

Supporting Information

Efficient conversion of microcrystalline cellulose to 1,2-alkanediols over supported Ni catalysts

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List of pioneer works concerning hydrogenolysis of cellulose over heterogeneous catalysts

Table S1 Recent advances on the catalytic conversion of cellulose into polyols on various heterogeneous catalyst*

Entry	Catalyst	Reaction Condition*	Cellulose (wt%)	Conversion (%)	Yield (%)						References
					S	M	Ery	Gly	1,2-P	EG	
1	2.5% Pt/Al ₂ O ₃ 0.21 g	463 K, 5 MPa H ₂ , 24 h	0.8 (0.48g + H ₂ O 60 mL)	n.r.	25	6	n.r.	n.r.	n.r.	n.r.	1, 2
2	60% Ni/SiO ₂ -Al ₂ O ₃ 0.009 g	463 K, 5 MPa H ₂ , 24 h	0.8 (0.16g + H ₂ O 50 mL)	n.r.	2	n.r.	n.r.	n.r.	n.r.	n.r.	
3	4 wt% Ru/C 0.1 g (0.04 mmol)	518 K, 6 MPa H ₂ , 0.5 h	2 (1g + H ₂ O 50 mL)	85.5	29.6	9.7	6.1	6.4	6.8	5.6	3
4	2% Ni-30% W ₂ C/AC 0.15 g	518 K, 6 MPa H ₂ , 0.5 h	1 (0.5 g + H ₂ O 50 mL)	100	3.9	1.9	2.3	n.r.	7.6	61.0	4, 5
5	3% Ni/AC 0.15 g	518 K, 6 MPa H ₂ , 0.5 h	1 (0.5 g + H ₂ O 50 mL)	69	3.8	1.2	0.7	n.r.	4.2	5.8	
6	Ni5-W15/SBA-15 0.3 g	518 K, 6 MPa H ₂ , 0.5 h	1 (1.0g + H ₂ O 100 mL)	100	5.8	2.2	6.0	n.r.	3.2	76.1	6
7	20 wt% Ni/AC 0.3 g	518 K, 6 MPa H ₂ , 0.5 h	1 (1.0g + H ₂ O 100 mL)	71.9	10.1	1.5	0	0	4.3	9.2	
8	WCx/MC 0.3 g	518 K, 6 MPa H ₂ , 0.5 h	1 (1.0g + H ₂ O 100 mL)	100	1.2	1.4	1.5	n.r.	5.1	72.9	7
9	16%Ni ₂ P/AC (1:2)	498 K, 6 MPa H ₂ , 1.5 h	1 (0.5 g + H ₂ O 50 mL)	100	48.4	4.7	n.r.	n.r.	1.2	8.2	8

10	1% Ni/CNT 0.05 g	458 K, 5 MPa H ₂ , 24h	0.8 0.16g + H ₂ O 20 mL)	n.r.	69	4.0r	5.0.	5.0	n.r.	n.r.	9
11	3 wt% Ni/ Al ₂ O ₃ 0.5 g	503 K, 4 MPa H ₂ ., 4 h	2 (1g + H ₂ O 50 mL)	78.0	4.7	1.2	1.5	0.0	1.3	12.3	10
12	3 wt% Ni/AC 0.5g	503 K, 4 MPa H ₂ , 4 h	2 (1g + H ₂ O 50 mL)	80.8	9.5	2.6	4.6	0.0	6.9	8.7	
13	3 wt% Ni/CNF 0.5 g	503 K, 6 MPa H ₂ , 4 h	2 (1g + H ₂ O 50 mL)	93.9	22.7	4.9	7.8	1.8	7.1	6.5	
14	3 wt% Ni/CNF 0.5 g	463 K, 6 MPa H ₂ , 24 h	2 (ball-milled) (1g + H ₂ O 50 mL)	92.2	50.3	6.2	12.8	1.0	1.2	2.5	
15	3 wt% Ni/CNF 2.5 g	463 K, 6 MPa H ₂ , 24 h	10 (ball-milled) (5g + H ₂ O 50 mL)	94.0	47.0	6.9	10.7	0.1	1.5	6.4	
16	5 wt% Ru/C 0.1 g+ H ₂ SO ₄	433 K, 5MPa H ₂ , 5h	5 (0.5 g + Acid 10 mL)	74.0	11.7	n.r.	0.0	n.r.	5.7	0.0	11
17	5 wt% Ru/C 0.25g+ H ₄ SiW ₁₂ O ₄₀	463 K, 9.5 MPa H ₂ , 1 h	2 (ball-milled) (5g + H ₂ O 50 mL)	100	85 (S+M)		n.r.	n.r.	n.r.	n.r.	12
18	5 wt% Ru/C 2.5g+ H ₄ SiW ₁₂ O ₄₀	463 K, 5 MPa H ₂ , 24 h	20 (ball-milled) (5g + H ₂ O 50 mL)	65	38 S+M	n.r.	n.r.	n.r.	n.r.	n.r.	
19	2 wt% Pt _(N) BP2000 1 mg	463 K, 5 MPa H ₂ , 24 h	0.8 (ball-milled) (0.324g + H ₂ O 40 mL)	101	52.7	12.1	n.r.	2.0 (C2-C3 polyols)			13
20	2 wt% Ru/AC(N) 0.05 g	463 K, 18 h	0.8 (ball-milled) (0.324g + H ₂ O 30 mL + 2-propanol 10 mL)	85.2	36.3	10.6	6.7 (C2-C4 polyols)				14

21	Pt/H-ZSM-5(23) 0.05	518 K, 6 MPa H ₂ , 2 h	0.17 (0.05g + H ₂ O 30 mL)	93	1.3	0.8	n.r.	n.r.	21.0	7.2	15
22	2 wt% Ru/C (0.2 g), 0.5 g Ca(OH) ₂	473 K, 6 MPa H ₂ , 0.5 h	4 (0.05g + H ₂ O 50 mL)	38.3	trace	trace	n.r.	n.r.	5.5	6.7	16

* Initial H₂ pressure measured at room temperature; abbreviations: n.r. = not reported, S = sorbitol; M = mannitol; Ery = erythritol; Gly = glycerol, 1,2-P = 1,2-propanediol, EG = ethylene glycol.

References

1. A. Fukuoka and P. L. Dhepe, *Angew. Chem.-Int. Edit.*, 2006, **45**, 5161-5163.
2. P. L. Dhepe and A. Fukuoka, *Catalysis Surveys from Asia*, 2007, **11**, 186-191.
3. C. Luo, S. Wang and H. Liu, *Angewandte Chemie*, 2007, **119**, 7780-7783.
4. N. Ji, T. Zhang, M. Y. Zheng, A. Q. Wang, H. Wang, X. D. Wang and J. G. G. Chen, *Angew. Chem.-Int. Edit.*, 2008, **47**, 8510-8513.
5. N. Ji, T. Zhang, M. Y. Zheng, A. Q. Wang, H. Wang, X. D. Wang, Y. Y. Shu, A. L. Stottlemeyer and J. G. G. Chen, *Catal. Today*, 2009, **147**, 77-85.
6. M. Y. Zheng, A. Q. Wang, N. Ji, J. F. Pang, X. D. Wang and T. Zhang, *ChemSusChem*, 2010, **3**, 63-66.
7. Y. H. Zhang, A. Q. Wang and T. Zhang, *Chem. Commun.*, 2010, **46**, 862-864.
8. L. N. Ding, A. Q. Wang, M. Y. Zheng and T. Zhang, *ChemSusChem*, 2010, **3**, 818-821.
9. W. P. Deng, X. S. Tan, W. H. Fang, Q. H. Zhang and Y. Wang, *Catal. Lett.*, 2009, **133**, 167-174.
10. S. Van de Vyver, J. Geboers, M. Dusselier, H. Schepers, T. Vosch, L. A. Zhang, G. Van Tendeloo, P. A. Jacobs and B. F. Sels, *ChemSusChem*, 2010, **3**, 698-701.
11. R. Palkovits, K. Tajvidi, J. Procelewska, R. Rinaldi and A. Ruppert, *Green Chem.*, 2010, **12**, 972-978.
12. J. Geboers, S. Van de Vyver, K. Carpentier, K. de Blochouse, P. Jacobs and B. Sels, *Chem. Commun.*, 2010, **46**, 3577-3579.
13. H. Kobayashi, Y. Ito, T. Komanoya, Y. Hosaka, P. L. Dhepe, K. Kasai, K. Hara and A. Fukuoka, *Green Chem.*, 2011, **13**, 326-333.
14. H. Kobayashi, H. Matsushashi, T. Komanoya, K. Hara and A. Fukuoka, *Chem. Commun.*, 2011, **47**, 2366-2368.
15. S. J. You, I. G. Baek, Y. T. Kim, K. E. Jeong, H. J. Chae, T. W. Kim, C. U. Kim, S. Y. Jeong, T. J. Kim, Y. M. Chung, S. H. Oh and E. D. Park, *Korean J. Chem. Eng.*, 2011, **28**, 744-750.
16. T. Y. Deng, J. Y. Sun and H. C. Liu, *Sci. China-Chem.*, 2010, **53**, 1476-1480.

