Supplementary Data

This supplementary data is a part of a paper entitled “Synthesis, Characterization, and Theoretical Study of a New Organotellurium Ligands Containing Amino Group”.

The spectra details (FT-IR and MS) of the prepared organotellurium compounds

(4-Amino-[1,1'-biphenyl]-3-yl)mercury(II) chloride (A): -

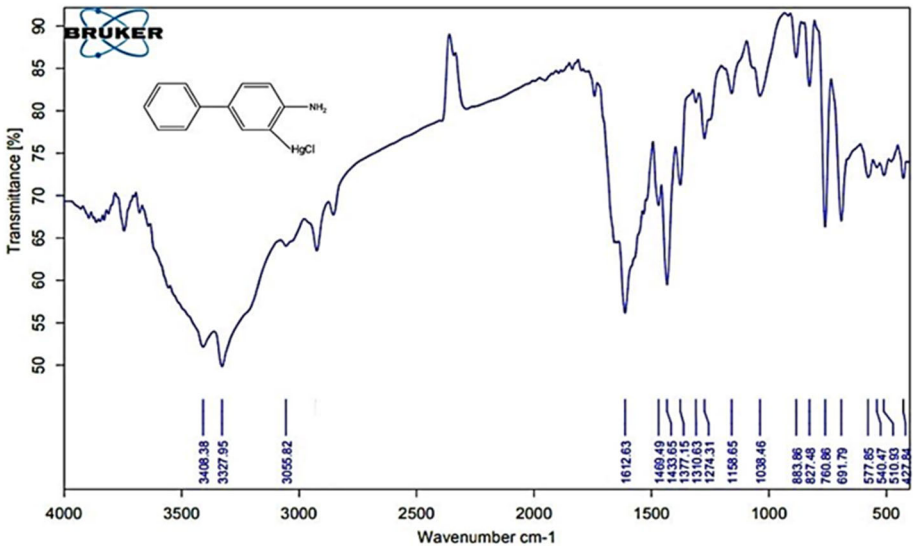


Fig S1. Infrared spectrum of the compound **A**

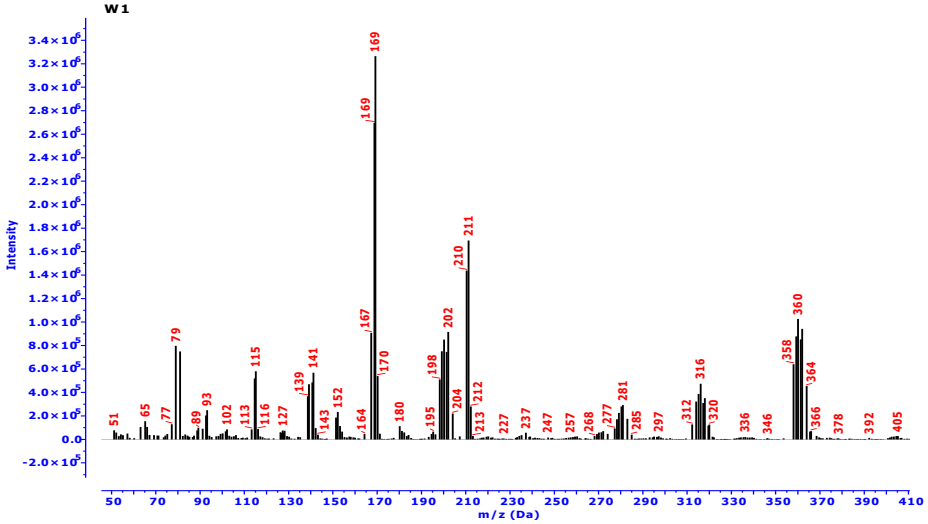


Fig S2. The mass spectrum of the compound **A**

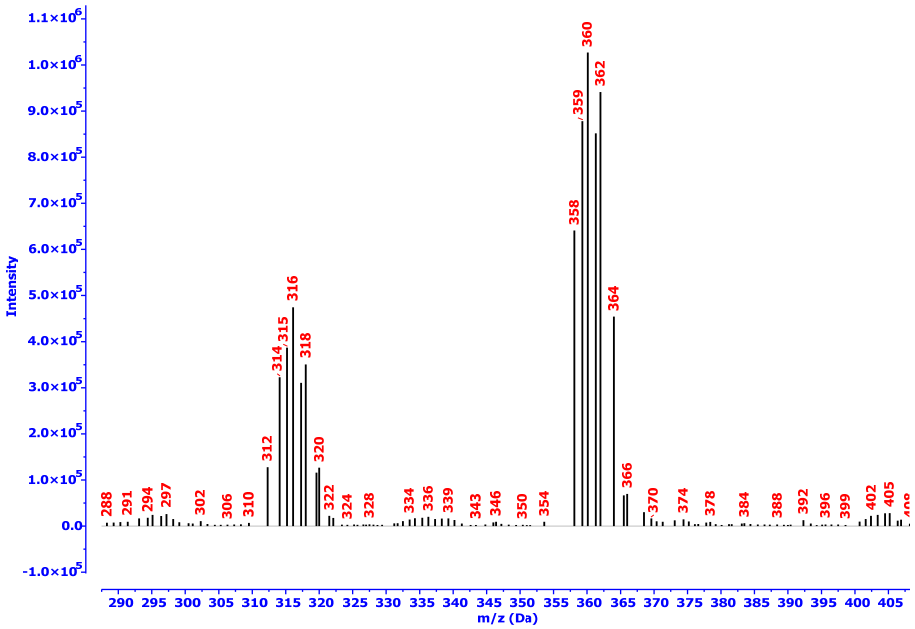
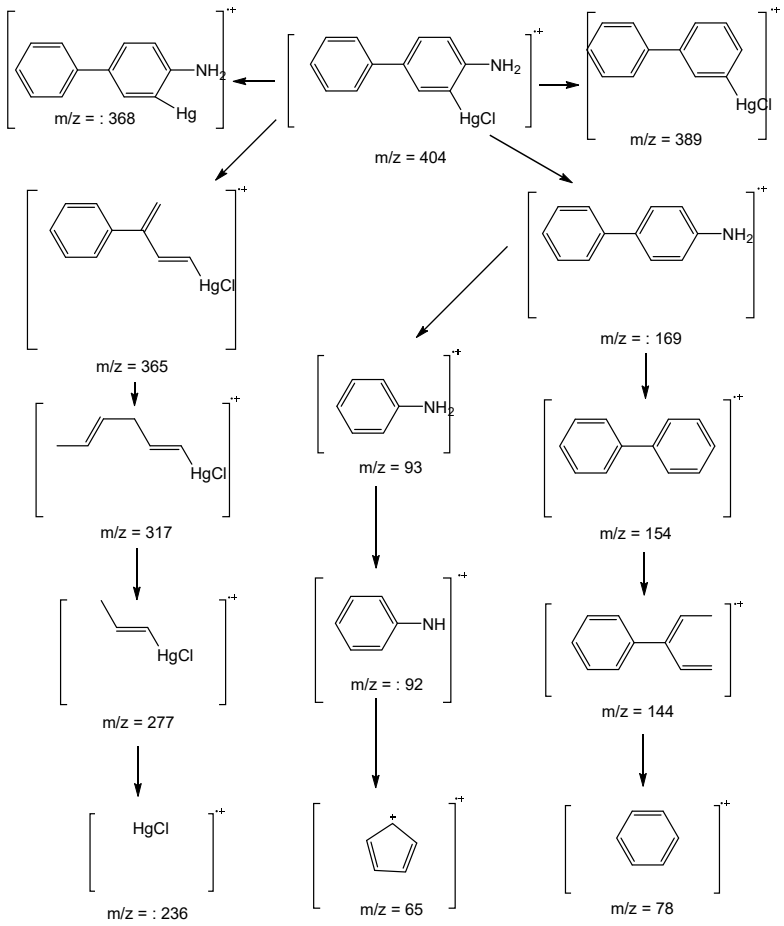


