

Timothy Ebbels

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

134 papers	9,422 citations	48 h-index	96 g-index
151 ext. papers	10,683 ext. citations	6.1 avg, IF	5.64 L-index

#	Paper	IF	Citations
134	Metabolic profiling, metabolomic and metabonomic procedures for NMR spectroscopy of urine, plasma, serum and tissue extracts. <i>Nature Protocols</i> , 2007 , 2, 2692-703	18.8	1536
133	Human metabolic phenotype diversity and its association with diet and blood pressure. <i>Nature</i> , 2008 , 453, 396-400	50.4	847
132	Contemporary issues in toxicology the role of metabonomics in toxicology and its evaluation by the COMET project. <i>Toxicology and Applied Pharmacology</i> , 2003 , 187, 137-46	4.6	342
131	Proposed minimum reporting standards for data analysis in metabolomics. <i>Metabolomics</i> , 2007 , 3, 231-241	4.7	317
130	High-resolution magic-angle-spinning NMR spectroscopy for metabolic profiling of intact tissues. <i>Nature Protocols</i> , 2010 , 5, 1019-32	18.8	309
129	Recursive segment-wise peak alignment of biological (1)h NMR spectra for improved metabolic biomarker recovery. <i>Analytical Chemistry</i> , 2009 , 81, 56-66	7.8	258
128	The Consortium for Metabonomic Toxicology (COMET): aims, activities and achievements. <i>Pharmacogenomics</i> , 2005 , 6, 691-9	2.6	255
127	Integrated pathway-level analysis of transcriptomics and metabolomics data with IMPaLA. <i>Bioinformatics</i> , 2011 , 27, 2917-8	7.2	239
126	Analytical reproducibility in (1)H NMR-based metabonomic urinalysis. <i>Chemical Research in Toxicology</i> , 2002 , 15, 1380-6	4	239
125	Optimized preprocessing of ultra-performance liquid chromatography/mass spectrometry urinary metabolic profiles for improved information recovery. <i>Analytical Chemistry</i> , 2011 , 83, 5864-72	7.8	201
124	Improved analysis of multivariate data by variable stability scaling: application to NMR-based metabolic profiling. <i>Analytica Chimica Acta</i> , 2003 , 490, 265-276	6.6	149
123	Prediction and classification of drug toxicity using probabilistic modeling of temporal metabolic data: the consortium on metabonomic toxicology screening approach. <i>Journal of Proteome Research</i> , 2007 , 6, 4407-22	5.6	146
122	Optimization and evaluation of metabolite extraction protocols for untargeted metabolic profiling of liver samples by UPLC-MS. <i>Analytical Chemistry</i> , 2010 , 82, 7779-86	7.8	144
121	Urinary metabolic signatures of human adiposity. <i>Science Translational Medicine</i> , 2015 , 7, 285ra62	17.5	141
120	Spectral editing and pattern recognition methods applied to high-resolution magic-angle spinning 1H nuclear magnetic resonance spectroscopy of liver tissues. <i>Analytical Biochemistry</i> , 2003 , 323, 26-32	3.1	134
119	Bayesian deconvolution and quantification of metabolites in complex 1D NMR spectra using BATMAN. <i>Nature Protocols</i> , 2014 , 9, 1416-27	18.8	132
118	Geometric trajectory analysis of metabolic responses to toxicity can define treatment specific profiles. <i>Chemical Research in Toxicology</i> , 2004 , 17, 579-87	4	131