Results

The qualitative results for liquid products from cellulose hydrogenolysis showed the products were very complex and included methanol, i-propanol, ethanol, n-propanol, n-butanol, 1,2-propanediol, ethylene glycol, 1,2-butanediol, 1,2-hexanediol, glycerol, erythritol, sorbitol, mannitol, glucose and so on (Fig. S1). A set of typical GC and IC spectra of cellulose degradation products were shown in Fig. S2.

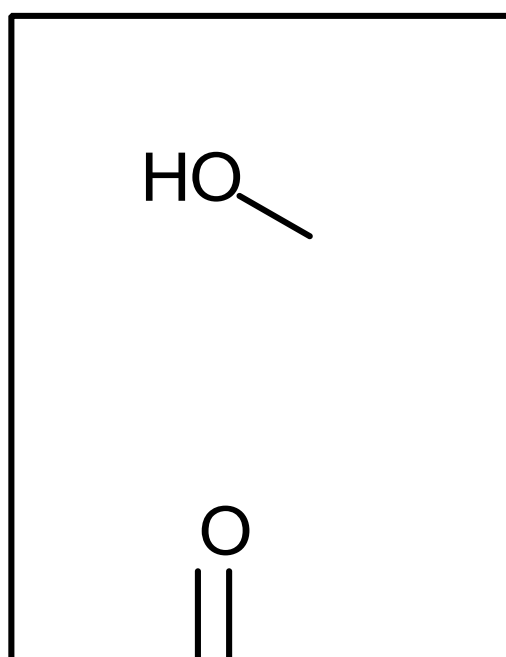


Fig. S1 The qualitative results for liquid products from cellulose hydrogenolysis

^a Based on GC-MS analysis, ^b based on the IC retention time

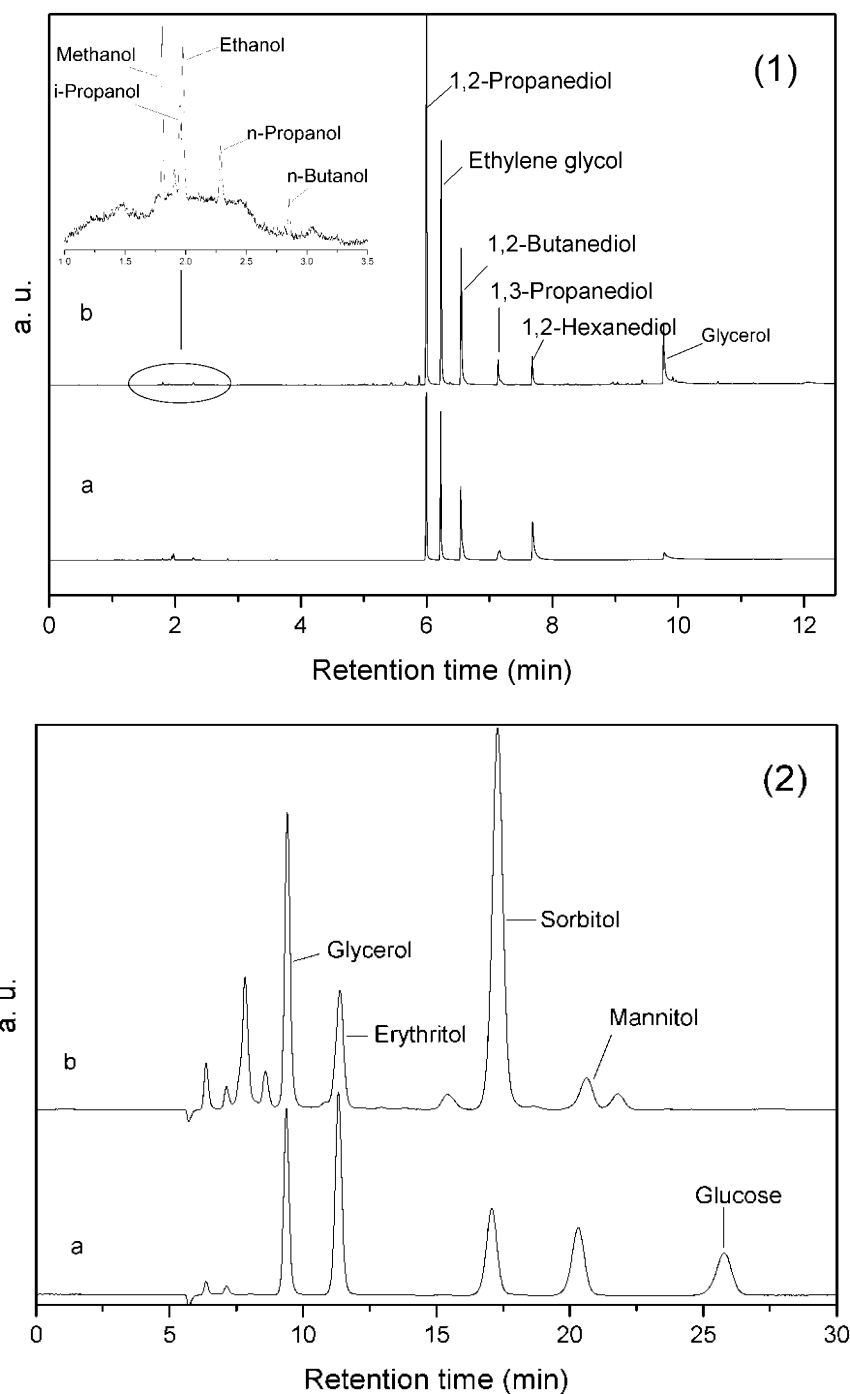


Fig. S2 GC and HPLC spectra of cellulose degradation products over 20% Ni/ZnO catalyst. (1) GC, (2) IC, ^a standard samples, ^b cellulose degradation products



Fig. S3 Comparison of the samples after reaction, reaction condition: microcrystalline cellulose (FMC PH-101, 20-100 mm, 83% crystallinity), 0.5 g; H₂O, 50 mL; temperature, 518 K; H₂ pressure, 6 MPa at room temperature; 800RPM; a without a catalyst, reaction time, 2 h; b partially conversion of cellulose over Ni/ZnO (0.15 g), reaction time, 0.5 h; c complete conversion over Ni/ZnO, reaction time, 2 h