Fig S3. Expanded mass spectrum of the compound **A**



Scheme S1. Mechanical fragmentation of the compound **A**

3-(Tribromo-λ^4-tellanyl)-[1,1'-biphenyl]-4-amine (B): -

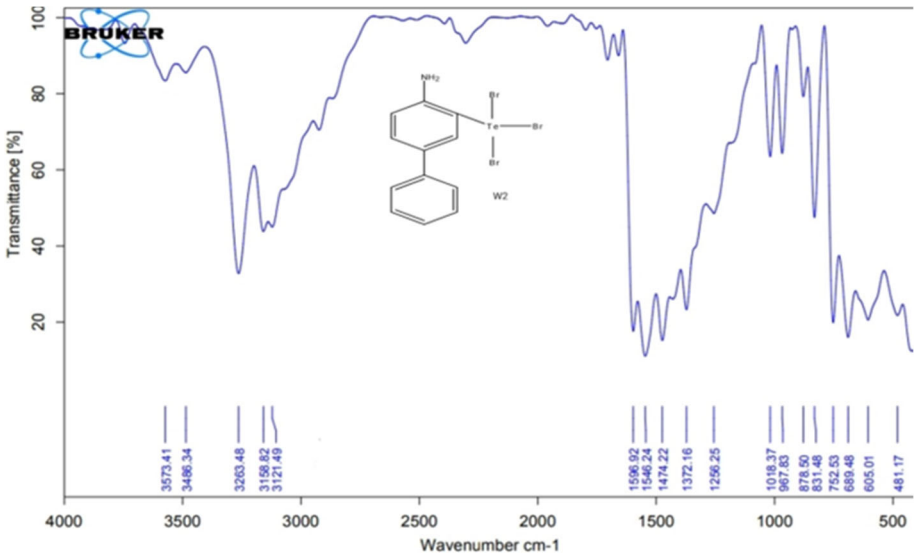


Fig S4. Infrared spectrum of the compound **B**

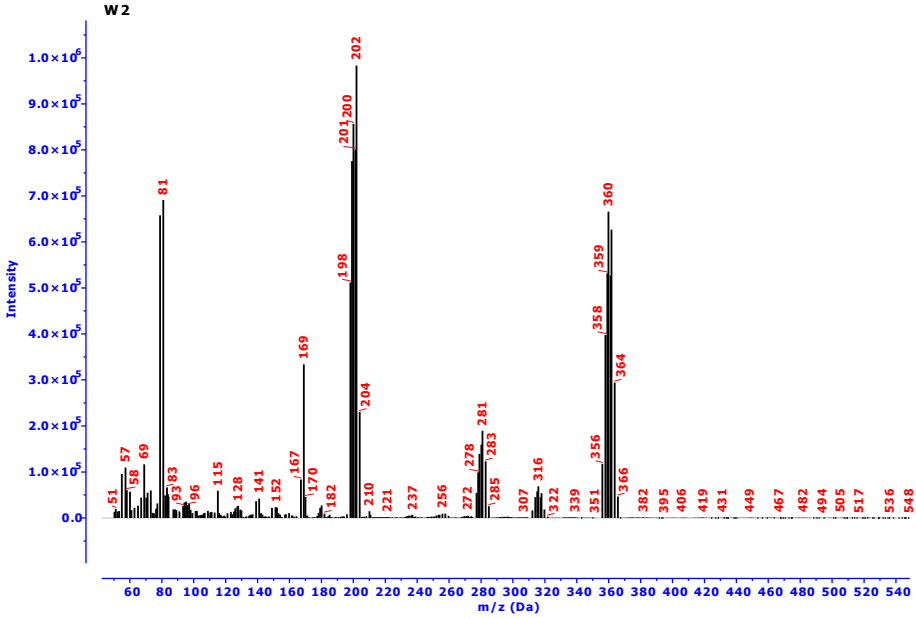


Fig S5. The mass spectrum of the compound **B**

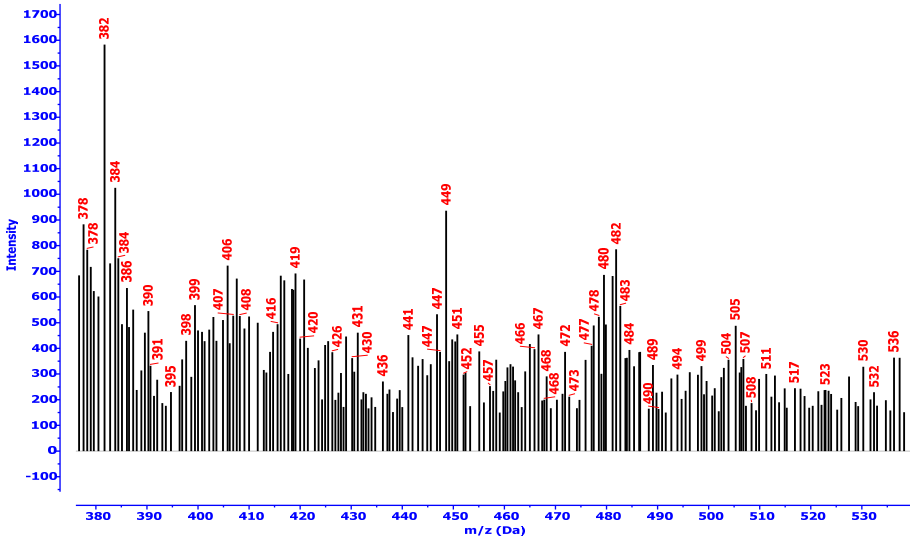
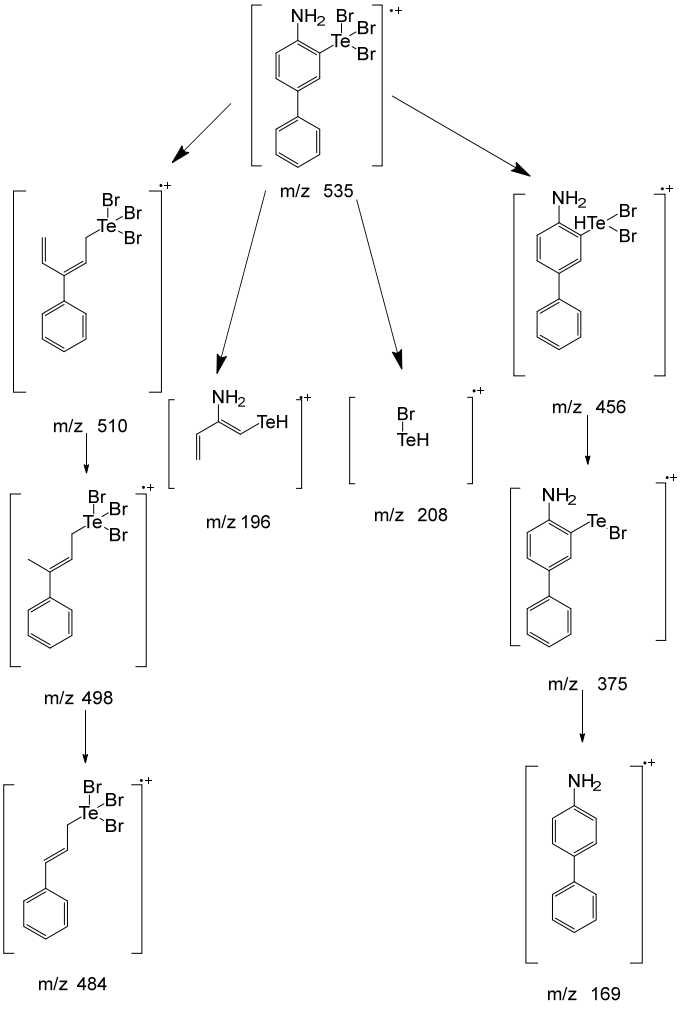


