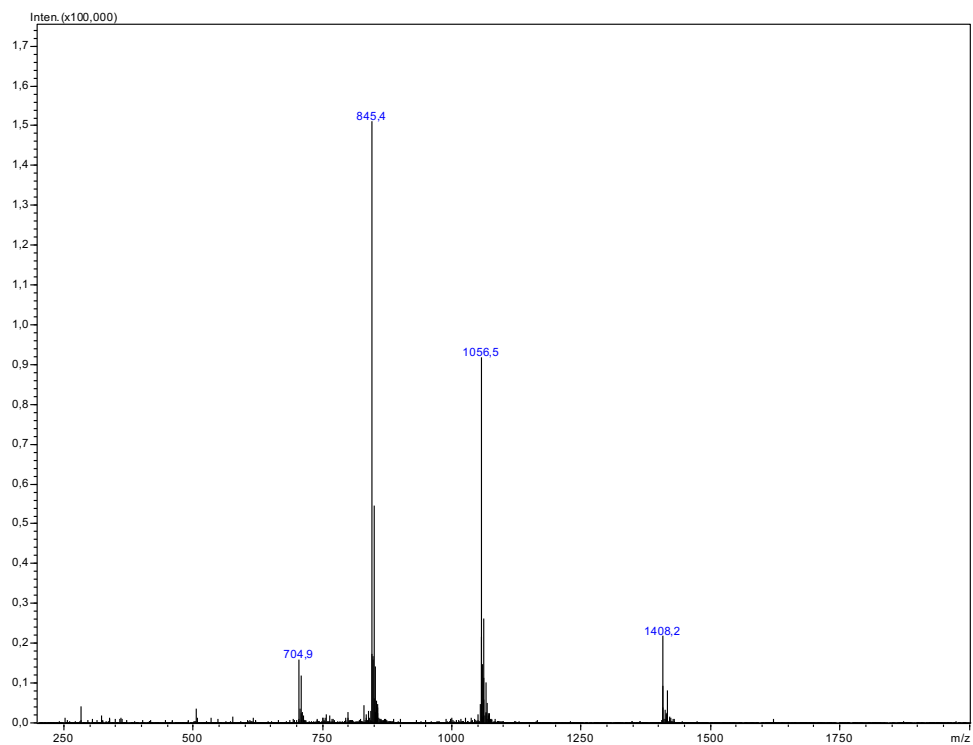


Figure S6: ESI-MS (positive mode) of **Y1F**. m/z corresponds to molecular composition as follows: 1408.2 $[M+3H]^{3+}$, 1056.5 $[M+4H]^{4+}$, 845.4 $[M+5H]^{5+}$, 704.9 $[M+6H]^{6+}$.

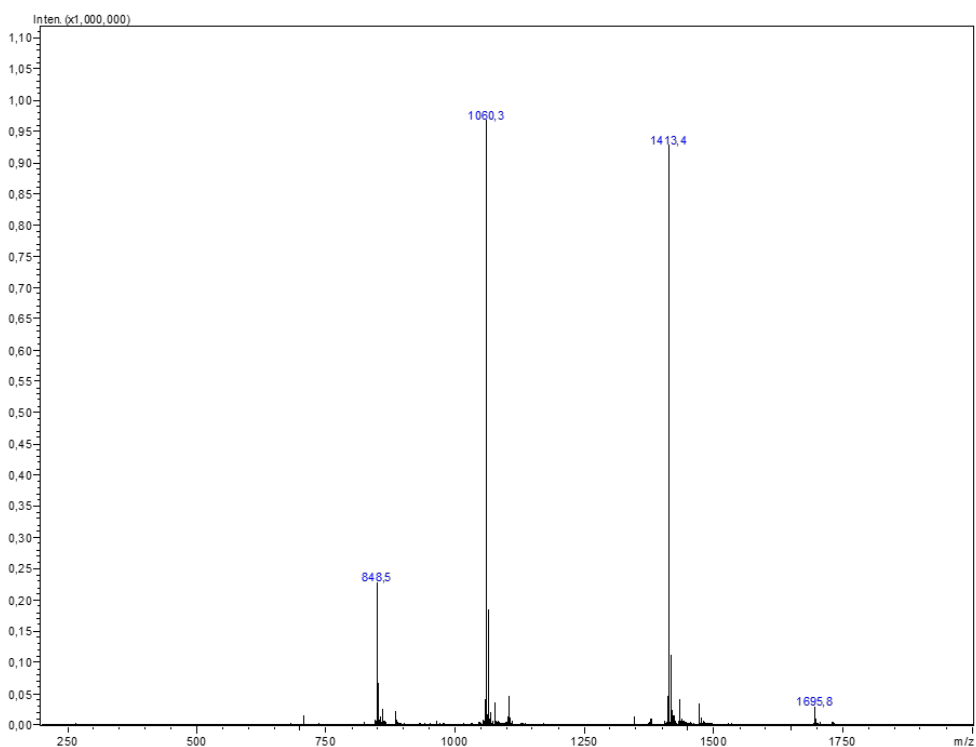


Figure S7: ESI-MS (positive mode) of Y2. m/z corresponds to molecular composition as follows: m/z corresponds to molecular composition as follows: 1695.8 $[2M+5H]^{5+}$, 1413.4 $[M+3H]^{3+}$, 1060.3 $[M+4H]^{4+}$, 848.5 $[M+5H]^{5+}$.

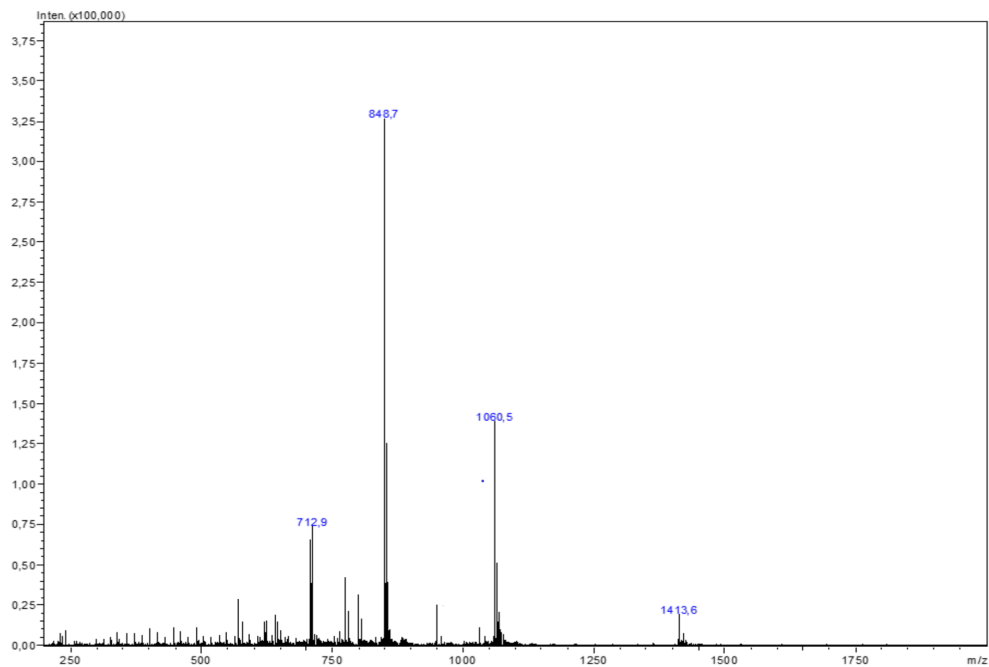


Figure S8: ESI-MS (positive mode) of Y2Y. m/z corresponds to molecular composition as follows: m/z corresponds to molecular composition as follows: 1413.6 $[M+3H]^{3+}$, 1060.5 $[M+4H]^{4+}$, 848.7 $[M+5H]^{5+}$, 712.9 $[M+6H]^{6+}$.

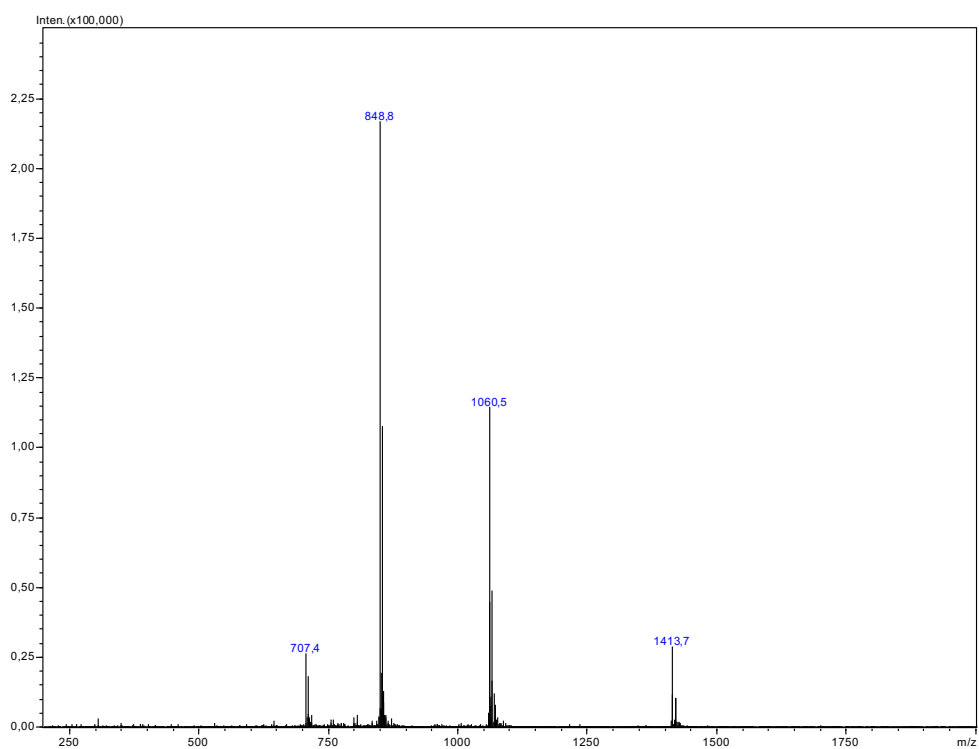


Figure S9: ESI-MS (positive mode) of Y2F. m/z corresponds to molecular composition as follows: m/z corresponds to molecular composition as follows: 1413.7 $[M+3H]^{3+}$, 1060.5 $[M+4H]^{4+}$, 848.8 $[M+5H]^{5+}$, 707.4 $[M+6H]^{6+}$.

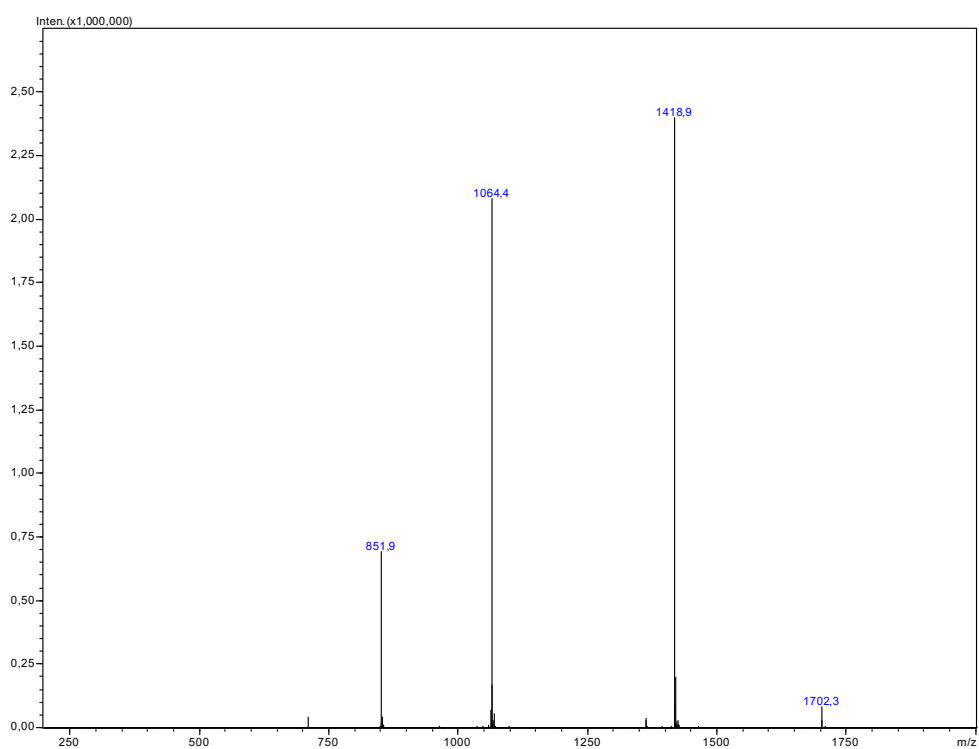


Figure 10: ESI-MS (positive mode) of Y3Y. m/z corresponds to molecular composition as follows: m/z corresponds to molecular composition as follows: 1702.3 $[2M+5H]^{5+}$, 1418.9 $[M+3H]^{3+}$, 1064.4 $[M+4H]^{4+}$, 851.9 $[M+5H]^{5+}$.