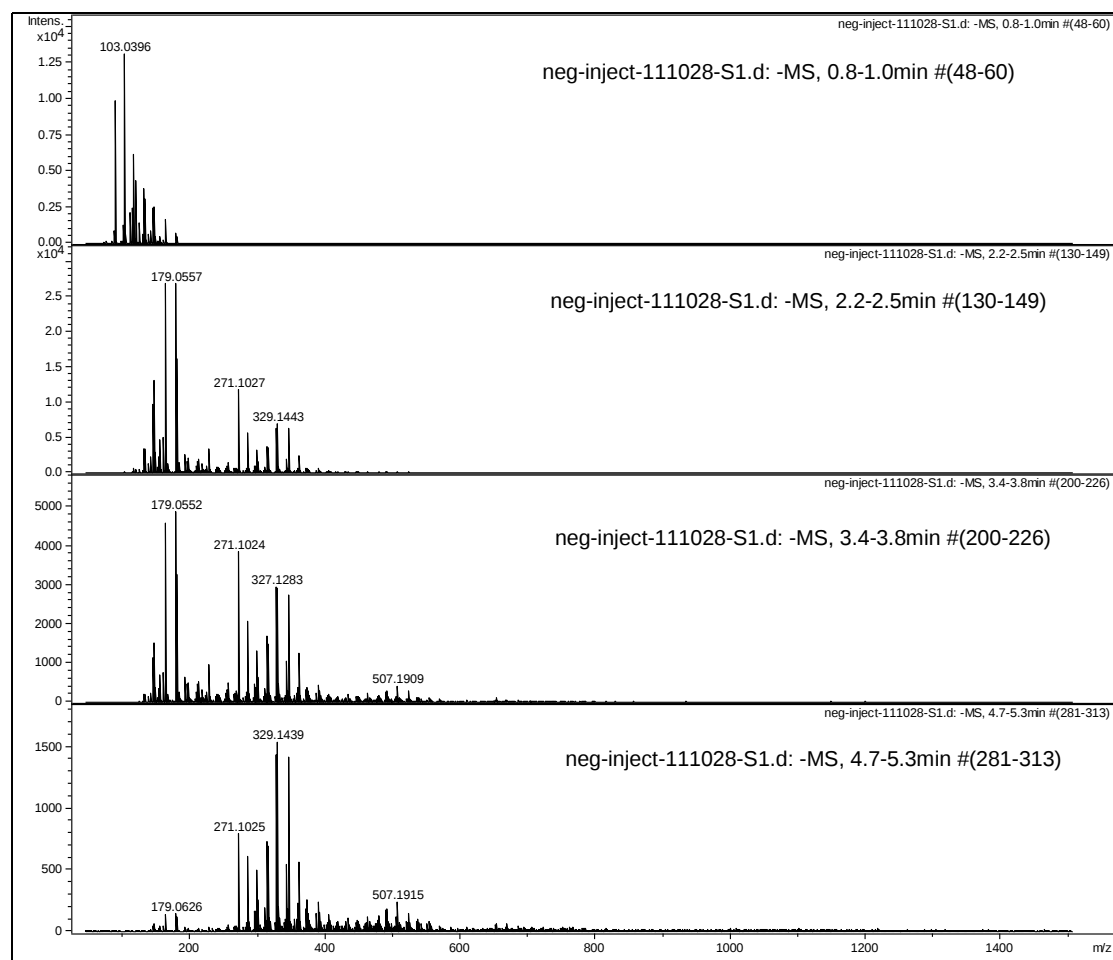


Fig S4 High-resolution ion chromatograms of degradation products of cellulose

Table S2 Results of cellulose conversion over supported catalysts^a

Entry	Catalyst ^b	Conv. ^c (%)	Yield based on carbon ^d (%)					
			1,2-PD ^e	EG	1,2-BD	1,3-PD	1,2-HD	Total ^f
20	Ni/Al ₂ O ₃ + ZnO	94	9.4	9.1	3.4	0.7	4.9	27.5
21	Ni/kieselguhr + ZnO	96	12.9	11.7	1.4	0.6	5.4	32.0
22	Ni/ZrO ₂ + ZnO	88	14.8	13.3	8.2	1.2	6.6	44.1
23	20% Ni/ZnO-leaching	75	0.8	1.1	0.5	0.2	0.3	2.9
24	NONE	68	-	-	-	-	-	-

^a *Reaction conditions*: catalyst, 0.15 g; microcrystalline cellulose (FMC ph-101, 20-100 mm, 83% crystallinity), 0.5 g; H₂O, 50 mL; temperature, 518 K; H₂ pressure, 6 MPa at room temperature; 800 RPM; reaction time, 2 h. ^b Metal loadings are referred to nominal values of Ni loading on the support analysed by ICP. Entries 17-20: 0.15g Ni catalyst and 0.12 g ZnO; Entry 21: filtrate of 0.15g 20% Ni/ZnO treated in water without cellulose under reaction conditions. ^c Cellulose conversions were calculated by the weight loss of cellulose in the reaction. ^d The yields of polyols were calculated using the equation: Yield (C%)=(moles of carbon in the products)/(moles of carbon in cellulose charged into the reactor)×100%. ^e Abbreviations: PD=propanediol, EG=ethylene glycol, BD=butanediol, HD=hexanediol; ^f sum of glycol yield.

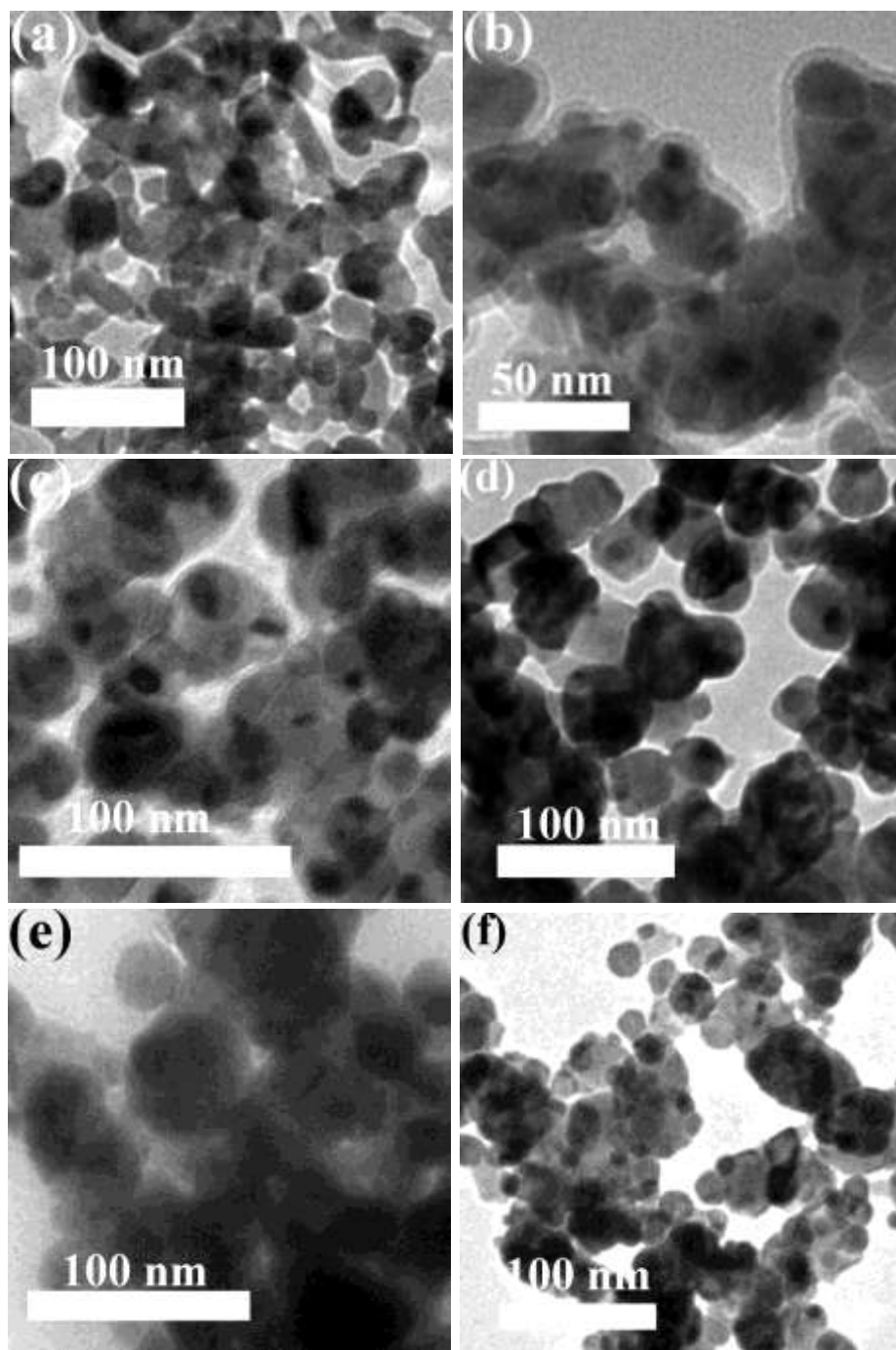


Fig. S5 TEM images of ZnO and Ni/ZnO catalysts (a) ZnO, (b) 15% Ni/ZnO, (c) 20% Ni/ZnO, (d) 30% Ni/ZnO; (e) 40% Ni/ZnO, (f) 20% Ni/ZnO-IM

