

Supplementary Information

Coumarin-Based Fluorescent Probe for Central Nervous System Disease Biomarker. *Sensors* 2014, 14, 21140-21150

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Table S1. Fluorescence data of homocysteine in standard sample.

Standard Concentration (μM)	Fluorescence Intensity (au)	Detected Concentration (μM)	Recovery (%)
10	74.49 ± 0.84	7.32	73
20	84.38 ± 1.44	27.36	137
50	96.05 ± 0.91	51.03	102
100	113.46 ± 6.25	86.32	86
150	148.81 ± 11.48	157.97	105

Table S2. LC-MS measurements of standard samples.

Compound	R ²	Standard Concentration (μ M or nM)	Standard Concentration (ppm)	Detected Concentration	Recovery (%)
Homocysteine	0.9996	0.741 μ M	0.1	0.516 $\pm$ 0.232 μ M	70
		3.71 μ M	0.5	2.319 $\pm$ 0.086 μ M	63
		7.41 μ M	1	6.420 $\pm$ 0.678 μ M	87
		37.1 μ M	5	34.481 $\pm$ 0.430 μ M	93
		74.1 μ M	10	69.770 $\pm$ 0.382 μ M	94
Methymalonic acid	0.9985	0.847 μ M	0.1	0.489 $\pm$ 0.095 μ M	58
		4.24 μ M	0.5	3.248 $\pm$ 0.160 μ M	77
		8.47 μ M	1	9.205 $\pm$ 0.269 μ M	109
		42.4 μ M	5	41.198 $\pm$ 0.972 μ M	96
		84.7 μ M	10	85.924 $\pm$ 1.456 μ M	101
Vitamin B12	0.9995	0.0737 nM	0.1	0.119 $\pm$ 0.005 nM	161
		0.369 nM	0.5	0.318 $\pm$ 0.030 nM	86
		0.737 nM	1	0.666 $\pm$ 0.111 nM	90
		3.69 nM	5	3.375 $\pm$ 0.044 nM	91
		7.37 nM	10	6.579 $\pm$ 0.016 nM	89

Table S3. Fluorescence and LC-MS data of homocysteine and methylmalonic acid in PD patient sera.

	No.	Homocysteine (Fluorescence) (μM)	Homocysteine $\pm$ Std Dev (LC-MS) (μM)	Methylmalonic Acid $\pm$ Std Dev (LC-MS) (μM)
Group 1	1	36.12	25.55 $\pm$ 1.33	2.37 $\pm$ 0.08
	2	95.69	34.66 $\pm$ 1.11	1.27 $\pm$ 0.01
	3	46.27	83.16 $\pm$ 4.52	1.61 $\pm$ 0.17
	4	72.91	23.55 $\pm$ 1.18	2.80 $\pm$ 0.17
	5	90.11	29.25 $\pm$ 2.07	0.93 $\pm$ 0.01
	6	94.09	33.47 $\pm$ 6.81	4.83 $\pm$ 0.08
	7	66.25	26.59 $\pm$ 6.37	2.29 $\pm$ 0.08
	8	48.79	47.25 $\pm$ 3.04	1.27 $\pm$ 0.17
	9	59.79	14.29 $\pm$ 0.30	3.47 $\pm$ 0.17
	10	61.57	54.28 $\pm$ 1.48	4.49 $\pm$ 0.01
	11	81.11	72.13 $\pm$ 1.11	1.61 $\pm$ 0.25
	12	50.61	35.10 $\pm$ 2.07	0.85 $\pm$ 0.08
	13	78.64	33.84 $\pm$ 1.56	3.39 $\pm$ 0.08
	14	101.38	25.62 $\pm$ 2.81	3.22 $\pm$ 0.25
Average		70.24	38.48	2.46
Standard deviation		20.68	19.40	1.29
Median		69.58	33.66	2.33
Max.		101.38	83.16	4.83
Min.		36.12	14.29	0.85
Group 2	1	86.52	68.28 $\pm$ 1.63	3.05 $\pm$ 0.17
	2	44.33	12.44 $\pm$ 2.89	2.03 $\pm$ 0.01
	3	50.57	65.54 $\pm$ 2.07	3.30 $\pm$ 0.17
	4	57.01	40.36 $\pm$ 1.41	2.03 $\pm$ 0.08
	5	57.37	54.28 $\pm$ 3.63	3.90 $\pm$ 0.25
	6	77.29	19.77 $\pm$ 0.52	4.58 $\pm$ 0.17
	7	46.57	40.36 $\pm$ 0.22	6.27 $\pm$ 0.17
	8	50.25	27.03 $\pm$ 2.22	7.71 $\pm$ 0.08
Average		58.74	41.01	4.11
Standard deviation		12.76	20.65	2.01
Median		53.79	40.36	3.60
Max.		86.52	68.28	7.71
Min.		44.33	12.44	2.03
Group 3	1	30.28	3.18 $\pm$ 0.52	2.03 $\pm$ 0.01
	2	57.22	11.85 $\pm$ 0.81	1.78 $\pm$ 0.08
	3	59.14	16.07 $\pm$ 0.96	2.12 $\pm$ 0.08
	4	67.87	26.29 $\pm$ 1.56	4.32 $\pm$ 0.08
	5	54.22	22.44 $\pm$ 0.44	3.47 $\pm$ 0.08
	6	59.03	34.51 $\pm$ 1.48	2.80 $\pm$ 0.08
Average		54.63	19.06	2.75
Standard deviation		12.76	11.10	0.98
Median		58.12	19.26	2.46
Max.		67.87	34.51	4.32
Min		30.28	3.18	1.78