Fig S6. Expanded mass spectrum of the compound **B**



Scheme S2. Mechanical fragmentation of the compound **B**

3,3'-(Dibromo-λ^4-tellanediyl)bis([1,1'-biphenyl]-4-amine) (C): -

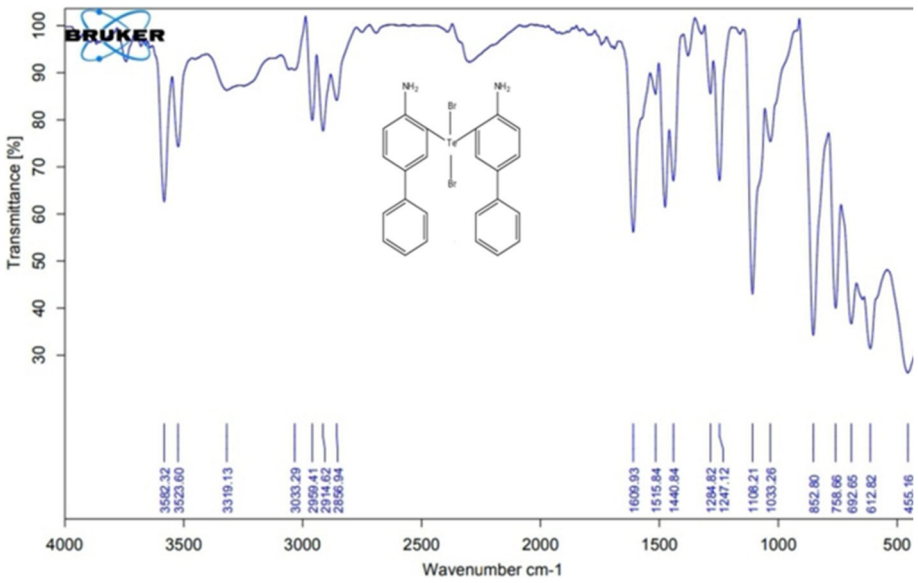


Fig S7. Infrared spectrum of the compound **C**

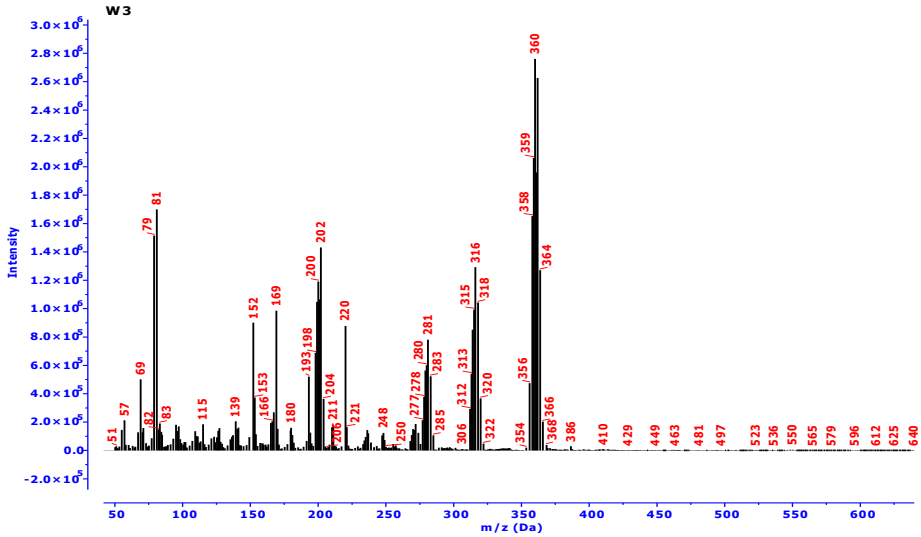


Fig S8. The mass spectrum of the compound **C**

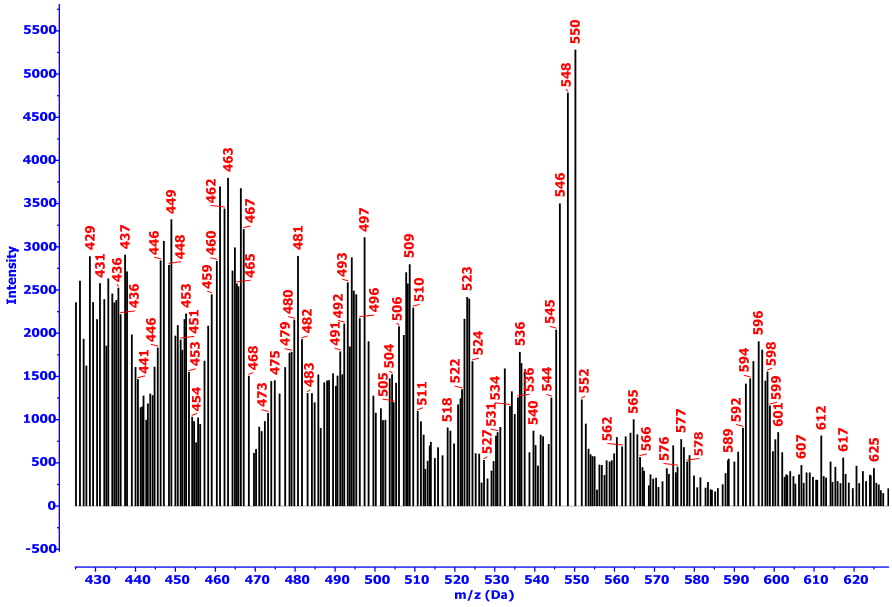
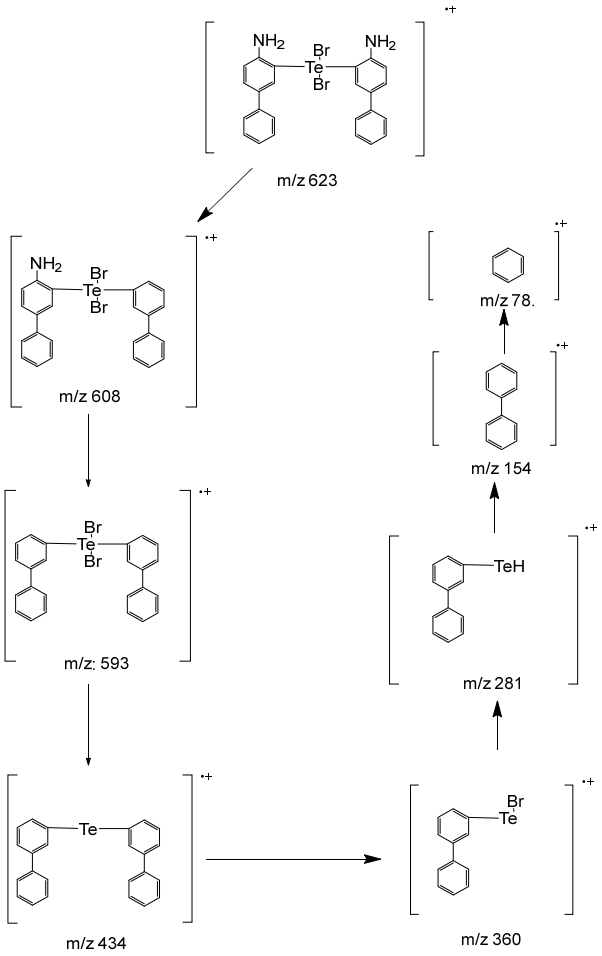


