XXV. Ulusal Klinik Biyokimya Kongresi, 08-11 Mayıs 2025, Antalya/TÜRKİYE

METABOLİK SENDROM VE METABOLOMİK ANALİZLERE YAKLAŞIM

Dr. Eren VURGUN

İstanbul Prof.Dr. Cemil Taşcıoğlu Şehir Hastanesi

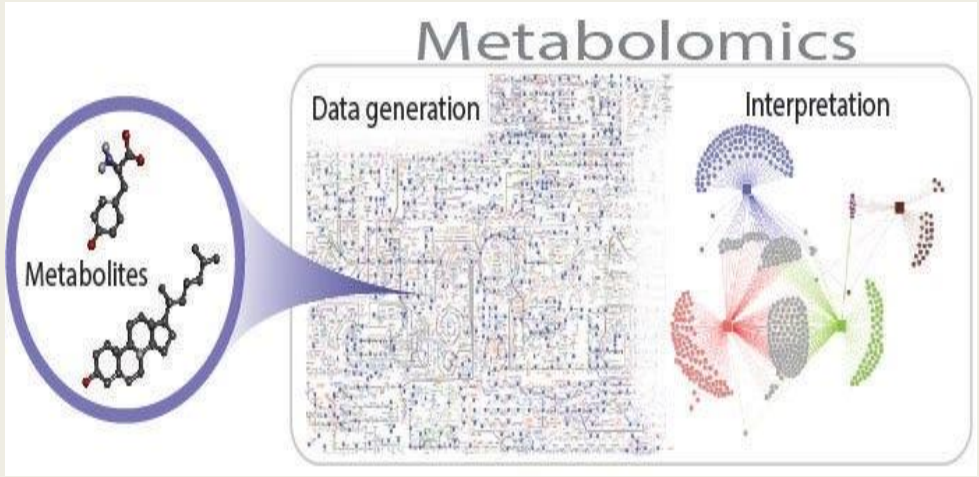
Tıbbi Biyokimya

10/05/2025

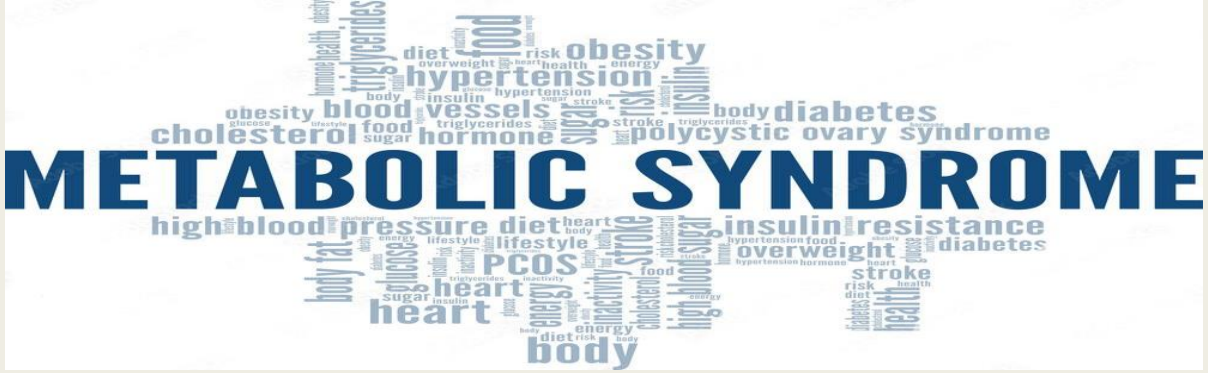
SUNUM İÇERİĞİ

- Metabolik Sendrom
  - Giriş ve Güncel Durum
  - Epidemiyoloji
  - Etiyoloji
  - Patofizyoloji
  - Tanı Kriterleri

- Metabolomik
  - Giriş ve Güncel Durum
  - Analizler ve Prosedür
  - Metabolik Sendromdaki Sonuçlar
  - Gelecekten Beklentiler
  - Yazılım ve Analiz Programları



GİRİŞ



- **Metabolik sendrom**; tip 2 diabetes mellitus, miyokard enfarktüsü, serebrovasküler olaylar, periferik vasküler hastalıklar gibi aterosklerotik kardiyovasküler hastalık riskini artıran çeşitli durumların bir araya gelmesiyle oluşan bir sendromdur.

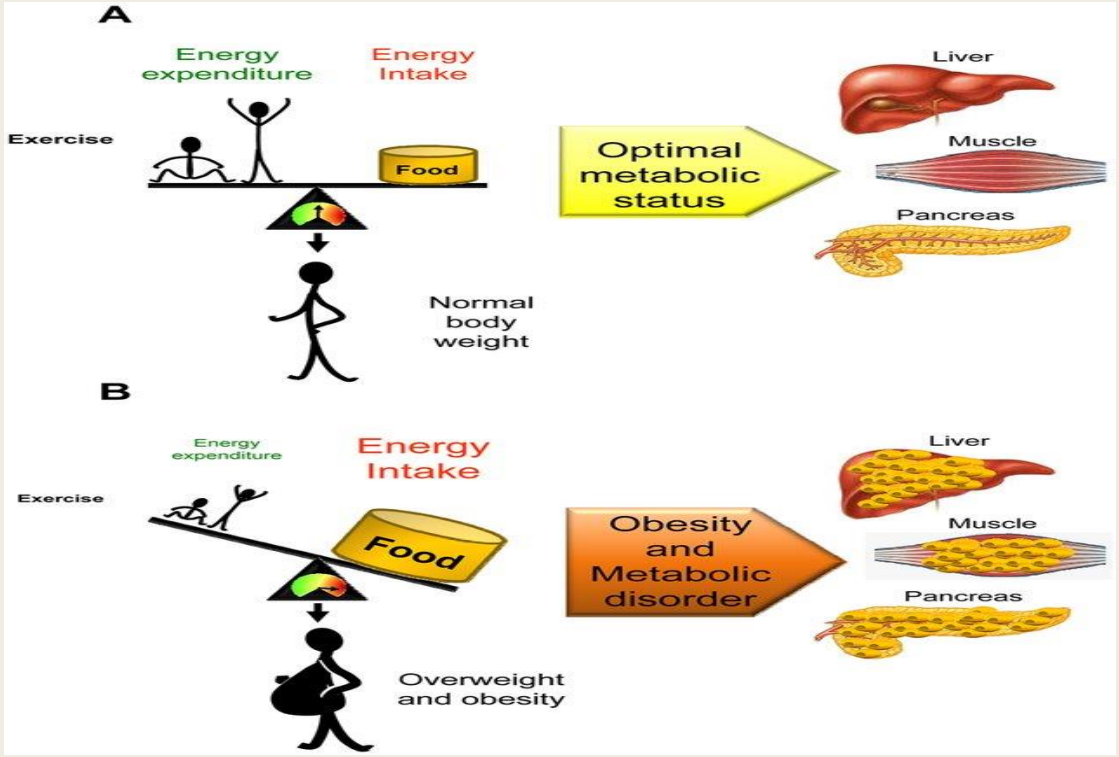
- Metabolik sendromu tanımlayan metabolik durumlar kümesi;
  - Abdominal obezite
  - İnsülin direnci
  - Hipertansiyon
  - Aterojenik dislipidemi

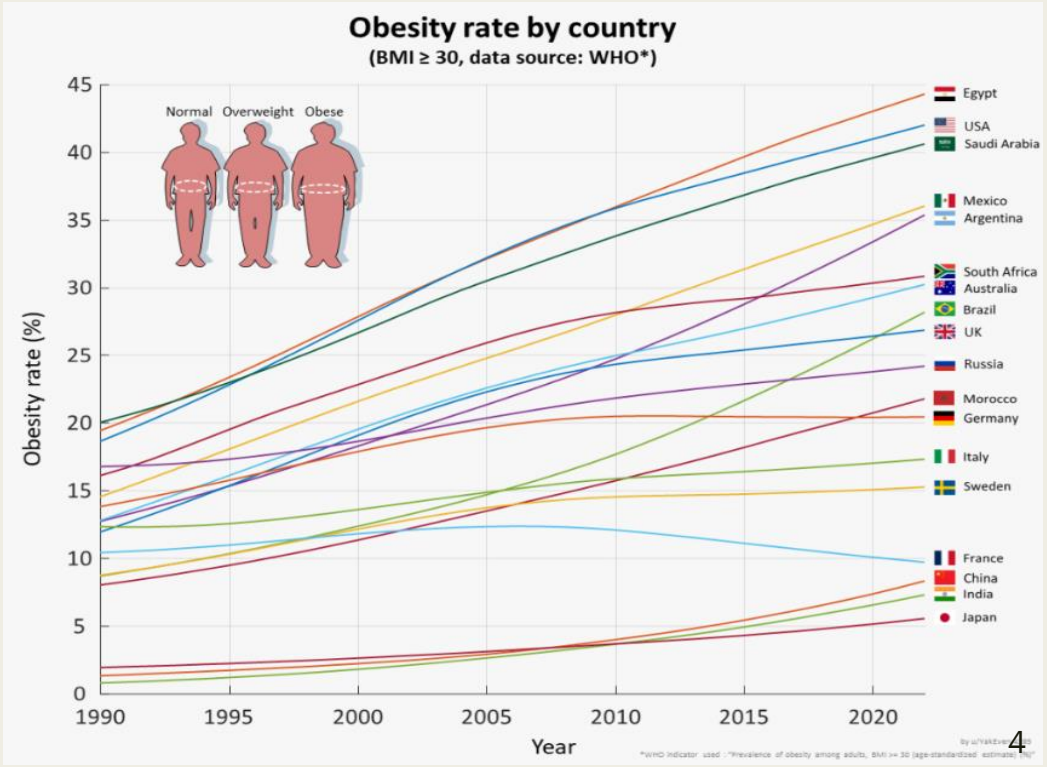
- Tip 2 DM riski ⇧ 2x
- Aterosklerotik kardiyovasküler hastalıklar riski ⇧ 5x

GÜNCEL DURUM

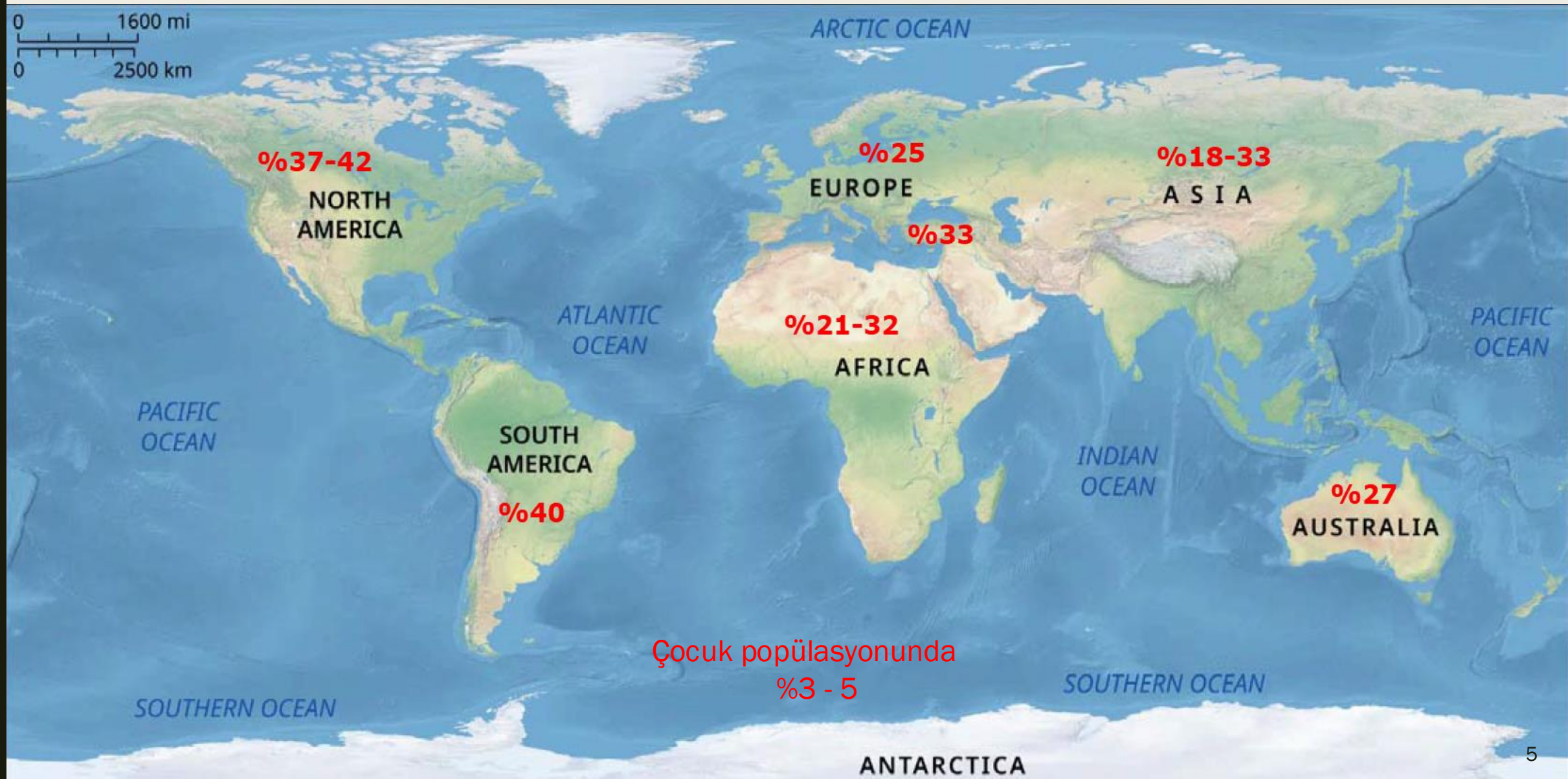
- Hareketsiz yaşam tarzı ve aşırı kalori alımı, son birkaç dekatta obezite prevalansında önemli bir artışa yol açmıştır.

- Dünya nüfusundaki obezite artışı nedeniyle de son 30 yılda metabolik sendrom insidansı da belirgin ölçüde artmıştır.



