Supplementary Materials

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1. Prisma Interface

Given the large number of molecules in the study, it was decided to develop the PRISMA software to automate some tasks, and its use allowed the rapid analysis of ORCA output, generation of IR spectra and normalization, and identification of possible errors, as well as the reduction of errors in the creation of the input files. Figures S.76 and S.77 and present the tool's interface and infrared spectrum visualization functionality.

Figure S1. PRISMA interface with open ORCA result file: i) suitable result; ii) result with negative frequency.

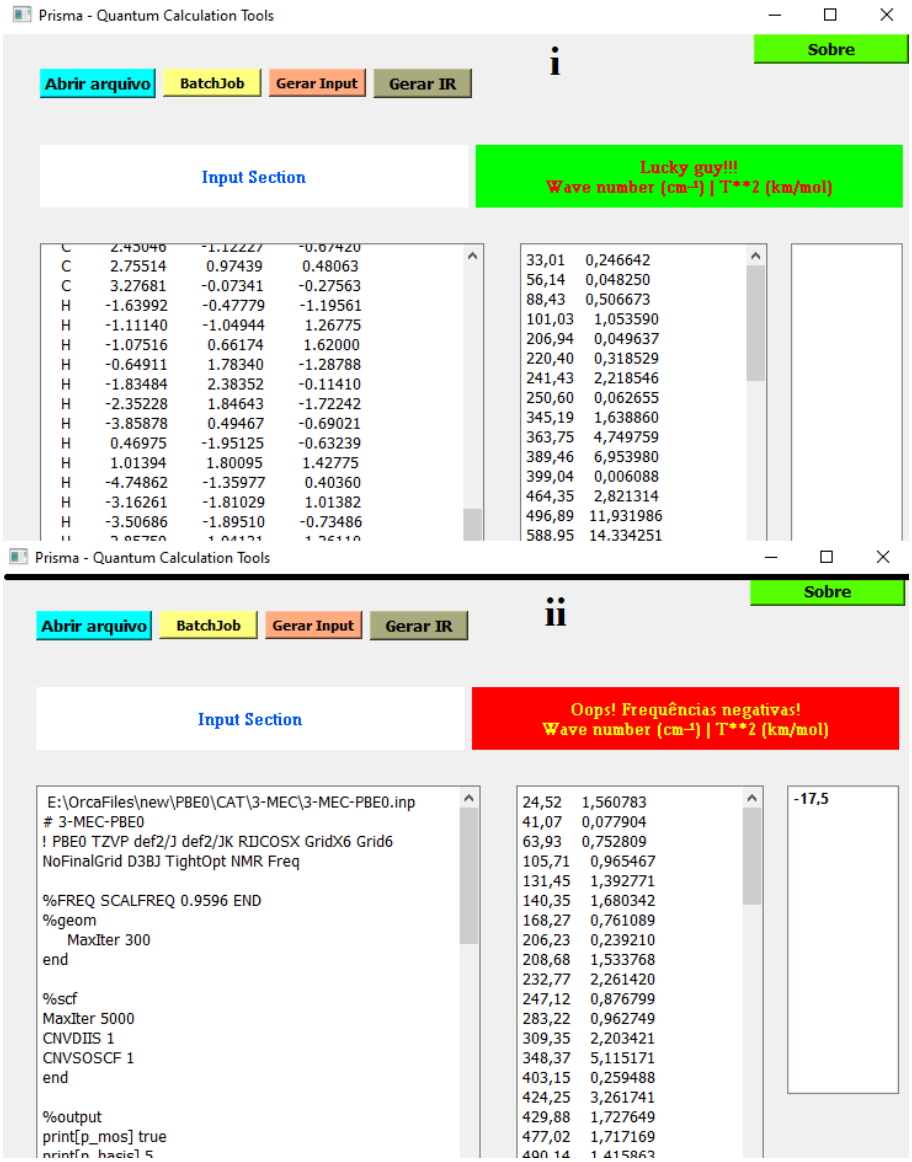
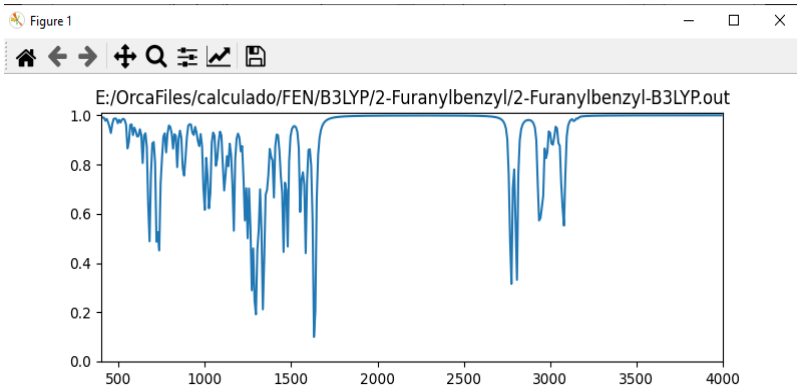
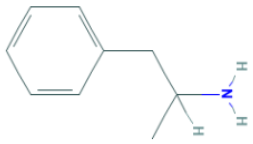
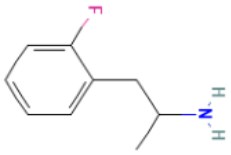
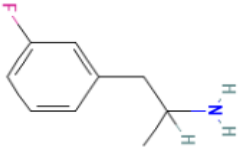
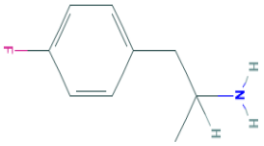
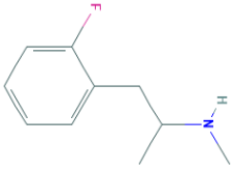
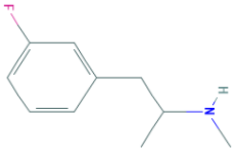
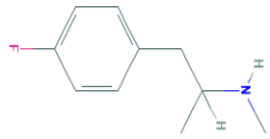
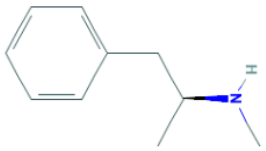
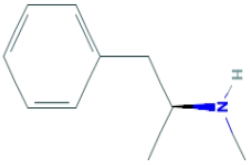
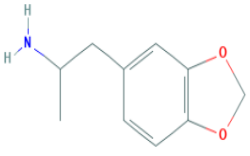
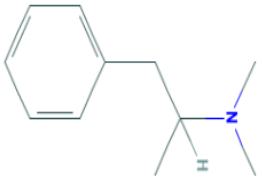
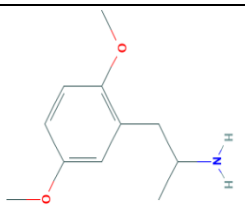