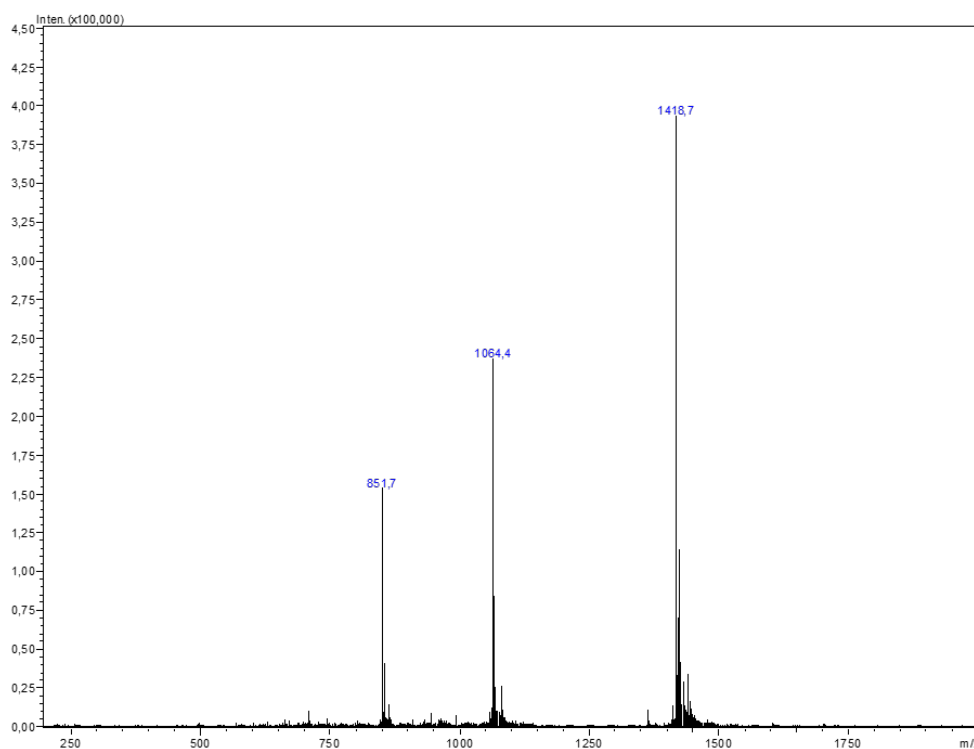


Figure S11: ESI-MS (positive mode) of **Y3F**. m/z corresponds to molecular composition as follows: m/z corresponds to molecular composition as follows: 1418.7 $[M+3H]^{3+}$, 1064.4 $[M+4H]^{4+}$, 851.7 $[M+5H]^{5+}$.

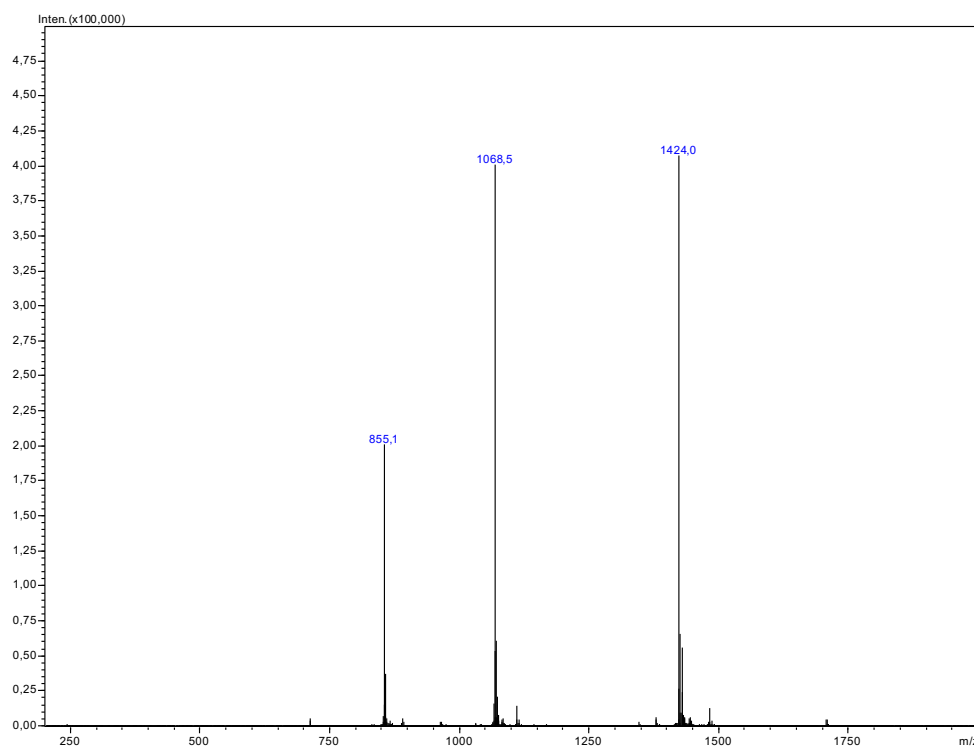


Figure S12: ESI-MS (positive mode) of **Y4**. m/z corresponds to molecular composition as follows: m/z corresponds to molecular composition as follows: 1424.0 $[M+3H]^{3+}$, 1068.5 $[M+4H]^{4+}$, 855.1 $[M+5H]^{5+}$.

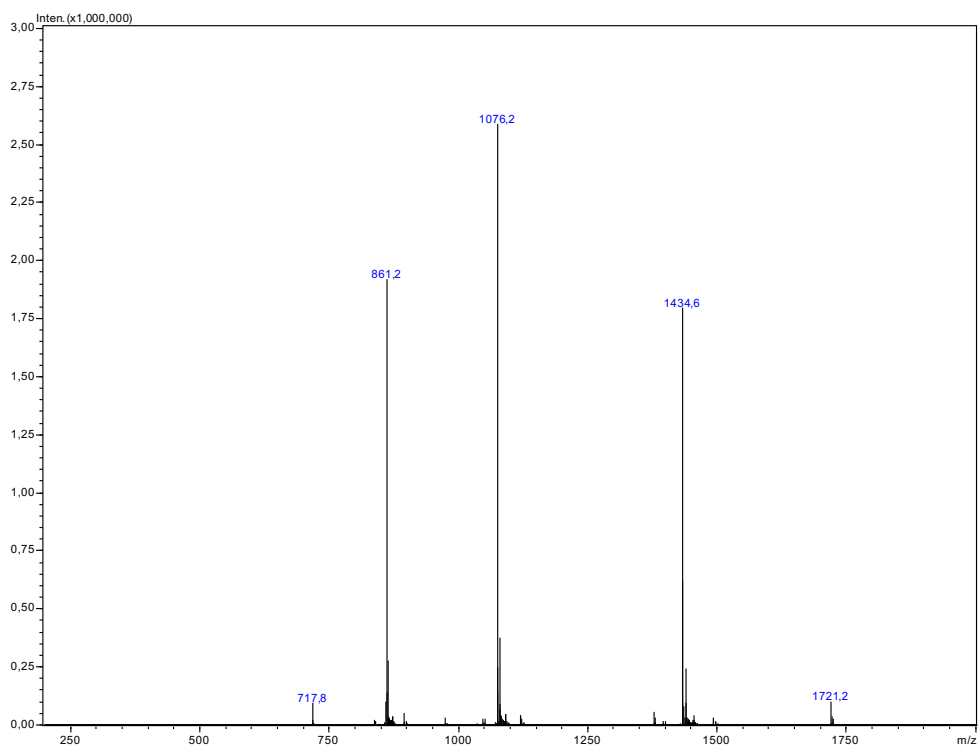


Figure 13: ESI-MS (positive mode) of **Y6**. m/z corresponds to molecular composition as follows: m/z corresponds to molecular composition as follows: 1721.2 $[2M+5H]^{5+}$, 1434.6 $[M+3H]^{3+}$, 1076.2 $[M+4H]^{4+}$, 861.2 $[M+5H]^{5+}$, 717.8 $[M+6H]^{6+}$.

3. HPLC Chromatograms of ^{nat}Ga-complexed trimers

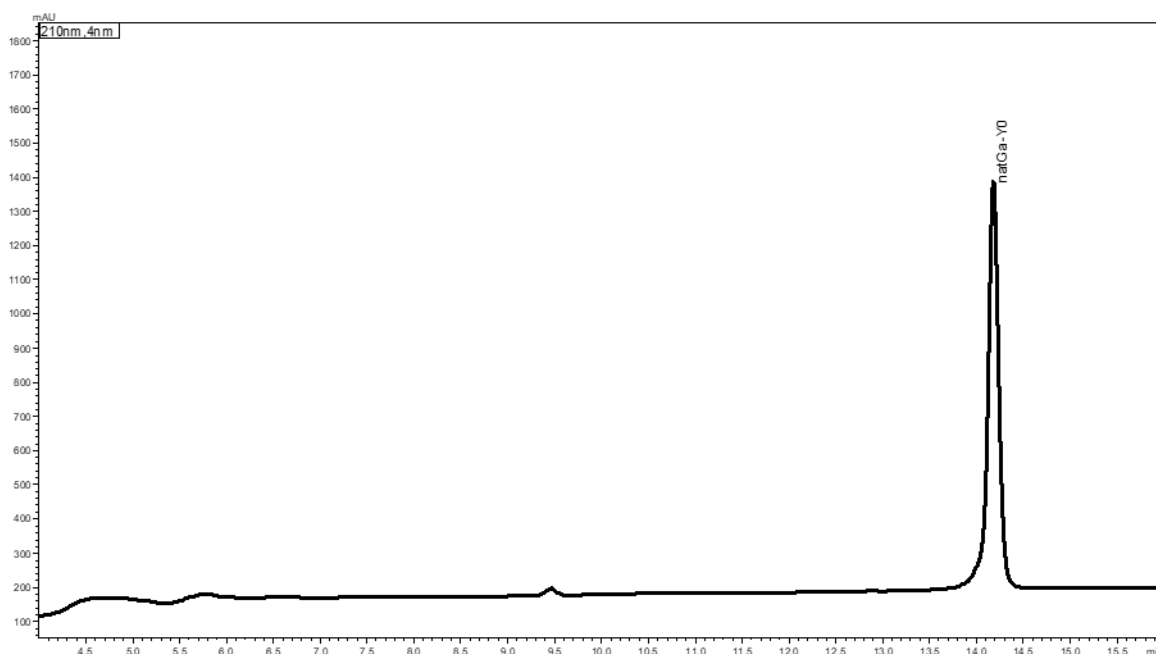


Figure S14: Analytical HPLC (UV 210 nm) of ^{nat}Ga-Y0. HPLC analysis was performed using analytical column C2, 0.75 mL/min; gradient: 10–50% MeCN in H₂O containing 0.1% TFA in 15 min. $t_R = 14.2$ min. Compound Purity = 98% determined by 210 nm wavelength.

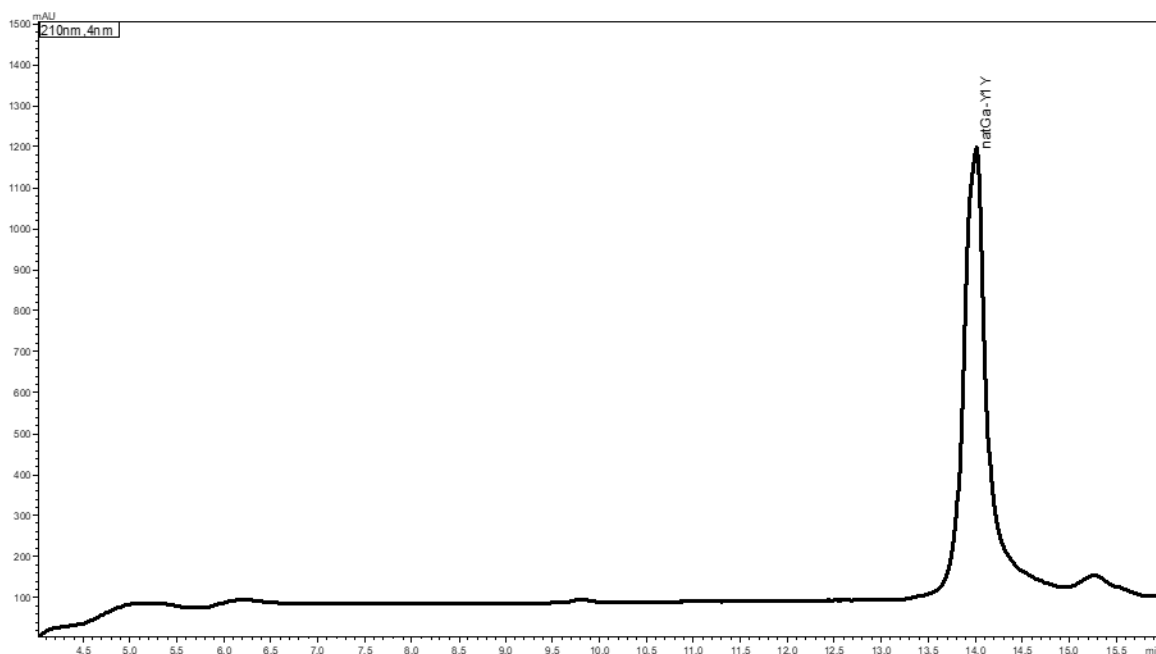


Figure S15: Analytical HPLC (UV 210 nm) of ^{nat}Ga-Y1Y. HPLC analysis was performed using analytical column C2, 0.75 mL/min; gradient: 10–50% MeCN in H₂O containing 0.1% TFA in 15 min. $t_R = 14.0$ min. Compound Purity = 96% determined by 210 nm wavelength.