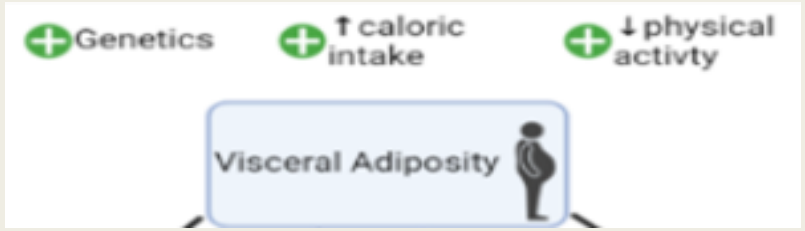


EPİDEMİYOLOJİ



ETİYOLOJİ

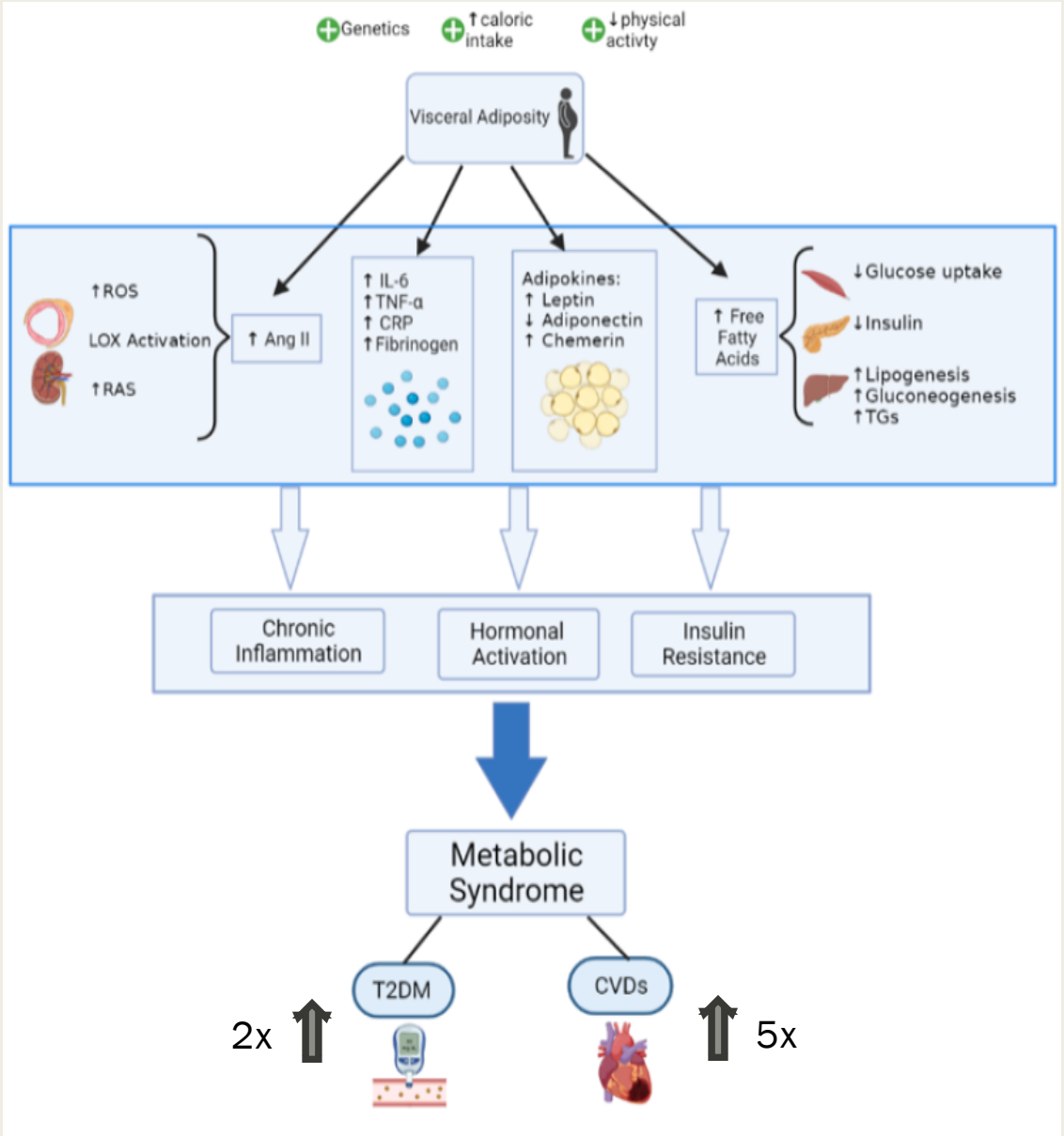
MULTİFAKTÖRYEL =

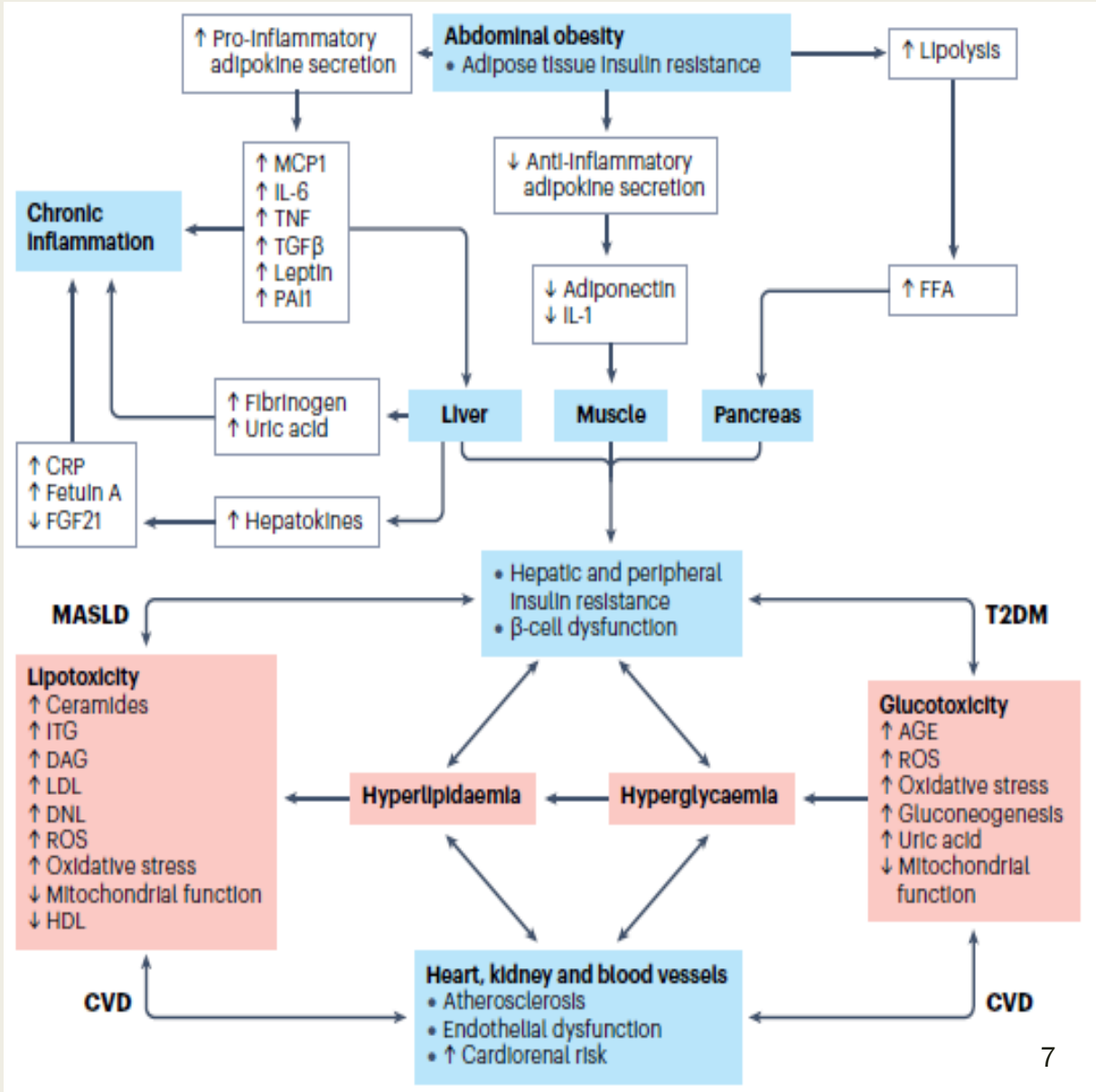


- Metabolik sendrom ve komponentlerinin kalıtsallık değerleri;

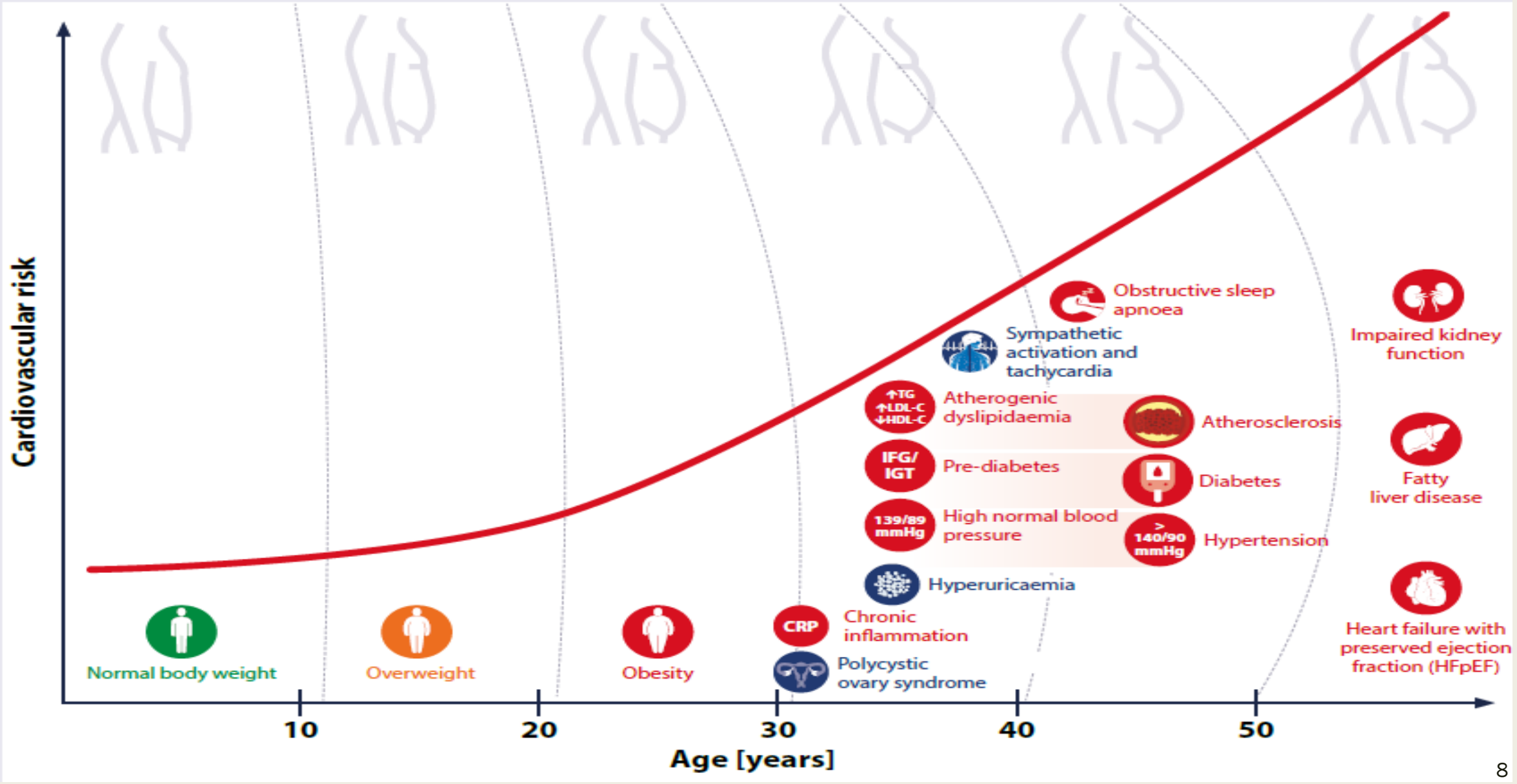
- HDL: %40-60
- Dislipidemi: %40-60
- Tip 2 DM: %30-70
- Hipertansiyon: %20-60
- MetS: %10-30

PATOFİZYOLOJİ





MetS gelişiminin zaman çizelgesi



PATOFİZYOLOJİNİN SONUÇLARI

İnsülin direnci ➡ Hiperglisemi

Abdominal obezite

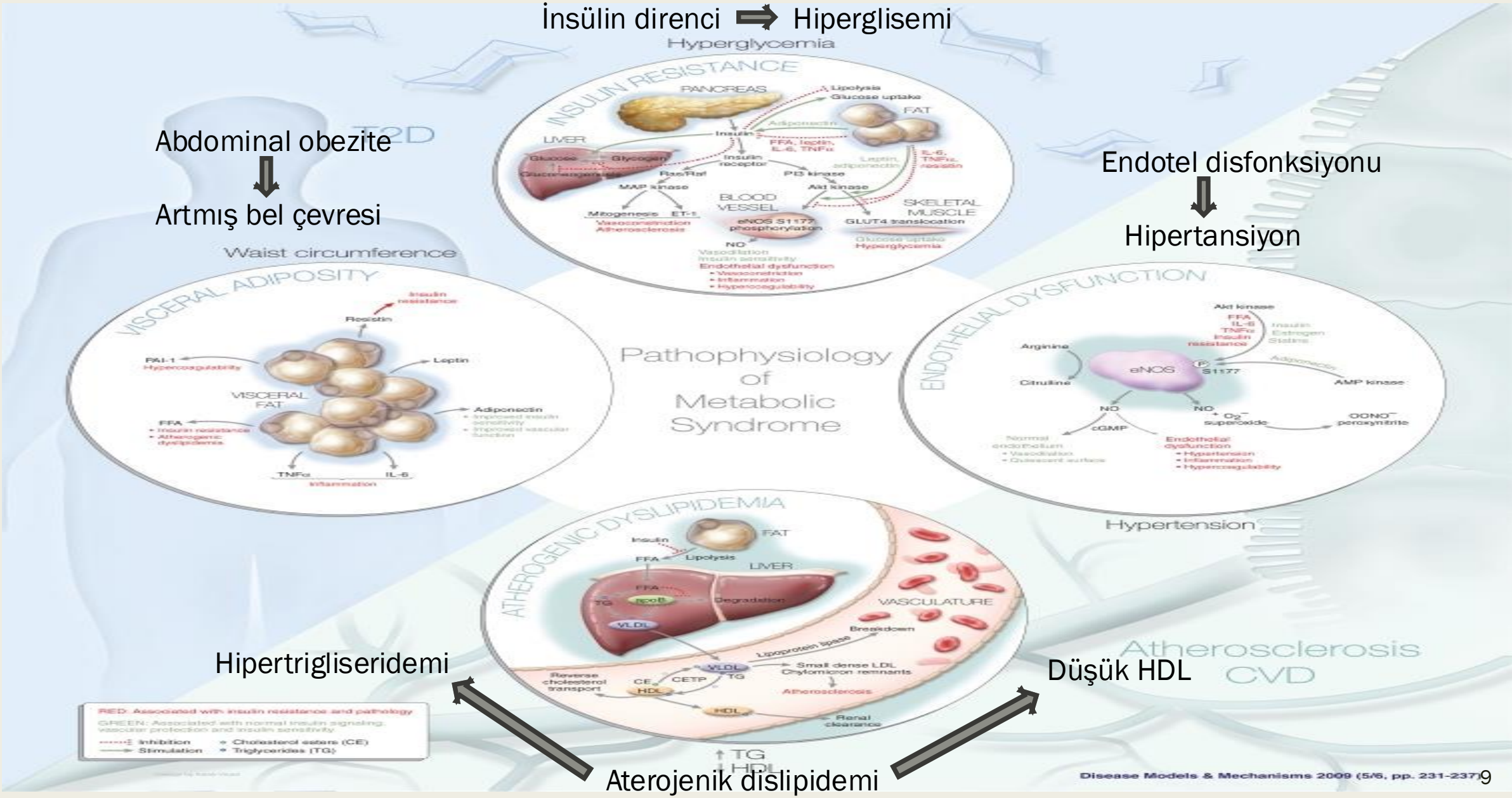
⬇

Artmış bel çevresi

Endotel disfonksiyonu

⬇

Hipertansiyon



Hipertrigliseridemi

Düşük HDL

Aterojenik dislipidemi

TANI KRİTERLERİ

Table 1 | Diagnostic criteria proposed for the clinical diagnosis of MetS by professional organizations