Figure S2. PRISMA: Infrared spectrum visualization module.



2. Studied System

Table S1 - Amphetamines

 Anfetamina [1] amphetamine $C_9H_{13}N$	 2-Fluoro-amphetamine [2] 2-FA $C_9H_{12}FN$	 3-Fluoro-amphetamine [3] 3-FA $C_9H_{12}FN$	 4-Fluoro-amphetamine [4] 4-FA $C_9H_{12}FN$
 2-Fluoro-methamphetamine 2-FMA [5] $C_{10}H_{14}FN$	 3-Fluoro-methamphetamine 3-FMA [6] $C_{10}H_{14}FN$	 4-Fluoro-methamphetamine 4-FMA [7] $C_{10}H_{14}FN$	 Metanfetamina [8] methamphetamine $C_{10}H_{15}N$
 4-Methyl-amphetamine 4-MA [9] $C_{10}H_{15}N$	 3,4- methylene-dioxyamphetamine 3,4 MDA [10] Tenamfetamine	 Dimetilanfetamina DMA [11] $C_{11}H_{17}N$	 2,5-Dimethoxy-amphetamine 2,5-DMA [12]

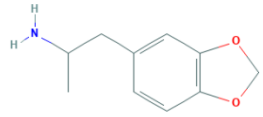
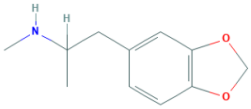
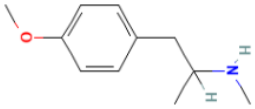
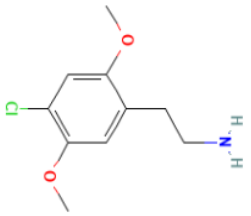
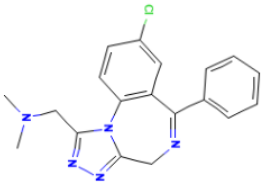
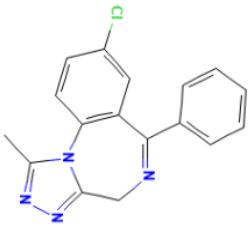
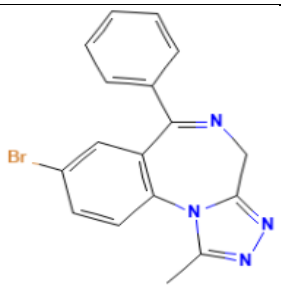
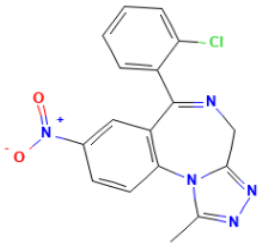
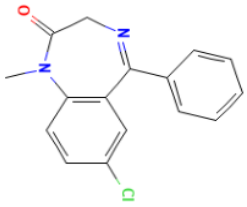
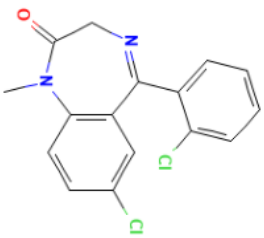
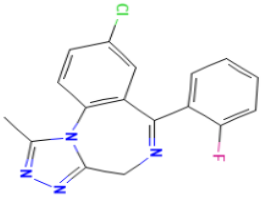
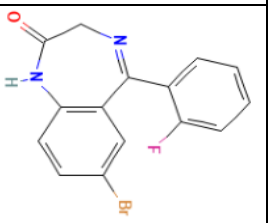
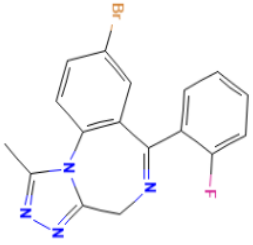
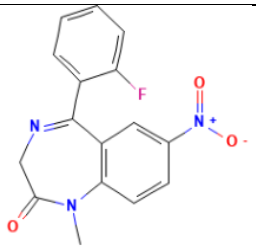
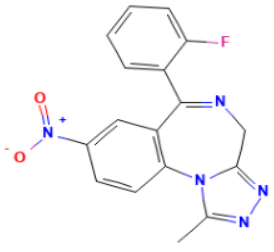
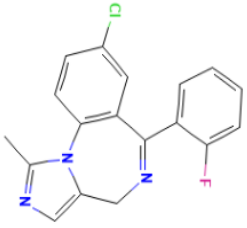
	$C_{10}H_{13}NO_2$		$C_{11}H_{17}NO_2$
 3,4-Methylenedioxy methamphetamine MDMA [13] Ecstasy $C_{11}H_{15}NO_2$	 p-Metoxy-amphetamine PMA [14] $C_{10}H_{15}NO$	 p-Methoxy-methamphetamine PMMA [15] $C_{11}H_{17}NO$	 1-(4-Chloro-2,5-dimethoxyphenyl)-2-aminoethane 2C-C [16] $C_{10}H_{14}ClNO_2$