Fig S9. Expanded mass spectrum of the compound **C**



Scheme S3. Mechanical fragmentation of the compound **C**

3,3''-tellurobis([1,1'-biphenyl]-4-amine) (D): -

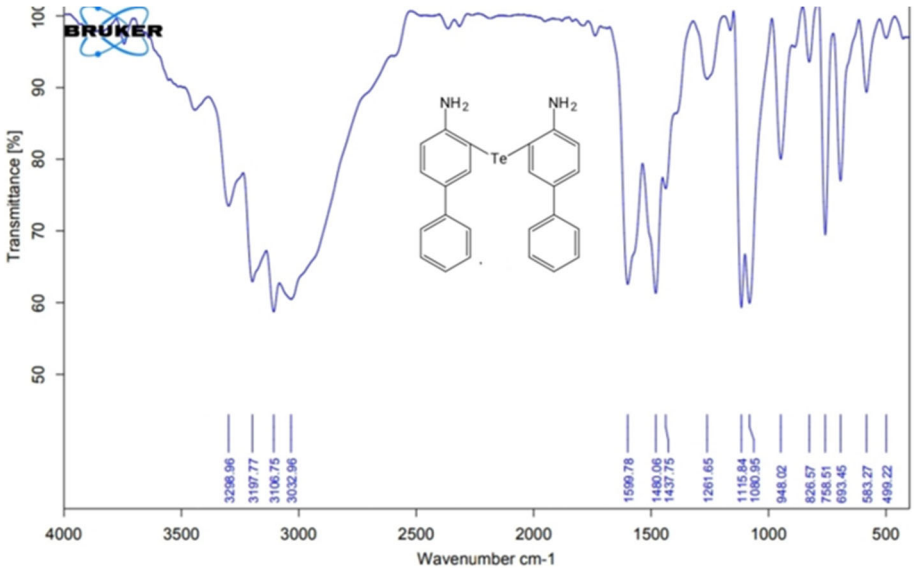


Fig S10. Infrared spectrum of the compound **D**

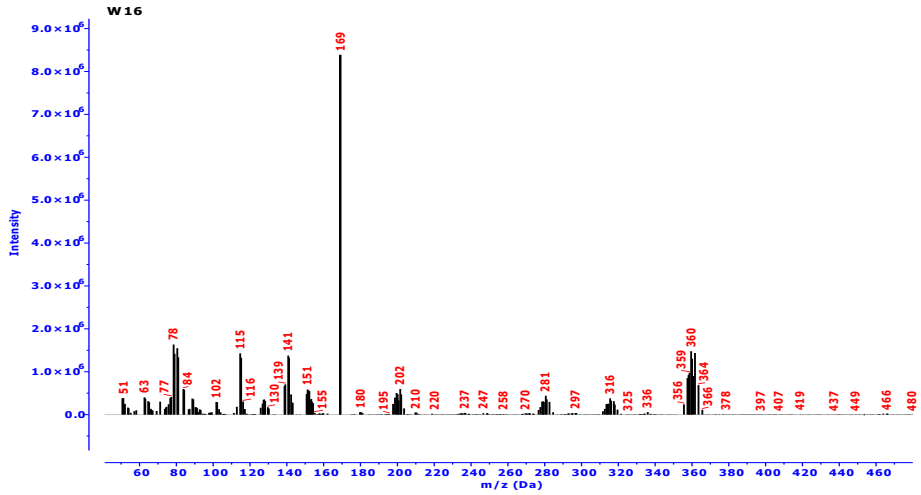


Fig S11. The mass spectrum of the compound **D**

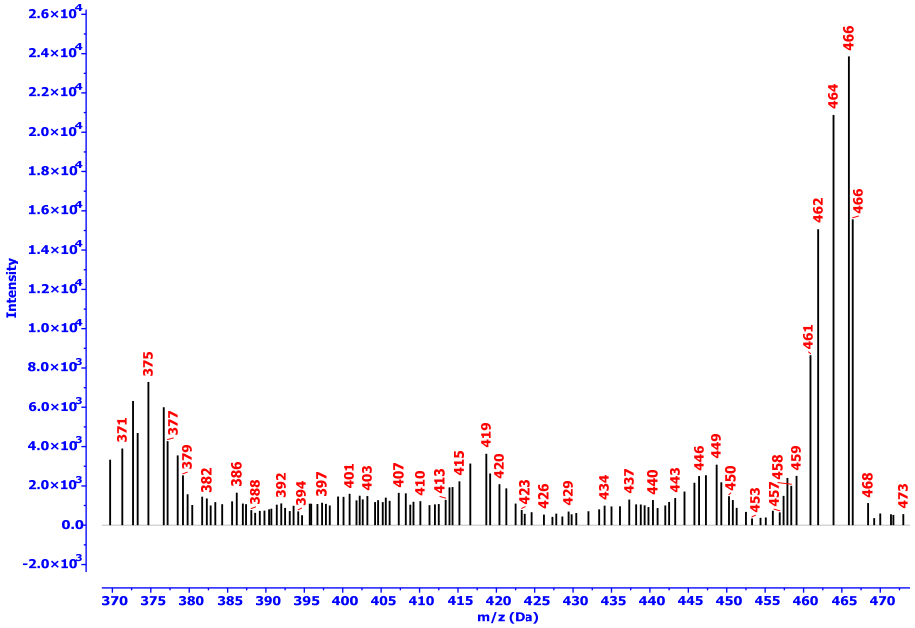
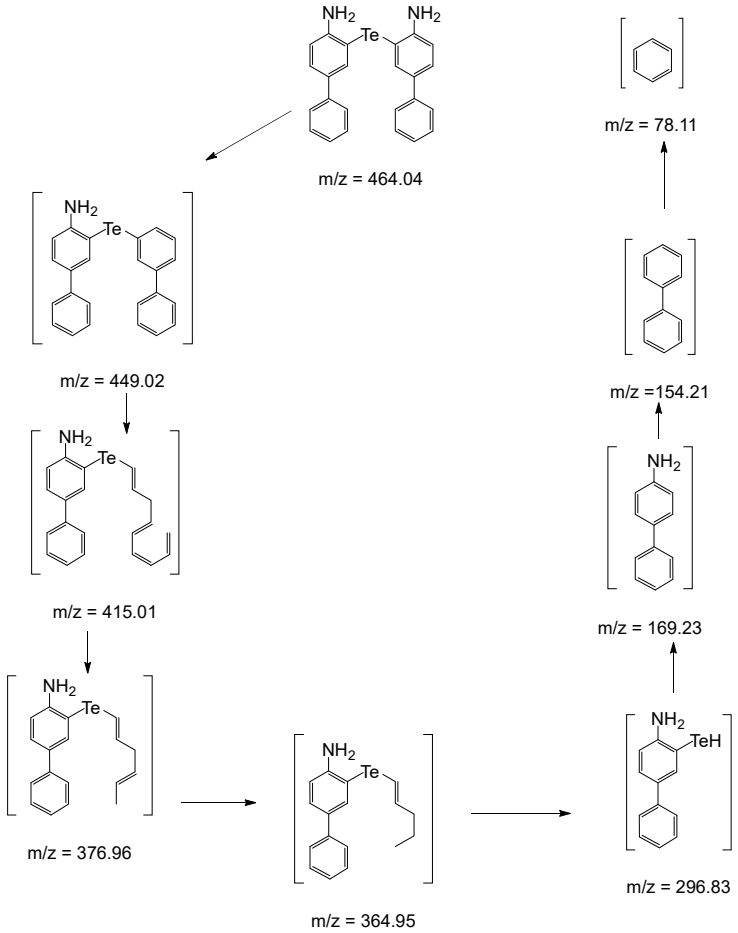