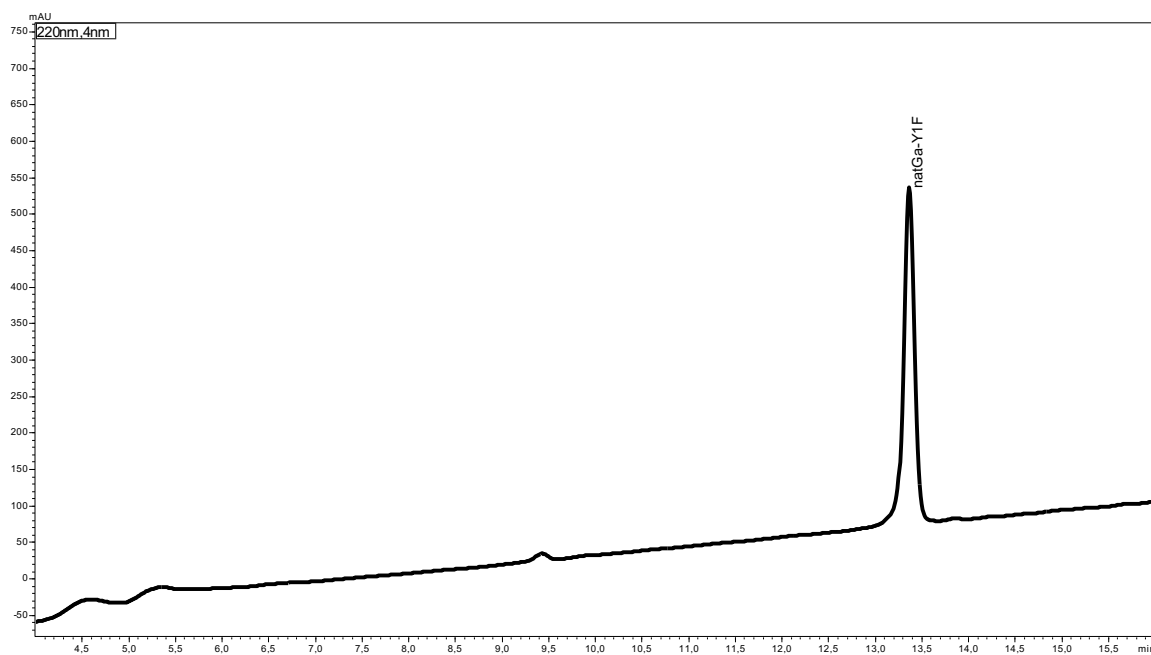


Figure S16: Analytical HPLC-UV (210 nm) of ^{nat}Ga-Y1F. HPLC analysis was performed using analytical column C2, 0.75 mL/min; gradient: 10–50% MeCN in H₂O containing 0.1% TFA in 15 min. t_R = 13.4 min. Compound Purity = 98% determined by 210 nm wavelength.

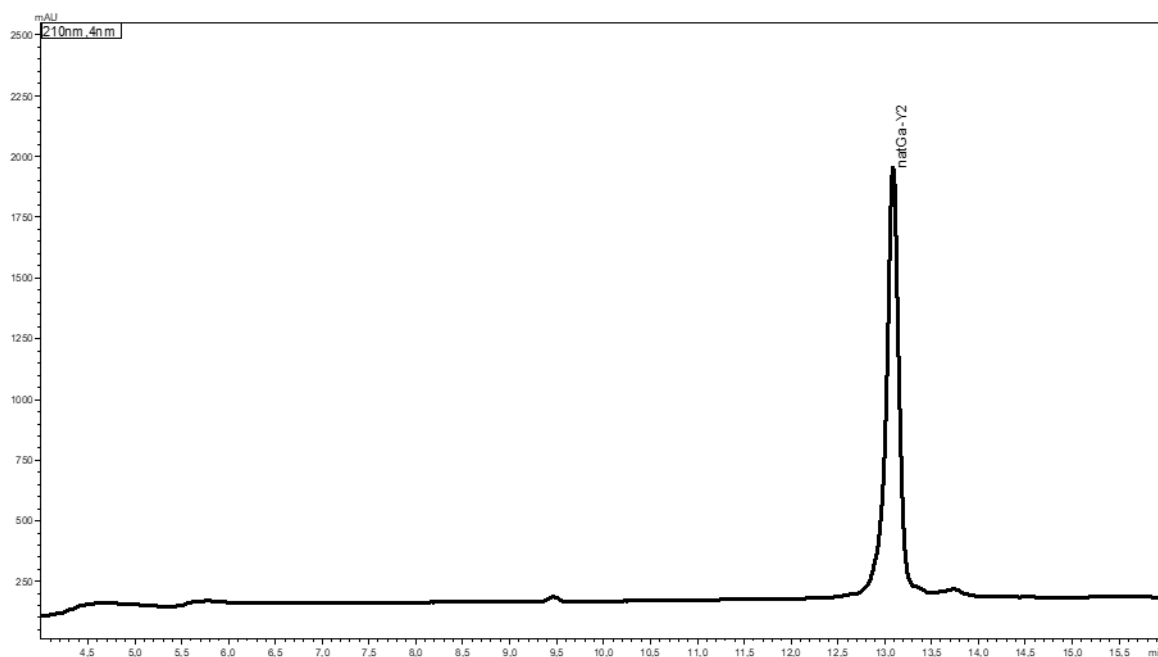


Figure S17: Analytical HPLC (UV 210 nm) of ^{nat}Ga-Y2. HPLC analysis was performed using analytical column C2, 0.75 mL/min; gradient: 10–50% MeCN in H₂O containing 0.1% TFA in 15 min. t_R = 13.1 min. Compound Purity = 98% determined by 210 nm wavelength.

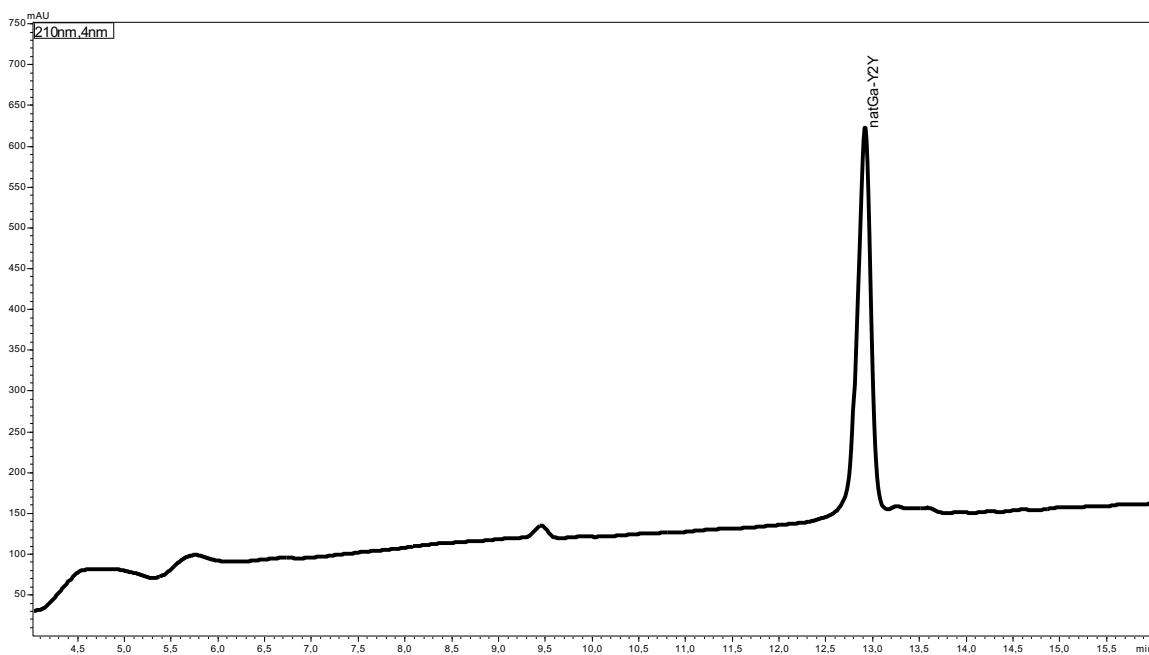


Figure S18: Analytical HPLC (UV 210 nm) of ^{nat}Ga-Y2Y. HPLC analysis was performed using analytical column C2, 0.75 mL/min; gradient: 10–50% MeCN in H₂O containing 0.1% TFA in 15 min. $t_R = 12.9$ min. Compound Purity = 95% determined by 210 nm wavelength.

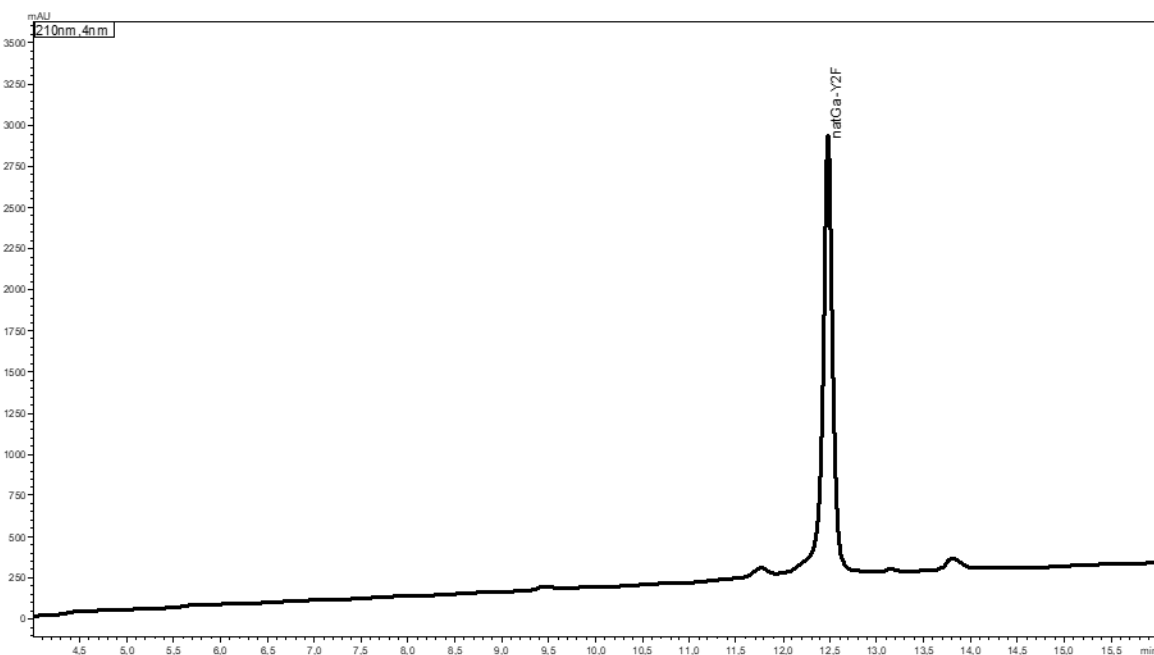


Figure S19: Analytical HPLC (UV 210 nm) of ^{nat}Ga-Y2F. HPLC analysis was performed using analytical column C2, 0.75 mL/min; gradient: 10–50% MeCN in H₂O containing 0.1% TFA in 15 min. $t_R = 12.5$ min. Compound Purity = 95% determined by 210 nm wavelength.

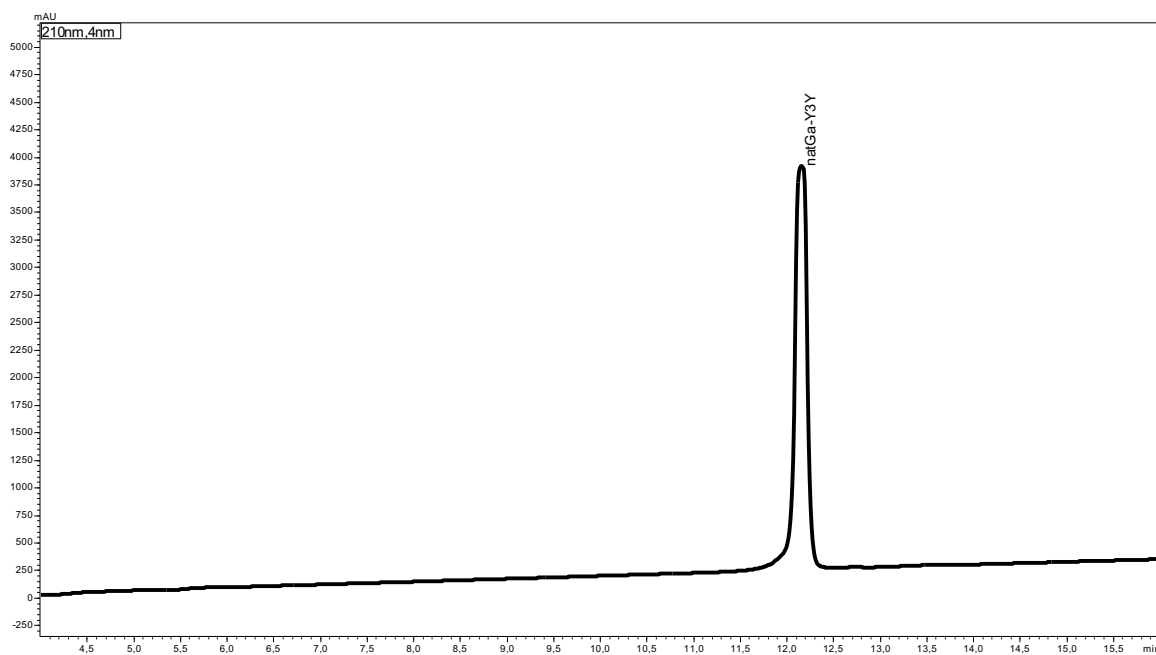


Figure S20: Analytical HPLC (UV 210 nm) of $^{nat}\text{Ga-Y3Y}$. HPLC analysis was performed using analytical column C2, 0.75 mL/min; gradient: 10–50% MeCN in H_2O containing 0.1% TFA in 15 min. $t_R = 12.2$ min. Compound Purity = 99% determined by 210 nm wavelength.