Organization (year)	MetS definition	Insulin resistance or hyperglycaemia	Adiposity	Dyslipidaemia	Elevated blood pressure	Other
WHO (1998)[5]	Insulin resistance plus any other two criteria	Impaired glucose regulation or diabetes mellitus, or lowered insulin sensitivity	Waist-to-hip ratio >0.90 in men, waist-to-hip ratio >0.85 in women and/or BMI >30 kg/m^2			
EGIR (1999)[6]	Insulin resistance plus any other two criteria	Plasma insulin >75th percentile, impaired glucose tolerance, or impaired fasting glucose	WC ≥94 cm in men or ≥80 cm in women			
ATP III (2001)[7]	Any three of five criteria	Fasting plasma glucose >110 mg/dl (6.11 mmol/l), which was modified in 2004 to >100 mg/dl (5.55 mmol/l), or diabetes mellitus	WC ≥102 cm in men or ≥88 cm in women			
AACE (2003)[138]	Insulin resistance plus any other two criteria	Impaired glucose tolerance or impaired fasting glucose (but not diabetes mellitus)	BMI ≥25 kg/m^2			
IDF (2005)[13]	Body weight plus any other two criteria	Fasting plasma glucose >100 mg/dl (5.55 mmol/l), diabetes mellitus	Increased WC (population-specific)			
AHA/NHLBI (2005)[15]	Any three of five criteria	Fasting plasma glucose >100 mg/dl (5.55 mmol/l) or on antihyperglycaemic therapy	WC ≥102 cm in men or ≥88 cm in women			
Joint Scientific Statement from IDF, NHLBI, AHA, WHF, IAS and IASO (2009)[10]	Any three of five criteria	Fasting plasma glucose >100 mg/dl (5.55 mmol/l) or on antihyperglycaemic therapy	Population-specific and country-specific definitions (see 'Other' cell)	TGs ≥150 mg/dl (1.69 mmol/l) or on lipid-lowering therapy, HDL-C <40 mg/dl (1.03 mmol/l) in men or <50 mg/dl (1.29 mmol/l) in women or on therapy	≥130/85 mmHg or on hypertension therapy	Recommended that the IDF cut points be used for people who are not of European origin and either the IDF or AHA/NHLBI cut points used for people of European origin until more data are available

AACE, American Association of Clinical Endocrinologists; AHA, American Heart Association; ATP III, National Cholesterol Education Program's Adult Treatment Panel III; EGIR, European Group for the Study of Insulin Resistance; HDL-C, HDL cholesterol; IAS, International Atherosclerosis Society; IASO, International Association for the Study of Obesity; IDF, International Diabetes Federation; MetS, the metabolic syndrome; NHLBI, National Heart, Lung, and Blood Institute; PCOS, polycystic ovary syndrome; TGs, triglycerides; WC, waist circumference; WHF, World Heart Federation; WHO, World Health Organization. Adapted with permission from ref. 11, Elsevier.

Practice Guideline > Circulation. 2009 Oct 20;120(16):1640-5.
doi: 10.1161/CIRCULATIONAHA.109.192644. Epub 2009 Oct 5.

Harmonizing the metabolic syndrome: a joint interim statement of the International Diabetes Federation Task Force on Epidemiology and Prevention; National Heart, Lung, and Blood Institute; American Heart Association; World Heart Federation; International Atherosclerosis Society; and International Association for the Study of Obesity

K G M M Alberti, Robert H Eckel, Scott M Grundy, Paul Z Zimmet, James I Cleeman, Karen A Donato, Jean-Charles Fruchart, W Philip T James, Catherine M Loria, Sidney C Smith Jr;
International Diabetes Federation Task Force on Epidemiology and Prevention;
National Heart, Lung, and Blood Institute; American Heart Association; World Heart Federation;
International Atherosclerosis Society; International Association for the Study of Obesity

PMID: 19805654 DOI: 10.1161/CIRCULATIONAHA.109.192644

Abstract

A cluster of risk factors for cardiovascular disease and type 2 diabetes mellitus, which occur together more often than by chance alone, have become known as the metabolic syndrome. The risk factors include raised blood pressure, dyslipidemia (raised triglycerides and lowered high-density lipoprotein cholesterol), raised fasting glucose, and central obesity. Various diagnostic criteria have been proposed by different organizations over the past decade. Most recently, these have come from the International Diabetes Federation and the American Heart Association/National Heart, Lung, and Blood Institute. The main difference concerns the measure for central obesity, with this being an obligatory component in the International Diabetes Federation definition, lower than in the American Heart Association/National Heart, Lung, and Blood Institute criteria, and ethnic specific. The present article represents the outcome of a meeting between several major organizations in an attempt to unify criteria. It was agreed that there should not be an obligatory component, but that waist measurement would continue to be a useful preliminary screening tool. Three abnormal findings out of 5 would qualify a person for the metabolic syndrome. A single set of cut points would be used for all components except waist circumference, for which further work is required. In the interim, national or regional cut points for waist circumference can be used.

ÜLKEMİZDEKİ TANI KRİTERLERİ – TEMD 2024

Tablo 2. Uluslararası Diyabet Federasyonu metabolik sendrom tanı kriterleri

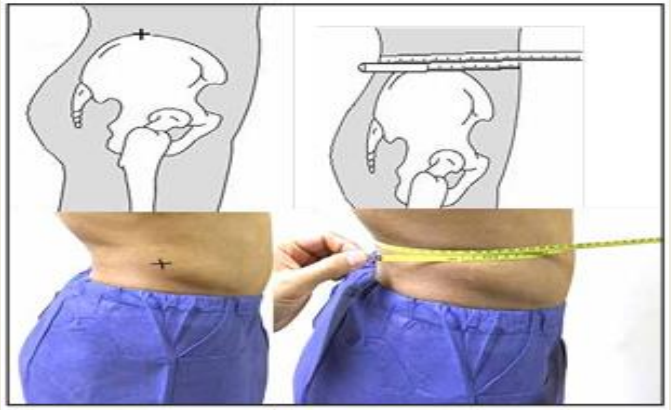
Parametre	Kriterler
Abdominal obezite	Bel çevresi erkeklerde ≥94 cm, kadınlarda ≥80 cm*
Plazma trigliserit düzeyi	≥150 mg/dl ya da TG yüksekliği için farmakolojik tedavi almak
Plazma HDL-kolesterol	Kadında <50 mg/dl, erkekte <40 mg/dl ya da düşük HDL-K nedeniyle farmakolojik tedavi almak
Kan basıncı	≥130/85 mmHg ya da antihipertansif tedavi almak
Açlık kan şekeri	≥100 mg/dl ya da kan şekeri yüksekliği için tedavi almak

Tanı için bel çevresi ve diğer kriterlerden en az iki tanesinin varlığı gerekir.
*Uluslararası Diyabet Federasyonu bel çevresi kesme noktaları için biliniyorsa ülkeye ait değerlerin kullanımını önermektedir. Ülkemiz için erkeklerde ≥100 cm ve kadınlarda ≥90 cm üzeri kesme noktaları santral obeziteyi gösterir.

Tablo 2. Türkiye ve diğer ülkelerde abdominal obeziteyi öngördüren bel çevresi değerleri

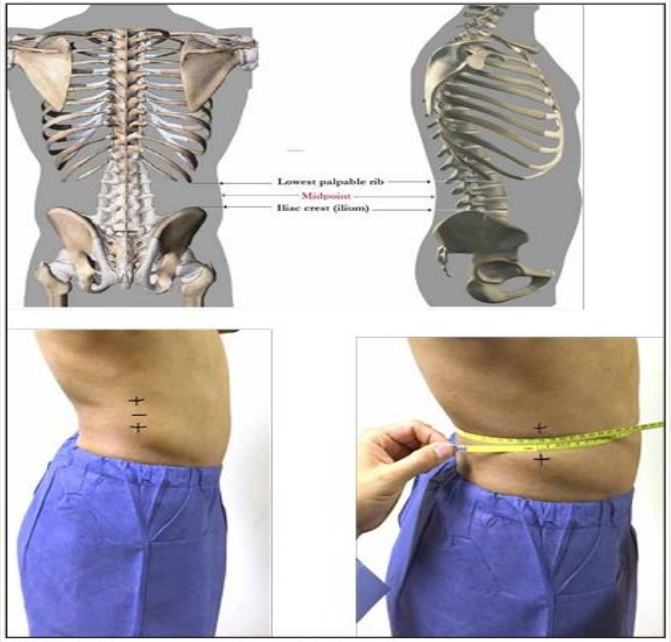
	Kadın (cm)	Erkek (cm)
Türkiye	≥90	≥100
ABD	≥88	≥102
Avrupa	≥80	≥94
Güney Asya ve Çin	≥80	≥90

Figure 3. National Heart, Lung, and Blood Institute waist circumference measurement at the iliac crest



SOURCE: NCHS, National Health and Nutrition Examination Survey, 2016.

Figure 9. World Health Organization waist circumference measurement



SOURCE: NCHS, National Health and Nutrition Examination Survey, 2016.

AFİŞ ve ÖNERİLER

OMİK

Table 7. Integration and Interoperability of Omics Data: Approaches, Tools, and Benefits.

Omics Type	Integration Approach	Interoperability Tools and Standards	Benefits	Limitations
Genomics	Cross-referencing genetic variants	VCF (Variant Call Format), dbSNP [109], Ensembl [110]	Identifies genetic variations and their effects	High data volume; interpretation of variants; privacy issues
Transcriptomics	Aligning RNA-seq data with genome	FASTQ, SAM/BAM, GTF/GFF, GEO (https://genome.ucsc.edu/ENCODE/, accessed on 1 June 2024)	Reveals gene expression patterns and alternative splicing	Data complexity; variability between samples
Proteomics	Correlating protein levels with gene expression	mzML [111], PRIDE [57], UniProt [112]	Understands protein abundance and functional roles	Sensitivity to sample preparation; high technical variability
Metabolomics	Linking metabolites to metabolic pathways	mzTab, HMDB [113], KEGG [114]	Provides insights into cellular metabolism and pathway activities	Complex data integration; diverse chemical properties
Epigenomics	Mapping epigenetic modifications	BED, WIG, GEO, ENCODE (https://genome.ucsc.edu/ENCODE/, accessed on 1 June 2024)	Studies DNA methylation, histone modifications and chromatin accessibility	High data complexity; dynamic nature of epigenetic changes
Lipidomics	Profiling lipid species	LIPID MAPS [115], mzXML [111]	Explores lipid composition and its role in cell biology	Heterogeneity of lipids; difficulty in quantifying low-abundance lipids
Glycomics	Characterizing glycan structures	GlyTouCan [116], UniCarb-DB [117]	Analyzes glycan functions and interactions	Structural complexity of glycans; limited analytical standards
Microbiomics	Integrating microbiome with host data	QIIME [118], MG-RAST [119]	Examines microbial communities and their impact on host health	Variability in sample preparation; complex data interpretation

Metabolomik

- **Metabolitler;** oligonükleotidler, şekerler, peptidler, nükleozidler, organik asitler, ketonlar, aldehitler, aminler, amino asitler, lipidler, steroidler, alkaloidler ve ilaçlar gibi kimyasal bileşiklerdir.
- Ne kimyasal olarak ne de fiziksel olarak birbirleriyle ilişkileri yoktur.
- Molekül ağırlıkları genellikle <1500 Da (<1700 Da)

- 2005 yılında İnsan Metabolom Projesi [Human Metabolome Project (HMP)]

1. Hastalıkların tanımlanması, teşhisi ve tedavisi ile tedaviye yanıt sürecini incelemede metabolomla hastalık arasında metabolik yolaklar üzerinden ilişki kurulması

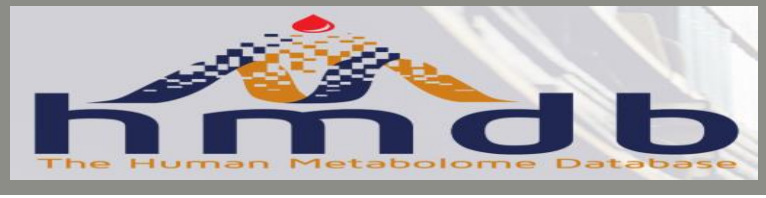
2. İlaç metabolizması ve toksikolojisinin değerlendirilmesi