Fig S12. Expanded mass spectrum of the compound **D**



Scheme S4. Mechanical fragmentation of the compound **D**

3,3''-ditellanediyl bis([1,1'-biphenyl]-4-amine) (E): -

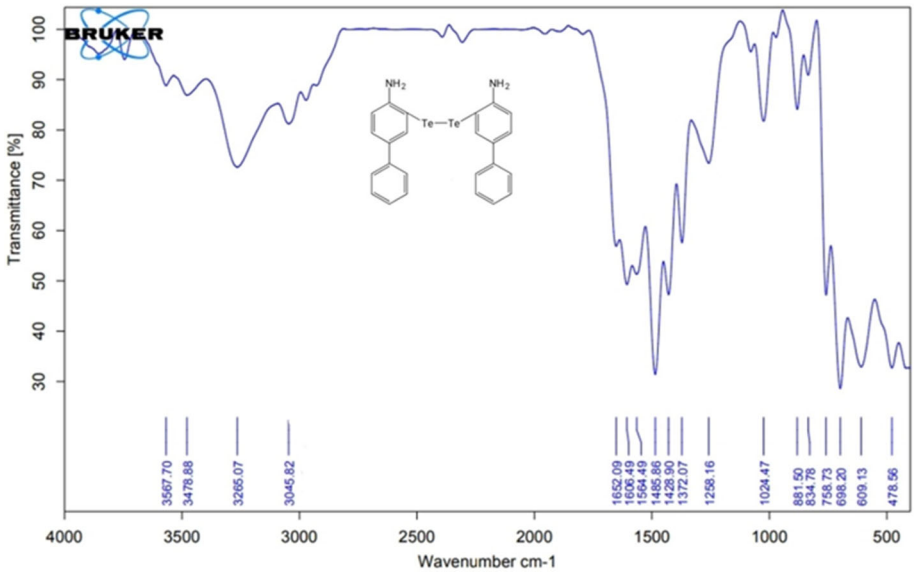