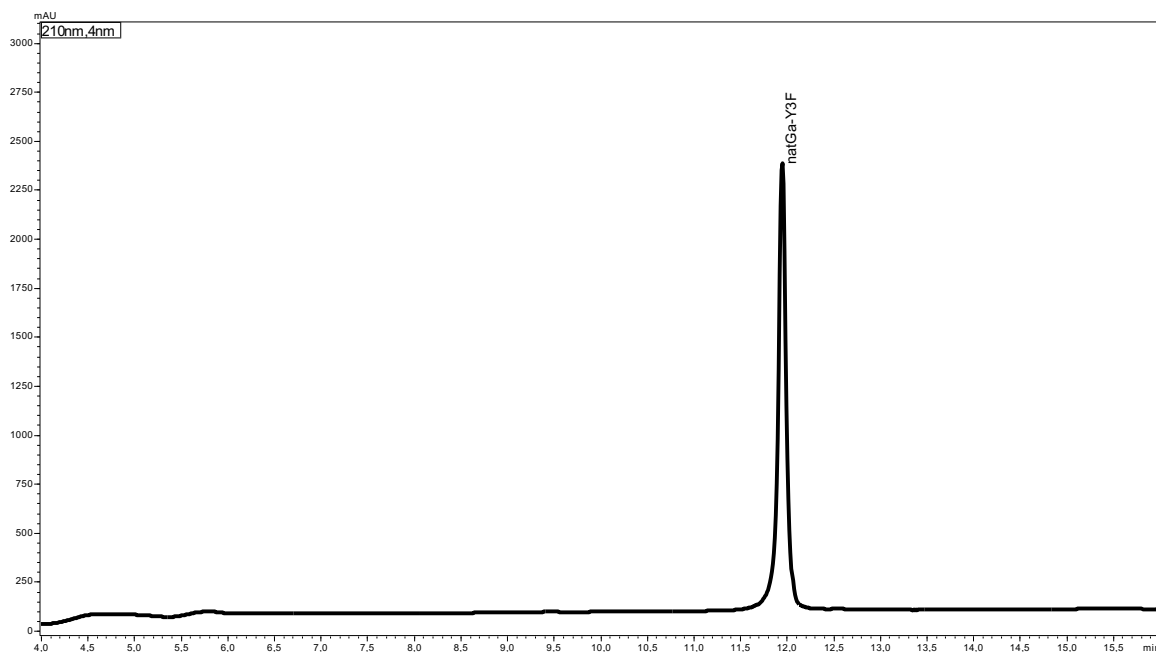


Figure S21: Analytical HPLC (UV 210 nm) of $^{nat}\text{Ga-Y3F}$. HPLC analysis was performed using analytical column C2, 0.75 mL/min; gradient: 10–50% MeCN in H_2O containing 0.1% TFA in 15 min. $t_R = 12$ min. Compound Purity = 99% determined by 210 nm wavelength.

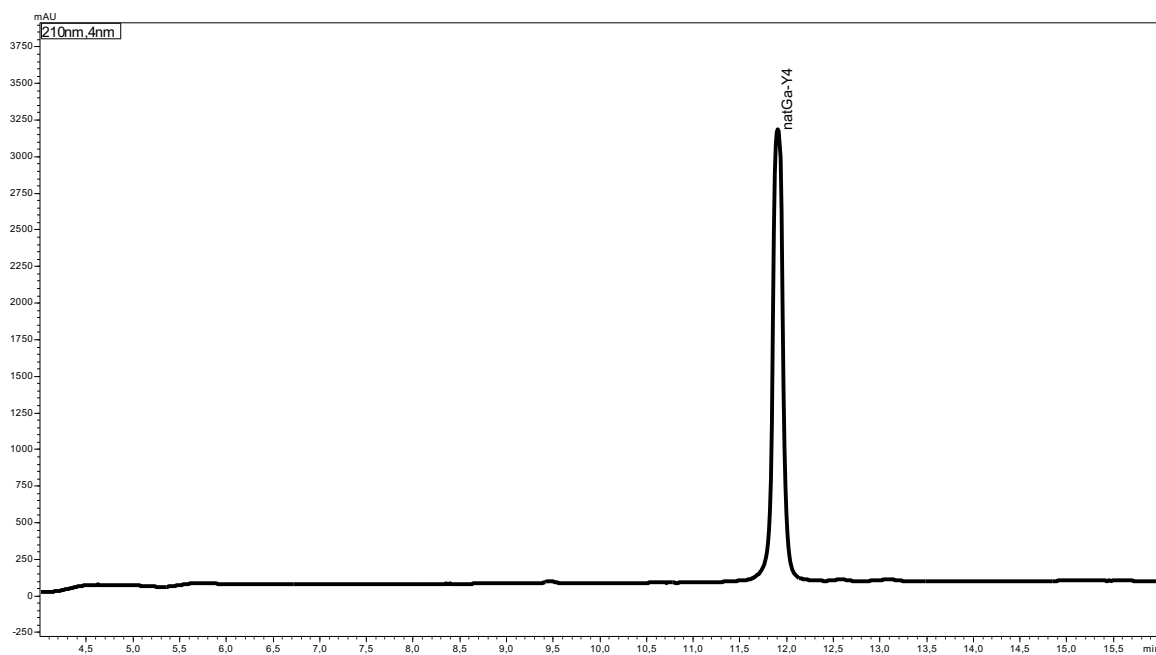


Figure S22: Analytical HPLC (UV 210 nm) of ^{nat}Ga-Y4. HPLC analysis was performed using analytical column C2, 0.75 mL/min; gradient: 10–50% MeCN in H₂O containing 0.1% TFA in 15 min. t_R = 11.9 min. Compound Purity = 98% determined by 210 nm wavelength.

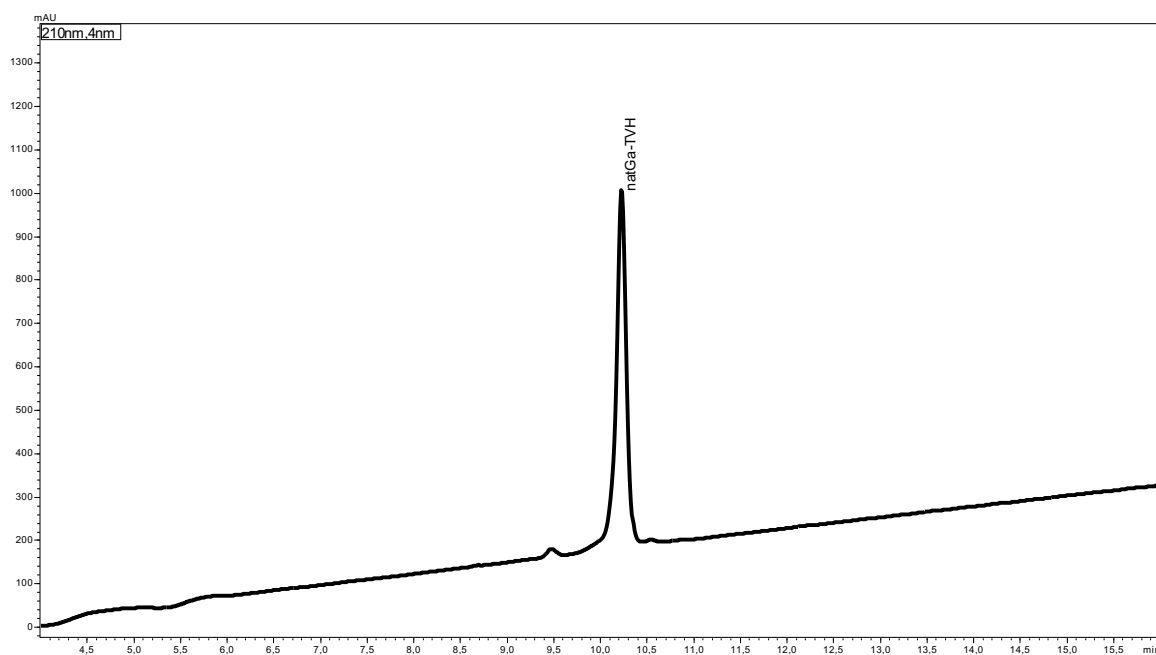


Figure S23: Analytical HPLC (UV 210 nm) of ^{nat}Ga-Y6 (^{nat}Ga-Trivehexin). HPLC analysis was performed using analytical column C2, 0.75 mL/min; gradient: 10–50% MeCN in H₂O containing 0.1% TFA in 15 min. t_R = 10.2 min. Compound Purity = 98% determined by 210 nm wavelength.

4. Biodistribution data

Table S1: Biodistribution data (90 min p.i.) for $^{68}\text{Ga-Y0}$ without ($n = 6$; 66 ± 8 pmol) and with ($n = 3$) addition of 50 nmol of TRAP(AvB6)₃, in H2009 bearing SCID mice. Data are given as averages \pm standard deviation. %IA/g = percent injected activity per gram tissue.

Organ/Tissue	$^{68}\text{Ga-Y0}$		+ 50 nmol cold 10 min prior to activity
	%IA/g	tumor/organ ratio	
Blood	4.01 \pm 0.74	2.2 \pm 0.5	2.39 \pm 0.79
Heart (myocard)	2.13 \pm 0.42	4.2 \pm 0.8	1.93 \pm 0.37
Lung	16.87 \pm 5.34	0.6 \pm 0.2	5.66 \pm 1.47
Liver	7.55 \pm 0.78	1.2 \pm 0.2	7.65 \pm 1.93
Spleen	5.21 \pm 1.05	1.7 \pm 0.4	2.56 \pm 0.29
Pancreas	0.91 \pm 0.22	10.1 \pm 2.8	0.99 \pm 0.15
Stomach (empty)	10.26 \pm 1.62	0.9 \pm 0.2	1.46 \pm 0.22
Small intestine (empty)	4.20 \pm 1.07	2.2 \pm 0.4	1.16 \pm 0.09
Large intestine (empty)	5.74 \pm 1.36	1.6 \pm 0.4	1.29 \pm 0.16
Kidneys	90.74 \pm 6.70	0.1 \pm 0.0	61.56 \pm 5.90
Adrenals	2.40 \pm 0.38	3.7 \pm 0.7	1.54 \pm 0.43
Muscle	1.10 \pm 0.22	8.1 \pm 1.3	0.50 \pm 0.11
Tumor H2009	8.73 \pm 0.81		2.51 \pm 0.24

Table S2: Biodistribution data (90 min p.i.) for $^{68}\text{Ga-Y1Y}$ without ($n = 5$; 95 ± 55 pmol) and with ($n = 3$) addition of 50 nmol of non-labeled compound, in H2009 bearing SCID mice. Data are given as averages \pm standard deviation. %IA/g = percent injected activity per gram tissue.

Organ/Tissue	$^{68}\text{Ga-Y1Y}$		+ 50 nmol cold 10 min prior to activity
	%IA/g	tumor/organ ratio	
Blood	2.54 \pm 0.37	3.2 \pm 0.7	1.64 \pm 0.67
Heart (myocard)	1.54 \pm 0.61	5.7 \pm 2.0	1.15 \pm 0.34
Lung	6.76 \pm 2.02	1.2 \pm 0.2	3.92 \pm 0.97
Liver	4.39 \pm 0.46	1.8 \pm 0.3	4.61 \pm 0.05
Spleen	3.85 \pm 0.86	2.2 \pm 0.5	2.08 \pm 0.25
Pancreas	0.64 \pm 0.11	12.7 \pm 2.9	0.65 \pm 0.12
Stomach (empty)	6.78 \pm 0.72	1.2 \pm 0.2	1.12 \pm 0.19
Small intestine (empty)	2.72 \pm 0.36	3.0 \pm 0.7	1.11 \pm 0.16
Large intestine (empty)	4.10 \pm 0.84	2.0 \pm 0.5	1.01 \pm 0.34
Kidneys	91.21 \pm 9.95	0.1 \pm 0.0	65.79 \pm 13.01
Adrenals	1.57 \pm 0.41	5.3 \pm 1.5	1.30 \pm 0.42
Muscle	0.75 \pm 0.17	11.2 \pm 3.4	0.34 \pm 0.08
Tumor H2009	8.16 \pm 2.01		1.50 \pm 0.64

Table S3: Biodistribution data (90 min p.i.) for ⁶⁸Ga-Y1F without (n = 5; 68 ± 26 pmol) and with (n = 3) addition of 50 nmol of non-labeled compound, in H2009 bearing SCID mice. Data are given as averages ± standard deviation. %IA/g = percent injected activity per gram tissue.

Organ/Tissue	⁶⁸ Ga-Y1F		+ 50 nmol cold
	%IA/g	tumor/organ ratio	10 min prior to activity
Blood	2.57 ± 0.33	3.2 ± 0.6	2.39 ± 0.35
Heart (myocard)	1.20 ± 0.16	6.8 ± 1.2	1.16 ± 0.14
Lung	8.81 ± 0.64	0.9 ± 0.1	4.10 ± 0.93
Liver	3.86 ± 0.17	2.1 ± 0.4	3.30 ± 0.40
Spleen	3.48 ± 0.49	2.4 ± 0.2	1.80 ± 0.47
Pancreas	0.61 ± 0.10	13.3 ± 2.3	0.57 ± 0.11
Stomach (empty)	7.37 ± 1.23	1.1 ± 0.3	1.07 ± 0.14
Small intestine (empty)	2.86 ± 0.57	2.9 ± 0.9	1.07 ± 0.10
Large intestine (empty)	4.43 ± 1.28	2.0 ± 0.9	0.95 ± 0.10
Kidneys	111.14 ± 15.33	0.1 ± 0.0	74.29 ± 4.22
Adrenals	1.26 ± 0.24	6.5 ± 0.8	1.51 ± 0.61
Muscle	0.97 ± 0.48	9.5 ± 3.2	0.36 ± 0.03
Tumor H2009	8.08 ± 1.35		1.80 ± 0.12

Table S4: Biodistribution data (90 min p.i.) for ⁶⁸Ga-Y2 without (n = 5; 153 ± 11 pmol) and with (n = 3) addition of 50 nmol of non-labeled compound, in H2009 bearing SCID mice. Data are given as averages ± standard deviation. %IA/g = percent injected activity per gram tissue.