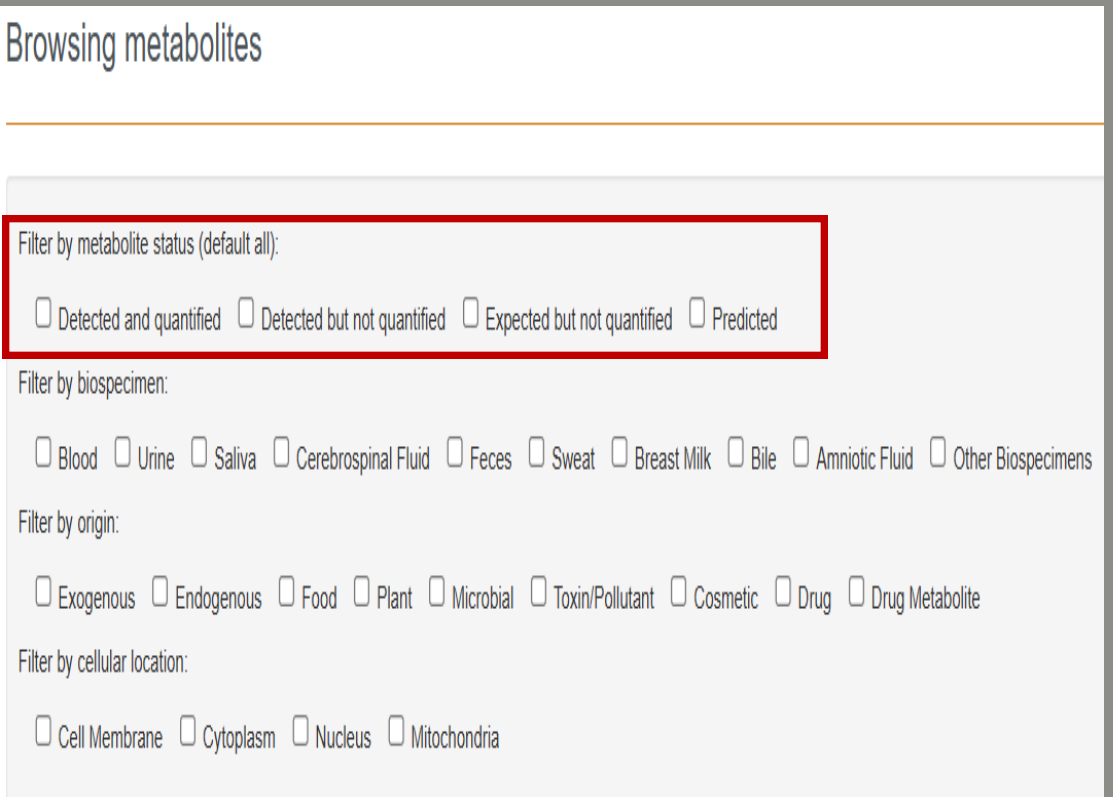
3. İnsan metabolizması ve insan genomu arasında bir bağlantı oluşturulması

4. Metabolomik çalışmalar için bir yazılım geliştirilmesi

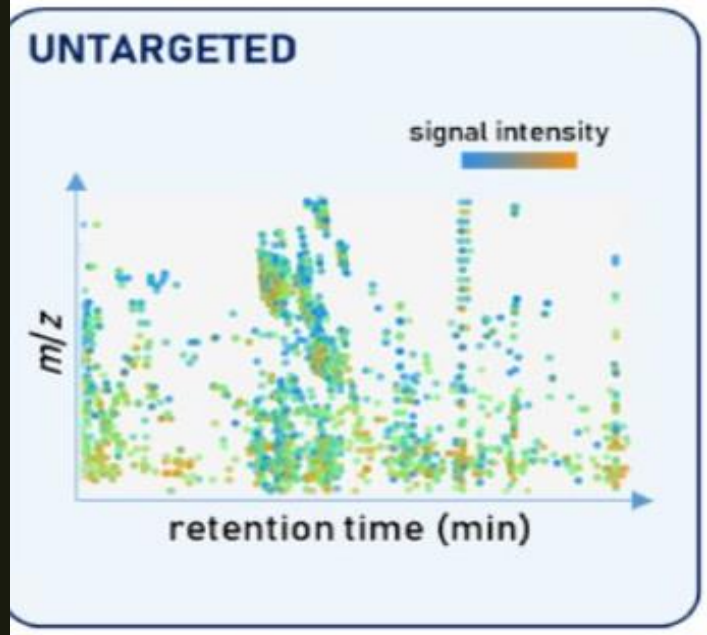
GÜNCEL DURUM

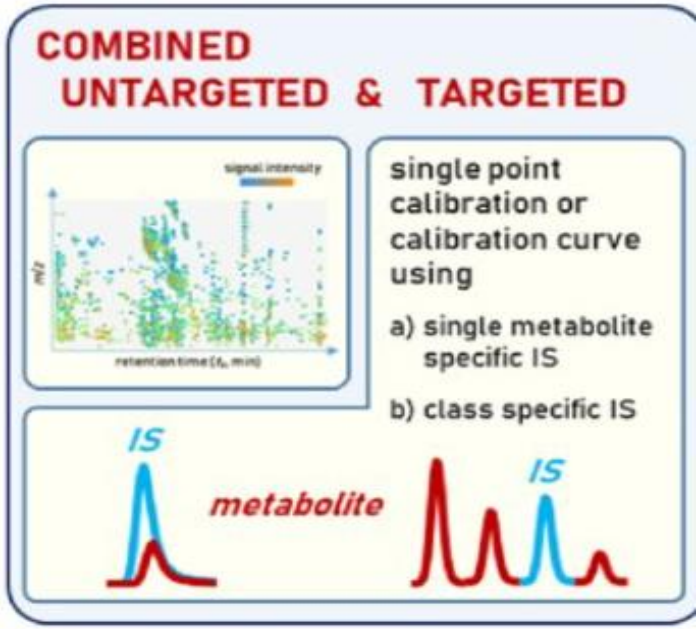
- ~ 248,136 metabolit
- ~ 132,335 insan metabolizma, ilaç ve hastalıklara ait yolak