Fig S13. Infrared spectrum of the compound **E**

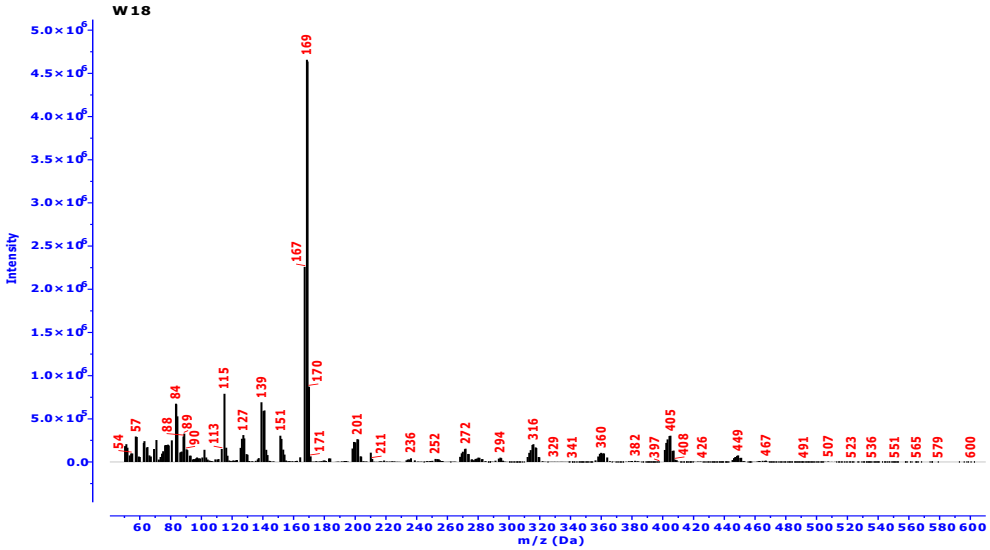


Fig S14. The mass spectrum of the compound **E**

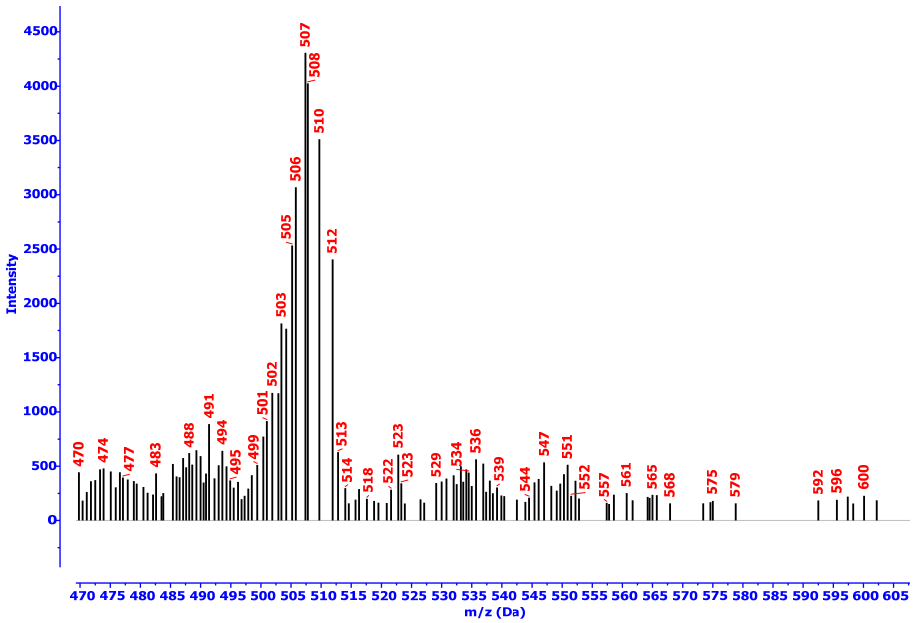
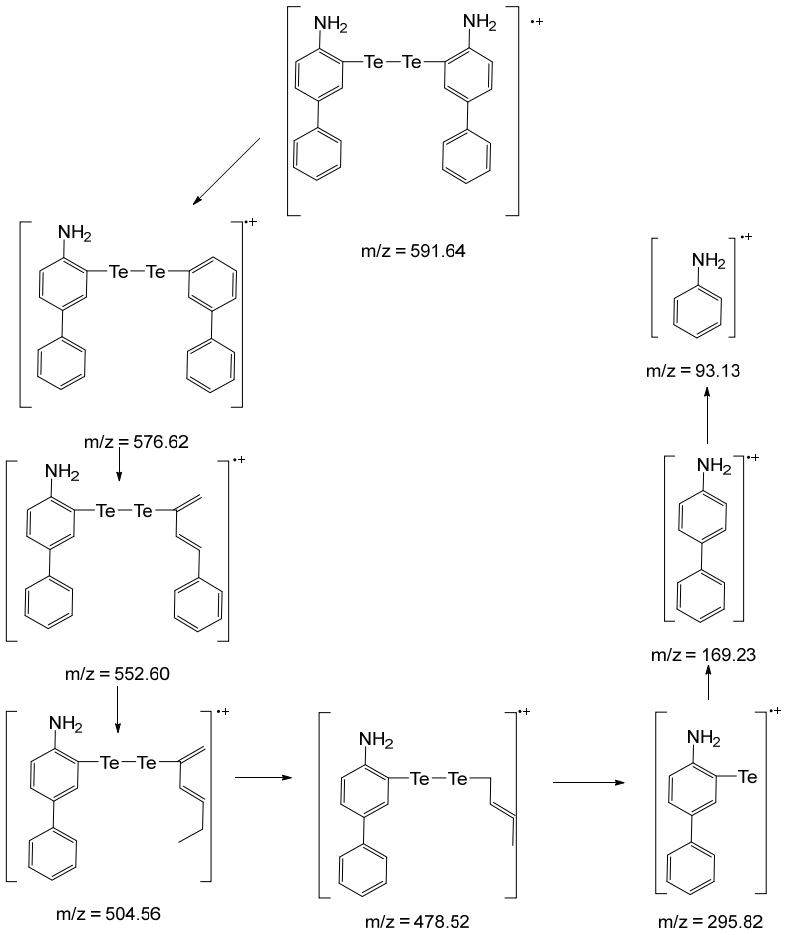