Figure S1. Standard calibration curve of homocysteine from the fluorescence study.

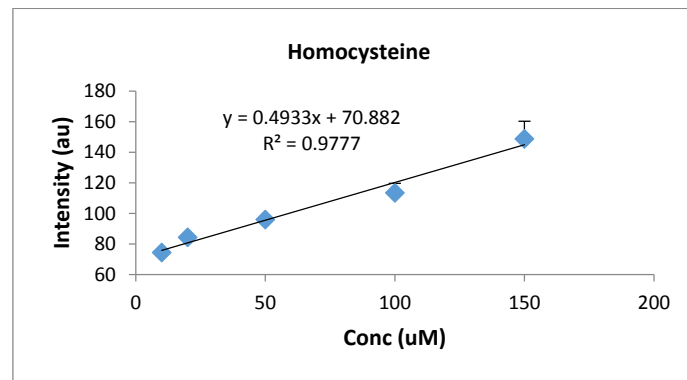


Figure S2. LC-MS EIC of homocysteine, methylmalonic acid, and vitamin B12.

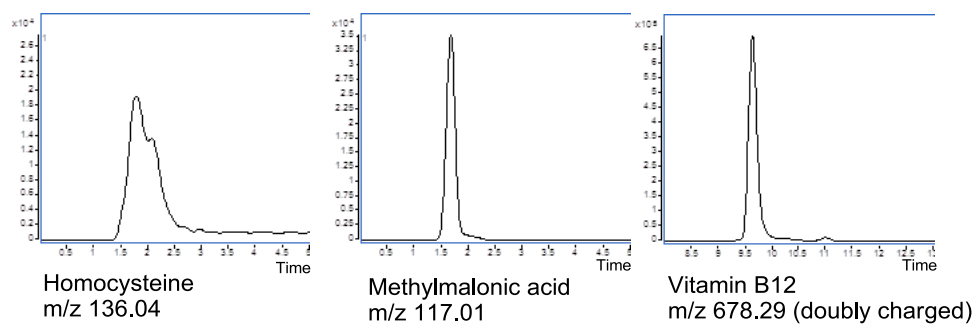


Figure S3. Standard calibration curve of homocysteine, methylmalonic acid, and vitamin B12 from LC-MS study.