117	NMR-based metabonomic toxicity classification: hierarchical cluster analysis and k-nearest-neighbour approaches. <i>Analytica Chimica Acta</i> , 2003 , 490, 3-15	6.6	127
116	Design and analysis of metabolomics studies in epidemiologic research: a primer on -omic technologies. <i>American Journal of Epidemiology</i> , 2014 , 180, 129-39	3.8	123
115	Correction of mass calibration gaps in liquid chromatography-mass spectrometry metabolomics data. <i>Bioinformatics</i> , 2010 , 26, 2488-9	7.2	119
114	BATMAN--an R package for the automated quantification of metabolites from nuclear magnetic resonance spectra using a Bayesian model. <i>Bioinformatics</i> , 2012 , 28, 2088-90	7.2	118
113	Opening up the "Black Box": metabolic phenotyping and metabolome-wide association studies in epidemiology. <i>Journal of Clinical Epidemiology</i> , 2010 , 63, 970-9	5.7	113
112	COordination of Standards in MetabOmicS (COSMOS): facilitating integrated metabolomics data access. <i>Metabolomics</i> , 2015 , 11, 1587-1597	4.7	109
111	Comparative metabonomics of differential hydrazine toxicity in the rat and mouse. <i>Toxicology and Applied Pharmacology</i> , 2005 , 204, 135-51	4.6	107
110	Metabolome-wide association study identifies multiple biomarkers that discriminate north and south Chinese populations at differing risks of cardiovascular disease: INTERMAP study. <i>Journal of Proteome Research</i> , 2010 , 9, 6647-54	5.6	106
109	Optimizing the use of quality control samples for signal drift correction in large-scale urine metabolic profiling studies. <i>Analytical Chemistry</i> , 2012 , 84, 2670-7	7.8	104
108	The evolution of partial least squares models and related chemometric approaches in metabonomics and metabolic phenotyping. <i>Journal of Chemometrics</i> , 2010 , 24, 636-649	1.6	104
107	Metabolic profiling and the metabolome-wide association study: significance level for biomarker identification. <i>Journal of Proteome Research</i> , 2010 , 9, 4620-7	5.6	102
106	Meeting-in-the-middle using metabolic profiling - a strategy for the identification of intermediate biomarkers in cohort studies. <i>Biomarkers</i> , 2011 , 16, 83-8	2.6	88
105	Data standards can boost metabolomics research, and if there is a will, there is a way. <i>Metabolomics</i> , 2016 , 12, 14	4.7	85
104	Bioinformatic methods in NMR-based metabolic profiling. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2009 , 55, 361-374	10.4	82
103	Batch statistical processing of 1H NMR-derived urinary spectral data. <i>Journal of Chemometrics</i> , 2002 , 16, 461-468	1.6	80
102	Applying 'omics technologies in chemicals risk assessment: Report of an ECETOC workshop. <i>Regulatory Toxicology and Pharmacology</i> , 2017 , 91 Suppl 1, S3-S13	3.4	74
101	Power Analysis and Sample Size Determination in Metabolic Phenotyping. <i>Analytical Chemistry</i> , 2016 , 88, 5179-88	7.8	70
100	Toxicity classification from metabonomic data using a density superposition approach: [CLOUDS] <i>Analytica Chimica Acta</i> , 2003 , 490, 109-122	6.6	69