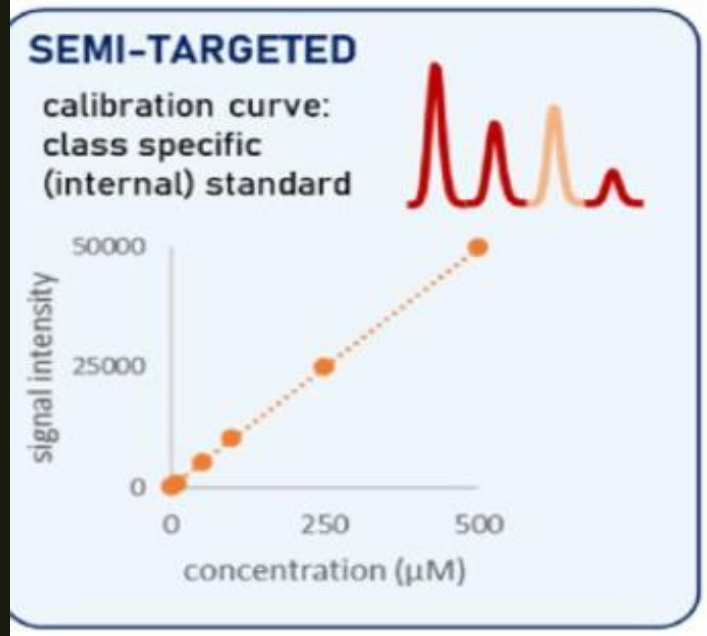


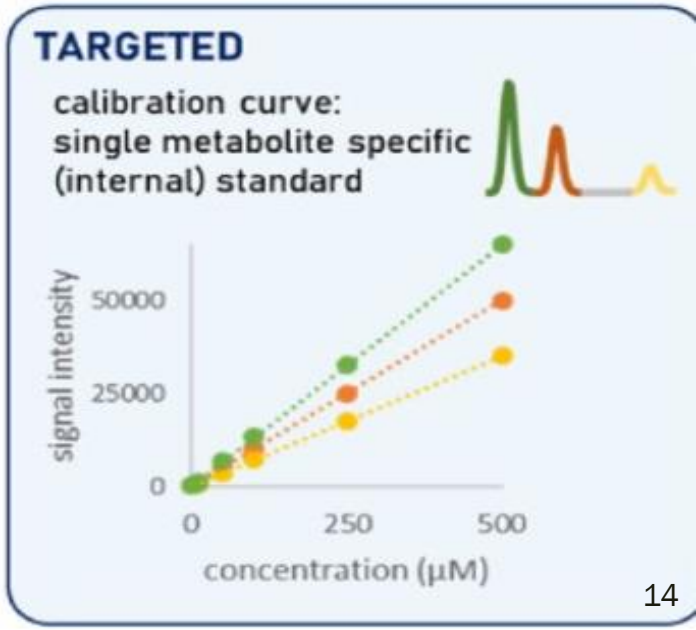


METABOLOMİK ÇALIŞMALAR

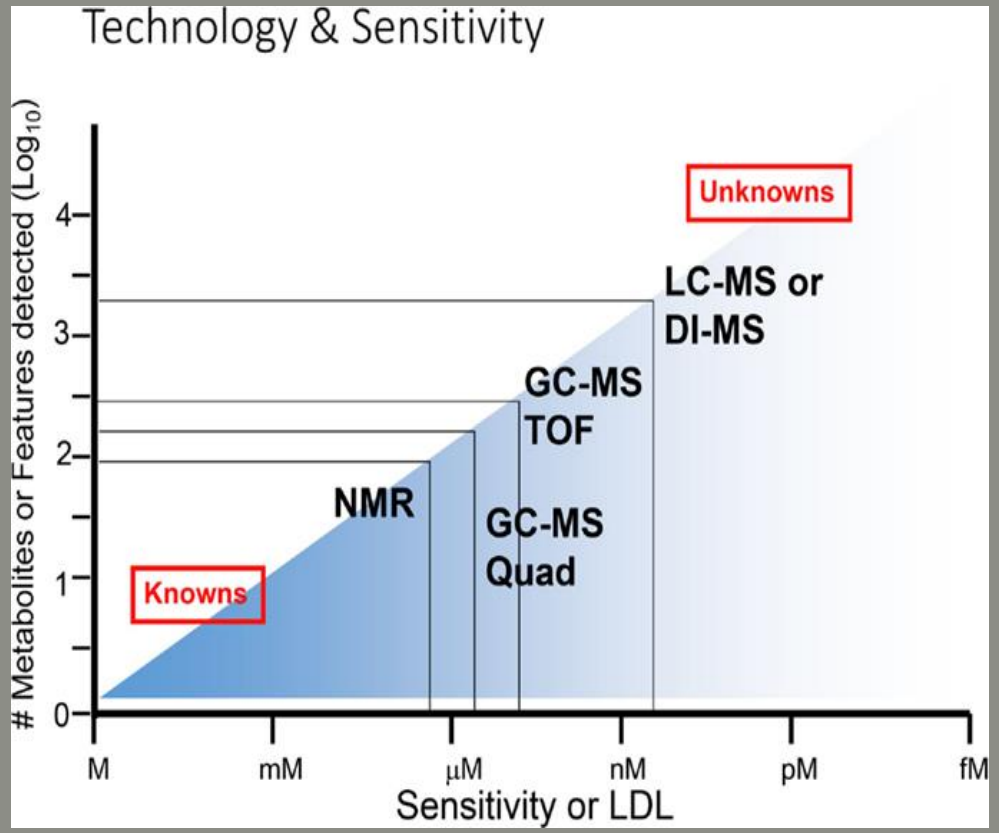








METABOLOMİK / LİPİDOMİK ANALİZLER



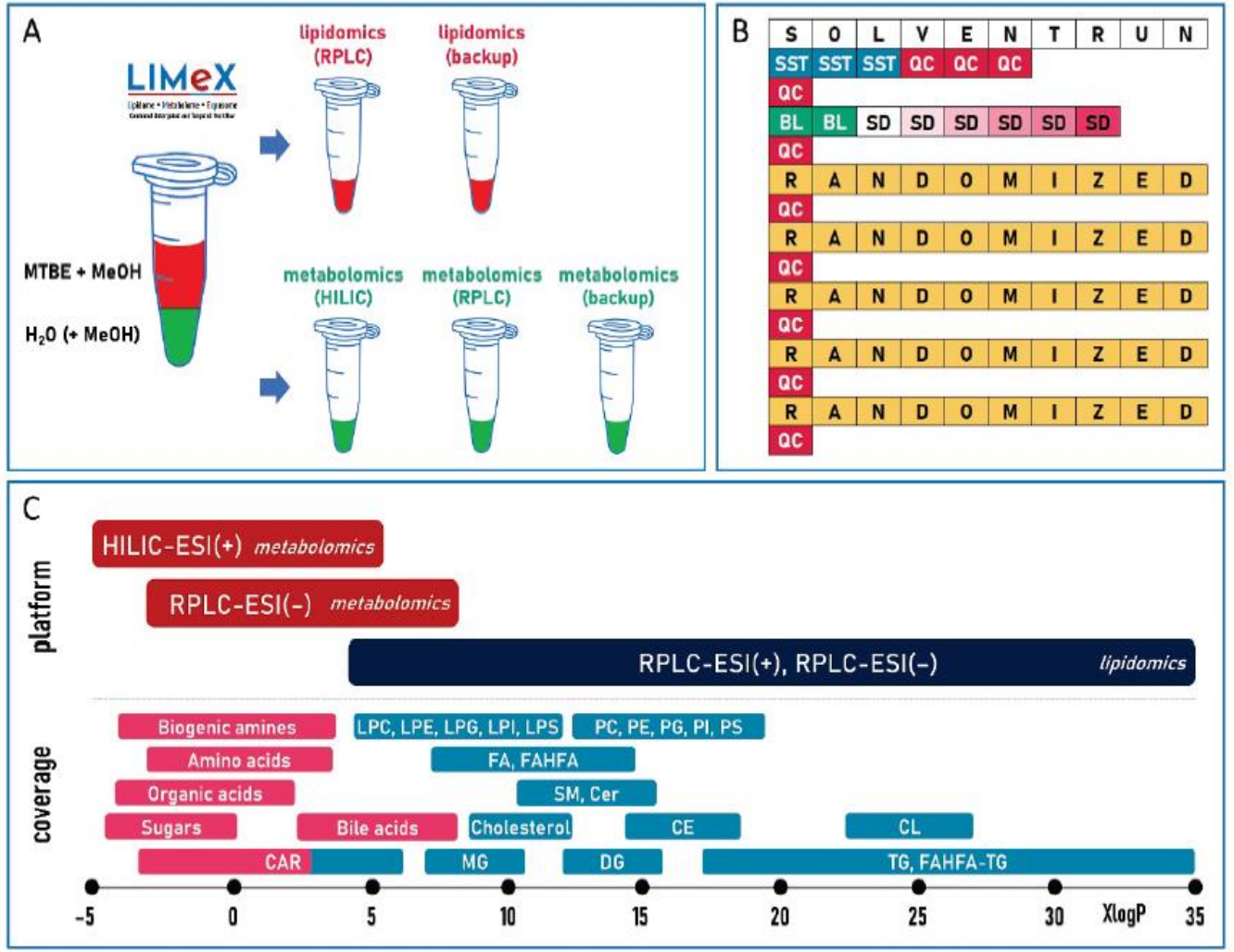
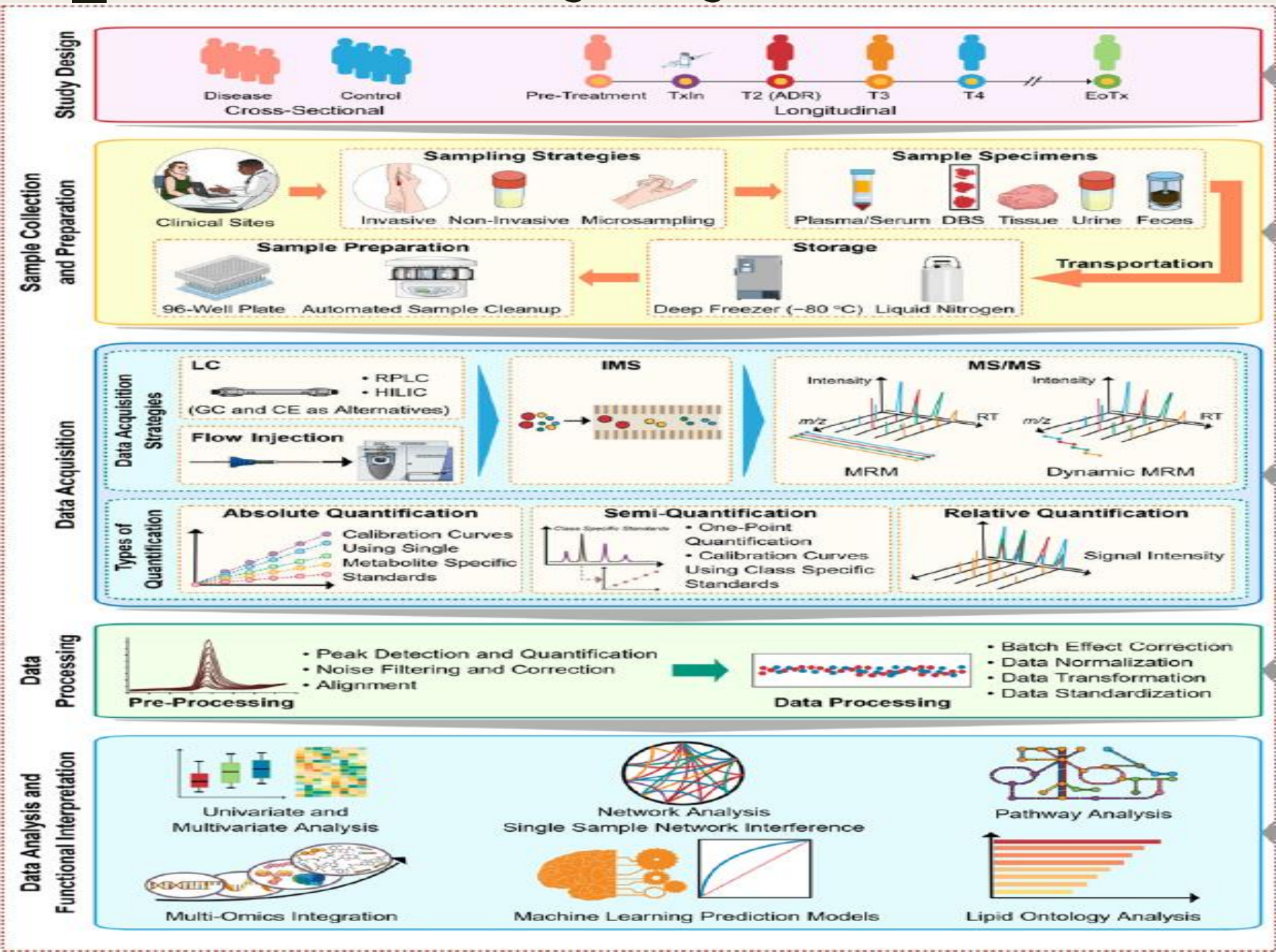


Fig. 2. (**A**) Example of sample extraction using MTBE, methanol, and water [41], leading to two phases for subsequent metabolomics and lipidomics platforms. (**B**) Example of a typical LC-MS sequence during metabolomics and lipidomic analysis, consisting of solvent injection for general platform equilibration, followed by a system suitability test (SST), platform equilibration using pooled QC samples, analysis of method blanks (BL), a diluted series of QC samples (SD), randomized study samples with regular QC sample injections after every 10 study samples. (**C**) Example of different LC-MS platforms [41,42] for metabolomic and lipidomic analysis in relation to the XlogP (predicted octanol/water partition coefficient) range of subgroups of polar metabolites and complex lipids.

ÇALIŞMA PROSEDÜRÜ



QA and Consideration

- Control Selection
- Sample Size
- Systemic Bias Removal

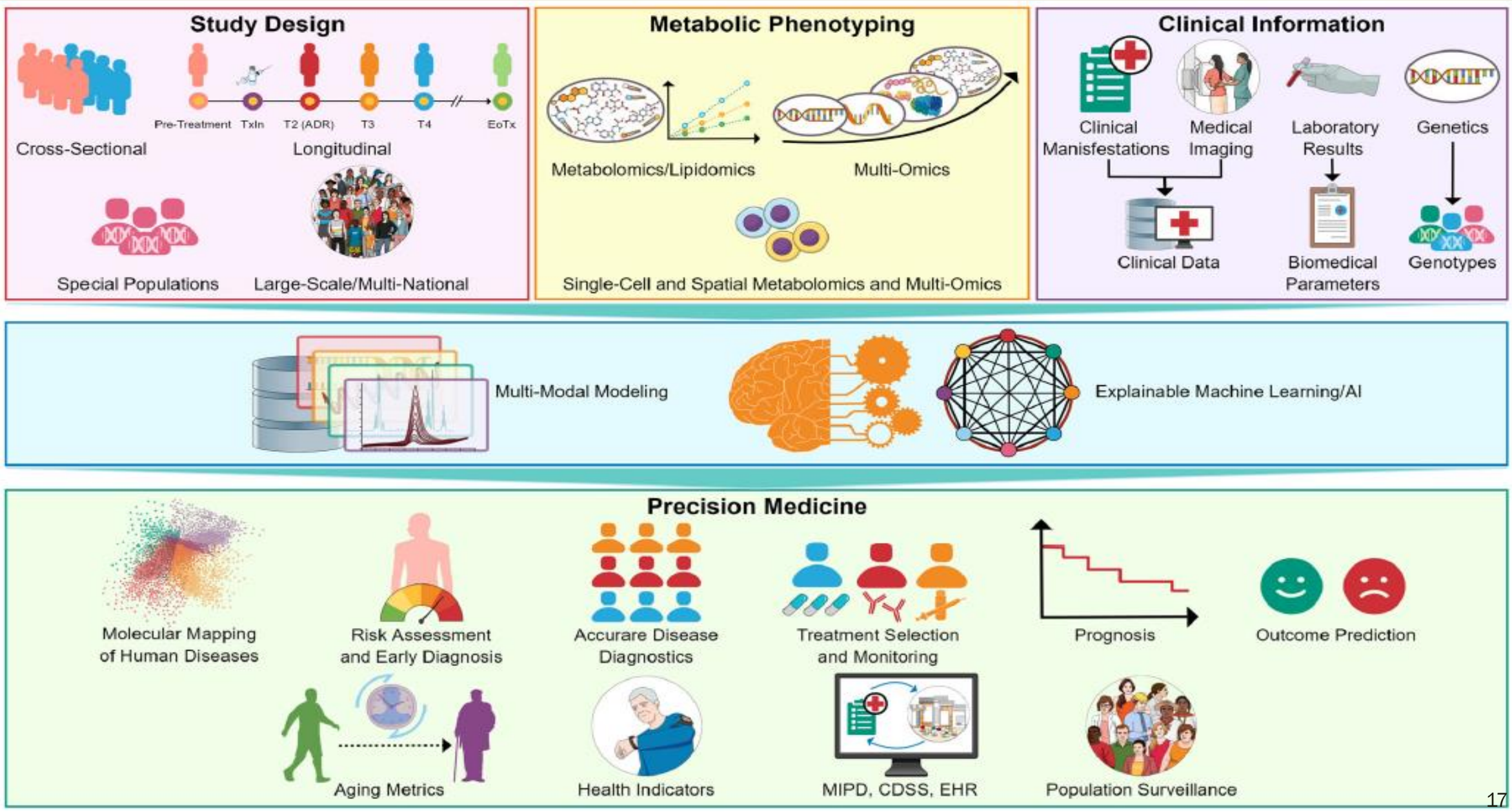
- Standardized Protocols
- Inclusion of QC Samples
- Inclusion of Reference Materials
- Standardized Biobanks

- System Suitability Test
- Routine Maintenance of Analytical Instruments
- Disease- and Sample-Specific Quantitative Assays

- Data Quality Control and Harmonization
- Standardization of Data Processing Workflow

- Standardized Computational Workflow
- Data Sharing with FAIR Principles
- Domain Expertise for Accurate Interpretation

OMİKLERİN HASSAS TIPA POTANSİYEL ENTEGRASYONU



› Methods Mol Biol. 2018:1730:3-28. doi: 10.1007/978-1-4939-7592-1_1.

Metabolomics as a Tool to Understand Pathophysiological Processes

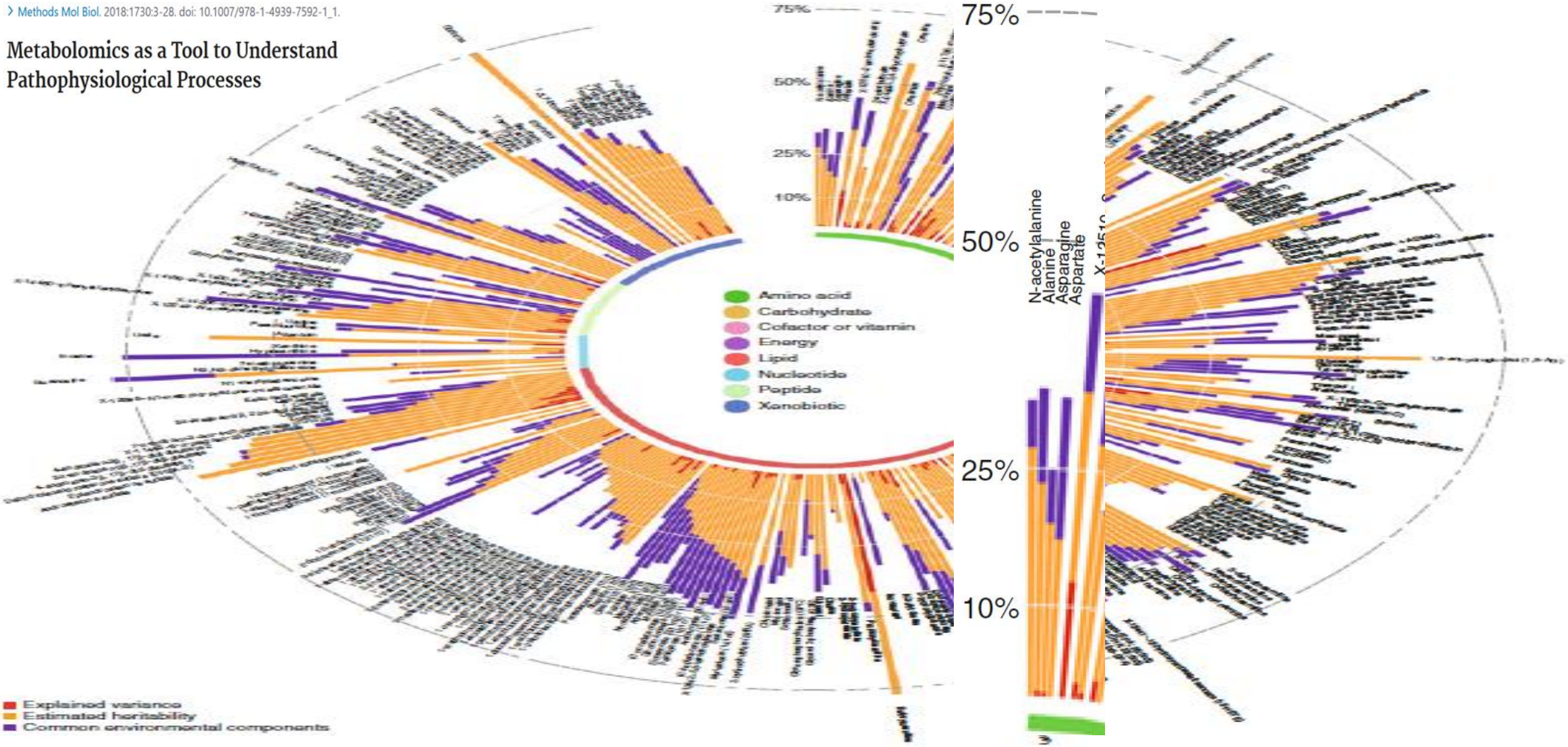
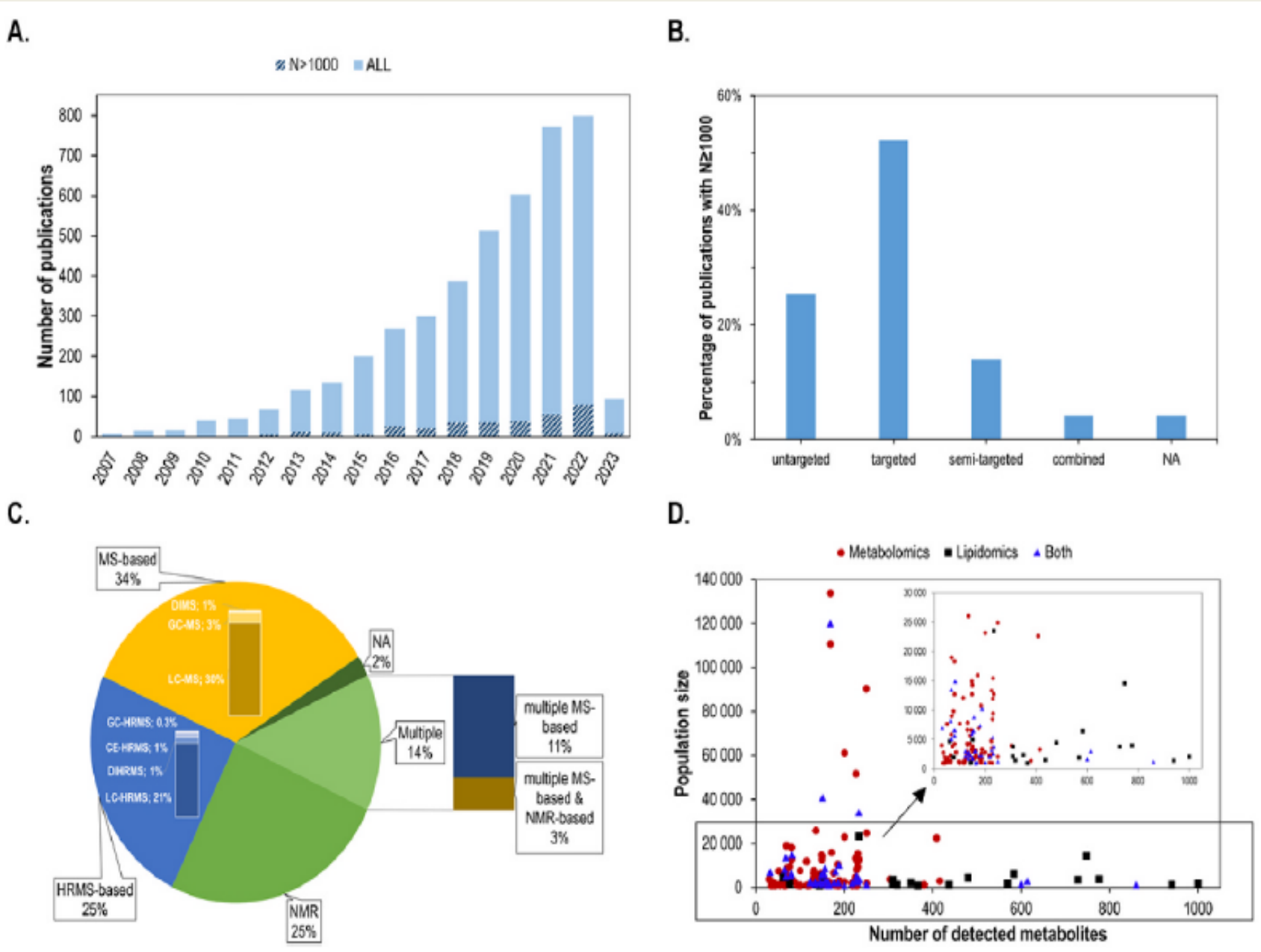