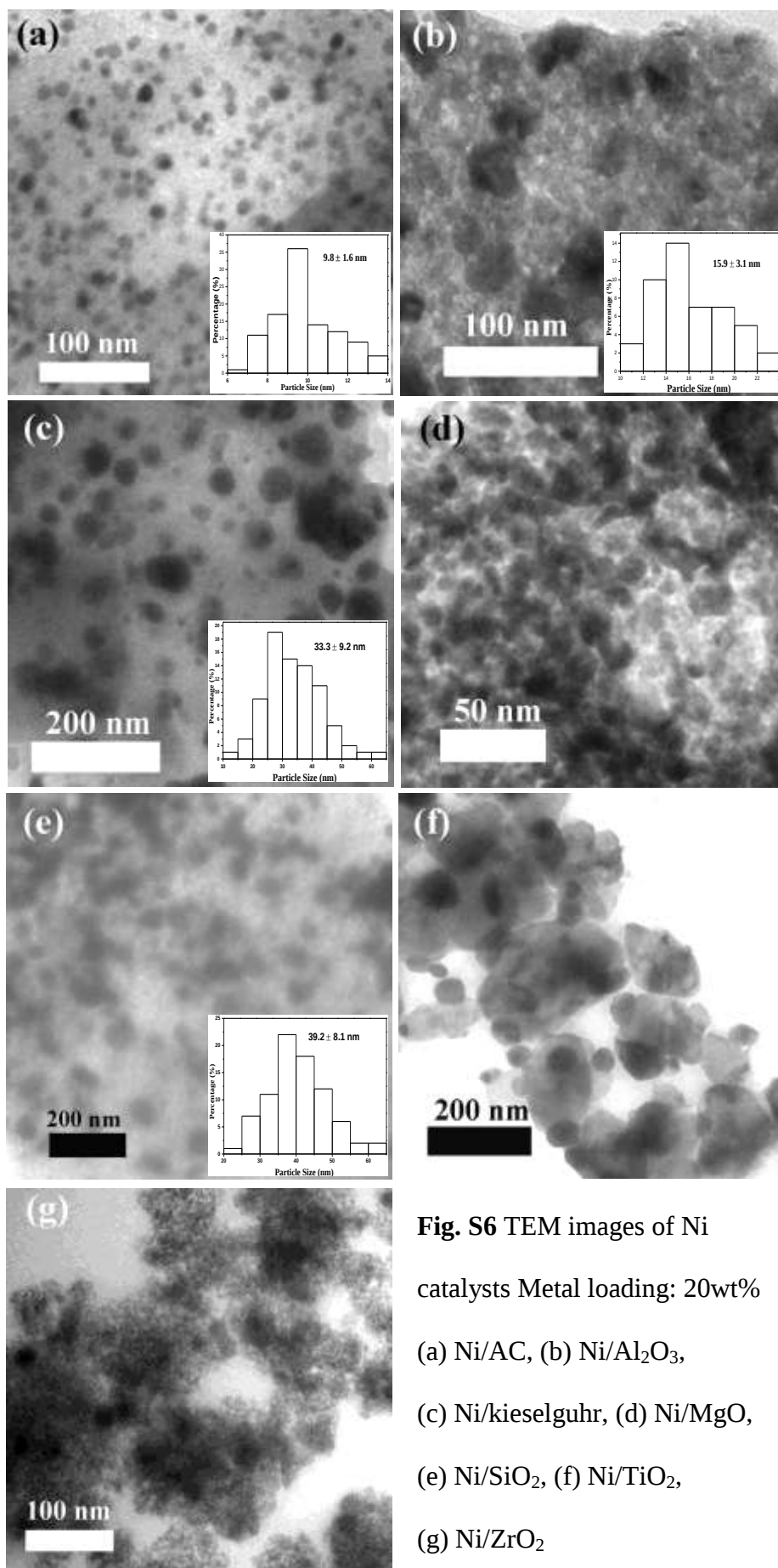


Fig. S6 TEM images of Ni catalysts Metal loading: 20wt%
(a) Ni/AC, (b) Ni/Al₂O₃,
(c) Ni/kieselguhr, (d) Ni/MgO,
(e) Ni/SiO₂, (f) Ni/TiO₂,
(g) Ni/ZrO₂

Table S3 Nickel particle size calculated calculated by the Scherrer's equation

Entry	Catalyst	Particle Size
1	20% Ni/Al ₂ O ₃	17.0
2	20% Ni/kieselguhr	23.9
3	20% Ni/SiO ₂	27.0
4	20% Ni/TiO ₂	19.2
5	20% Ni/AC	18.3
6	20% Ni/ZrO ₂	18.2
7	20% Ni/MgO	9.5

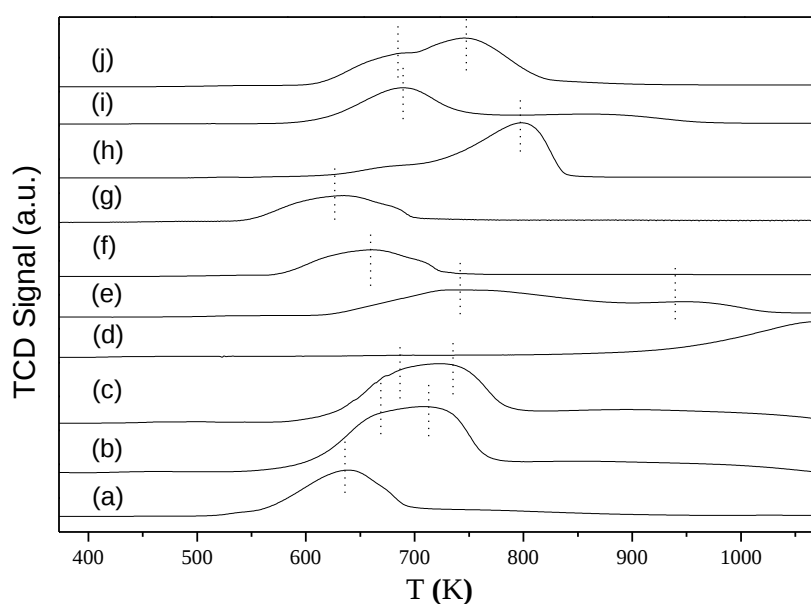


Fig. S7 Comparison of the temperature-programmed reduction (TPR) profiles of Ni samples (a) NiO_x (calcination of Ni(NO₃)₂ at 773 K for three hours), (b) 20% Ni/ZnO-IM, (c) 20% Ni/ZnO, (d) 20% Ni/Al₂O₃, (e) 20% Ni/kieselguhr, (f) 20% Ni/SiO₂, (g) 20% Ni/AC, (h) 20% Ni/TiO₂, (i) 20% Ni/ZrO₂, (j) 20% Ni/MgO

Appendix: Mass Spectrum SmartFormula Report

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\LSHXPWANGXC\neg-inject-111028-S1.d
Method tune_low_neg.m
Sample Name TuneMix
Comment

