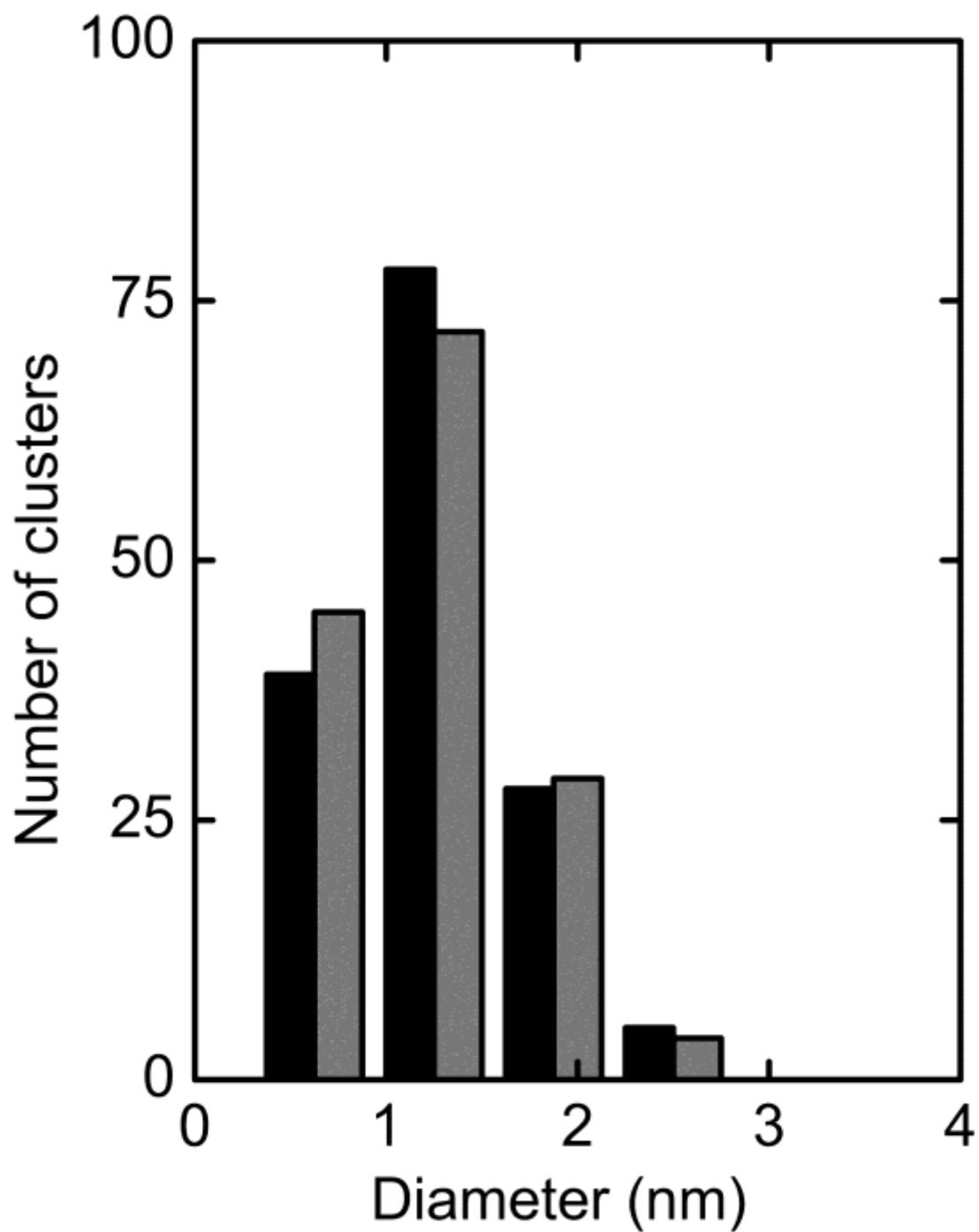


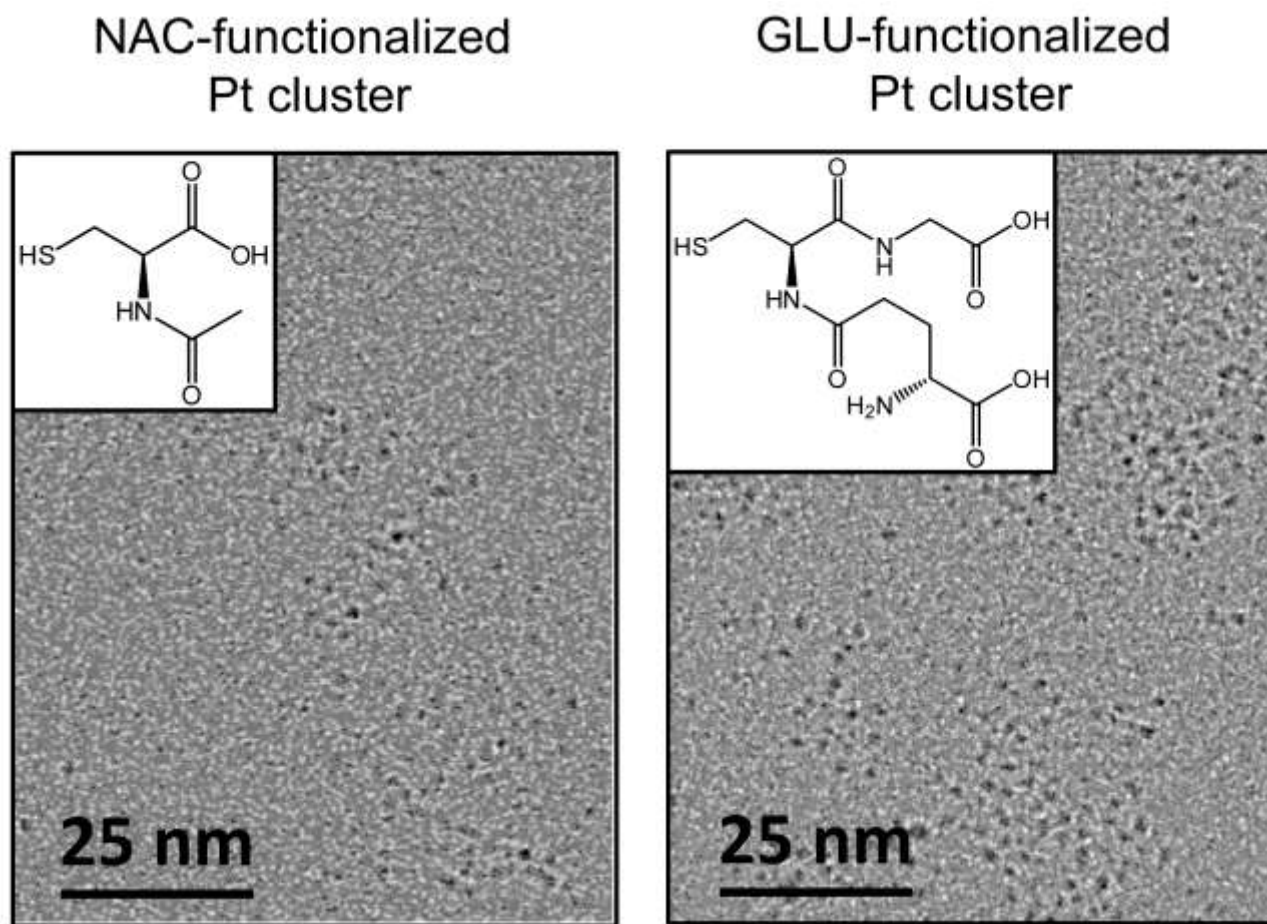
## Supplementary Information

### **Rational design, characterization and catalytic application of metal clusters functionalized with hydrophilic, chiral ligands: a proof of principle study**

Sebastian Kunz\*, Patrick Schreiber, Martin Ludwig, Mark M. Maturi, Olaf Ackermann, Martin Tschurl  
and Ueli Heiz