99	NMR-based metabolic profiling identifies biomarkers of liver regeneration following partial hepatectomy in the rat. <i>Journal of Proteome Research</i> , 2010 , 9, 59-69	5.6	68
98	Consensus-phenotype integration of transcriptomic and metabolomic data implies a role for metabolism in the chemosensitivity of tumour cells. <i>PLoS Computational Biology</i> , 2011 , 7, e1001113	5	65
97	Subset optimization by reference matching (STORM): an optimized statistical approach for recovery of metabolic biomarker structural information from ¹ H NMR spectra of biofluids. <i>Analytical Chemistry</i> , 2012 , 84, 10694-701	7.8	64
96	Use cases, best practice and reporting standards for metabolomics in regulatory toxicology. <i>Nature Communications</i> , 2019 , 10, 3041	17.4	62
95	Serum metabolic signatures of coronary and carotid atherosclerosis and subsequent cardiovascular disease. <i>European Heart Journal</i> , 2019 , 40, 2883-2896	9.5	58
94	Statistical experimental design and partial least squares regression analysis of biofluid metabonomic NMR and clinical chemistry data for screening of adverse drug effects. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2004 , 73, 139-149	3.8	57
93	Computational tools and workflows in metabolomics: An international survey highlights the opportunity for harmonisation through Galaxy. <i>Metabolomics</i> , 2017 , 13, 12	4.7	52
92	Robust algorithms for automated chemical shift calibration of 1D ¹ H NMR spectra of blood serum. <i>Analytical Chemistry</i> , 2008 , 80, 7158-62	7.8	52
91	Analytic properties of statistical total correlation spectroscopy based information recovery in ¹ H NMR metabolic data sets. <i>Analytical Chemistry</i> , 2009 , 81, 2075-84	7.8	51
90	Genetic algorithms for simultaneous variable and sample selection in metabonomics. <i>Bioinformatics</i> , 2009 , 25, 112-8	7.2	50
89	The carcinoGENOMICS project: critical selection of model compounds for the development of omics-based in vitro carcinogenicity screening assays. <i>Mutation Research - Reviews in Mutation Research</i> , 2008 , 659, 202-10	7	50
88	Temporal metabonomic modeling of l-arginine-induced exocrine pancreatitis. <i>Journal of Proteome Research</i> , 2008 , 7, 4435-45	5.6	49
87	Metabolic response to low-level toxicant exposure in a novel renal tubule epithelial cell system. <i>Molecular BioSystems</i> , 2011 , 7, 247-57		48
86	Intra- and inter-omic fusion of metabolic profiling data in a systems biology framework. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2010 , 104, 121-131	3.8	48
85	Time-resolved metabolic footprinting for nonlinear modeling of bacterial substrate utilization. <i>Applied and Environmental Microbiology</i> , 2009 , 75, 2453-63	4.8	46
84	Validation of metabolomics for toxic mechanism of action screening with the earthworm <i>Lumbricus rubellus</i> . <i>Metabolomics</i> , 2009 , 5, 72-83	4.7	46
83	Identification of a gravitationally lensed $z = 2.515$ star-forming galaxy. <i>Monthly Notices of the Royal Astronomical Society</i> , 1996 , 281, L75-L81	4.3	45
82	Correlation Network Analysis reveals a sequential reorganization of metabolic and transcriptional states during germination and gene-metabolite relationships in developing seedlings of <i>Arabidopsis</i> . <i>BMC Systems Biology</i> , 2010 , 4, 62	3.5	41

81	PhenoMeNal: processing and analysis of metabolomics data in the cloud. <i>GigaScience</i> , 2019 , 8,	7.6	41
80	Reliability of plasma polar metabolite concentrations in a large-scale cohort study using capillary electrophoresis-mass spectrometry. <i>PLoS ONE</i> , 2018 , 13, e0191230	3.7	40
79	nmrML: A Community Supported Open Data Standard for the Description, Storage, and Exchange of NMR Data. <i>Analytical Chemistry</i> , 2018 , 90, 649-656	7.8	37
78	Statistical total correlation spectroscopy editing of 1H NMR spectra of biofluids: application to drug metabolite profile identification and enhanced information recovery. <i>Analytical Chemistry</i> , 2009 , 81, 6458-66	7.8	37
77	Intra- and interlaboratory reproducibility of ultra performance liquid chromatography-time-of-flight mass spectrometry for urinary metabolic profiling. <i>Analytical Chemistry</i> , 2012 , 84, 2424-32	7.8	36
76	Metabolic profiling and population screening of analgesic usage in nuclear magnetic resonance spectroscopy-based large-scale epidemiologic studies. <i>Analytical Chemistry</i> , 2009 , 81, 5119-29	7.8	36
75	A statistical framework for biomarker discovery in metabolomic time course data. <i>Bioinformatics</i> , 2011 , 27, 1979-85	7.2	36
74	Data-driven approach for metabolite relationship recovery in biological 1H NMR data sets using iterative statistical total correlation spectroscopy. <i>Analytical Chemistry</i> , 2011 , 83, 2075-82	7.8	35
73	A Bayesian Model of NMR Spectra for the Deconvolution and Quantification of Metabolites in Complex Biological Mixtures. <i>Journal of the American Statistical Association</i> , 2012 , 107, 1259-1271	2.8	34
72	Evaluation of metabolic variation in normal rat strains from a statistical analysis of 1H NMR spectra of urine. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2004 , 36, 823-33	3.5	32
71	Cluster analysis statistical spectroscopy using nuclear magnetic resonance generated metabolic data sets from perturbed biological systems. <i>Analytical Chemistry</i> , 2009 , 81, 6581-9	7.8	30
70	Workflow for Integrated Processing of Multicohort Untargeted H NMR Metabolomics Data in Large-Scale Metabolic Epidemiology. <i>Journal of Proteome Research</i> , 2016 , 15, 4188-4194	5.6	28
69	diXa: a data infrastructure for chemical safety assessment. <i>Bioinformatics</i> , 2015 , 31, 1505-7	7.2	27
68	Bidirectional correlation of NMR and capillary electrophoresis fingerprints: a new approach to investigating <i>Schistosoma mansoni</i> infection in a mouse model. <i>Analytical Chemistry</i> , 2010 , 82, 203-10	7.8	27
67	A differential network approach to exploring differences between biological states: an application to prediabetes. <i>PLoS ONE</i> , 2011 , 6, e24702	3.7	27
66	Modelling the acid/base H NMR chemical shift limits of metabolites in human urine. <i>Metabolomics</i> , 2016 , 12, 152	4.7	24
65	Untargeted metabolome quantitative trait locus mapping associates variation in urine glycerate to mutant glycerate kinase. <i>Journal of Proteome Research</i> , 2012 , 11, 631-42	5.6	23
64	Piecewise multivariate modelling of sequential metabolic profiling data. <i>BMC Bioinformatics</i> , 2008 , 9, 105	3.6	23