Acquisition Date 10/28/2011 11:51:53 AM

Operator QIBEBT

Instrument / Ser# maXis 10161

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	2800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
71.0497	1	C ₄ H ₇ O		71.0502	7.6		n.a.	1.5	even	ok
73.0291	1	C ₃ H ₅ O ₂	100.00	73.0295	5.6	5.5	18.9	1.5	even	ok
75.0083	1	C ₂ H ₃ O ₃	100.00	75.0088	5.9	5.8	13.0	1.5	even	ok
83.0500	1	C ₅ H ₇ O		83.0502	2.9		n.a.	2.5	even	ok
85.0293	1	C ₄ H ₅ O ₂	100.00	85.0295	2.8	2.7	25.1	2.5	even	ok
85.0655	1	C ₅ H ₉ O	100.00	85.0659	4.2	4.2	31.2	1.5	even	ok
87.0447	1	C ₄ H ₇ O ₂	100.00	87.0452	5.6	5.6	25.1	1.5	even	ok
87.0816	1	C ₅ H ₁₁ O		87.0815	-0.7		n.a.	0.5	even	ok
88.0480	1	C ₄ H ₇ O ₂		87.0452	6.5		n.a.	1.5	even	ok
89.0240	1	C ₃ H ₅ O ₃	100.00	89.0244	4.6	4.6	8.0	1.5	even	ok
90.0273	1	C ₃ H ₅ O ₃	100.00	89.0244	4.6	4.6	8.0	1.5	even	ok
99.0081	1	C ₄ H ₃ O ₃	100.00	99.0088	6.5	6.4	25.2	3.5	even	ok
99.0448	1	C ₅ H ₇ O ₂	100.00	99.0452	3.9	3.9	31.3	2.5	even	ok
99.0820	1	C ₆ H ₁₁ O		99.0815	-4.7		n.a.	1.5	even	ok
101.0240	1	C ₄ H ₅ O ₃	100.00	101.0244	4.2	4.1	25.2	2.5	even	ok
101.0603	1	C ₅ H ₉ O ₂	100.00	101.0608	4.5	4.5	31.3	1.5	even	ok
102.0264	1	C ₄ H ₅ O ₃		101.0244	14.0		n.a.	2.5	even	ok
103.0397	1	C ₄ H ₇ O ₃	100.00	103.0401	4.0	4.0	7.4	1.5	even	ok
103.0765	1	C ₅ H ₁₁ O ₂		103.0765	-0.5		n.a.	0.5	even	ok
105.0190	1	C ₃ H ₅ O ₄	100.00	105.0193	2.9	2.9	19.3	1.5	even	ok
105.0557	1	C ₄ H ₉ O ₃		105.0557	0.2		n.a.	0.5	even	ok
112.0481	1	C ₆ H ₇ O ₂	100.00	111.0452	4.0	4.0	2.9	3.5	even	ok
113.0233	1	C ₅ H ₅ O ₃		113.0244	9.9		n.a.	3.5	even	ok
113.0599	1	C ₆ H ₉ O ₂	100.00	113.0608	7.6	7.5	37.5	2.5	even	ok
115.0396	1	C ₅ H ₇ O ₃	100.00	115.0401	4.2	4.2	6.6	2.5	even	ok
115.0761	1	C ₆ H ₁₁ O ₂	100.00	115.0765	3.1	3.1	37.5	1.5	even	ok
117.0188	1	C ₄ H ₅ O ₄	100.00	117.0193	4.7	4.7	25.4	2.5	even	ok
117.0552	1	C ₅ H ₉ O ₃	100.00	117.0557	4.7	4.7	3.7	1.5	even	ok
119.0344	1	C ₄ H ₇ O ₄	100.00	119.0350	4.6	4.6	9.4	1.5	even	ok
119.0704	1	C ₅ H ₁₁ O ₃		119.0714	8.1		n.a.	0.5	even	ok
121.0313	1	C ₇ H ₅ O ₂		121.0295	-14.8		n.a.	5.5	even	ok
121.0501	1	C ₄ H ₉ O ₄	100.00	121.0506	4.2	4.2	25.4	0.5	even	ok
125.0602	1	C ₇ H ₉ O ₂	100.00	125.0608	5.1	5.2	10.3	3.5	even	ok
125.0955	1	C ₈ H ₁₃ O		125.0972	13.5		n.a.	2.5	even	ok
127.0402	1	C ₆ H ₇ O ₃		127.0401	-1.0		n.a.	3.5	even	ok

Appendix: Mass Spectrum SmartFormula Report

Mass Spectrum SmartFormula Report										
Meas. m/z	#	Formula	Score	m/z	err (ppm)	Mean err (ppm)	mSigma	rdb	e ⁻ Conf	N-Rule
127.0751	1	C 7 H 11 O 2		127.0765	10.6		n.a.	2.5	even	ok
129.0190	1	C 5 H 5 O 4		129.0193	2.6		n.a.	3.5	even	ok
129.0550	1	C 6 H 9 O 3	100.00	129.0557	5.2	5.2	37.6	2.5	even	ok
129.0925	1	C 7 H 13 O 2		129.0921	-3.1		n.a.	1.5	even	ok
131.0342	1	C 5 H 7 O 4	100.00	131.0350	5.8	5.8	31.6	2.5	even	ok
131.0708	1	C 6 H 11 O 3	100.00	131.0714	4.7	4.7	4.0	1.5	even	ok
132.0394	1	C 5 H 7 O 4		131.0350	-7.6		n.a.	2.5	even	ok
133.0500	1	C 5 H 9 O 4	100.00	133.0506	4.9	4.8	7.4	1.5	even	ok
133.0859	1	C 6 H 13 O 3		133.0870	8.4		n.a.	0.5	even	ok
134.0535	1	C 5 H 9 O 4	100.00	133.0506	3.9	4.8	7.4	1.5	even	ok
135.0277	1	C 4 H 7 O 5		135.0299	16.3		n.a.	1.5	even	ok
135.0653	1	C 5 H 11 O 4		135.0663	7.3		n.a.	0.5	even	ok
139.0756	1	C 8 H 11 O 2	100.00	139.0765	6.2	6.2	50.0	3.5	even	ok
141.0551	1	C 7 H 9 O 3	100.00	141.0557	4.6	4.6	43.9	3.5	even	ok
143.0348	1	C 6 H 7 O 4		143.0350	1.3		n.a.	3.5	even	ok
143.0718	1	C 7 H 11 O 3		143.0714	-3.0		n.a.	2.5	even	ok
143.1072	1	C 8 H 15 O 2		143.1078	3.9		n.a.	1.5	even	ok
145.0498	1	C 6 H 9 O 4	100.00	145.0506	5.9	5.9	5.9	2.5	even	ok
145.0866	1	C 7 H 13 O 3		145.0870	2.9		n.a.	1.5	even	ok
146.0185	1	C 5 H 5 O 5		145.0142	-5.7		n.a.	3.5	even	ok
147.0301	1	C 5 H 7 O 5		147.0299	-1.4		n.a.	2.5	even	ok
147.0655	1	C 6 H 11 O 4	100.00	147.0663	5.5	5.5	4.8	1.5	even	ok
149.0449	1	C 5 H 9 O 5	100.00	149.0455	4.1	4.1	31.8	1.5	even	ok
149.0691	1	C 6 H 11 O 4		147.0663	13.0		n.a.	1.5	even	ok
149.0811	1	C 6 H 13 O 4	100.00	149.0819	5.9	5.8	37.8	0.5	even	ok
150.0481	1	C 5 H 9 O 5		149.0455	5.9		n.a.	1.5	even	ok
151.0602	1	C 5 H 11 O 5	100.00	151.0612	6.3	6.2	31.8	0.5	even	ok
155.1053	1	C 9 H 15 O 2		155.1078	15.8		n.a.	2.5	even	ok
157.0899	1	C 8 H 13 O 3		157.0870	-18.3		n.a.	2.5	even	ok
159.0676	1	C 7 H 11 O 4		159.0663	-8.3		n.a.	2.5	even	ok
159.1031	1	C 8 H 15 O 3		159.1027	-2.7		n.a.	1.5	even	ok
161.0447	1	C 6 H 9 O 5	100.00	161.0455	5.5	5.5	37.9	2.5	even	ok
161.0791	1	C 7 H 13 O 4		161.0819	17.6		n.a.	1.5	even	ok
163.0603	1	C 6 H 11 O 5	100.00	163.0612	5.6	5.6	37.9	1.5	even	ok
165.0768	1	C 6 H 13 O 5		165.0768	0.3		n.a.	0.5	even	ok
165.0913	1	C 10 H 13 O 2		165.0921	4.9		n.a.	4.5	even	ok
166.1124	1	C 7 H 17 O 4		165.1132	25.7		n.a.	-0.5	even	ok
167.1077	1	C 10 H 15 O 2		167.1078	0.3		n.a.	3.5	even	ok
169.0869	1	C 9 H 13 O 3		169.0870	0.7		n.a.	3.5	even	ok
171.1017	1	C 9 H 15 O 3		171.1027	5.7		n.a.	2.5	even	ok
172.1413	1	C 10 H 19 O 2		171.1391	6.8		n.a.	1.5	even	ok
173.0821	1	C 8 H 13 O 4		173.0819	-1.0		n.a.	2.5	even	ok
179.0551	1	C 6 H 11 O 6	100.00	179.0561	5.6	5.6	38.1	1.5	even	ok
179.1070	1	C 11 H 15 O 2		179.1078	4.2		n.a.	4.5	even	ok
181.0708	1	C 6 H 13 O 6	100.00	181.0718	5.4	5.4	38.1	0.5	even	ok
181.1236	1	C 11 H 17 O 2		181.1234	-1.1		n.a.	3.5	even	ok
183.1002	1	C 10 H 15 O 3		183.1027	13.5		n.a.	3.5	even	ok
187.0970	1	C 9 H 15 O 4		187.0976	3.1		n.a.	2.5	even	ok
193.1203	1	C 12 H 17 O 2		193.1234	16.1		n.a.	4.5	even	ok
195.0864	1	C 7 H 15 O 6		195.0874	5.2		n.a.	0.5	even	ok
195.1060	1	C 11 H 15 O 3		195.1027	-17.1		n.a.	4.5	even	ok
195.1394	1	C 12 H 19 O 2		195.1391	-1.8		n.a.	3.5	even	ok
197.1157	1	C 11 H 17 O 3		197.1183	13.3		n.a.	3.5	even	ok
205.0722	1	C 8 H 13 O 6		205.0718	-2.1		n.a.	2.5	even	ok
207.1365	1	C 13 H 19 O 2		207.1391	12.3		n.a.	4.5	even	ok
213.1101	1	C 11 H 17 O 4		213.1132	14.7		n.a.	3.5	even	ok
227.1297	1	C 12 H 19 O 4		227.1289	-3.6		n.a.	3.5	even	ok
229.1443	1	C 12 H 21 O 4		229.1445	1.0		n.a.	2.5	even	ok
237.0946	1	C 9 H 17 O 7		237.0980	14.2		n.a.	1.5	even	ok
239.1115	1	C 9 H 19 O 7		239.1136	8.9		n.a.	0.5	even	ok
253.1219	1	C 10 H 19 O 7		251.1136	-12.9		n.a.	1.5	even	ok
257.0882	1	C 8 H 17 O 9		257.0878	-1.5		n.a.	0.5	even	ok