Fig. 3 Map of associations between the single-nucleotide polymorphism (SNP) and metabolite levels in blood. The contribution of genetic vs. environmental factors to metabolite level variance was estimated on the basis of GWAS study results. The proportion of heritability explained by all SNPs associated with a given metabolite at the genome-wide level is shown in red. *Figure was reproduced from Shin et al. Nature genetics 2014 with the permission for re-use from Nature publishing group* [116]

METABOLOMİK ÇALIŞMALARININ DURUMU



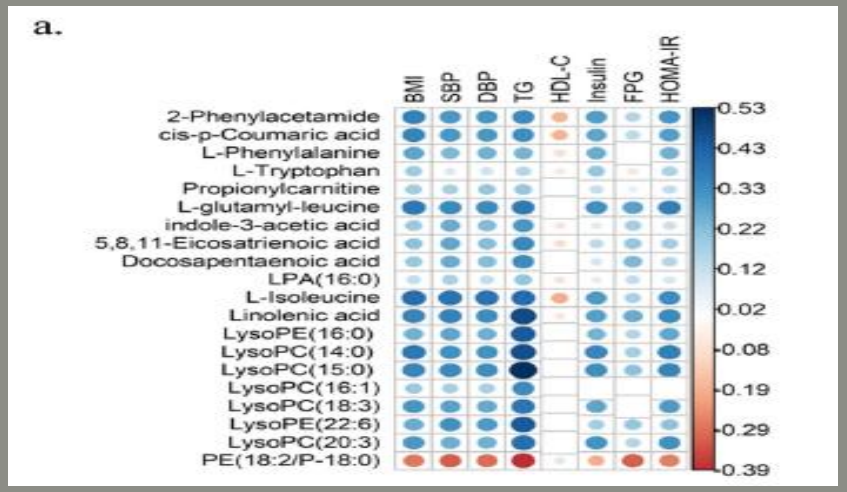
TrAC Trends in Analytical Chemistry
Volume 167, October 2023, 117225

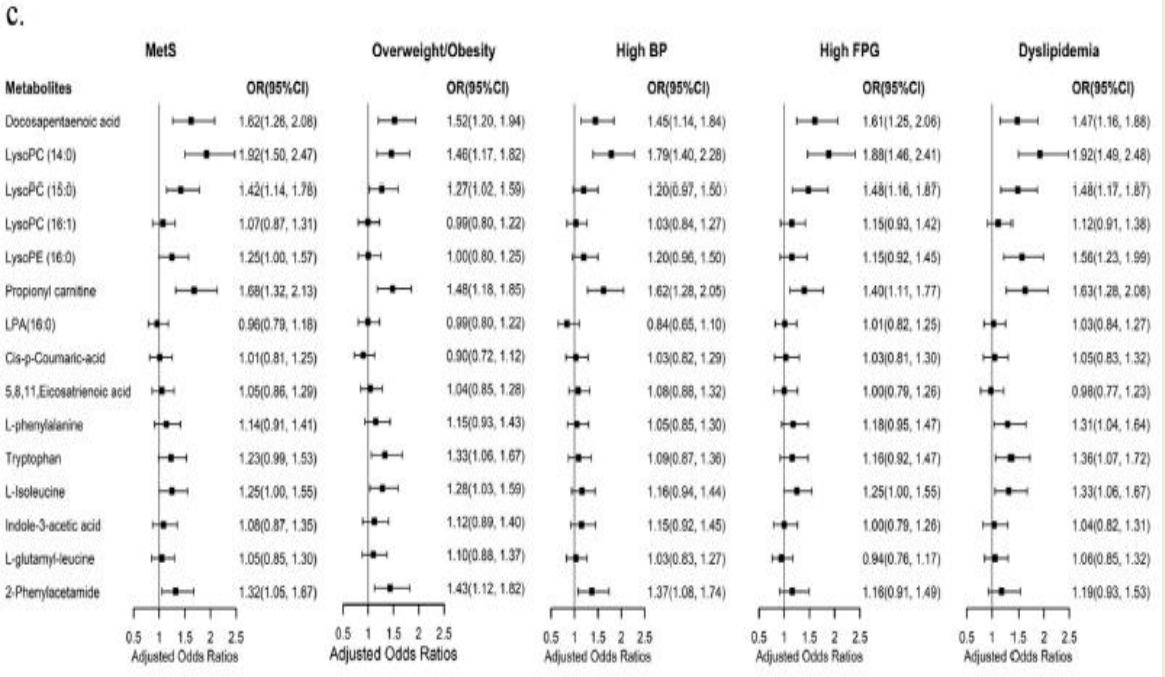
Scaling-up metabolomics: Current state and perspectives

Fig. 1. **A.** Evolution of publication number, including metabolomics analyses of human cohorts (N = 4385), of which are studies involving over 1000 individuals (N = 335). **B.** Distribution of metabolomics approaches among studies involving over 1000 individuals. **C.** Distribution of analytical platforms used in metabolomics/lipidomics studies involving over 1000 individuals. NA indicates that information was not available in the paper. 'Combined' approach refers to studies that use more than one approach, for example targeted and untargeted methods. **D.** Number of detected metabolites in terms of population size analysed by targeted either metabolomics, lipidomics or both (N = 157).

EBioMedicine. 2021 Dec:74:103707. doi: 10.1016/j.ebiom.2021.103707. Epub 2021 Nov 18.

Multi-stage metabolomics and genetic analyses identified metabolite biomarkers of metabolic syndrome and their genetic determinants





Cardiovasc Diabetol. 2023 Jun 16;22(1):141. doi: 10.1186/s12933-023-01862-z.

Identification of candidate metabolite biomarkers for metabolic syndrome and its five components in population-based human cohorts

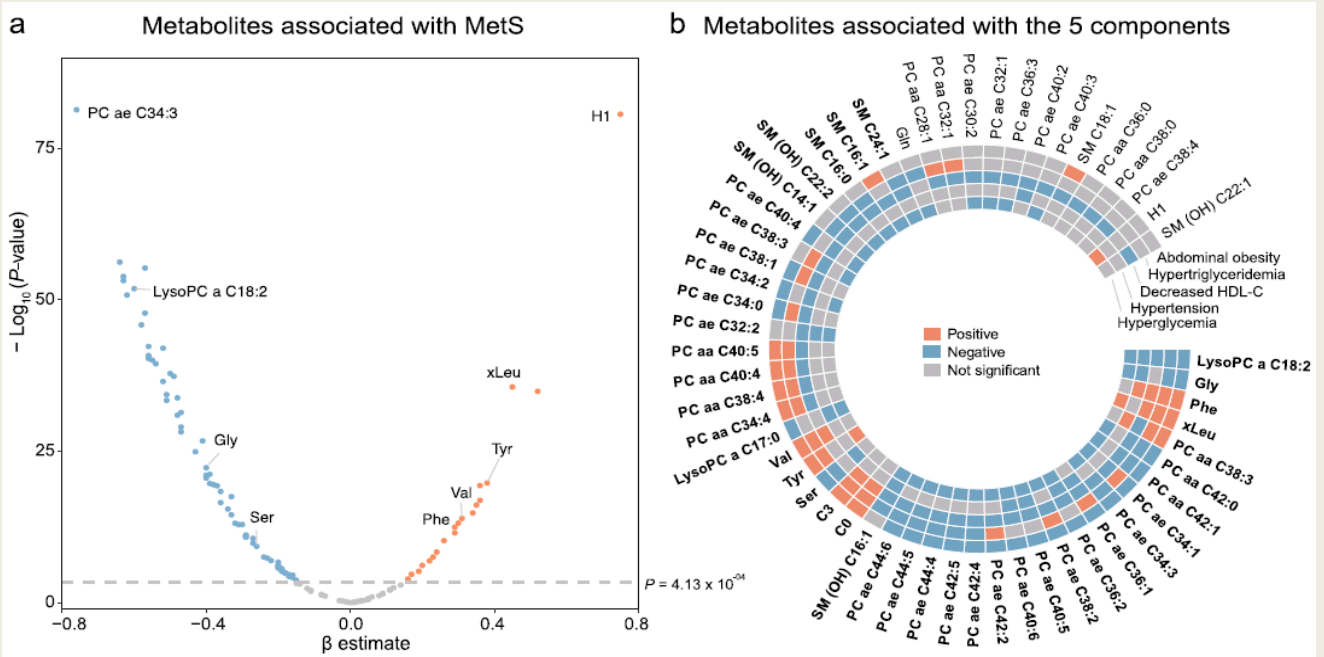
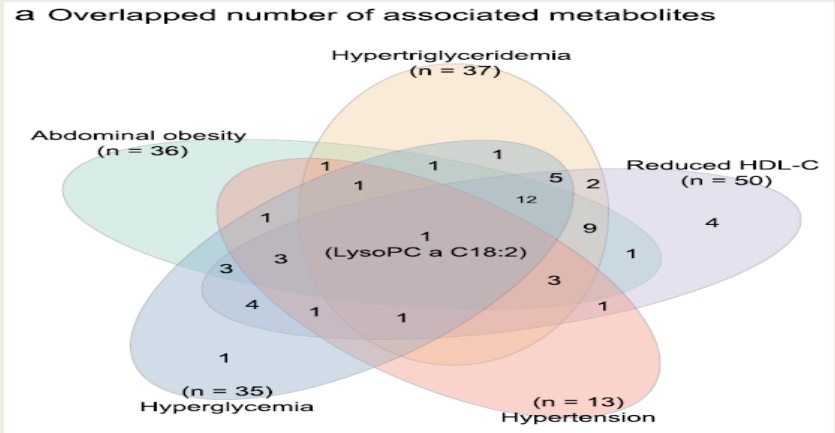


Fig. 2 The metabolites associated with MetS and its five components. **a** Volcano plot of regression results of 121 metabolites. The horizontal dashed lines represent the Bonferroni cut-off value. Orange dots: positively associated, blue dots: negatively associated, gray dots: not significant. **b** Circle plot of the association between 56 replicated MetS-associated metabolites and 5 components of MetS. Metabolites with bold font indicate significant association with three or more components



Sci Rep. 2020 Jan 20;10(1):669. doi: 10.1038/s41598-019-56909-7.