Table S2. Benzodyazepines

 Adinazolam [17] Deracyn $C_{19}H_{18}ClN_5$	 Alprazolam [18] Xanax $C_{17}H_{13}ClN_4$	 Bromazolam [19] $C_{17}H_{13}BrN_4$	 Clonazolam [20] $C_{17}H_{12}ClN_5O_2$
 Diazepam [21] Valium $C_{16}H_{13}ClN_2O$	 Diclazepam [22] 2-Chlorodiazepam $C_{16}H_{12}Cl_2N_2O$	 Flualprazolam [23] $C_{17}H_{12}ClFN_4$	 Flubromazepam [24] $C_{15}H_{10}BrFN_2O$
 Flubromazolam [25] $C_{17}H_{12}BrFN_4$	 Flunitrazepam [26] Narcozep	 Flunitrazolam [27] UNII-OK0I6HTR1Y	 Midazolam [28] Dormicum

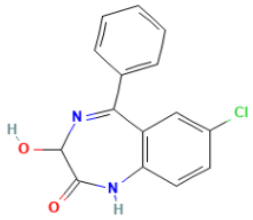
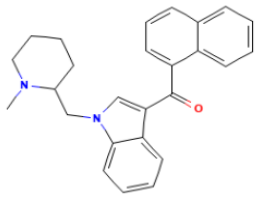
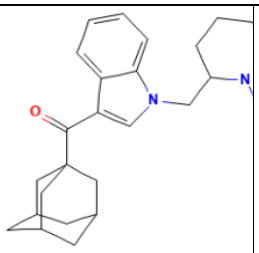
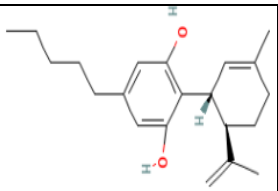
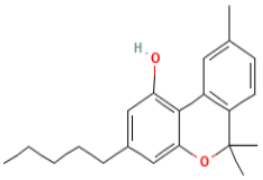
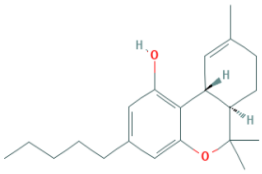
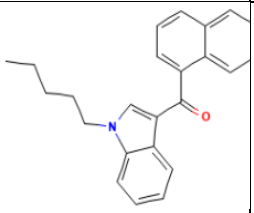
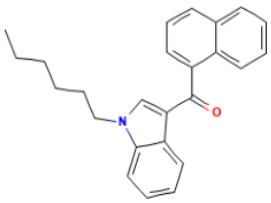
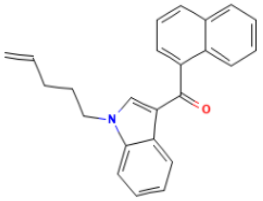
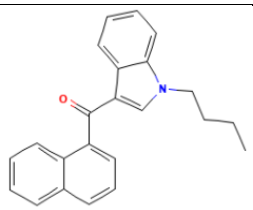
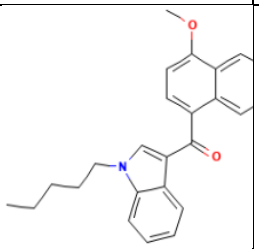
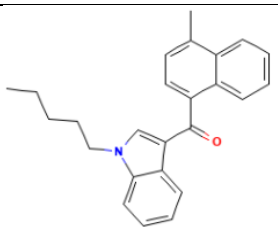
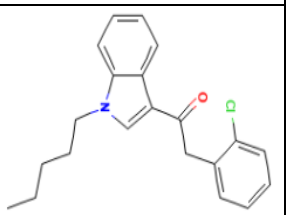
	$C_{16}H_{12}FN_3O_3$	$C_{17}H_{12}FN_5O_2$	$C_{18}H_{13}ClFN_3$
 Oxazepam [29] Tazepam, Serax, Adumbran $C_{15}H_{11}ClN_2O_2$			