Appendix: Mass Spectrum SmartFormula Report

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\LSHXPWANGXC\neg-inject-111028-S1.d
Method tune_low_neg.m
Sample Name TuneMix
Comment

Acquisition Date 10/28/2011 11:51:53 AM

Operator QIBEBT

Instrument / Ser# maXis 10161

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	2800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
131.0710	1	C ₆ H ₁₁ O ₃	100.00	131.0714	2.7	2.7	10.2	1.5	even	ok
133.0503	1	C ₅ H ₉ O ₄	100.00	133.0506	2.3	2.4	5.2	1.5	even	ok
145.0503	1	C ₆ H ₉ O ₄	100.00	145.0506	2.5	2.4	6.4	2.5	even	ok
147.0659	1	C ₆ H ₁₁ O ₄	100.00	147.0663	2.6	2.5	4.9	1.5	even	ok
149.0452	1	C ₅ H ₉ O ₅	100.00	149.0455	2.1	2.0	5.9	1.5	even	ok
153.0917	1	C ₉ H ₁₃ O ₂	100.00	153.0921	2.7	2.8	6.8	3.5	even	ok
161.0452	1	C ₆ H ₉ O ₅	100.00	161.0455	2.4	2.4	7.3	2.5	even	ok
163.0608	1	C ₆ H ₁₁ O ₅	100.00	163.0612	2.3	2.2	7.9	1.5	even	ok
167.1073	1	C ₁₀ H ₁₅ O ₂	100.00	167.1078	2.6	2.5	7.3	3.5	even	ok
179.0557	1	C ₆ H ₁₁ O ₆	100.00	179.0561	2.4	2.4	7.7	1.5	even	ok
180.0590	1	C ₆ H ₁₁ O ₆	100.00	179.0561	3.0	2.4	7.7	1.5	even	ok
183.1023	1	C ₁₀ H ₁₅ O ₃	100.00	183.1027	2.2	2.2	9.2	3.5	even	ok
188.1009	1	C ₉ H ₁₅ O ₄		187.0976	0.5		n.a.	2.5	even	ok
188.1357	1	C ₁₀ H ₁₉ O ₃		187.1340	9.0		n.a.	1.5	even	ok
189.0760	1	C ₈ H ₁₃ O ₅	100.00	189.0768	4.7	4.6	50.3	2.5	even	ok
191.0571	1	C ₇ H ₁₁ O ₆		191.0561	-5.2		n.a.	2.5	even	ok
191.0727	1	C ₈ H ₁₃ O ₅		189.0768	47.5		n.a.	2.5	even	ok
191.0918	1	C ₈ H ₁₅ O ₅	100.00	191.0925	3.6	3.5	50.3	1.5	even	ok
193.0714	1	C ₇ H ₁₃ O ₆		193.0718	1.9		n.a.	1.5	even	ok
193.1085	1	C ₈ H ₁₇ O ₅		193.1081	-1.8		n.a.	0.5	even	ok
193.1229	1	C ₁₂ H ₁₇ O ₂	100.00	193.1234	2.4	2.4	9.6	4.5	even	ok
195.0871	1	C ₇ H ₁₅ O ₆	100.00	195.0874	1.4	1.4	44.3	0.5	even	ok
195.1385	1	C ₁₂ H ₁₉ O ₂	100.00	195.1391	3.0	2.9	7.4	3.5	even	ok
196.1056	1	C ₁₁ H ₁₅ O ₃		195.1027	2.4		n.a.	4.5	even	ok
197.1178	1	C ₁₁ H ₁₇ O ₃	100.00	197.1183	2.5	2.4	7.5	3.5	even	ok
200.0998	1	C ₁₀ H ₁₅ O ₄		199.0976	6.0		n.a.	3.5	even	ok
200.1357	1	C ₁₁ H ₁₉ O ₃		199.1340	8.4		n.a.	2.5	even	ok
201.0763	1	C ₉ H ₁₃ O ₅		201.0768	2.7		n.a.	3.5	even	ok
209.1172	1	C ₁₂ H ₁₇ O ₃	100.00	209.1183	5.6	5.4	9.3	4.5	even	ok
211.1335	1	C ₁₂ H ₁₉ O ₃	100.00	211.1340	2.3	2.3	9.7	3.5	even	ok
213.1127	1	C ₁₁ H ₁₇ O ₄	100.00	213.1132	2.6	2.7	10.4	3.5	even	ok
225.1124	1	C ₁₂ H ₁₇ O ₄	100.00	225.1132	3.6	3.6	9.2	4.5	even	ok
227.1283	1	C ₁₂ H ₁₉ O ₄	100.00	227.1289	2.6	2.7	9.3	3.5	even	ok
255.1077	1	C ₉ H ₁₉ O ₈	100.00	255.1085	3.1	3.1	12.1	0.5	even	ok
257.0871	1	C ₈ H ₁₇ O ₉	100.00	257.0878	2.8	2.9	14.3	0.5	even	ok