Fig S15. Expanded mass spectrum of the compound **E**



Scheme S5. Mechanical fragmentation of the compound **E**

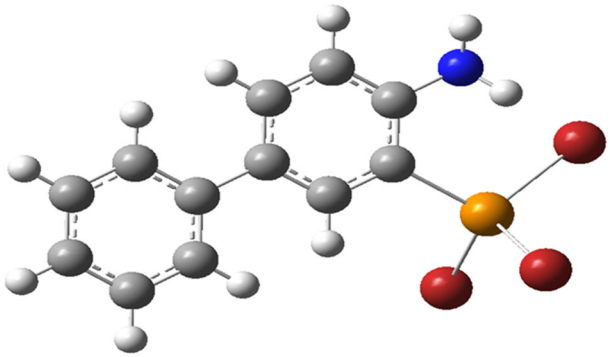


Fig S16. Molecular structure of compound **B**

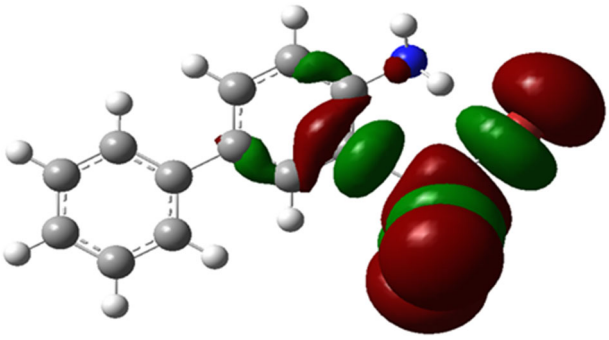


Fig S17. Molecular orbital (HOMO) of compound **B**

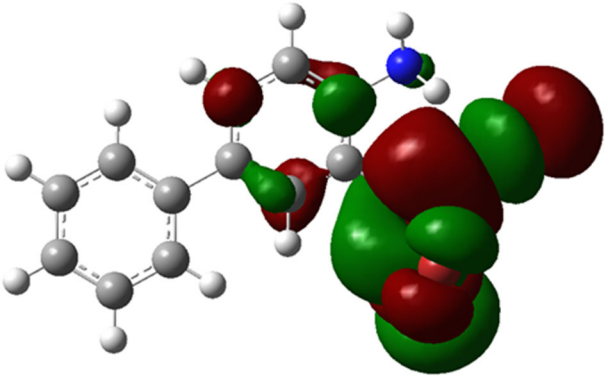


Fig S18. Molecular orbital (LUMO) of compound **C**

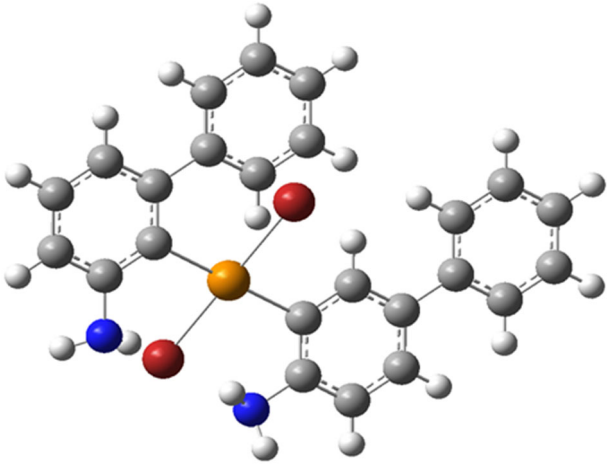


Fig S19. Molecular structure of compound **C**

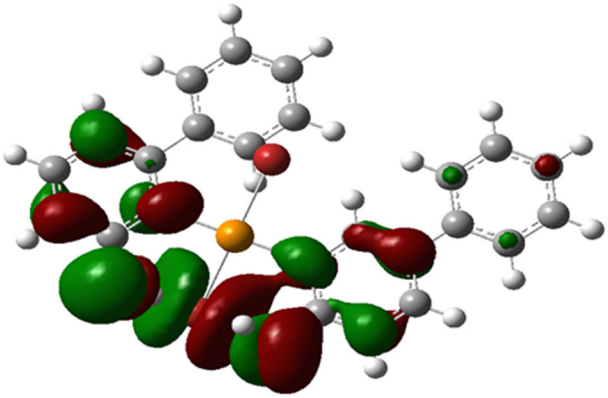


Fig S20. Molecular orbital (HOMO) of compound **C**

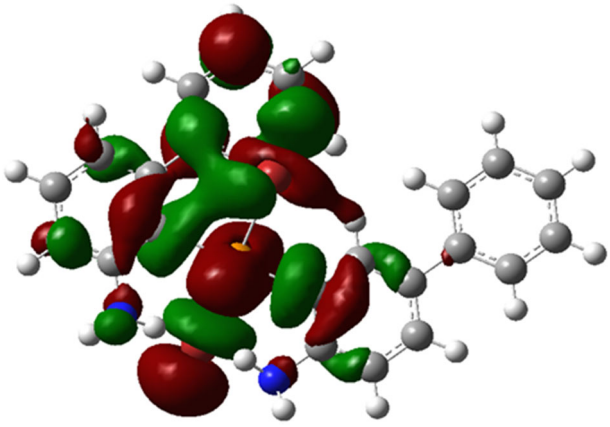


Fig S21. Molecular orbital (LUMO) of compound **C**

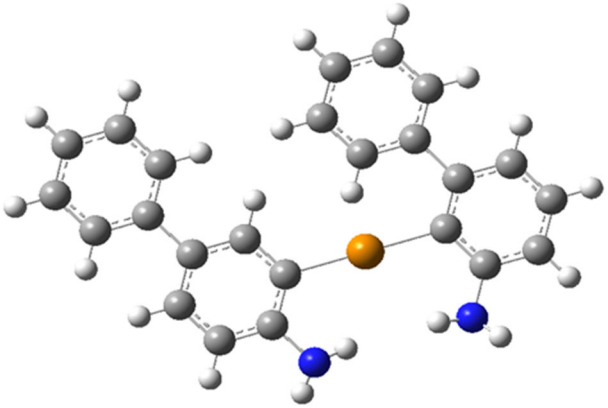


Fig S22. Molecular structure of compound **D**

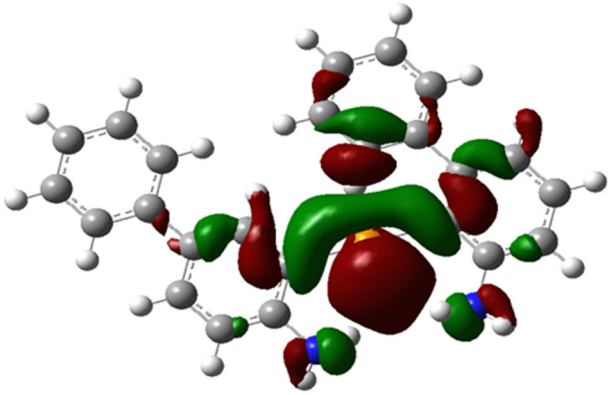


Fig S23. Molecular orbital (HOMO) of compound **D**

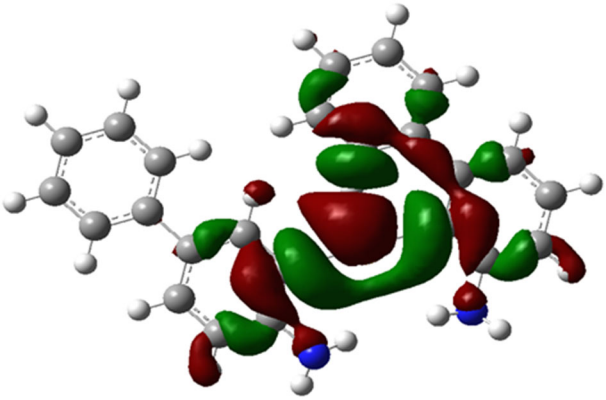


Fig S24. Molecular orbital (LUMO) of compound **D**

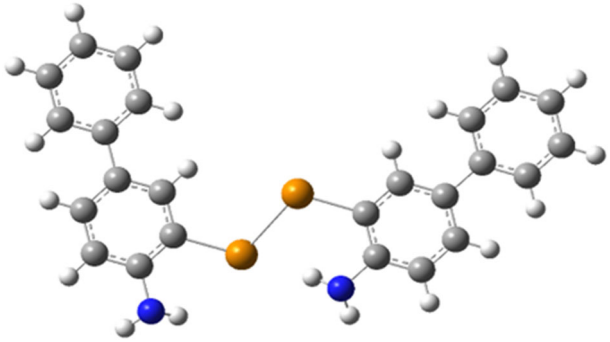


Fig S25. Molecular structure of compound **E**

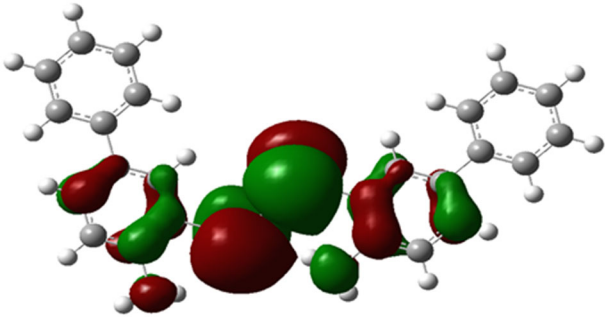


Fig 26. Molecular orbital (HOMO) of compound **E**

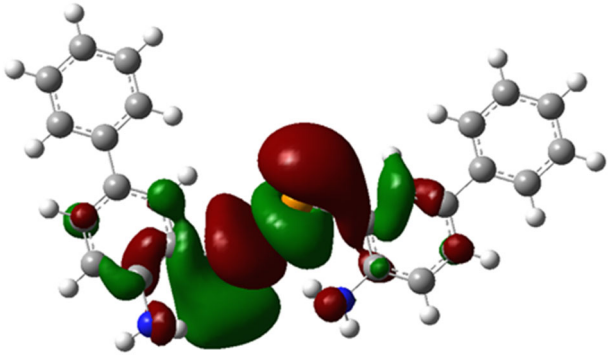


Fig S27. Molecular orbital (LUMO) of compound **E**