Table S3. Cannabinoids

 AM-1220 [30] Methanone $C_{26}H_{26}N_2O$	 AM1248 [31] $C_{26}H_{34}N_2O$	 Cannabidiol [32] Epidiolex $C_{21}H_{30}O_2$	 Cannabinol [33] $C_{21}H_{26}O_2$
 Δ9-THC [34] Δ9-tetrahydro-cannabinol Marinol, Dronabinol $C_{21}H_{30}O_2$	 JWH-018 [35] 1-Pentyl-3-(1-naphthoyl)índole $C_{24}H_{23}NO$	 JWH-019 [36] 1-Hexyl-3-(naphthalen-1-oyl)índole $C_{25}H_{25}NO$	 JWH-022 [37] naphthalen-1-yl(1-(pent-4-en-1-yl)-1H-indol-3-yl)methanone $C_{24}H_{21}NO$
 JWH-073 [38] 1-Butyl-3-(1-naphthoyl)índole $C_{23}H_{21}NO$	 JWH-081 [39] 1-Pentyl-3-(4-methoxynaphthoyl)indole $C_{25}H_{25}NO_2$	 JWH-122 [40] CHEMBL557004, UNII-44147RI31X $C_{25}H_{25}NO$	 JWH-203 [41] UNII-52CP80V8FY $C_{21}H_{22}ClNO$

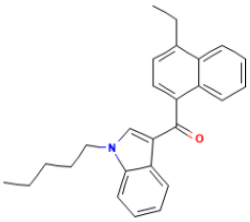
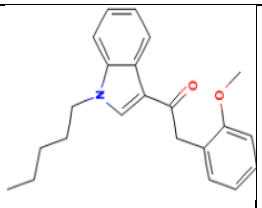
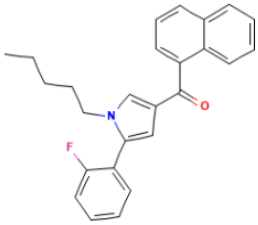
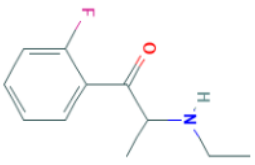
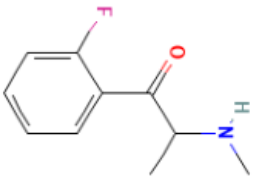
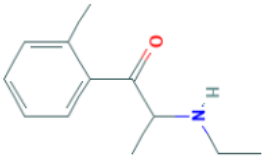
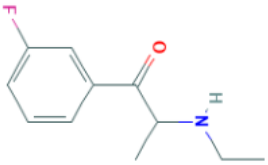
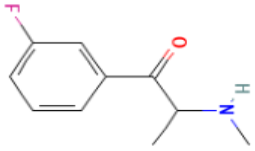
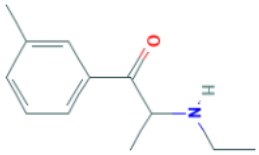
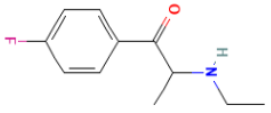
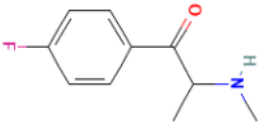
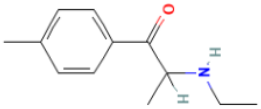
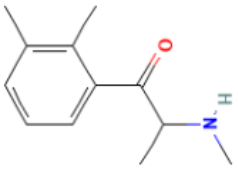
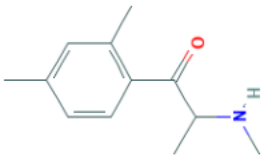
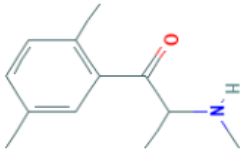
 JWH-210 [42] UNII-R18JYO04PY $C_{26}H_{27}NO$	 JWH-250 [43] UNII-IP9911R8A0 $C_{22}H_{25}NO_2$	 JWH-307 [44] 06QTR14ONW $C_{26}H_{24}FNO$	