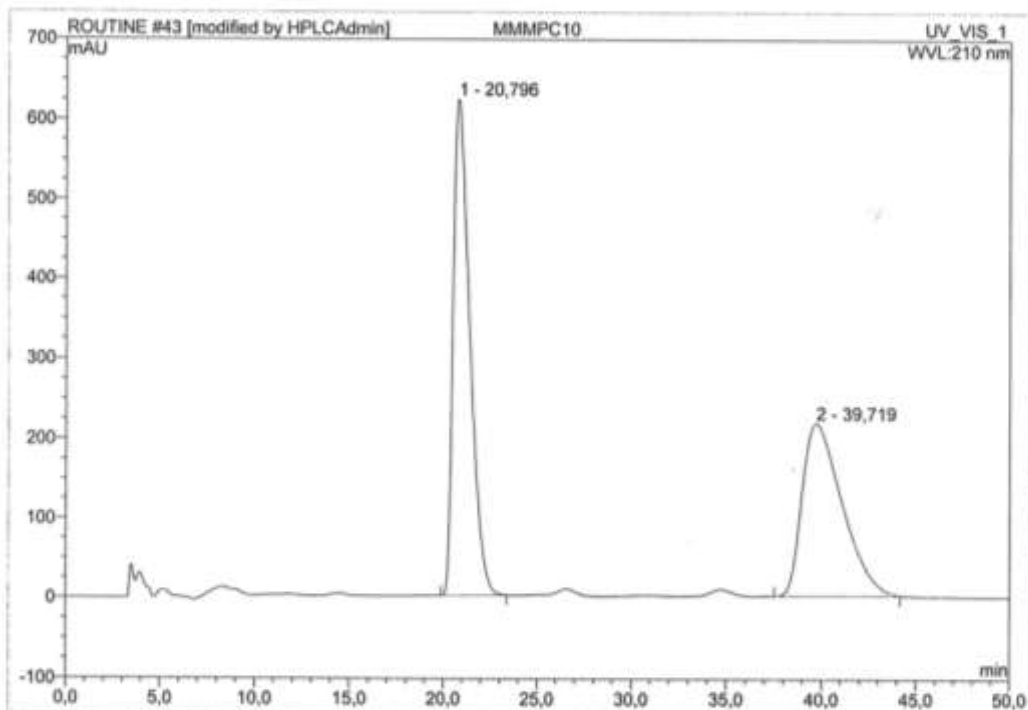


**Figure S1.** Particle size distributions of CYS-functionalized clusters (grey bars) prepared from “unprotected” Pt clusters (black bars). The statistics clearly show that cluster size is preserved after functionalization. In addition, no agglomerates of clusters are found.



**Figure S2.** TEM images of NAC- and GLU-functionalized clusters, prepared from the same “unprotected” cluster batch as the CYS-clusters.

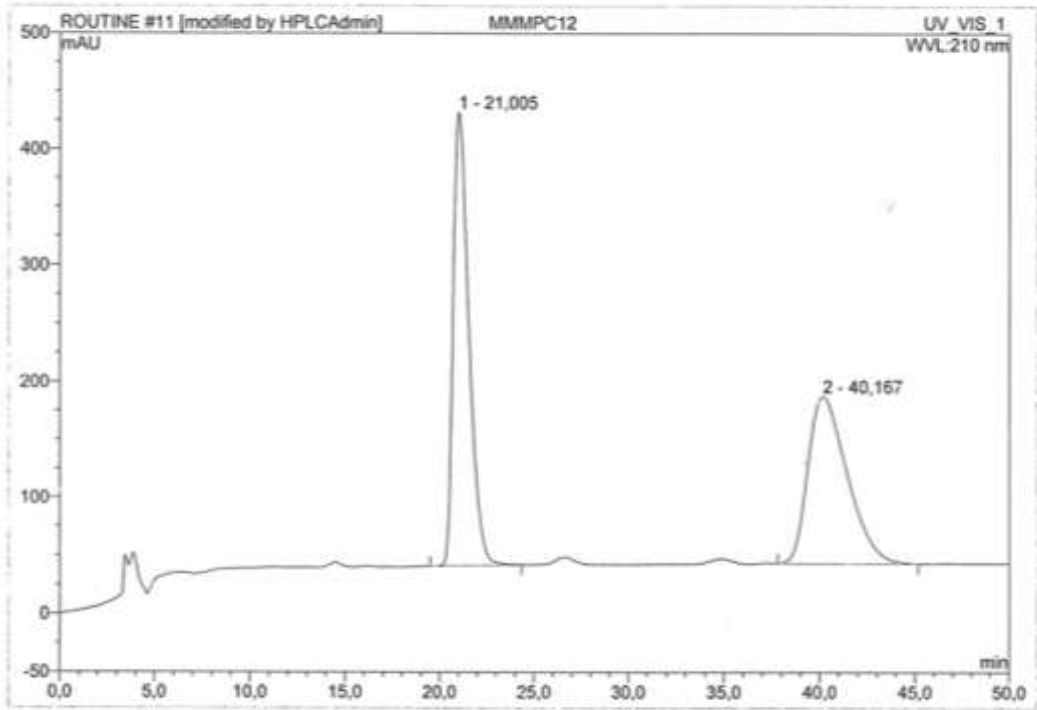
43 MMMPC10			
Daicel Chiralcel, OJ-H, 250x4.6			
Sample Name:	MMMPC10	Injection Volume:	50,0
Vial Number:	GB11	Channel:	UV_VIS_1
Sample Type:	unknown	Wavelength:	210
Control Program:	Säule5_NP_ISO_90_10_1_50	Bandwidth:	1
Quantif. Method:	gradA	Dilution Factor:	1,0000
Recording Time:	16.11.2012 15:05	Sample Weight:	1,0000
Run Time (min):	50,00	Sample Amount:	1,0000



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	20,80	n.a.	621,586	640,851	54,69	n.a.	BMB
2	39,72	n.a.	217,043	530,937	45,31	n.a.	BMB*
<b>Total:</b>			838,628	1171,788	100,00	0,000	

**Figure S3.** Representative HPLC chromatogram of derivatized reaction product from catalytic investigations of CYS-functionalized clusters.