63	Processing and modeling of nuclear magnetic resonance (NMR) metabolic profiles. <i>Methods in Molecular Biology</i> , 2011 , 708, 365-88	1.4	23
62	Dietary and urinary metabonomic factors possibly accounting for higher blood pressure of black compared with white Americans: results of International Collaborative Study on macro-/micronutrients and blood pressure. <i>Hypertension</i> , 2013 , 62, 1074-80	8.5	22
61	A statistically rigorous test for the identification of parent-fragment pairs in LC-MS datasets. <i>Analytical Chemistry</i> , 2010 , 82, 1766-78	7.8	21
60	Synergistic and Antagonistic Mutation Responses of Human MCL-5 Cells to Mixtures of Benzo[a]pyrene and 2-Amino-1-Methyl-6-Phenylimidazo[4,5-b]pyridine: Dose-Related Variation in the Joint Effects of Common Dietary Carcinogens. <i>Environmental Health Perspectives</i> , 2016 , 124, 88-96	8.4	21
59	Framework for the quality assurance of 'omics technologies considering GLP requirements. <i>Regulatory Toxicology and Pharmacology</i> , 2017 , 91 Suppl 1, S27-S35	3.4	20
58	Optimized Phenotypic Biomarker Discovery and Confounder Elimination via Covariate-Adjusted Projection to Latent Structures from Metabolic Spectroscopy Data. <i>Journal of Proteome Research</i> , 2018 , 17, 1586-1595	5.6	20
57	A comparison of human serum and plasma metabolites using untargeted H NMR spectroscopy and UPLC-MS. <i>Metabolomics</i> , 2018 , 14, 32	4.7	20
56	Statistical Correlations between NMR Spectroscopy and Direct Infusion FT-ICR Mass Spectrometry Aid Annotation of Unknowns in Metabolomics. <i>Analytical Chemistry</i> , 2016 , 88, 2583-9	7.8	20
55	¹ H NMR-based profiling reveals differential immune-metabolic networks during influenza virus infection in obese mice. <i>PLoS ONE</i> , 2014 , 9, e97238	3.7	20
54	Genome metabolome integrated network analysis to uncover connections between genetic variants and complex traits: an application to obesity. <i>Journal of the Royal Society Interface</i> , 2014 , 11, 20130908	4.1	18
53	Bayesian inference for multiple Gaussian graphical models with application to metabolic association networks. <i>Annals of Applied Statistics</i> , 2017 , 11,	2.1	18
52	Combining spectral ordering with peak fitting for one-dimensional NMR quantitative metabolomics. <i>Analytical Chemistry</i> , 2013 , 85, 4605-12	7.8	18
51	The future of metabolomics in ELIXIR. <i>F1000Research</i> , 2017 , 6,	3.6	18
50	The association of fish consumption and its urinary metabolites with cardiovascular risk factors: the International Study of Macro-/Micronutrients and Blood Pressure (INTERMAP). <i>American Journal of Clinical Nutrition</i> , 2020 , 111, 280-290	7	18
49	Improving Visualization and Interpretation of Metabolome-Wide Association Studies: An Application in a Population-Based Cohort Using Untargeted H NMR Metabolic Profiling. <i>Journal of Proteome Research</i> , 2017 , 16, 3623-3633	5.6	17
48	MetAssimulo: simulation of realistic NMR metabolic profiles. <i>BMC Bioinformatics</i> , 2010 , 11, 496	3.6	17
47	Metabolomics: The Stethoscope for the Twenty-First Century. <i>Medical Principles and Practice</i> , 2021 , 30, 301-310	2.1	17
46	springScape: visualisation of microarray and contextual bioinformatic data using spring embedding and an 'information landscape'. <i>Bioinformatics</i> , 2006 , 22, e99-107	7.2	16