Table S4. Cathinones

 2-Fluoroethcathinone 2-FEC [45] 127C7F28AS $C_{11}H_{14}FNO$	 2-Fluoro-methcathinone 2-FMC [46] $C_{10}H_{12}FNO$	 2-Methyleth-cathinone 2-MEC [47] $C_{12}H_{17}NO$	 3-Fluoro-ethcathinone 3-FEC [48] $C_{11}H_{14}FNO$
 3-Fluoro-methcathinone 3-FMC [49] 3-Flephedrone $C_{10}H_{12}FNO$	 3-methyl-ethcathinone 3-MEC [50] $C_{12}H_{17}NO$	 4-Fluoro-ethcathinone 4-FEC [51] ML7H977FPM $C_{11}H_{14}FNO$	 4-Fluoro-methcathinone 4-FMC [52] Flephedrone $C_{10}H_{12}FNO$
 4-methyl-ethcathinone 4-MEC [53] $C_{12}H_{17}NO$	 2,3-Dimethyl-methcathinone 2,3-DMMC [54] $C_{12}H_{17}NO$	 2,4-Dimethyl-methcathinone 2,4-DMMC [55] $C_{12}H_{17}NO$	 2,5-DMMC [56] 1-(2,5-Dimethyl-phenyl)-2-(methylamino) propan-1-one $C_{12}H_{17}NO$

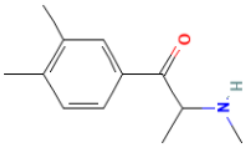
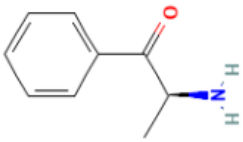
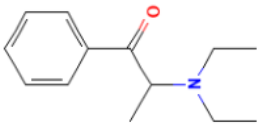
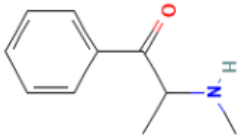
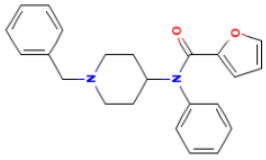
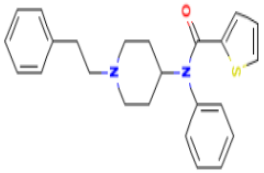
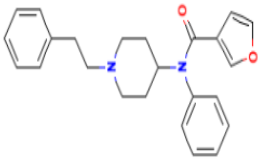
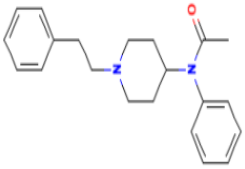
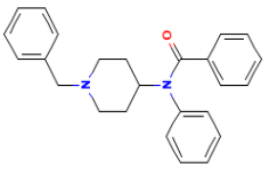
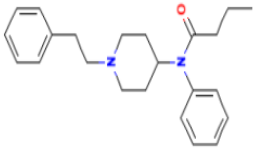
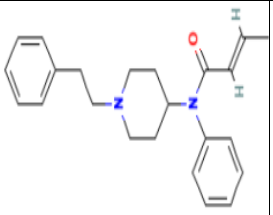
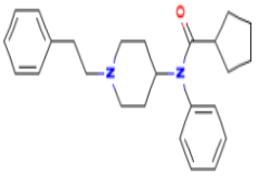
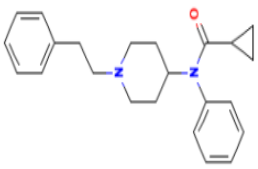
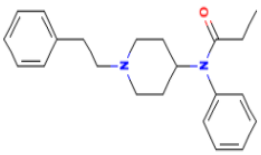
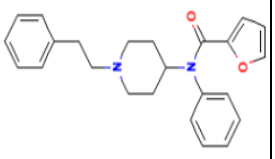
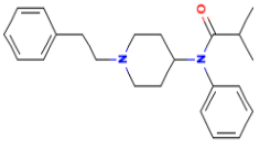
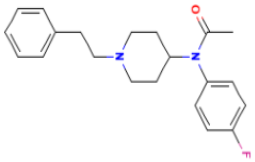
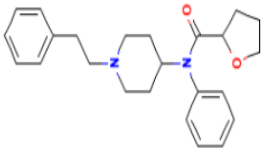
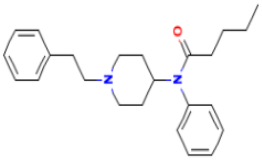
 3,4-Dimethyl-methcathinone 3,4-DMMC [57] $C_{12}H_{17}NO$	 Cathinone [58] Norephedrone $C_9H_{11}NO$	 Diethylcathinone [59] Amfepramone Diethylpropion $C_{13}H_{19}NO$	 Methcathinone, Ephedrone [60] $C_{10}H_{13}NO$