Table S1. The most important fissions of the compound **A**

Molecular ion	*m/z*	Molecular ion	*m/z*
$[C_{12}H_{10}NHgCl]^+$	404	$[C_6H_9HgCl]^+$	317
$[C12H11N]^+$	169	$[C_{12}H_{10}]^+$	154
$[C_{10}H_9HgCl]^+$	365	$[C_3H_5HgCl]^+$	277

Table S2. The most important fissions of the compound **B**

Molecular ion	*m/z*	Molecular ion	*m/z*
$[C_{12}H_{10}Br_3NTe]^+$	535	$[C_4H_7NTe]^+$	196
$[TeHBr]^+$	202	$[C_{12}H_{11}Br_2NTe]^+$	456
$[C_{11}H_{11}Br_3Te]^+$	510	$[C_{12}H_{11}N]^+$	169

Table S3. The most important fissions of the compound **C**

Molecular ion	*m/z*	Molecular ion	*m/z*
$[C_{24}H_{20}N_2Br_2Te]^+$	623	$[C_{24}H_{18}Br_2Te]^+$	593
$[C_{12}H_9BrTe]^+$	360	$[C_{24}H_{18}Te]^+$	434
$[C_{24}H_{19}Br_2NTe]^+$	608	$[C_{12}H_{10}Te]^+$	281

Table S4. The most important fissions of the compound **D**

Molecular ion	*m/z*	Molecular ion	*m/z*
$[C_{24}H_{20}N_2Te]^+$	464	$[C_{21}H_{21}NTe]^+$	415
$[C_{12}H_{11}N]^+$	169	$[C_{17}H_{19}NTe]^+$	364
$[C_{24}H_{19}NTe]^+$	449	$[C_6H_6]^+$	77

Table S5. The most important fissions of the compound **E**

Molecular ion	*m/z*	Molecular ion	*m/z*
$[C_{24}H_{20}N_2Te_2]^+$	591	$[C_{22}H_{19}NTe_2]^+$	552
$[C_{12}H_{11}N]^+$	169	$[C_{12}H_{10}NTe]^+$	296
$[C_{24}H_{19}NTe_2]^+$	576	$[C_6H_7N]^+$	93