Organ/Tissue	⁶⁸ Ga-Y2		+ 50 nmol cold
	%IA/g	tumor/organ ratio	10 min prior to activity
Blood	2.26 ± 0.26	3.5 ± 0.5	1.75 ± 0.34
Heart (myocard)	1.08 ± 0.13	7.4 ± 0.6	0.83 ± 0.03
Lung	4.80 ± 0.50	1.7 ± 0.2	3.15 ± 0.32
Liver	3.37 ± 0.68	2.4 ± 0.4	3.43 ± 0.59
Spleen	2.51 ± 0.33	3.2 ± 0.7	1.91 ± 0.39
Pancreas	0.65 ± 0.12	12.7 ± 2.9	0.57 ± 0.12
Stomach (empty)	7.17 ± 0.58	1.1 ± 0.1	1.15 ± 0.12
Small intestine (empty)	2.55 ± 0.27	3.1 ± 0.5	0.78 ± 0.11
Large intestine (empty)	3.81 ± 0.53	2.1 ± 0.2	0.96 ± 0.13
Kidneys	91.99 ± 12.24	0.1 ± 0.0	71.99 ± 7.05
Adrenals	1.50 ± 1.28	8.8 ± 6.2	1.46 ± 0.35
Muscle	0.72 ± 0.15	11.4 ± 2.4	0.24 ± 0.05
Tumor H2009	7.95 ± 1.02		1.47 ± 0.19

Table S5: Biodistribution data (90 min p.i.) for ⁶⁸Ga-Y2Y without (n = 5; 101 ± 35 pmol) and with (n = 3) addition of 50 nmol of non-labeled compound, in H2009 bearing SCID mice. Data are given as averages ± standard deviation. %IA/g = percent injected activity per gram tissue.

Organ/Tissue	⁶⁸ Ga-Y2Y		+ 50 nmol cold
	%IA/g	tumor/organ ratio	10 min prior to activity
Blood	1.91 ± 0.49	4.4 ± 1.1	1.21 ± 0.13
Heart (myocard)	0.85 ± 0.16	9.6 ± 1.8	0.74 ± 0.10
Lung	7.02 ± 1.34	1.2 ± 0.2	3.15 ± 0.69
Liver	2.59 ± 0.35	3.1 ± 0.3	2.37 ± 0.34
Spleen	4.36 ± 0.79	1.9 ± 0.4	1.55 ± 0.15
Pancreas	0.44 ± 0.07	18.2 ± 2.3	0.45 ± 0.10
Stomach (empty)	6.55 ± 1.48	1.3 ± 0.3	0.83 ± 0.18
Small intestine (empty)	2.23 ± 0.41	3.6 ± 0.7	0.52 ± 0.05
Large intestine (empty)	3.89 ± 0.73	2.1 ± 0.4	0.65 ± 0.17
Kidneys	80.77 ± 5.12	0.1 ± 0.0	57.09 ± 6.23
Adrenals	1.07 ± 0.27	7.8 ± 1.7	1.11 ± 0.34
Muscle	0.63 ± 0.12	13.0 ± 2.5	0.27 ± 0.14
Tumor H2009	7.93 ± 0.28		1.21 ± 0.17

Table S6: Biodistribution data (90 min p.i.) for ⁶⁸Ga-Y2F without (n = 5; 110 ± 24 pmol) and with (n = 3) addition of 50 nmol of non-labeled compound, in H2009 bearing SCID mice. Data are given as averages ± standard deviation. %IA/g = percent injected activity per gram tissue.

Organ/Tissue	⁶⁸ Ga-Y2F		+ 50 nmol cold
	%IA/g	tumor/organ ratio	10 min prior to activity
Blood	1.62 ± 0.20	4.9 ± 1.0	0.82 ± 0.08
Heart (myocard)	0.76 ± 0.06	10.6 ± 2.0	0.46 ± 0.04
Lung	5.62 ± 1.34	1.4 ± 0.2	2.03 ± 0.09
Liver	2.09 ± 0.17	3.8 ± 0.9	1.86 ± 0.25
Spleen	3.84 ± 1.14	2.2 ± 0.5	1.02 ± 0.38
Pancreas	0.38 ± 0.04	20.8 ± 3.9	0.26 ± 0.06
Stomach (empty)	6.99 ± 3.40	1.3 ± 0.3	0.65 ± 0.13
Small intestine (empty)	2.51 ± 0.50	3.2 ± 0.4	0.55 ± 0.05
Large intestine (empty)	3.96 ± 1.16	2.1 ± 0.5	0.54 ± 0.08
Kidneys	107.37 ± 7.49	0.1 ± 0.0	75.63 ± 7.06
Adrenals	0.84 ± 0.07	9.6 ± 2.2	0.64 ± 0.12
Muscle	0.66 ± 0.12	12.2 ± 1.5	0.14 ± 0.02
Tumor H2009	7.99 ± 1.62		1.03 ± 0.35

Table S7: Biodistribution data (90 min p.i.) for $^{68}\text{Ga-Y3Y}$ without ($n = 5$; 109 ± 7 pmol) and with ($n = 3$) addition of 50 nmol of non-labeled compound, in H2009 bearing SCID mice. Data are given as averages \pm standard deviation. %IA/g = percent injected activity per gram tissue.

Organ/Tissue	$^{68}\text{Ga-Y3Y}$		+ 50 nmol cold 10 min prior to activity
	%IA/g	tumor/organ ratio	
Blood	1.13 \pm 0.25	4.9 \pm 0.5	0.56 \pm 0.18
Heart (myocard)	0.66 \pm 0.16	8.5 \pm 1.1	0.45 \pm 0.12
Lung	4.96 \pm 0.48	1.0 \pm 0.2	2.24 \pm 0.57
Liver	1.23 \pm 0.19	4.4 \pm 0.7	1.40 \pm 0.43
Spleen	3.82 \pm 0.82	1.4 \pm 0.2	1.06 \pm 0.12
Pancreas	0.33 \pm 0.07	17.0 \pm 1.4	0.20 \pm 0.07
Stomach (empty)	4.03 \pm 1.36	1.5 \pm 0.7	0.47 \pm 0.12
Small intestine (empty)	1.69 \pm 0.20	3.2 \pm 0.6	0.41 \pm 0.15
Large intestine (empty)	3.94 \pm 1.85	1.8 \pm 1.1	0.58 \pm 0.24
Kidneys	72.57 \pm 5.25	0.1 \pm 0.0	57.16 \pm 3.56
Adrenals	0.81 \pm 0.41	6.7 \pm 3.0	0.29 \pm 0.15
Muscle	0.51 \pm 0.11	10.7 \pm 1.1	0.14 \pm 0.08
Tumor H2009	5.92 \pm 2.07		0.95 \pm 0.14

Table S8: Biodistribution data (90 min p.i.) for $^{68}\text{Ga-Y3F}$ without ($n = 5$; 93 ± 6 pmol) and with ($n = 3$) addition of 50 nmol of non-labeled compound, in H2009 bearing SCID mice. Data are given as averages \pm standard deviation. %IA/g = percent injected activity per gram tissue.

Organ/Tissue	$^{68}\text{Ga-Y3F}$		+ 50 nmol cold 10 min prior to activity
	%IA/g	tumor/organ ratio	
Blood	0.96 \pm 0.30	7.2 \pm 1.1	0.43 \pm 0.16
Heart (myocard)	0.62 \pm 0.15	10.9 \pm 0.8	0.34 \pm 0.09
Lung	4.83 \pm 1.54	1.5 \pm 0.3	1.60 \pm 0.60
Liver	0.95 \pm 0.22	7.1 \pm 0.7	1.00 \pm 0.40
Spleen	2.38 \pm 0.31	2.8 \pm 0.4	1.04 \pm 0.22
Pancreas	0.34 \pm 0.11	20.4 \pm 3.1	0.15 \pm 0.06
Stomach (empty)	5.64 \pm 1.94	1.3 \pm 0.3	0.55 \pm 0.08
Small intestine (empty)	2.60 \pm 0.90	2.7 \pm 0.5	0.33 \pm 0.07
Large intestine (empty)	5.15 \pm 2.63	1.6 \pm 0.7	0.42 \pm 0.09
Kidneys	71.11 \pm 15.01	0.1 \pm 0.0	49.29 \pm 4.36
Adrenals	0.77 \pm 0.42	10.3 \pm 3.8	0.75 \pm 0.46
Muscle	0.66 \pm 0.25	10.9 \pm 3.0	0.12 \pm 0.07
Tumor H2009	6.69 \pm 1.21		0.89 \pm 0.29

Table S9: Biodistribution data (90 min p.i.) for ⁶⁸Ga-Y4 without (n = 5; 94 ± 14 pmol) and with (n = 3) addition of 50 nmol of non-labeled compound, in H2009 bearing SCID mice. Data are given as averages ± standard deviation. %IA/g = percent injected activity per gram tissue.

Organ/Tissue	⁶⁸ Ga-Y4		+ 50 nmol cold
	%IA/g	tumor/organ ratio	10 min prior to activity
Blood	0.86 ± 0.26	5.5 ± 1.4	0.36 ± 0.02
Heart (myocard)	0.47 ± 0.12	9.6 ± 1.3	0.19 ± 0.04
Lung	3.22 ± 0.63	1.4 ± 0.2	1.31 ± 0.36
Liver	0.93 ± 0.14	5.0 ± 0.5	0.84 ± 0.08
Spleen	1.57 ± 0.57	3.0 ± 0.7	1.00 ± 0.17
Pancreas	0.28 ± 0.08	16.5 ± 1.6	0.12 ± 0.00
Stomach (empty)	4.92 ± 1.06	1.0 ± 0.3	0.47 ± 0.03
Small intestine (empty)	1.35 ± 0.53	3.7 ± 1.0	0.27 ± 0.05
Large intestine (empty)	2.29 ± 0.59	2.1 ± 0.6	0.34 ± 0.01
Kidneys	91.29 ± 8.28	0.1 ± 0.0	65.31 ± 8.22
Adrenals	0.71 ± 0.37	7.1 ± 1.9	0.32 ± 0.01
Muscle	01.41 ± 0.06	12.2 ± 2.8	0.07 ± 0.01
Tumor H2009	4.47 ± 0.96		0.82 ± 0.09

Table S10: Biodistribution data (90 min p.i.) for ⁶⁸Ga-Y6 (⁶⁸Ga-Trivehexin) without (n = 5; 97 ± 13 pmol) and with (n = 3) addition of 50 nmol of Trivehexin, in H2009 bearing SCID mice. Data are given as averages ± standard deviation. %IA/g = percent injected activity per gram tissue.

Organ/Tissue	⁶⁸ Ga-Y6		+ 50 nmol cold
	%IA/g	tumor/organ ratio	10 min prior to activity
Blood	1.03 ± 0.21	7.5 ± 1.7	0.25 ± 0.15
Heart (myocard)	0.59 ± 0.11	13.2 ± 3.1	0.27 ± 0.03
Lung	4.47 ± 1.12	1.8 ± 0.6	0.98 ± 0.25
Liver	0.73 ± 0.11	10.5 ± 2.2	0.59 ± 0.08
Spleen	3.91 ± 0.91	2.0 ± 0.5	1.14 ± 0.13
Pancreas	0.27 ± 0.04	28.5 ± 4.2	0.10 ± 0.03
Stomach (empty)	6.24 ± 1.24	1.2 ± 0.2	0.37 ± 0.09
Small intestine (empty)	2.72 ± 1.15	3.1 ± 1.1	0.25 ± 0.06
Large intestine (empty)	4.36 ± 0.77	1.8 ± 0.5	0.35 ± 0.08
Kidneys	95.73 ± 12.59	0.1 ± 0.0	80.45 ± 17.63
Adrenals	0.50 ± 0.11	15.9 ± 4.3	0.37 ± 0.13
Muscle	0.68 ± 0.18	11.4 ± 2.6	0.07 ± 0.02
Tumor H2009	7.52 ± 1.21		0.69 ± 0.17

5. Kinetic data

Table S11: Kinetic data for $^{68}\text{Ga-YO}$, derived from ROI analysis of 90 min dynamic PET scans ($n = 3$).