11 MMMPC12			
Daicel Chiralcel OJ-H, 250x4.6			
Sample Name:	MMMPC12	Injection Volume:	50,0
Vial Number:	GA9	Channel:	UV_VIS_1
Sample Type:	unknown	Wavelength:	210
Control Program:	Säule5_NP_ISO_90_10_1_50	Bandwidth:	1
Quantif. Method:	gradA	Dilution Factor:	1,0000
Recording Time:	27.11.2012 10:21	Sample Weight:	1,0000
Run Time (min):	50,00	Sample Amount:	1,0000



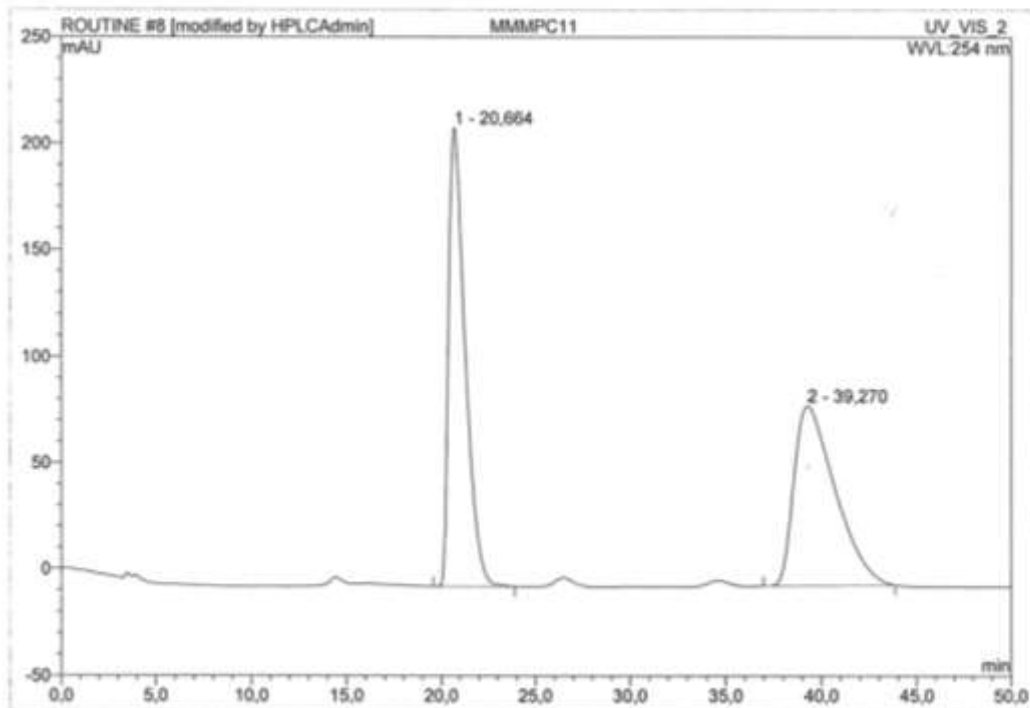
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	21,01	n.a.	390,632	379,667	52,48	n.a.	BMB*
2	40,17	n.a.	144,270	343,726	47,52	n.a.	BMB*
<b>Total:</b>			534,902	723,394	100,00	0,000	

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Chromeleon (c) Dionex 1996-2006  
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**Figure S4.** Representative HPCL chromatogram of derivatized reaction product from catalytic investigations of GLU-functionalized clusters.

<b>8 MMMPC11</b>			
<b>Daicel Chiralcel, OJ-H, 250x4.6</b>			
Sample Name:	MMMPC11	Injection Volume:	50,0
Vial Number:	GA12	Channel:	UV_VIS_2
Sample Type:	unknown	Wavelength:	254
Control Program:	Säule5_NP_ISO_90_10_1_50	Bandwidth:	1
Quantif. Method:	gradA	Dilution Factor:	1,0000
Recording Time:	22.11.2012 17:28	Sample Weight:	1,0000
Run Time (min):	50,00	Sample Amount:	1,0000



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	20,66	n.a.	215,575	219,108	50,93	n.a.	BMB
2	39,27	n.a.	84,601	211,075	49,07	n.a.	BMB*
<b>Total:</b>			300,176	430,183	100,00	0,000	

**Figure S5.** Representative HPLC chromatogram of derivatized reaction product from catalytic investigations of NAC-functionalized clusters.

**Table S1.** Number of ligands per Pt atom and per Pt surface atom for all three ligand-functionalized clusters. The ligand (determined by EA) to Pt (determined by AAS) ratio was calculated by using the sulfur content for estimation of the number of ligands within the sample. Based on the dispersion of the metal cluster, estimated as described within the article (see 3. Results and Discussion), the ligand coverage was calculated under the assumption that a full monolayer consists of one ligand per Pt surface atom.

<b>Ligand</b>	<b>Ligands / Pt<sub>atom</sub></b>	<b>Ligands / Pt<sub>surface atom</sub></b>
CYS	0.57	0.60
NAC	0.57	0.60
GLU	0.44	0.46