Metabolomic and Lipidomic Signatures of Metabolic Syndrome and its Physiological Components in Adults: A Systematic Review

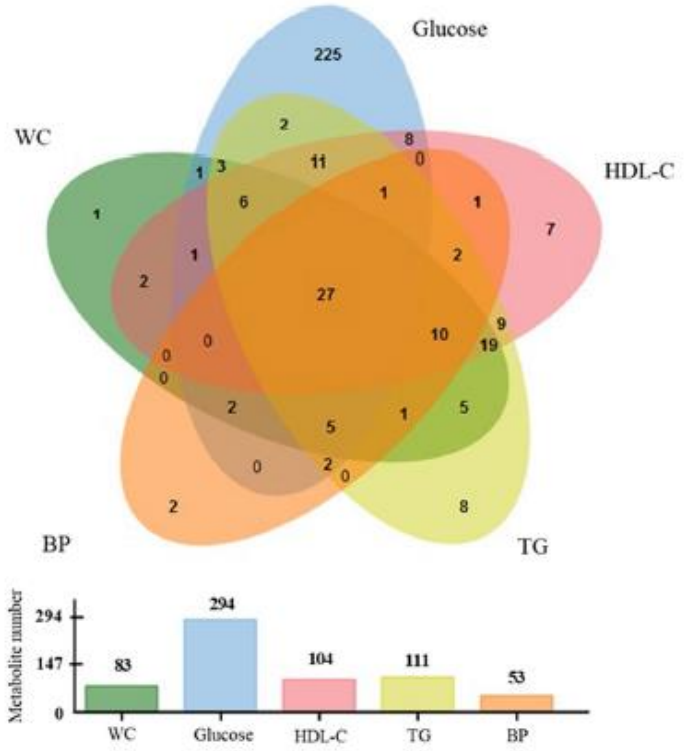
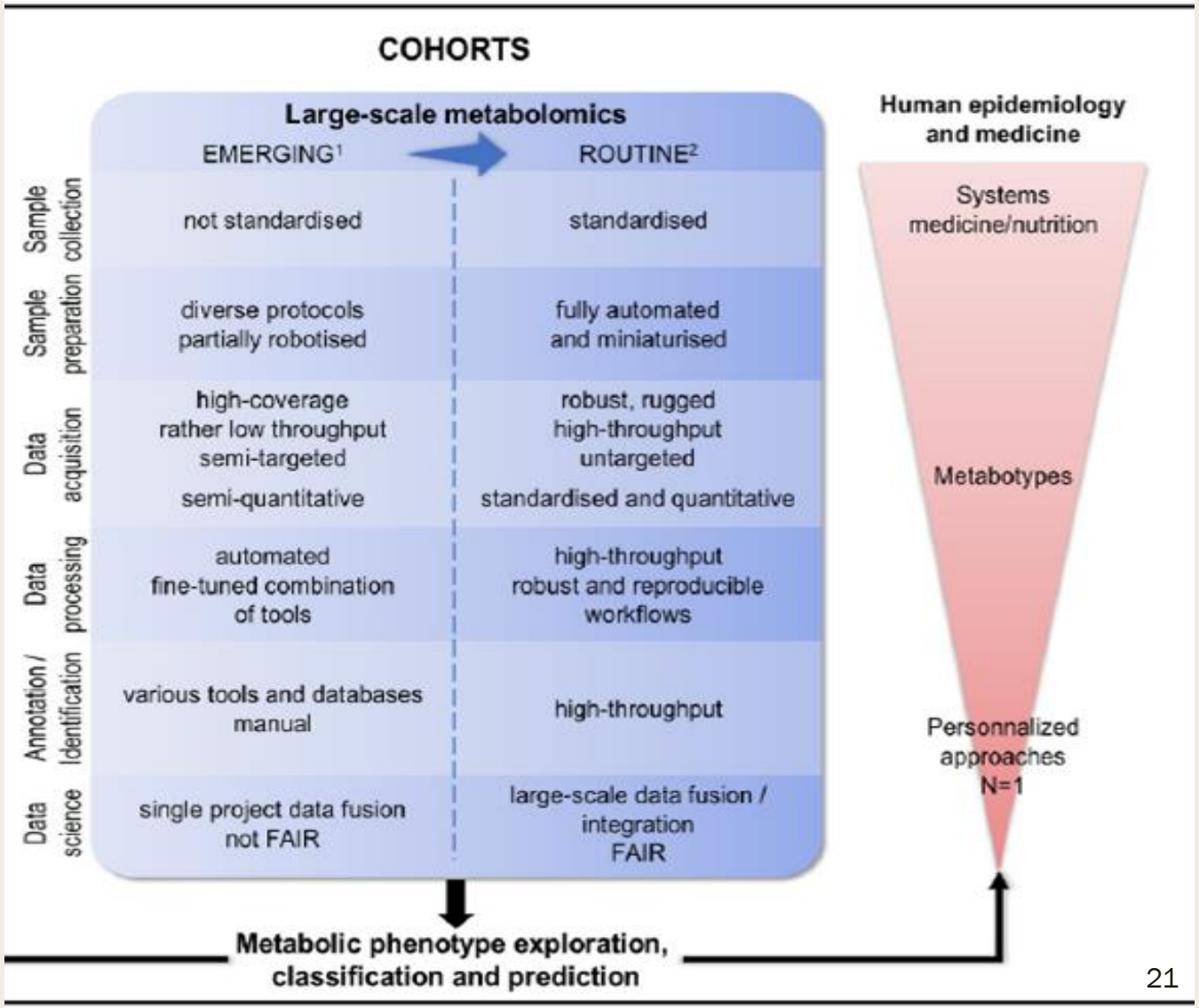


Figure 2. Venn diagram showing the number of metabolites significantly correlated with MetS components, together with respective histogram representing the number of significant metabolites for each clinical MetS components. WC = waist circumference; BP = blood pressure; TG = triglycerides; HDL-C = high-density lipoprotein cholesterol.

TrAC Trends in Analytical Chemistry
Volume 167, October 2023, 117225

Scaling-up metabolomics: Current state and perspectives



Yazılım ve Analiz Programları

proteowizard

XCMS

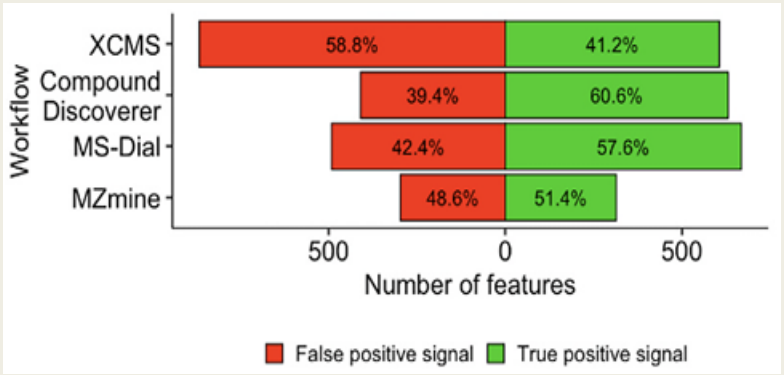
OPENMS

MZmine 3

MS-DIAL

MetaboAnalyst R

COMPOUND DISCOVERER



❖1. Lipid oriented databases
- LIPID MAPS® Structure Database
- LIPID MAPS® Computationally-generated Bulk Lipids
- LIPID MAPS® Lipidomics Ion Mobility Database
- LIPID MAPS® In-Silico Structure Database
- SwissLipids Knowlegebase

❖2. Lipidomics data repositories
- Metabolomics Workbench
- MetaboLights

❖3. Analysis of targeted lipidomics datasets
- LipidCreator
- METLIN-MRM/XCMS-MRM

❖4. Lipid identification from untargeted lipidomics datasets

❑4.1 Full MS (HRAM LC-MS)
- Lipid Data Analyzer (LDA)
- LipidFinder
- MS-DIAL
- XCMS Online

❑4.2 Data dependent acquisition (DDA)
- Lipid Data Analyzer (LDA)
- LipidHunter2
- LipidXplorer
- Lipostar 2.0
- MS-DIAL
- MZmine

❑4.3 Data independent acquisition (DIA)
- Lipostar 2.0
- MS-DIAL

❑4.4 Tools considering ion mobility separation
- Lipostar 2.0
- MS-DIAL

❑4.5 Identification of oxidized lipids
- Lipid Data Analyzer (LDA)
- Lipostar 2.0
- LPPtiger
- MS-DIAL

❖5. Lipid quantification from untargeted lipidomics datasets
- Lipid Data Analyzer (LDA)
- Lipostar 2.0
- MS-DIAL
- MZmine
- XCMS Online

❖6. Analysis and visualization of lipidomics data
- Lipid Data Analyzer (LDA)
- LIPID MAPS Statistical Analysis Tools
- Lipostar 2.0
- MetaboAnalyst 5.0
- MS-DIAL
- MZmine
- XCMS Online

❖7. Data integration solutions

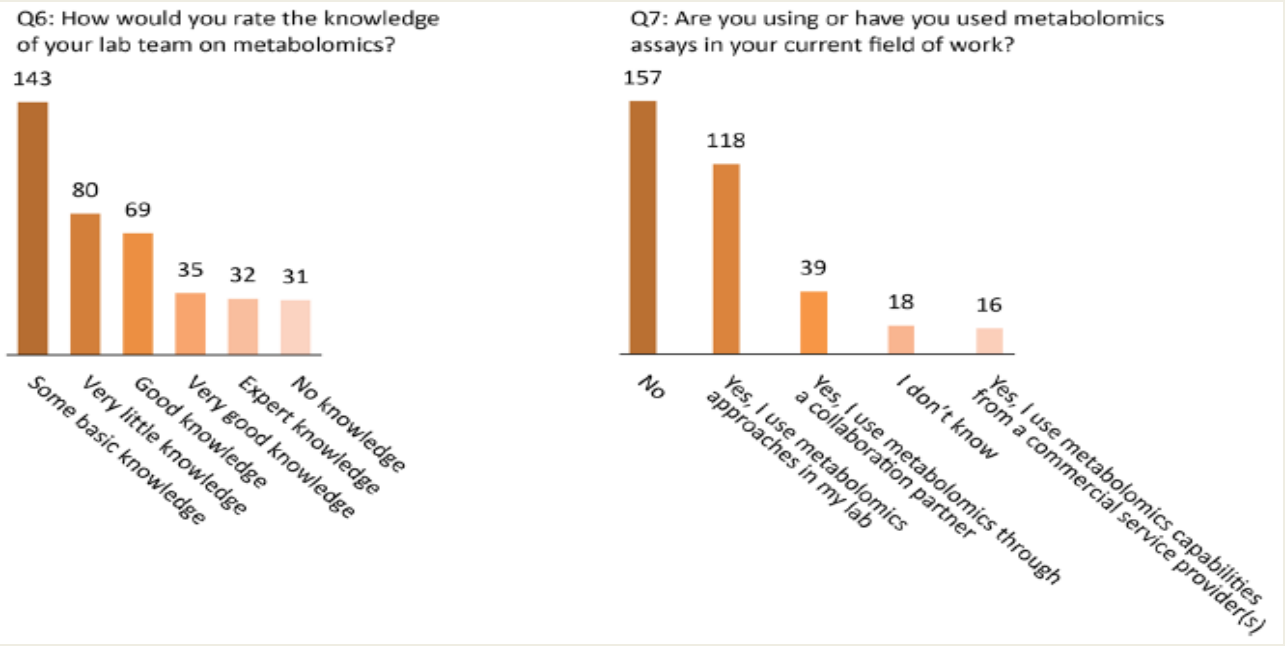
❑7.1 Lipid annotations and ID converters
- BridgeDb
- Goslin
- LipidLynxX
- RefMet

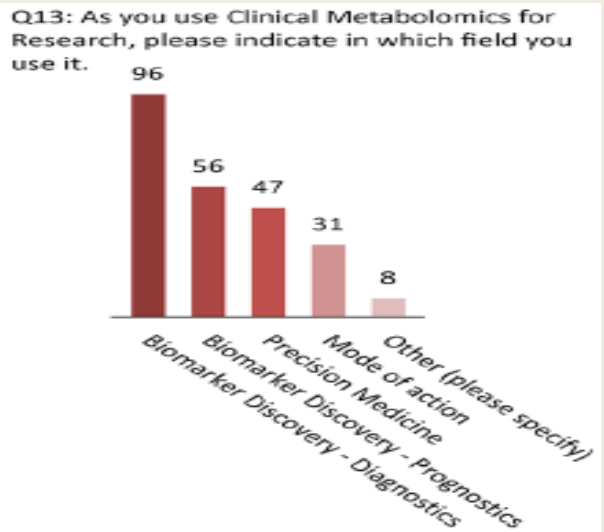
❑7.2 Lipid ontology enrichment analysis
- LION web
- Lipid Mini-On

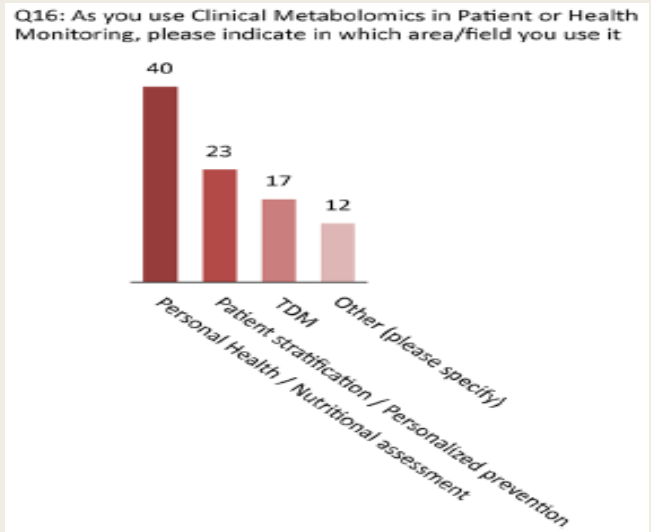
❑7.3 Pathway and network solutions
- BioPAN
- Lipostar 2.0
- WikiPathways (Lipid portal)

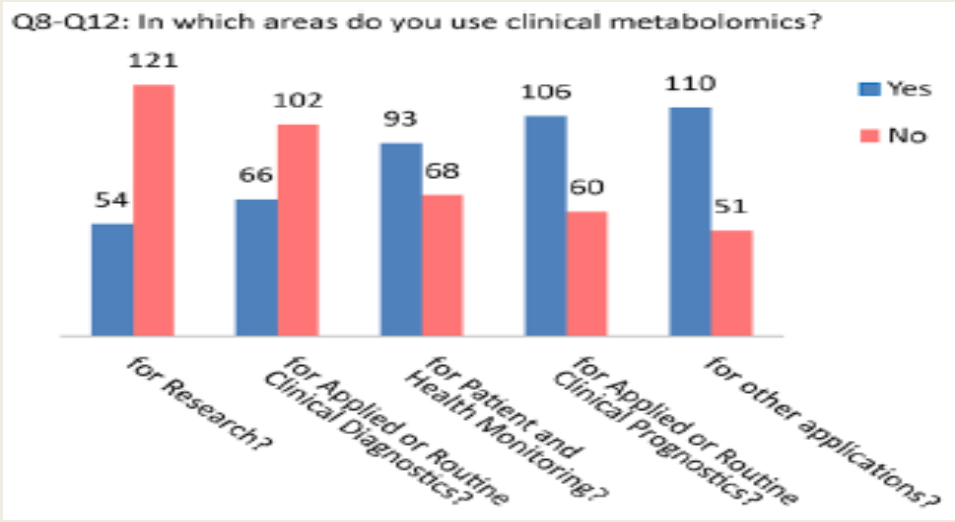
> Clin Chem Lab Med. 2024 Jun 26;62(10):1950-1961. doi: 10.1515/cclm-2024-0550. Print 2024 Sep 25.