Time (min)	Blood	Muscle	Tumor
0.0	0.01 ± 0.00	0.01 ± 0.00	0.01 ± 0.00
0.1	2.15 ± 1.38	0.01 ± 0.00	0.15 ± 0.19
0.2	5.88 ± 1.38	0.01 ± 0.00	0.68 ± 0.17
0.3	9.89 ± 2.02	0.01 ± 0.00	1.26 ± 0.47
0.4	16.32 ± 5.17	0.09 ± 0.07	1.99 ± 0.90
0.5	21.40 ± 8.11	0.51 ± 0.19	2.48 ± 1.32
0.6	23.76 ± 6.69	0.62 ± 0.25	2.75 ± 1.16
0.8	25.90 ± 1.75	0.81 ± 0.08	3.23 ± 1.02
0.9	24.58 ± 0.88	1.01 ± 0.39	3.32 ± 1.08
1.1	23.49 ± 1.06	1.17 ± 0.31	3.44 ± 1.15
1.3	23.00 ± 1.03	1.23 ± 0.24	3.46 ± 1.12
1.4	22.50 ± 1.06	1.36 ± 0.24	3.51 ± 1.19
1.6	22.05 ± 1.16	1.34 ± 0.23	3.59 ± 1.31
1.8	21.75 ± 1.34	1.42 ± 0.15	3.62 ± 1.08
1.9	21.36 ± 1.34	1.25 ± 0.16	3.61 ± 1.09
2.1	21.04 ± 1.42	1.57 ± 0.11	3.53 ± 1.08
2.3	20.81 ± 1.51	1.25 ± 0.06	3.70 ± 1.21
2.4	20.58 ± 1.55	1.36 ± 0.19	3.70 ± 1.22
2.6	20.38 ± 1.59	1.06 ± 0.19	3.74 ± 1.23
2.8	20.08 ± 1.58	1.43 ± 0.08	3.81 ± 1.10
2.9	19.92 ± 1.67	1.13 ± 0.23	3.81 ± 1.20
3.1	19.69 ± 1.44	1.41 ± 0.10	3.86 ± 1.28
3.3	19.56 ± 1.63	1.31 ± 0.26	3.82 ± 1.24
3.4	19.55 ± 1.65	1.37 ± 0.18	3.96 ± 1.27
3.6	19.30 ± 1.81	1.50 ± 0.02	3.96 ± 1.26
3.8	19.17 ± 1.78	1.54 ± 0.12	4.07 ± 1.17
3.9	19.03 ± 1.84	1.18 ± 0.06	4.08 ± 1.36
5.0	18.14 ± 2.04	1.47 ± 0.10	4.29 ± 1.29
7.0	16.72 ± 2.33	1.47 ± 0.11	4.64 ± 1.39
9.0	15.63 ± 2.41	1.55 ± 0.12	4.95 ± 1.53
11.0	14.73 ± 2.45	1.54 ± 0.13	5.21 ± 1.54
13.0	13.97 ± 2.38	1.55 ± 0.16	5.44 ± 1.56
15.0	13.32 ± 2.34	1.65 ± 0.23	5.62 ± 1.62
17.0	12.82 ± 2.24	1.65 ± 0.17	5.79 ± 1.62
19.0	12.39 ± 2.23	1.63 ± 0.18	5.96 ± 1.60
22.5	11.85 ± 2.11	1.68 ± 0.19	6.18 ± 1.62
27.5	11.16 ± 2.00	1.68 ± 0.21	6.45 ± 1.60
32.5	10.64 ± 1.89	1.70 ± 0.25	6.66 ± 1.53
37.5	10.21 ± 1.80	1.69 ± 0.20	6.80 ± 1.52
42.5	9.88 ± 1.75	1.71 ± 0.20	6.92 ± 1.47
47.5	9.63 ± 1.74	1.73 ± 0.19	7.01 ± 1.46
52.5	9.34 ± 1.71	1.71 ± 0.19	7.13 ± 1.36
57.5	9.07 ± 1.68	1.72 ± 0.14	7.20 ± 1.30
65.0	8.72 ± 1.62	1.69 ± 0.17	7.28 ± 1.25
75.0	8.29 ± 1.62	1.68 ± 0.16	7.38 ± 1.10
85.0	7.93 ± 1.58	1.67 ± 0.17	7.45 ± 1.03

Table S12: Kinetic data for ⁶⁸Ga-Y1Y, derived from ROI analysis of 90 min dynamic PET scans (n = 4).

Time (min)	Blood	Muscle	Tumor
0.0	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
0.1	2.64 ± 2.62	0.00 ± 0.00	0.13 ± 0.23
0.2	11.28 ± 7.21	0.00 ± 0.00	0.87 ± 0.89
0.3	17.71 ± 9.52	0.00 ± 0.00	1.66 ± 1.34
0.4	24.35 ± 12.49	0.00 ± 0.00	2.35 ± 1.70
0.5	24.10 ± 8.21	0.05 ± 0.09	2.58 ± 1.40
0.6	23.33 ± 5.72	0.82 ± 0.15	2.54 ± 1.20
0.8	24.09 ± 3.75	0.91 ± 0.28	2.77 ± 1.11
0.9	22.88 ± 2.77	1.13 ± 0.26	2.89 ± 1.05
1.1	21.71 ± 2.45	1.15 ± 0.25	3.03 ± 1.00
1.3	23.25 ± 2.43	1.21 ± 0.14	3.20 ± 0.82
1.4	22.69 ± 2.49	1.31 ± 0.14	3.29 ± 0.74
1.6	21.86 ± 1.75	1.44 ± 0.15	3.37 ± 0.76
1.8	21.37 ± 1.57	1.39 ± 0.26	3.40 ± 0.75
1.9	21.10 ± 1.57	1.43 ± 0.11	3.47 ± 0.71
2.1	20.81 ± 1.65	1.44 ± 0.08	3.58 ± 0.76
2.3	20.41 ± 1.52	1.46 ± 0.12	3.58 ± 0.67
2.4	20.39 ± 1.72	1.43 ± 0.11	3.60 ± 0.69
2.6	20.12 ± 1.53	1.48 ± 0.15	3.67 ± 0.65
2.8	19.95 ± 1.39	1.40 ± 0.17	3.67 ± 0.63
2.9	19.66 ± 1.57	1.35 ± 0.10	3.75 ± 0.58
3.1	19.51 ± 1.51	1.38 ± 0.20	3.81 ± 0.59
3.3	19.37 ± 1.65	1.51 ± 0.09	3.80 ± 0.67
3.4	19.05 ± 1.62	1.60 ± 0.16	3.88 ± 0.53
3.6	18.87 ± 1.66	1.56 ± 0.11	3.82 ± 0.61
3.8	18.95 ± 1.92	1.54 ± 0.05	3.94 ± 0.53
3.9	18.56 ± 1.47	1.51 ± 0.16	3.98 ± 0.48
5.0	17.59 ± 1.69	1.43 ± 0.15	4.17 ± 0.43
7.0	15.92 ± 1.72	1.47 ± 0.14	4.54 ± 0.32
9.0	14.60 ± 1.72	1.55 ± 0.16	4.84 ± 0.26
11.0	13.53 ± 1.56	1.56 ± 0.16	5.04 ± 0.23
13.0	12.65 ± 1.46	1.59 ± 0.15	5.27 ± 0.21
15.0	11.88 ± 1.51	1.60 ± 0.14	5.40 ± 0.22
17.0	11.26 ± 1.55	1.61 ± 0.14	5.56 ± 0.23
19.0	10.72 ± 1.59	1.60 ± 0.11	5.70 ± 0.22
22.5	9.90 ± 1.50	1.60 ± 0.10	5.85 ± 0.19
27.5	8.92 ± 1.45	1.59 ± 0.10	6.05 ± 0.19
32.5	8.26 ± 1.37	1.60 ± 0.08	6.18 ± 0.20
37.5	7.76 ± 1.28	1.59 ± 0.06	6.25 ± 0.21
42.5	7.37 ± 1.20	1.58 ± 0.06	6.33 ± 0.24
47.5	7.08 ± 1.18	1.54 ± 0.05	6.36 ± 0.25
52.5	6.80 ± 1.11	1.52 ± 0.04	6.41 ± 0.27
57.5	6.53 ± 1.03	1.52 ± 0.07	6.43 ± 0.30
65.0	6.18 ± 0.98	1.47 ± 0.06	6.45 ± 0.32
75.0	5.74 ± 0.87	1.43 ± 0.07	6.49 ± 0.37
85.0	5.45 ± 0.81	1.41 ± 0.09	6.52 ± 0.42

Table S13: Kinetic data for ^{68}Ga -Y1F, derived from ROI analysis of 90 min dynamic PET scans (n = 2).

Time (min)	Blood	Muscle	Tumor
0.0	0.99 ± 1.41	0.00 ± 0.00	0.00 ± 0.00
0.1	11.30 ± 5.10	0.00 ± 0.00	0.35 ± 0.49
0.2	18.40 ± 4.37	0.03 ± 0.05	0.73 ± 1.03
0.3	21.84 ± 8.22	0.17 ± 0.29	0.91 ± 1.29
0.4	19.27 ± 8.57	0.31 ± 0.54	1.19 ± 0.86
0.5	17.66 ± 7.93	0.34 ± 0.59	1.93 ± 0.16
0.6	22.31 ± 4.99	0.55 ± 0.41	2.11 ± 0.08
0.8	24.88 ± 1.69	0.59 ± 0.54	2.27 ± 0.02
0.9	23.21 ± 0.58	0.73 ± 0.63	2.20 ± 0.17
1.1	20.72 ± 2.42	0.66 ± 0.57	2.27 ± 0.19
1.3	20.92 ± 1.47	0.75 ± 0.66	2.29 ± 0.18
1.4	20.67 ± 1.62	0.82 ± 0.48	2.17 ± 0.42
1.6	20.11 ± 1.34	0.92 ± 0.37	2.36 ± 0.16
1.8	19.56 ± 1.48	1.03 ± 0.22	2.46 ± 0.36
1.9	19.36 ± 1.43	1.18 ± 0.16	2.40 ± 0.23
2.1	18.91 ± 1.27	1.19 ± 0.08	2.50 ± 0.35
2.3	18.69 ± 1.28	1.33 ± 0.09	2.49 ± 0.13
2.4	18.54 ± 1.35	1.23 ± 0.10	2.54 ± 0.42
2.6	18.29 ± 1.43	1.36 ± 0.20	2.65 ± 0.23
2.8	18.04 ± 1.39	1.30 ± 0.14	2.52 ± 0.37
2.9	17.81 ± 0.99	1.31 ± 0.13	2.74 ± 0.23
3.1	17.74 ± 1.28	1.44 ± 0.12	2.93 ± 0.11
3.3	17.31 ± 1.22	1.38 ± 0.22	2.82 ± 0.18
3.4	17.07 ± 1.20	1.37 ± 0.22	2.98 ± 0.24
3.6	16.89 ± 1.20	1.49 ± 0.12	2.88 ± 0.02
3.8	16.66 ± 1.35	1.41 ± 0.14	3.08 ± 0.14
3.9	16.61 ± 1.35	1.47 ± 0.29	2.97 ± 0.06
5.0	15.58 ± 1.52	1.41 ± 0.19	3.35 ± 0.05
7.0	13.91 ± 1.59	1.51 ± 0.17	3.74 ± 0.08
9.0	12.47 ± 1.40	1.49 ± 0.19	4.09 ± 0.10
11.0	11.25 ± 0.99	1.51 ± 0.17	4.37 ± 0.07
13.0	10.31 ± 0.73	1.55 ± 0.15	4.61 ± 0.02
15.0	9.70 ± 0.57	1.58 ± 0.19	4.78 ± 0.00
17.0	9.24 ± 0.42	1.57 ± 0.18	4.96 ± 0.06
19.0	8.85 ± 0.19	1.60 ± 0.17	5.09 ± 0.03
22.5	8.42 ± 0.05	1.59 ± 0.21	5.23 ± 0.11
27.5	7.87 ± 0.24	1.59 ± 0.20	5.46 ± 0.07
32.5	7.49 ± 0.37	1.57 ± 0.22	5.62 ± 0.09
37.5	7.19 ± 0.48	1.58 ± 0.20	5.78 ± 0.11
42.5	6.95 ± 0.48	1.57 ± 0.25	5.86 ± 0.09
47.5	6.71 ± 0.47	1.58 ± 0.20	5.97 ± 0.14
52.5	6.50 ± 0.38	1.55 ± 0.24	6.03 ± 0.12
57.5	6.38 ± 0.38	1.54 ± 0.20	6.05 ± 0.11
65.0	6.20 ± 0.36	1.52 ± 0.24	6.16 ± 0.07
75.0	5.94 ± 0.33	1.51 ± 0.24	6.24 ± 0.06
85.0	5.71 ± 0.31	1.47 ± 0.22	6.35 ± 0.05

Table S14: Kinetic data for ^{68}Ga -Y2, derived from ROI analysis of 90 min dynamic PET scans (n = 3).

Time (min)	Blood	Muscle	Tumor
0.0	0.75 ± 1.28	0.00 ± 0.00	0.00 ± 0.00
0.1	6.94 ± 7.46	0.00 ± 0.00	0.11 ± 0.09
0.2	19.50 ± 10.00	0.00 ± 0.00	0.89 ± 0.49
0.3	27.64 ± 8.30	0.01 ± 0.01	1.66 ± 0.53
0.4	30.18 ± 1.67	0.26 ± 0.42	2.37 ± 0.50
0.5	28.66 ± 2.23	0.58 ± 0.58	2.83 ± 0.40
0.6	24.65 ± 0.43	0.95 ± 0.20	2.95 ± 0.86
0.8	22.29 ± 1.32	1.21 ± 0.06	3.16 ± 1.06
0.9	21.50 ± 1.21	1.44 ± 0.09	3.41 ± 0.99
1.1	20.61 ± 0.90	1.33 ± 0.06	3.52 ± 0.76
1.3	20.30 ± 1.16	1.46 ± 0.25	3.51 ± 0.79
1.4	19.74 ± 0.67	1.43 ± 0.20	3.60 ± 0.82
1.6	19.02 ± 1.14	1.24 ± 0.14	3.62 ± 0.74
1.8	18.98 ± 0.96	1.46 ± 0.07	3.69 ± 0.85
1.9	18.48 ± 0.84	1.53 ± 0.15	3.82 ± 0.80
2.1	18.41 ± 0.96	1.67 ± 0.25	3.88 ± 0.75
2.3	17.83 ± 0.69	1.58 ± 0.32	3.86 ± 0.82
2.4	17.59 ± 0.71	1.54 ± 0.14	4.08 ± 0.63
2.6	17.29 ± 0.72	1.49 ± 0.19	4.03 ± 0.79
2.8	16.94 ± 0.73	1.72 ± 0.11	4.03 ± 0.70
2.9	16.67 ± 0.49	1.63 ± 0.09	4.10 ± 0.69
3.1	16.46 ± 0.56	1.72 ± 0.12	4.14 ± 0.78
3.3	16.32 ± 0.39	1.72 ± 0.34	4.26 ± 0.67
3.4	15.95 ± 0.32	1.72 ± 0.03	4.24 ± 0.76
3.6	15.88 ± 0.28	1.81 ± 0.16	4.36 ± 0.75
3.8	15.65 ± 0.27	1.69 ± 0.03	4.36 ± 0.66
3.9	15.27 ± 0.16	1.82 ± 0.34	4.53 ± 0.52
5.0	14.17 ± 0.22	1.68 ± 0.13	4.62 ± 0.64
7.0	12.45 ± 0.51	1.71 ± 0.15	4.88 ± 0.57
9.0	11.30 ± 0.68	1.74 ± 0.16	5.09 ± 0.54
11.0	10.48 ± 0.75	1.73 ± 0.20	5.23 ± 0.52
13.0	9.85 ± 0.79	1.71 ± 0.20	5.30 ± 0.53
15.0	9.34 ± 0.81	1.68 ± 0.15	5.35 ± 0.54
17.0	8.95 ± 0.81	1.65 ± 0.14	5.44 ± 0.52
19.0	8.59 ± 0.86	1.65 ± 0.14	5.44 ± 0.58
22.5	8.16 ± 0.84	1.64 ± 0.17	5.46 ± 0.59
27.5	7.70 ± 0.87	1.61 ± 0.16	5.50 ± 0.61
32.5	7.26 ± 0.87	1.57 ± 0.17	5.48 ± 0.65
37.5	6.92 ± 0.84	1.54 ± 0.15	5.48 ± 0.65
42.5	6.62 ± 0.82	1.49 ± 0.17	5.47 ± 0.67
47.5	6.33 ± 0.80	1.49 ± 0.18	5.47 ± 0.70
52.5	6.09 ± 0.81	1.44 ± 0.15	5.43 ± 0.70
57.5	5.83 ± 0.80	1.42 ± 0.14	5.44 ± 0.69
65.0	5.51 ± 0.81	1.38 ± 0.16	5.45 ± 0.69
75.0	5.13 ± 0.86	1.34 ± 0.16	5.41 ± 0.67
85.0	4.80 ± 0.84	1.30 ± 0.17	5.40 ± 0.66

Table S15: Kinetic data for ^{68}Ga -Y2Y, derived from ROI analysis of 90 min dynamic PET scans (n = 3).