45	Spectroscopic confirmation of redshifts predicted by gravitational lensing. <i>Monthly Notices of the Royal Astronomical Society</i> , 1998 , 295, 75	4.3	16
44	Integrated histopathological and urinary metabonomic investigation of the pathogenesis of microcystin-LR toxicosis. <i>Veterinary Pathology</i> , 2013 , 50, 159-71	2.8	13
43	Metabolic phenotyping for discovery of urinary biomarkers of diet, xenobiotics and blood pressure in the INTERMAP Study: an overview. <i>Hypertension Research</i> , 2017 , 40, 336-345	4.7	12
42	Embedding standards in metabolomics: the Metabolomics Society data standards task group. <i>Metabolomics</i> , 2015 , 11, 782-783	4.7	12
41	Identifying biochemical phenotypic differences between cryptic species. <i>Biology Letters</i> , 2014 , 10,	3.6	12
40	Effect of the histone deacetylase inhibitor trichostatin a on the metabolome of cultured primary hepatocytes. <i>Journal of Proteome Research</i> , 2010 , 9, 413-9	5.6	12
39	A combined metabonomic and transcriptomic approach to investigate metabolism during development in the chick chorioallantoic membrane. <i>Journal of Proteome Research</i> , 2010 , 9, 3126-34	5.6	12
38	Metabonomic investigations into the global biochemical sequelae of exposure to the pancreatic toxin 1-cyano-2-hydroxy-3-butene in the rat. <i>Magnetic Resonance in Chemistry</i> , 2009 , 47 Suppl 1, S26-35	2.1	12
37	Modelling short time series in metabolomics: a functional data analysis approach. <i>Advances in Experimental Medicine and Biology</i> , 2011 , 696, 307-15	3.6	11
36	Proteomic and metabolomic responses to connexin43 silencing in primary hepatocyte cultures. <i>Archives of Toxicology</i> , 2013 , 87, 883-94	5.8	10
35	The future of metabolomics in ELIXIR. <i>F1000Research</i> , 2017 , 6, 1649	3.6	10
34	Construction of confidence regions for isotopic abundance patterns in LC/MS data sets for rigorous determination of molecular formulas. <i>Analytical Chemistry</i> , 2010 , 82, 7319-28	7.8	9
33	Statistical Techniques in Metabolic Profiling 2008 , 347-373		9
32	Predictive modelling using pathway scores: robustness and significance of pathway collections. <i>BMC Bioinformatics</i> , 2019 , 20, 543	3.6	8
31	Statistical analysis in metabolic phenotyping. <i>Nature Protocols</i> , 2021 , 16, 4299-4326	18.8	8
30	Quantitative Investigation of Probabilistic Spectral Processing Methods Using Simulated NMR Data. <i>Applied Spectroscopy</i> , 2001 , 55, 1214-1224	3.1	6
29	Progress towards an OECD reporting framework for transcriptomics and metabolomics in regulatory toxicology. <i>Regulatory Toxicology and Pharmacology</i> , 2021 , 125, 105020	3.4	6
28	Targeted realignment of LC-MS profiles by neighbor-wise compound-specific graphical time warping with misalignment detection. <i>Bioinformatics</i> , 2020 , 36, 2862-2871	7.2	5