A global perspective on the status of clinical metabolomics in laboratory medicine – a survey by the IFCC metabolomics working group







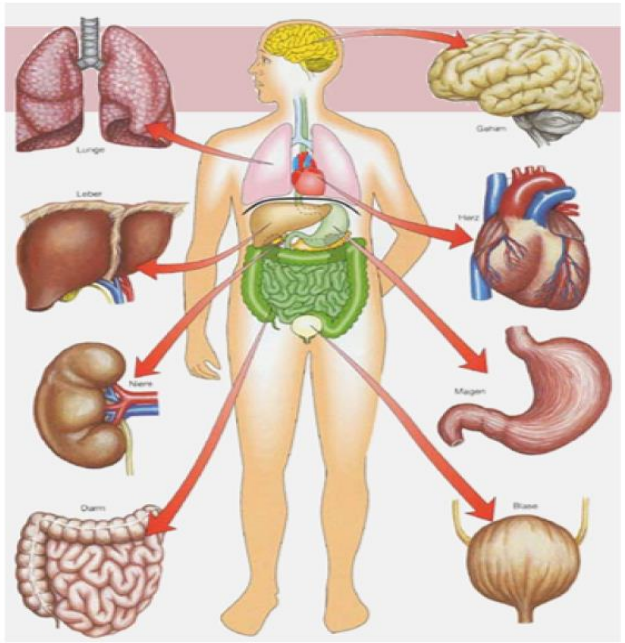


SONUÇLAR

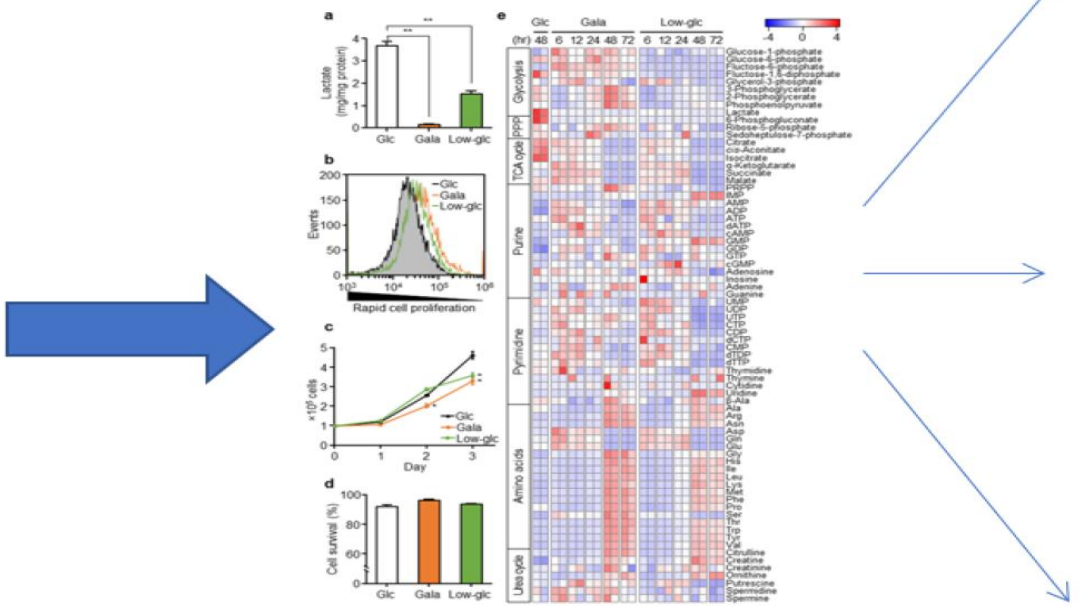
- İlgi ve halihazırda metabolomik faaliyetlerde bulunan katılımcıların yüksek sayısı karşısında olumlu yönde şaşırmışlardır.
- Anketin başında metabolomiklere dair bir tanım sunulmuş olsa da; metabolomiklerin başladığı ve klasik klinik biyokimya panellerinin sona erdiği sınır net olarak tanımlanmamıştır. Bu durum, metabolomikleri rutin testler olarak kullandığını bildiren katılımcı sayısının yüksek olmasını açıklayabilir.

KAYNAKLAR

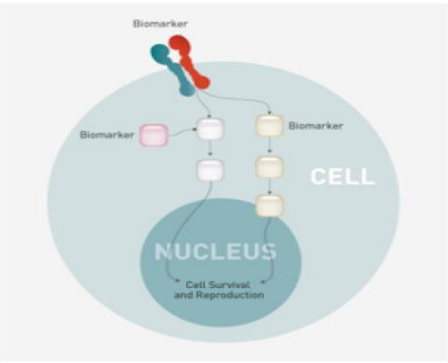
1. Swarup S, Ahmed I, Grigorova Y, et al. Metabolic Syndrome. [Updated 2024 Mar 7]. In: StatPearls [Internet]. Treasure Island (FL): StatPearls Publishing; 2025 Jan-. Available from: https://www.ncbi.nlm.nih.gov/books/NBK459248/
2. Abacı, A., Kılıçkap, M., Göksülük, H., Karaaslan, D., Barçın, C., Kayıkçıoğlu, M., Özer, N., Yılmaz, M. B., Şahin, M., & Tokgözoğlu, L. (2018). Türkiye'de metabolik sendrom sıklığı verileri: Kardiyovasküler risk faktörlerine yönelik epidemiyolojik çalışmaların sistematik derleme, meta-analiz ve meta-regresyonu. Turk Kardiyol Dern Ars, 46(7), 591-601. https://doi.org/10.5543/tkda.2018.00878.
3. Reisinger C, Nkeh-Chungag BN, Fredriksen PM, Goswami N. The prevalence of pediatric metabolic syndrome-a critical look on the discrepancies between definitions and its clinical importance. Int J Obes (Lond). 2021 Jan;45(1):12-24. doi: 10.1038/s41366-020-00713-1. Epub 2020 Nov 18.
4. Fahed G, Aoun L, Bou Zerdan M, Allam S, Bou Zerdan M, Bouferraa Y, Assi HI. Metabolic Syndrome: Updates on Pathophysiology and Management in 2021. Int J Mol Sci. 2022 Jan 12;23(2):786. doi: 10.3390/ijms23020786.
5. Neeland, I.J., Lim, S., Tchernof, A. et al. Metabolic syndrome. Nat Rev Dis Primers 10, 77 (2024). https://doi.org/10.1038/s41572-024-00563-5
6. Huang PL. A comprehensive definition for metabolic syndrome. Dis Model Mech. 2009 May-Jun;2(5-6):231-7. doi: 10.1242/dmm.001180.
7. Park S, Kim S, Kim B, Kim DS, Kim J, Ahn Y, Kim H, Song M, Shim I, Jung SH, Cho C, Lim S, Hong S, Jo H, Fahed AC, Natarajan P, Ellinor PT, Torkamani A, Park WY, Yu TY, Myung W, Won HH. Multivariate genomic analysis of 5 million people elucidates the genetic architecture of shared components of the metabolic syndrome. Nat Genet. 2024 Nov;56(11):2380-2391. doi: 10.1038/s41588-024-01933-1. Epub 2024 Sep 30.
8. Rana S, Ali S, Wani HA, Mushtaq QD, Sharma S, Rehman MU. Metabolic syndrome and underlying genetic determinants-A systematic review. J Diabetes Metab Disord. 2022 Mar 3;21(1):1095-1104. doi: 10.1007/s40200-022-01009-z.
9. Dobrowolski P, Prejbisz A, Kuryłowicz A, et al. Metabolic syndrome - a new definition and management guidelines: A joint position paper by the Polish Society of Hypertension, Polish Society for the Treatment of Obesity, Polish Lipid Association, Polish Association for Study of Liver, Polish Society of Family Medicine, Polish Society of Lifestyle Medicine, Division of Prevention and Epidemiology Polish Cardiac Society, "Club 30" Polish Cardiac Society, and Division of Metabolic and Bariatric Surgery Society of Polish Surgeons. Arch Med Sci. 2022;18(5):1133-1156. Published 2022 Aug 30. doi:10.5114/aoms/152921
10. Türkiye Endokrinoloji ve Metabolizma Derneği, Obezite Tanı ve Tedavi Kılavuzu 2024, chromeextension://efaidnbmnnnibpcajpcglclefindmkaj/https://file.temd.org.tr/Uploads/publications/guides/documents/obezitetanitedavikilavizu-2024.pdf
11. Vitorino R. Transforming Clinical Research: The Power of High-Throughput Omics Integration. Proteomes. 2024; 12(3):25. https://doi.org/10.3390/proteomes12030025
12. Rakusanova S, Cajka T. Metabolomics and Lipidomics for Studying Metabolic Syndrome: Insights into Cardiovascular Diseases, Type 1 & 2 Diabetes, and Metabolic Dysfunction-Associated Steatotic Liver Disease. Physiol Res. 2024 Aug 30;73(S1):S165-S183. doi: 10.33549/physiolres.935443.
13. Anh NK, Thu NQ, Tien NTN, Long NP, Nguyen HT. Advancements in Mass Spectrometry-Based Targeted Metabolomics and Lipidomics: Implications for Clinical Research. Molecules. 2024; 29(24):5934. https://doi.org/10.3390/molecules29245934



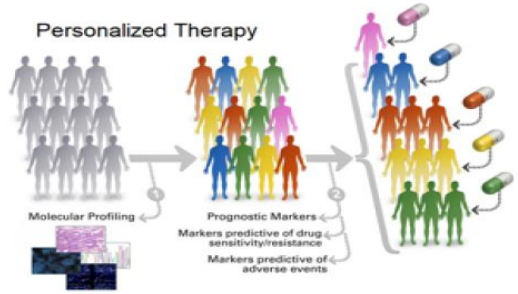
Human diseases



Metabolic profile



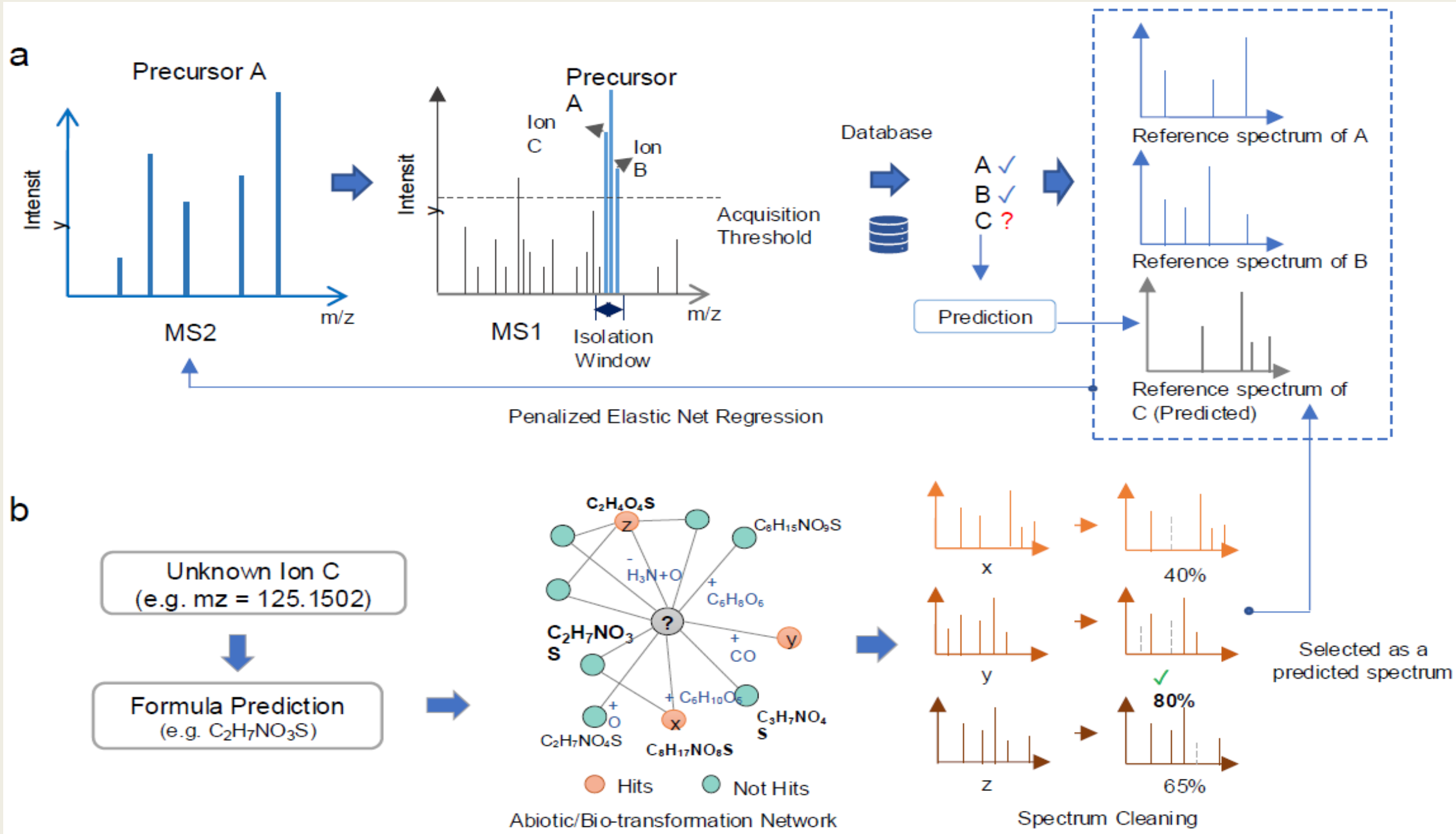
Diagnostic biomarkers



Personalised treatment

Precision medicine

TEŞEKKÜRLER...


a
Precursor A
Intensit
y
m/z
MS2
Precursor A
Ion C
Ion B
Intensit
y
Acquisition Threshold
m/z
MS1
Isolation Window
Database
A ✓
B ✓
C ?
Prediction
Reference spectrum of A
Reference spectrum of B
Reference spectrum of C (Predicted)
Penalized Elastic Net Regression
b
Unknown Ion C (e.g. mz = 125.1502)
Formula Prediction (e.g. C2H7NO3S)
C2H4O4S
C8H15NO3S
- H3N+O
+ C6H8O6
C2H7NO3S
+ CO
+ C6H10O6
+ O
C2H7NO4S
C8H17NO8S
C3H7NO4S
Hits
Not Hits
Abiotic/Bio-transformation Network
x
40%
y
80%
z
65%
Spectrum Cleaning
Selected as a predicted spectrum