Time (min)	Blood	Muscle	Tumor
0.0	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
0.1	3.95 ± 1.48	0.00 ± 0.00	0.12 ± 0.12
0.2	12.14 ± 0.76	0.00 ± 0.00	0.81 ± 0.13
0.3	18.86 ± 0.49	0.11 ± 0.18	1.65 ± 0.26
0.4	24.31 ± 3.17	0.18 ± 0.29	2.40 ± 0.57
0.5	24.43 ± 6.95	0.61 ± 0.34	2.73 ± 0.89
0.6	20.59 ± 4.39	1.09 ± 0.26	2.65 ± 0.84
0.8	19.62 ± 3.96	1.18 ± 0.31	2.90 ± 0.96
0.9	19.12 ± 3.65	1.21 ± 0.23	2.93 ± 0.89
1.1	18.76 ± 3.55	1.27 ± 0.31	3.03 ± 0.90
1.3	18.14 ± 3.49	1.43 ± 0.42	3.11 ± 0.91
1.4	17.95 ± 3.53	1.37 ± 0.41	3.15 ± 0.89
1.6	17.48 ± 3.42	1.39 ± 0.28	3.23 ± 0.92
1.8	17.34 ± 3.31	1.30 ± 0.31	3.33 ± 0.88
1.9	16.86 ± 3.40	1.37 ± 0.33	3.38 ± 0.89
2.1	16.69 ± 3.33	1.46 ± 0.32	3.40 ± 0.94
2.3	16.43 ± 3.26	1.38 ± 0.40	3.45 ± 0.89
2.4	16.34 ± 3.32	1.51 ± 0.26	3.47 ± 0.90
2.6	16.09 ± 3.32	1.43 ± 0.34	3.52 ± 0.87
2.8	15.78 ± 3.08	1.37 ± 0.36	3.60 ± 0.89
2.9	15.67 ± 3.34	1.61 ± 0.41	3.66 ± 0.87
3.1	15.42 ± 3.24	1.39 ± 0.22	3.74 ± 0.90
3.3	15.35 ± 3.23	1.49 ± 0.53	3.77 ± 0.90
3.4	15.11 ± 3.22	1.47 ± 0.28	3.77 ± 0.89
3.6	14.84 ± 3.21	1.40 ± 0.39	3.83 ± 0.94
3.8	14.82 ± 3.35	1.56 ± 0.46	3.87 ± 0.90
3.9	14.64 ± 3.04	1.53 ± 0.33	3.93 ± 0.90
5.0	13.69 ± 3.02	1.52 ± 0.33	4.14 ± 0.91
7.0	12.37 ± 2.81	1.59 ± 0.38	4.52 ± 0.96
9.0	11.31 ± 2.64	1.62 ± 0.41	4.79 ± 1.01
11.0	10.42 ± 2.48	1.63 ± 0.41	5.00 ± 1.04
13.0	9.73 ± 2.44	1.65 ± 0.45	5.19 ± 1.07
15.0	9.10 ± 2.33	1.63 ± 0.43	5.34 ± 1.11
17.0	8.53 ± 2.26	1.65 ± 0.47	5.47 ± 1.19
19.0	8.09 ± 2.17	1.65 ± 0.46	5.56 ± 1.21
22.5	7.47 ± 2.03	1.63 ± 0.46	5.74 ± 1.29
27.5	6.77 ± 1.88	1.62 ± 0.49	5.90 ± 1.36
32.5	6.24 ± 1.75	1.58 ± 0.53	6.01 ± 1.41
37.5	5.82 ± 1.65	1.57 ± 0.52	6.10 ± 1.44
42.5	5.54 ± 1.61	1.55 ± 0.53	6.18 ± 1.50
47.5	5.31 ± 1.60	1.54 ± 0.52	6.23 ± 1.52
52.5	5.10 ± 1.58	1.52 ± 0.51	6.26 ± 1.53
57.5	4.89 ± 1.50	1.47 ± 0.49	6.29 ± 1.55
65.0	4.54 ± 1.35	1.44 ± 0.50	6.35 ± 1.62
75.0	4.16 ± 1.22	1.40 ± 0.49	6.38 ± 1.66
85.0	3.94 ± 1.19	1.37 ± 0.51	6.39 ± 1.70

Table S16: Kinetic data for ⁶⁸Ga-Y2F, derived from ROI analysis of 90 min dynamic PET scans (n = 3).

Time (min)	Blood	Muscle	Tumor
0.0	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
0.1	4.42 ± 0.92	0.00 ± 0.00	0.13 ± 0.16
0.2	15.31 ± 0.79	0.00 ± 0.00	1.08 ± 0.43
0.3	25.08 ± 0.69	0.00 ± 0.00	2.04 ± 0.41
0.4	27.51 ± 2.57	0.15 ± 0.14	2.37 ± 0.22
0.5	25.75 ± 1.66	0.32 ± 0.42	2.68 ± 0.09
0.6	24.07 ± 2.09	1.04 ± 0.20	2.61 ± 0.24
0.8	22.36 ± 1.75	1.11 ± 0.17	2.55 ± 0.36
0.9	21.49 ± 1.36	1.30 ± 0.29	2.66 ± 0.35
1.1	20.30 ± 0.91	1.43 ± 0.24	2.82 ± 0.33
1.3	19.58 ± 0.87	1.43 ± 0.25	2.90 ± 0.31
1.4	19.23 ± 1.07	1.40 ± 0.30	3.00 ± 0.31
1.6	18.49 ± 0.98	1.44 ± 0.19	3.05 ± 0.44
1.8	18.11 ± 0.95	1.47 ± 0.28	3.07 ± 0.24
1.9	17.41 ± 0.89	1.46 ± 0.16	3.23 ± 0.39
2.1	17.15 ± 1.03	1.51 ± 0.22	3.31 ± 0.36
2.3	16.96 ± 1.13	1.54 ± 0.27	3.32 ± 0.44
2.4	16.51 ± 1.25	1.57 ± 0.08	3.43 ± 0.31
2.6	16.15 ± 1.25	1.79 ± 0.31	3.50 ± 0.26
2.8	15.96 ± 1.21	1.68 ± 0.54	3.61 ± 0.46
2.9	15.60 ± 1.33	1.55 ± 0.25	3.63 ± 0.31
3.1	15.36 ± 1.50	1.60 ± 0.15	3.63 ± 0.41
3.3	14.93 ± 1.43	1.76 ± 0.27	3.64 ± 0.34
3.4	14.83 ± 1.48	1.52 ± 0.17	3.86 ± 0.38
3.6	14.51 ± 1.53	1.71 ± 0.27	3.74 ± 0.46
3.8	14.22 ± 1.58	1.65 ± 0.33	3.89 ± 0.40
3.9	14.08 ± 1.43	1.59 ± 0.18	3.99 ± 0.39
5.0	12.61 ± 1.82	1.56 ± 0.02	4.22 ± 0.39
7.0	10.80 ± 2.03	1.62 ± 0.03	4.61 ± 0.44
9.0	9.63 ± 2.01	1.63 ± 0.05	4.91 ± 0.49
11.0	8.84 ± 2.02	1.63 ± 0.04	5.12 ± 0.48
13.0	8.26 ± 1.93	1.57 ± 0.02	5.30 ± 0.54
15.0	7.71 ± 1.77	1.61 ± 0.05	5.39 ± 0.61
17.0	7.26 ± 1.56	1.58 ± 0.02	5.52 ± 0.62
19.0	6.83 ± 1.34	1.56 ± 0.06	5.60 ± 0.65
22.5	6.28 ± 1.05	1.54 ± 0.04	5.74 ± 0.73
27.5	5.72 ± 0.68	1.48 ± 0.06	5.85 ± 0.79
32.5	5.44 ± 0.42	1.47 ± 0.07	5.93 ± 0.80
37.5	5.11 ± 0.29	1.43 ± 0.09	5.96 ± 0.87
42.5	4.90 ± 0.21	1.38 ± 0.08	5.99 ± 0.86
47.5	4.70 ± 0.17	1.36 ± 0.10	6.04 ± 0.88
52.5	4.46 ± 0.10	1.34 ± 0.10	6.05 ± 0.89
57.5	4.27 ± 0.14	1.29 ± 0.08	6.09 ± 0.91
65.0	3.99 ± 0.16	1.25 ± 0.09	6.12 ± 0.91
75.0	3.69 ± 0.20	1.18 ± 0.10	6.12 ± 0.98
85.0	3.48 ± 0.18	1.13 ± 0.09	6.10 ± 1.00

Table S17: Kinetic data for ^{68}Ga -**Y3Y**, derived from ROI analysis of 90 min dynamic PET scans (n = 3).

Time (min)	Blood	Muscle	Tumor
0.0	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
0.1	4.00 ± 3.37	0.00 ± 0.00	0.09 ± 0.15
0.2	12.05 ± 8.54	0.00 ± 0.00	0.50 ± 0.64
0.3	17.19 ± 10.42	0.00 ± 0.00	0.88 ± 0.97
0.4	20.19 ± 7.27	0.00 ± 0.00	1.11 ± 0.93
0.5	23.10 ± 3.56	0.00 ± 0.00	1.33 ± 0.77
0.6	21.19 ± 3.30	0.76 ± 0.14	1.42 ± 0.67
0.8	19.10 ± 1.93	0.90 ± 0.30	1.58 ± 0.70
0.9	20.22 ± 5.07	1.00 ± 0.22	1.73 ± 0.69
1.1	19.00 ± 4.17	1.08 ± 0.15	1.80 ± 0.58
1.3	17.50 ± 3.37	1.19 ± 0.17	1.88 ± 0.64
1.4	16.18 ± 2.29	1.24 ± 0.30	1.99 ± 0.68
1.6	15.36 ± 1.85	1.28 ± 0.20	2.10 ± 0.68
1.8	14.87 ± 1.74	1.29 ± 0.13	2.18 ± 0.64
1.9	14.39 ± 1.56	1.45 ± 0.20	2.26 ± 0.63
2.1	13.96 ± 1.51	1.49 ± 0.05	2.38 ± 0.63
2.3	13.45 ± 1.55	1.45 ± 0.14	2.39 ± 0.55
2.4	13.08 ± 1.24	1.41 ± 0.27	2.52 ± 0.53
2.6	12.62 ± 1.51	1.57 ± 0.19	2.56 ± 0.51
2.8	12.21 ± 1.39	1.62 ± 0.15	2.64 ± 0.44
2.9	11.94 ± 1.15	1.59 ± 0.20	2.70 ± 0.57
3.1	11.67 ± 1.30	1.60 ± 0.21	2.74 ± 0.49
3.3	11.42 ± 1.22	1.58 ± 0.31	2.77 ± 0.42
3.4	11.15 ± 1.21	1.60 ± 0.33	2.82 ± 0.43
3.6	10.93 ± 1.09	1.71 ± 0.13	2.94 ± 0.47
3.8	10.64 ± 1.18	1.60 ± 0.27	2.95 ± 0.38
3.9	10.55 ± 1.08	1.56 ± 0.18	3.06 ± 0.35
5.0	9.24 ± 1.09	1.61 ± 0.28	3.22 ± 0.34
7.0	7.65 ± 0.88	1.63 ± 0.24	3.51 ± 0.25
9.0	6.63 ± 0.83	1.63 ± 0.27	3.69 ± 0.22
11.0	5.93 ± 0.80	1.64 ± 0.27	3.81 ± 0.20
13.0	5.38 ± 0.75	1.59 ± 0.22	3.91 ± 0.19
15.0	4.96 ± 0.70	1.52 ± 0.24	3.96 ± 0.16
17.0	4.60 ± 0.70	1.53 ± 0.23	4.00 ± 0.17
19.0	4.30 ± 0.65	1.49 ± 0.18	4.02 ± 0.15
22.5	3.93 ± 0.62	1.44 ± 0.18	4.09 ± 0.14
27.5	3.49 ± 0.56	1.35 ± 0.17	4.11 ± 0.15
32.5	3.15 ± 0.51	1.29 ± 0.17	4.12 ± 0.14
37.5	2.89 ± 0.52	1.23 ± 0.17	4.11 ± 0.13
42.5	2.68 ± 0.47	1.16 ± 0.18	4.10 ± 0.14
47.5	2.49 ± 0.44	1.15 ± 0.14	4.10 ± 0.11
52.5	2.33 ± 0.46	1.10 ± 0.18	4.06 ± 0.14
57.5	2.16 ± 0.43	1.06 ± 0.15	4.05 ± 0.14
65.0	2.01 ± 0.40	0.99 ± 0.16	3.98 ± 0.18
75.0	1.82 ± 0.37	0.93 ± 0.17	3.91 ± 0.20
85.0	1.65 ± 0.34	0.89 ± 0.15	3.84 ± 0.24

Table S18: Kinetic data for ^{68}Ga -Y3F, derived from ROI analysis of 90 min dynamic PET scans (n = 3).