Appendix: Mass Spectrum SmartFormula Report

Mass Spectrum SmartFormula Report										
Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
271.1026	1	C 9 H 19 O 9	100.00	271.1035	3.0	3.0	1.8	0.5	even	ok
273.1074	1	C 9 H 19 O 9	100.00	271.1035	3.0	3.0	1.8	0.5	even	ok
275.0743	1	C 11 H 15 O 8		275.0772	10.7		n.a.	4.5	even	ok
275.1116	1	C 12 H 19 O 7		275.1136	7.4		n.a.	3.5	even	ok
275.1513	1	C 13 H 23 O 6		275.1500	-4.7		n.a.	2.5	even	ok
	2	C 17 H 21 O 3		273.1496	16.1		n.a.	7.5	even	ok
275.1653	1	C 17 H 23 O 3		275.1653	-0.1		n.a.	6.5	even	ok
275.2026	1	C 18 H 27 O 2		275.2017	-3.4		n.a.	5.5	even	ok
277.0918	1	C 11 H 17 O 8		277.0929	3.9		n.a.	3.5	even	ok
277.1457	1	C 16 H 21 O 4		277.1445	-4.2		n.a.	6.5	even	ok
277.1644	1	C 13 H 25 O 6		277.1657	4.6		n.a.	1.5	even	ok
277.1808	1	C 17 H 25 O 3		277.1809	0.4		n.a.	5.5	even	ok
277.2159	1	C 18 H 29 O 2		277.2173	5.1		n.a.	4.5	even	ok
278.1326	1	C 12 H 21 O 7		277.1293	0.4		n.a.	2.5	even	ok
278.1819	1	C 17 H 25 O 3		277.1809	8.7		n.a.	5.5	even	ok
279.1590	1	C 16 H 23 O 4		279.1602	4.2		n.a.	5.5	even	ok
279.1942	1	C 17 H 27 O 3		279.1966	8.5		n.a.	4.5	even	ok
280.1495	1	C 12 H 23 O 7		279.1449	-4.1		n.a.	1.5	even	ok
281.1749	1	C 16 H 25 O 4		281.1758	3.3		n.a.	4.5	even	ok
281.2126	1	C 17 H 29 O 3		281.2122	-1.4		n.a.	3.5	even	ok
281.2504	1	C 18 H 33 O 2		281.2486	-6.4		n.a.	2.5	even	ok
282.1288	1	C 11 H 21 O 8		281.1242	-4.2		n.a.	1.5	even	ok
282.1619	1	C 12 H 25 O 7		281.1606	7.5		n.a.	0.5	even	ok
283.1033	1	C 10 H 19 O 9		283.1035	0.6		n.a.	1.5	even	ok
284.1435	1	C 11 H 23 O 8		283.1398	-0.8		n.a.	0.5	even	ok
285.1182	1	C 10 H 21 O 9	100.00	285.1191	3.2	3.0	7.2	0.5	even	ok
285.1690	1	C 15 H 25 O 5		285.1707	6.1		n.a.	3.5	even	ok
285.2070	1	C 16 H 29 O 4		285.2071	0.5		n.a.	2.5	even	ok
286.1392	1	C 14 H 21 O 6		285.1344	-5.0		n.a.	4.5	even	ok
287.0968	1	C 9 H 19 O 10		287.0984	5.5		n.a.	0.5	even	ok
287.1234	1	C 10 H 21 O 9	100.00	285.1191	2.0	3.0	7.2	0.5	even	ok
289.1268	1	C 13 H 21 O 7		289.1293	8.6		n.a.	3.5	even	ok
289.1459	1	C 17 H 21 O 4		289.1445	-4.7		n.a.	7.5	even	ok
289.1674	1	C 14 H 25 O 6		289.1657	-6.0		n.a.	2.5	even	ok
289.1794	1	C 18 H 25 O 3		289.1809	5.3		n.a.	6.5	even	ok
291.1062	1	C 12 H 19 O 8		291.1085	8.0		n.a.	3.5	even	ok
291.1951	1	C 18 H 27 O 3		291.1966	5.0		n.a.	5.5	even	ok
293.0901	1	C 11 H 17 O 9		293.0878	-7.8		n.a.	3.5	even	ok
293.1383	1	C 16 H 21 O 5		293.1394	3.9		n.a.	6.5	even	ok
293.1768	1	C 17 H 25 O 4		293.1758	-3.3		n.a.	5.5	even	ok
293.2105	1	C 18 H 29 O 3		293.2122	5.9		n.a.	4.5	even	ok
294.1292	1	C 12 H 21 O 8		293.1242	-5.4		n.a.	2.5	even	ok
295.0541	1	C 10 H 13 O 10		293.0514	7.3		n.a.	4.5	even	ok
295.1024	1	C 11 H 19 O 9		295.1035	3.6		n.a.	2.5	even	ok
295.1390	1	C 12 H 23 O 8	100.00	295.1396	2.8	2.7	14.2	1.5	even	ok
295.1894	1	C 17 H 27 O 4		295.1915	7.1		n.a.	4.5	even	ok
297.1182	1	C 11 H 21 O 9	100.00	297.1191	3.0	3.0	17.5	1.5	even	ok
297.2065	1	C 17 H 29 O 4		297.2071	2.1		n.a.	3.5	even	ok
299.1339	1	C 11 H 23 O 9	100.00	299.1348	3.0	3.0	14.9	0.5	even	ok
301.1131	1	C 10 H 21 O 10	100.00	301.1140	3.2	3.2	29.0	0.5	even	ok
307.1384	1	C 13 H 23 O 8		307.1398	4.7		n.a.	2.5	even	ok
307.1754	1	C 14 H 27 O 7		307.1762	2.7		n.a.	1.5	even	ok
309.1563	1	C 13 H 25 O 8		309.1555	-2.6		n.a.	1.5	even	ok
309.2082	1	C 18 H 29 O 4		309.2071	-3.5		n.a.	4.5	even	ok
310.1218	1	C 12 H 21 O 9		309.1191	2.4		n.a.	2.5	even	ok
311.0963	1	C 11 H 19 O 10		311.0984	6.7		n.a.	2.5	even	ok
311.1337	1	C 12 H 23 O 9	100.00	311.1348	3.4	3.2	19.4	1.5	even	ok
311.1683	1	C 13 H 27 O 8		311.1711	9.1		n.a.	0.5	even	ok
311.1881	1	C 17 H 27 O 5		311.1864	-5.5		n.a.	4.5	even	ok
311.2204	1	C 18 H 31 O 4		311.2228	7.7		n.a.	3.5	even	ok
313.0076	1	C 8 H 9 O 13		313.0049	-8.7		n.a.	4.5	even	ok
313.1493	1	C 12 H 25 O 9	100.00	313.1504	3.5	3.3	18.0	0.5	even	ok
313.1993	1	C 17 H 29 O 5		313.2020	8.8		n.a.	3.5	even	ok

Appendix: Mass Spectrum SmartFomula Report

Mass Spectrum SmartFormula Report										
Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
313.2392	1	C 18 H 33 O 4		313.2384	-2.4		n.a.	2.5	even	ok
314.0465	1	C 9 H 13 O 12		313.0412	-5.8		n.a.	3.5	even	ok
315.1286	1	C 11 H 23 O 10	100.00	315.1297	3.3	3.3	0.7	0.5	even	ok
315.1545	1	C 12 H 25 O 9		313.1504	3.1		n.a.	0.5	even	ok
315.2544	1	C 18 H 35 O 4		315.2541	-1.0		n.a.	1.5	even	ok
317.1330	1	C 11 H 23 O 10	100.00	315.1297	5.0	3.3	0.7	0.5	even	ok
321.1549	1	C 14 H 25 O 8		321.1555	1.8		n.a.	2.5	even	ok
321.1902	1	C 15 H 29 O 7		321.1919	5.2		n.a.	1.5	even	ok
323.0488	1	C 7 H 15 O 14		323.0467	-6.4		n.a.	0.5	even	ok
323.0968	1	C 12 H 19 O 10		323.0984	4.9		n.a.	3.5	even	ok
323.1322	1	C 13 H 23 O 9		323.1348	7.9		n.a.	2.5	even	ok
323.1727	1	C 14 H 27 O 8		323.1711	-4.8		n.a.	1.5	even	ok
325.0625	1	C 7 H 17 O 14	100.00	325.0624	-0.5	-0.5	49.7	-0.5	even	ok
325.1486	1	C 13 H 25 O 9		325.1504	5.6		n.a.	1.5	even	ok
325.2019	1	C 18 H 29 O 5		325.2020	0.5		n.a.	4.5	even	ok
326.1159	1	C 12 H 21 O 10		325.1140	4.8		n.a.	2.5	even	ok
327.1286	1	C 12 H 23 O 10	100.00	327.1297	3.3	3.3	16.6	1.5	even	ok
327.1636	1	C 13 H 27 O 9		327.1661	7.5		n.a.	0.5	even	ok
327.2145	1	C 18 H 31 O 5		327.2177	9.8		n.a.	3.5	even	ok
328.1320	1	C 12 H 23 O 10	100.00	327.1297	3.3	3.3	16.6	1.5	even	ok
329.1442	1	C 12 H 25 O 10	100.00	329.1453	3.5	3.6	1.3	0.5	even	ok
331.1487	1	C 12 H 25 O 10	100.00	329.1453	4.8	3.6	1.3	0.5	even	ok
332.1270	1	C 11 H 23 O 11		331.1246	3.1		n.a.	0.5	even	ok
343.1235	1	C 12 H 23 O 11	100.00	343.1246	3.2	3.1	21.1	1.5	even	ok
345.1391	1	C 12 H 25 O 11	100.00	345.1402	3.4	3.3	2.7	0.5	even	ok
361.1339	1	C 12 H 25 O 12	100.00	361.1351	3.4	3.3	19.7	0.5	even	ok
362.1376	1	C 12 H 25 O 12	100.00	361.1351	2.7	3.3	19.7	0.5	even	ok