27	A combination of transcriptomics and metabolomics uncovers enhanced bile acid biosynthesis in HepG2 cells expressing CCAAT/enhancer-binding protein α (C/EBP α) hepatocyte nuclear factor 4 β (HNF4 β) and constitutive androstane receptor (CAR). <i>Journal of Proteome Research</i> , 2013 , 12, 2732-41	5.6	5
26	Integrative analysis of time course metabolic data and biomarker discovery. <i>BMC Bioinformatics</i> , 2020 , 21, 11	3.6	4
25	Orders of magnitude extension of the effective dynamic range of TDC-based TOFMS data through maximum likelihood estimation. <i>Journal of the American Society for Mass Spectrometry</i> , 2014 , 25, 1824-7	3.5	4
24	Variance and covariance heterogeneity analysis for detection of metabolites associated with cadmium exposure. <i>Statistical Applications in Genetics and Molecular Biology</i> , 2014 , 13, 191-201	1.2	4
23	Pathway analysis in metabolomics: Recommendations for the use of over-representation analysis. <i>PLoS Computational Biology</i> , 2021 , 17, e1009105	5	4
22	Characterization of data analysis methods for information recovery from metabolic ¹ H NMR spectra using artificial complex mixtures. <i>Metabolomics</i> , 2012 , 8, 1170-1180	4.7	3
21	Prospects for a statistical theory of LC/TOFMS data. <i>Journal of the American Society for Mass Spectrometry</i> , 2012 , 23, 779-91	3.5	3
20	Non-linear Methods for the Analysis of Metabolic Profiles 2007 , 201-226		3
19	Comparison of Bi- and Tri-Linear PLS Models for Variable Selection in Metabolomic Time-Series Experiments. <i>Metabolites</i> , 2019 , 9,	5.6	2
18	Over-representation of correlation analysis (ORCA): a method for identifying associations between variable sets. <i>Bioinformatics</i> , 2015 , 31, 102-8	7.2	2
17	Extraction and Integration of Genetic Networks from Short-Profile Omic Data Sets. <i>Metabolites</i> , 2020 , 10,	5.6	2
16	Bayesian estimation of the number of protonation sites for urinary metabolites from NMR spectroscopic data. <i>Metabolomics</i> , 2018 , 14, 56	4.7	2
15	Data mining and visualisation: general discussion. <i>Faraday Discussions</i> , 2019 , 218, 354-371	3.6	2
14	Statistical Data Analysis in Metabolomics 2011 , 163-180		2
13	Response to Comment on Optimized Preprocessing of Ultra-Performance Liquid Chromatography/Mass Spectrometry Urinary Metabolic Profiles for Improved Information Recovery <i>Analytical Chemistry</i> , 2011 , 83, 9721-9722	7.8	2
12	Semiempirical Molecular-Orbital Properties of Some Polycyclic Aromatic Hydrocarbons and Correlation with Environmental Toxic Equivalency Factors. <i>Polycyclic Aromatic Compounds</i> , 2003 , 23, 23-47	1.3	2
11	Processing and Analysis of Untargeted Multicohort NMR Data. <i>Methods in Molecular Biology</i> , 2019 , 2037, 453-470	1.4	2
10	Big Data and Databases for Metabolic Phenotyping 2019 , 329-367		2

9	PhenoMeNal: Processing and analysis of Metabolomics data in the Cloud		1
8	Statistical Methods in Metabolomics 2019 , 949-976		1
7	CHAPTER 12:Advances in Computational Analysis of Metabolomic NMR Data. <i>New Developments in NMR</i> , 2018 , 310-323	0.9	1
6	Estimation of permutation-based metabolome-wide significance thresholds		1
5	Bayesian Deconvolution and Quantification of Metabolites from J-Resolved NMR Spectroscopy. <i>Bayesian Analysis</i> , 2021 , 16,	2.3	1
4	Urinary hippurate and proline betaine relative to fruit intake, blood pressure, and body mass index. <i>Proceedings of the Nutrition Society</i> , 2016 , 75,	2.9	1
3	Multiple-testing correction in metabolome-wide association studies. <i>BMC Bioinformatics</i> , 2021 , 22, 67	3.6	1
2	Blood pressure interactions with the DASH dietary pattern, sodium, and potassium: The International Study of Macro-/Micronutrients and Blood Pressure (INTERMAP).. <i>American Journal of Clinical Nutrition</i> , 2022 ,	7	1
1	Report on the 9th Annual International Conference of the Metabolomics Society. <i>Metabolomics</i> , 2013 , 9, 935-937	4.7	