Time (min)	Blood	Muscle	Tumor
0.0	0.85 ± 1.47	0.00 ± 0.00	0.00 ± 0.00
0.1	9.72 ± 5.35	0.00 ± 0.00	0.14 ± 0.16
0.2	18.84 ± 7.99	0.00 ± 0.00	0.64 ± 0.31
0.3	26.89 ± 7.33	0.01 ± 0.02	1.27 ± 0.20
0.4	29.52 ± 4.86	0.24 ± 0.42	1.71 ± 0.31
0.5	27.07 ± 3.36	0.46 ± 0.65	1.89 ± 0.52
0.6	21.14 ± 1.36	0.83 ± 0.10	1.84 ± 0.40
0.8	18.68 ± 0.81	1.16 ± 0.17	2.02 ± 0.42
0.9	17.58 ± 0.96	1.14 ± 0.06	2.18 ± 0.45
1.1	16.50 ± 1.08	1.23 ± 0.10	2.36 ± 0.40
1.3	15.68 ± 1.13	1.21 ± 0.17	2.47 ± 0.39
1.4	14.80 ± 1.05	1.59 ± 0.29	2.56 ± 0.34
1.6	14.22 ± 1.14	1.48 ± 0.65	2.65 ± 0.39
1.8	13.73 ± 1.07	1.57 ± 0.20	2.75 ± 0.43
1.9	13.28 ± 1.30	1.68 ± 0.32	2.85 ± 0.43
2.1	12.60 ± 1.28	1.49 ± 0.39	2.93 ± 0.38
2.3	12.14 ± 1.44	1.49 ± 0.28	3.03 ± 0.38
2.4	11.75 ± 1.30	1.50 ± 0.50	3.02 ± 0.34
2.6	11.58 ± 1.34	1.53 ± 0.23	3.27 ± 0.47
2.8	11.06 ± 1.25	1.41 ± 0.07	3.17 ± 0.38
2.9	10.74 ± 1.48	1.48 ± 0.10	3.26 ± 0.30
3.1	10.49 ± 1.25	1.51 ± 0.02	3.31 ± 0.29
3.3	10.20 ± 1.33	1.84 ± 0.35	3.37 ± 0.31
3.4	9.91 ± 1.32	1.61 ± 0.33	3.52 ± 0.39
3.6	9.68 ± 1.34	1.57 ± 0.49	3.48 ± 0.33
3.8	9.46 ± 1.33	1.84 ± 0.17	3.51 ± 0.25
3.9	9.14 ± 1.27	1.64 ± 0.18	3.62 ± 0.31
5.0	7.93 ± 1.18	1.67 ± 0.16	3.73 ± 0.20
7.0	6.35 ± 0.96	1.72 ± 0.22	4.03 ± 0.10
9.0	5.38 ± 0.85	1.69 ± 0.19	4.17 ± 0.05
11.0	4.72 ± 0.75	1.62 ± 0.07	4.30 ± 0.08
13.0	4.24 ± 0.71	1.62 ± 0.09	4.33 ± 0.17
15.0	3.89 ± 0.66	1.67 ± 0.11	4.40 ± 0.17
17.0	3.59 ± 0.61	1.56 ± 0.01	4.44 ± 0.23
19.0	3.37 ± 0.50	1.51 ± 0.06	4.45 ± 0.24
22.5	3.01 ± 0.47	1.47 ± 0.04	4.48 ± 0.28
27.5	2.65 ± 0.39	1.42 ± 0.03	4.46 ± 0.34
32.5	2.37 ± 0.34	1.36 ± 0.10	4.46 ± 0.36
37.5	2.14 ± 0.32	1.28 ± 0.12	4.42 ± 0.39
42.5	1.97 ± 0.30	1.21 ± 0.14	4.39 ± 0.41
47.5	1.82 ± 0.28	1.23 ± 0.10	4.37 ± 0.41
52.5	1.71 ± 0.26	1.19 ± 0.09	4.32 ± 0.40
57.5	1.60 ± 0.24	1.12 ± 0.18	4.28 ± 0.44
65.0	1.45 ± 0.25	1.09 ± 0.14	4.21 ± 0.44
75.0	1.30 ± 0.22	1.04 ± 0.17	4.13 ± 0.44
85.0	1.19 ± 0.22	0.97 ± 0.18	4.03 ± 0.46

Table S19: Kinetic data for ^{68}Ga -Y4, derived from ROI analysis of 90 min dynamic PET scans (n = 3).

Time (min)	Blood	Muscle	Tumor
0.0	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
0.1	3.33 ± 1.82	0.00 ± 0.00	0.01 ± 0.02
0.2	18.09 ± 4.10	0.00 ± 0.00	0.97 ± 0.87
0.3	29.77 ± 6.66	0.00 ± 0.00	1.98 ± 1.35
0.4	34.25 ± 5.16	0.58 ± 0.24	2.61 ± 1.68
0.5	30.05 ± 3.71	1.15 ± 0.29	3.02 ± 1.71
0.6	25.44 ± 1.65	1.24 ± 0.25	3.06 ± 1.41
0.8	22.62 ± 0.89	1.48 ± 0.15	3.24 ± 1.50
0.9	21.13 ± 0.65	1.51 ± 0.25	3.25 ± 1.16
1.1	19.86 ± 1.10	1.55 ± 0.23	2.96 ± 0.39
1.3	18.77 ± 0.83	1.51 ± 0.16	3.16 ± 0.64
1.4	18.24 ± 1.26	1.64 ± 0.12	3.09 ± 0.40
1.6	17.61 ± 1.30	1.66 ± 0.05	3.21 ± 0.40
1.8	17.08 ± 1.30	1.72 ± 0.19	3.27 ± 0.49
1.9	16.35 ± 1.56	1.72 ± 0.07	3.33 ± 0.47
2.1	16.02 ± 1.48	1.78 ± 0.11	3.37 ± 0.46
2.3	15.42 ± 1.59	1.75 ± 0.06	3.50 ± 0.48
2.4	15.29 ± 1.59	1.87 ± 0.02	3.49 ± 0.40
2.6	14.90 ± 1.76	1.87 ± 0.17	3.59 ± 0.41
2.8	14.51 ± 1.69	1.77 ± 0.06	3.60 ± 0.28
2.9	14.20 ± 1.85	1.87 ± 0.20	3.71 ± 0.32
3.1	13.82 ± 1.71	1.81 ± 0.14	3.75 ± 0.35
3.3	13.65 ± 1.88	1.89 ± 0.07	3.77 ± 0.32
3.4	13.30 ± 1.79	1.93 ± 0.09	3.88 ± 0.33
3.6	13.00 ± 1.75	1.95 ± 0.12	3.82 ± 0.31
3.8	12.70 ± 1.69	1.88 ± 0.18	3.81 ± 0.25
3.9	12.53 ± 1.81	2.06 ± 0.22	3.86 ± 0.29
5.0	11.13 ± 1.74	1.90 ± 0.09	4.00 ± 0.20
7.0	9.43 ± 1.74	1.87 ± 0.05	4.12 ± 0.17
9.0	8.21 ± 1.75	1.80 ± 0.09	4.18 ± 0.26
11.0	7.32 ± 1.76	1.77 ± 0.16	4.23 ± 0.30
13.0	6.61 ± 1.76	1.72 ± 0.14	4.20 ± 0.29
15.0	6.01 ± 1.66	1.68 ± 0.11	4.22 ± 0.31
17.0	5.59 ± 1.57	1.63 ± 0.08	4.16 ± 0.33
19.0	5.25 ± 1.51	1.59 ± 0.14	4.15 ± 0.35
22.5	4.75 ± 1.32	1.52 ± 0.13	4.08 ± 0.37
27.5	4.22 ± 1.08	1.42 ± 0.09	4.02 ± 0.39
32.5	3.82 ± 0.92	1.33 ± 0.11	3.94 ± 0.36
37.5	3.52 ± 0.80	1.26 ± 0.08	3.87 ± 0.39
42.5	3.24 ± 0.69	1.21 ± 0.07	3.79 ± 0.36
47.5	3.01 ± 0.62	1.15 ± 0.08	3.72 ± 0.40
52.5	2.81 ± 0.54	1.10 ± 0.06	3.68 ± 0.38
57.5	2.64 ± 0.47	1.05 ± 0.07	3.62 ± 0.40
65.0	2.43 ± 0.39	1.00 ± 0.06	3.54 ± 0.36
75.0	2.17 ± 0.30	0.92 ± 0.05	3.45 ± 0.38
85.0	1.94 ± 0.24	0.86 ± 0.03	3.35 ± 0.36

Table S20: Kinetic data for $^{68}\text{Ga-Y6}$ ($^{68}\text{Ga-Trivehexin}$), derived from ROI analysis of 90 min dyn. PET scans (n = 3).

Time (min)	Blood	Muscle	Tumor
0.0	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
0.1	3.40 ± 2.13	0.00 ± 0.00	0.16 ± 0.24
0.2	7.35 ± 4.77	0.26 ± 0.45	0.51 ± 0.60
0.3	11.96 ± 7.68	0.69 ± 1.20	0.87 ± 0.92
0.4	17.23 ± 11.03	0.61 ± 1.05	1.45 ± 1.19
0.5	19.30 ± 10.77	1.00 ± 1.72	1.80 ± 1.18
0.6	20.51 ± 10.61	1.15 ± 1.26	1.99 ± 1.07
0.8	19.30 ± 4.45	1.19 ± 1.01	2.45 ± 1.03
0.9	20.40 ± 2.40	1.52 ± 1.24	2.85 ± 0.83
1.1	18.82 ± 2.36	1.59 ± 1.15	2.98 ± 0.91
1.3	17.62 ± 2.21	1.83 ± 1.09	3.26 ± 0.82
1.4	16.65 ± 2.12	1.82 ± 0.98	3.37 ± 0.77
1.6	16.00 ± 2.12	2.07 ± 1.35	3.50 ± 0.78
1.8	15.43 ± 2.26	1.90 ± 1.41	3.70 ± 0.75
1.9	14.84 ± 2.05	2.01 ± 1.15	3.68 ± 0.80
2.1	14.30 ± 2.01	1.92 ± 1.14	3.99 ± 0.80
2.3	13.77 ± 1.90	1.95 ± 0.94	4.06 ± 0.85
2.4	13.40 ± 2.08	1.90 ± 1.06	4.16 ± 0.85
2.6	13.14 ± 1.99	1.93 ± 0.91	4.31 ± 0.80
2.8	12.75 ± 1.84	2.00 ± 1.00	4.40 ± 0.77
2.9	12.54 ± 1.97	2.34 ± 1.17	4.46 ± 0.66
3.1	12.04 ± 1.74	2.12 ± 1.26	4.48 ± 0.80
3.3	11.94 ± 1.93	2.17 ± 1.19	4.70 ± 0.83
3.4	11.44 ± 1.87	1.81 ± 0.97	4.75 ± 0.74
3.6	11.26 ± 1.76	2.33 ± 1.46	4.61 ± 0.80
3.8	10.99 ± 1.86	2.06 ± 1.24	4.80 ± 0.65
3.9	10.79 ± 1.86	2.30 ± 1.00	4.88 ± 0.72
5.0	9.54 ± 1.67	2.12 ± 1.06	5.14 ± 0.73
7.0	7.89 ± 1.29	2.16 ± 0.92	5.60 ± 0.62
9.0	6.86 ± 1.16	2.05 ± 0.79	5.87 ± 0.63
11.0	6.09 ± 1.01	2.02 ± 0.75	6.07 ± 0.61
13.0	5.56 ± 0.88	1.99 ± 0.62	6.20 ± 0.62
15.0	5.12 ± 0.85	1.94 ± 0.65	6.28 ± 0.68
17.0	4.78 ± 0.79	1.89 ± 0.63	6.37 ± 0.72
19.0	4.49 ± 0.75	1.81 ± 0.51	6.38 ± 0.75
22.5	4.10 ± 0.69	1.77 ± 0.51	6.47 ± 0.80
27.5	3.66 ± 0.64	1.66 ± 0.43	6.49 ± 0.84
32.5	3.32 ± 0.59	1.57 ± 0.39	6.50 ± 0.92
37.5	3.06 ± 0.53	1.50 ± 0.35	6.46 ± 0.97
42.5	2.85 ± 0.52	1.46 ± 0.31	6.41 ± 0.99
47.5	2.67 ± 0.50	1.40 ± 0.31	6.34 ± 1.02
52.5	2.53 ± 0.49	1.34 ± 0.32	6.31 ± 1.07
57.5	2.40 ± 0.48	1.34 ± 0.29	6.24 ± 1.11
65.0	2.26 ± 0.49	1.26 ± 0.28	6.17 ± 1.13
75.0	2.11 ± 0.50	1.20 ± 0.26	6.05 ± 1.17
85.0	1.99 ± 0.54	1.14 ± 0.24	5.93 ± 1.21