Appendix: Mass Spectrum SmartFormula Report

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\LSHXPWANGXC\neg-inject-111028-S1.d
Method tune_low_neg.m
Sample Name TuneMix
Comment

Acquisition Date 10/28/2011 11:51:53 AM

Operator QIBEBT

Instrument / Ser# maXis 10161

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	2800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
179.0552	1	C ₆ H ₁₁ O ₆	100.00	179.0561	5.2	5.1	7.4	1.5	even	ok
181.0708	1	C ₆ H ₁₃ O ₆	100.00	181.0718	5.5	5.5	7.5	0.5	even	ok
201.1122	1	C ₁₀ H ₁₇ O ₄		201.1132	5.1		n.a.	2.5	even	ok
221.0639	1	C ₈ H ₁₃ O ₇		221.0667	12.6		n.a.	2.5	even	ok
227.1280	1	C ₁₂ H ₁₉ O ₄	100.00	227.1289	3.8	3.8	10.6	3.5	even	ok
231.1250	1	C ₁₁ H ₁₉ O ₅		231.1238	-5.2		n.a.	2.5	even	ok
240.1154	1	C ₉ H ₁₉ O ₇		239.1136	6.9		n.a.	0.5	even	ok
	2	C ₁₆ H ₁₅ O ₂		239.1078	-17.7		n.a.	9.5	even	ok
251.1491	1	C ₁₁ H ₂₃ O ₆		251.1500	3.6		n.a.	0.5	even	ok
261.1353	1	C ₁₂ H ₂₁ O ₆		261.1344	-3.6		n.a.	2.5	even	ok
	2	C ₁₆ H ₁₉ O ₃		259.1340	18.0		n.a.	7.5	even	ok
271.1023	1	C ₉ H ₁₉ O ₉	100.00	271.1035	4.1	4.1	14.0	0.5	even	ok
	2	C ₁₆ H ₁₅ O ₄	1.62	271.0976	-17.5	-17.6	40.9	9.5	even	ok
272.1059	1	C ₁₆ H ₁₅ O ₄	1.62	271.0976	-17.9	-17.6	40.9	9.5	even	ok
277.1292	1	C ₁₂ H ₂₁ O ₇		277.1293	0.3		n.a.	2.5	even	ok
	2	C ₁₆ H ₁₉ O ₄		275.1289	20.1		n.a.	7.5	even	ok
285.1180	1	C ₁₀ H ₂₁ O ₉	100.00	285.1191	3.9	3.8	14.7	0.5	even	ok
295.0178	1	C ₁₆ H ₅ O ₆		293.0092	-10.3		n.a.	14.5	even	ok
296.1426	1	C ₁₂ H ₂₃ O ₈		295.1398	2.3		n.a.	1.5	even	ok
299.1335	1	C ₁₁ H ₂₃ O ₉	100.00	299.1348	4.1	4.0	15.2	0.5	even	ok
302.1166	1	C ₁₀ H ₂₁ O ₁₀		301.1140	2.9		n.a.	0.5	even	ok
313.0076	1	C ₁₂ H ₇ O ₁₀		311.0045	5.9		n.a.	9.5	even	ok
313.1493	1	C ₁₂ H ₂₅ O ₉	100.00	313.1504	3.6	3.7	15.3	0.5	even	ok
314.1525	1	C ₁₂ H ₂₅ O ₉	100.00	313.1504	4.3	3.7	15.3	0.5	even	ok
315.1284	1	C ₁₁ H ₂₃ O ₁₀	100.00	315.1297	4.2	4.0	15.9	0.5	even	ok
325.0257	1	C ₆ H ₁₃ O ₁₅	100.00	325.0260	0.9	0.9	44.6	0.5	even	ok
325.1130	1	C ₁₂ H ₂₁ O ₁₀		325.1140	3.1		n.a.	2.5	even	ok
327.0422	1	C ₆ H ₁₅ O ₁₅	100.00	327.0416	-1.7	-1.7	44.6	-0.5	even	ok
327.1284	1	C ₁₂ H ₂₃ O ₁₀	100.00	327.1297	3.9	3.9	16.9	1.5	even	ok
328.1319	1	C ₁₂ H ₂₃ O ₁₀	100.00	327.1297	3.9	3.9	16.9	1.5	even	ok
329.1439	1	C ₁₂ H ₂₅ O ₁₀	100.00	329.1453	4.4	4.3	18.4	0.5	even	ok
343.1233	1	C ₁₂ H ₂₃ O ₁₁	100.00	343.1246	3.8	3.8	18.2	1.5	even	ok
345.1388	1	C ₁₂ H ₂₅ O ₁₁	100.00	345.1402	4.1	4.1	21.9	0.5	even	ok
361.1337	1	C ₁₂ H ₂₅ O ₁₂	100.00	361.1351	4.1	4.0	19.1	0.5	even	ok
362.1373	1	C ₁₂ H ₂₅ O ₁₂	100.00	361.1351	3.6	4.0	19.1	0.5	even	ok

Appendix: Mass Spectrum SmartFomula Report

Mass Spectrum SmartFormula Report										
Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
367.1969	1	C 16 H 31 O 9		367.1974	1.2		n.a.	1.5	even	ok
413.0787	1	C 10 H 21 O 17		413.0784	-0.7		n.a.	0.5	even	ok
425.2024	1	C 18 H 33 O 11		425.2028	1.0		n.a.	2.5	even	ok
429.0728	1	C 10 H 21 O 18		429.0733	1.3		n.a.	0.5	even	ok
453.0613	1	C 12 H 19 O 18		451.0577	2.5		n.a.	3.5	even	ok
455.1240	1	C 24 H 21 O 9		453.1191	2.2		n.a.	14.5	even	ok
	2	C 20 H 23 O 12		455.1195	-9.9		n.a.	9.5	even	ok
459.0827	1	C 22 H 17 O 11		457.0776	1.3		n.a.	14.5	even	ok
464.0794	1	C 10 H 23 O 20		463.0788	6.2		n.a.	-0.5	even	ok
465.0741	1	C 24 H 15 O 10		463.0671	-2.6		n.a.	17.5	even	ok
475.1165	1	C 16 H 25 O 16		473.1148	7.2		n.a.	4.5	even	ok
495.0689	1	C 10 H 23 O 22		495.0686	-0.5		n.a.	-0.5	even	ok
	2	C 14 H 21 O 19		493.0683	8.5		n.a.	4.5	even	ok
497.0839	1	C 14 H 23 O 19		495.0839	9.8		n.a.	3.5	even	ok
509.0852	1	C 22 H 19 O 14		507.0780	-3.2		n.a.	13.5	even	ok
511.0967	1	C 22 H 21 O 14		509.0937	4.9		n.a.	12.5	even	ok
527.0955	1	C 22 H 21 O 15		525.0886	-2.7		n.a.	12.5	even	ok
551.0952	1	C 24 H 21 O 15		549.0886	-1.8		n.a.	14.5	even	ok
609.2243	1	C 22 H 41 O 19		609.2248	0.7		n.a.	2.5	even	ok
651.2335	1	C 24 H 43 O 20		651.2353	2.8		n.a.	3.5	even	ok
669.2480	1	C 24 H 45 O 21		669.2459	-3.2		n.a.	2.5	even	ok
685.2376	1	C 24 H 45 O 22		685.2408	4.7		n.a.	2.5	even	ok

Appendix: Mass Spectrum SmartFormula Report

Mass Spectrum SmartFormula Report										
Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
477.1826	1	C 17 H 33 O 15		477.1825	-0.2		n.a.	1.5	even	ok
651.2370	1	C 24 H 43 O 20		651.2353	-2.6		n.a.	3.5	even	ok
653.2528	1	C 24 H 45 O 20		653.2510	-2.8		n.a.	2.5	even	ok
669.2406	1	C 31 H 41 O 16		669.2400	-0.9		n.a.	11.5	even	ok
815.2956	1	C 30 H 53 O 25		813.2881	-2.3		n.a.	4.5	even	ok
	2	C 37 H 51 O 20		815.2979	2.8		n.a.	12.5	even	ok