Table S5. Fentanys

 2-Furanylbenzyl fentanyl [61] 2- Furanylbenzyl Benzyl fu-f $C_{23}H_{24}N_2O_2$	 2-Thiophenoyl Fentanyl [62] 5JNS36UH4R $C_{24}H_{26}N_2OS$	 3-Furanyl fentanyl 3fuf [63] $C_{24}H_{26}N_2O_2$	 Acetyl Fentanyl Acetilfen [64] $C_{21}H_{26}N_2O$
 Benzoylbenzyl fentanyl Benzoylbenzyl Benzamide [65] $C_{25}H_{26}N_2O$	 Butyryl fentanyl Butyrfentanyl Butanamide [66] $C_{23}H_{30}N_2O$	 Crotonylfentanyl [67] UNII-R0XLG8CO63 $C_{23}H_{28}N_2O$	 Cyclopentanoyl Fentanyl Cyclopentyl-fentanyl [68] $C_{25}H_{33}ClN_2O$
 Cyclopropyl Fentanyl [69] DEA No. 9845	 Fentanyl [70] Fentora $C_{22}H_{28}N_2O$	 Furanyl Fentanyl [71] UNII-3F7C9J1LS7 $C_{24}H_{26}N_2O_2$	 Isobutyryl fentanyl Isobutyrfentanyl [72]

$C_{23}H_{28}N_2O$			$C_{23}H_{30}N_2O$
 para-Fluoroacetyl fentanyl [73] Acetyl 4'-fluorofentanyl $C_{21}H_{25}FN_2O$	 Tetrahydrofuran Fentanyl [74] Thf-f $C_{24}H_{30}N_2O_2$	 Valeryl fentanyl Pentanamide [75] $C_{24}H_{32}N_2O$	

3. Theoretical Spectra

Figure S3. Infrared Theoretical Spectra for 2C-C:

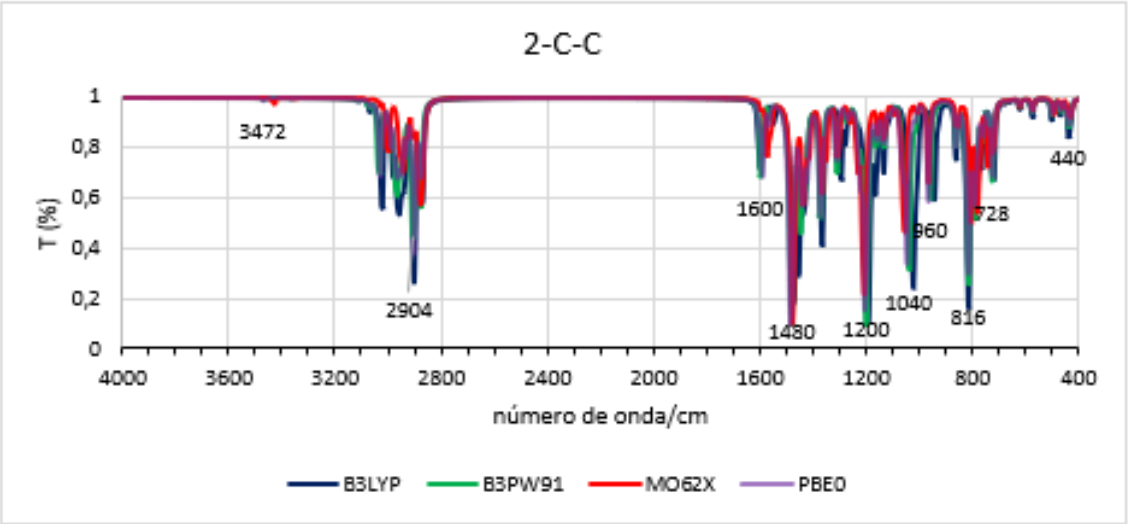


Figure S4. Infrared Theoretical Spectra for 2-FA:

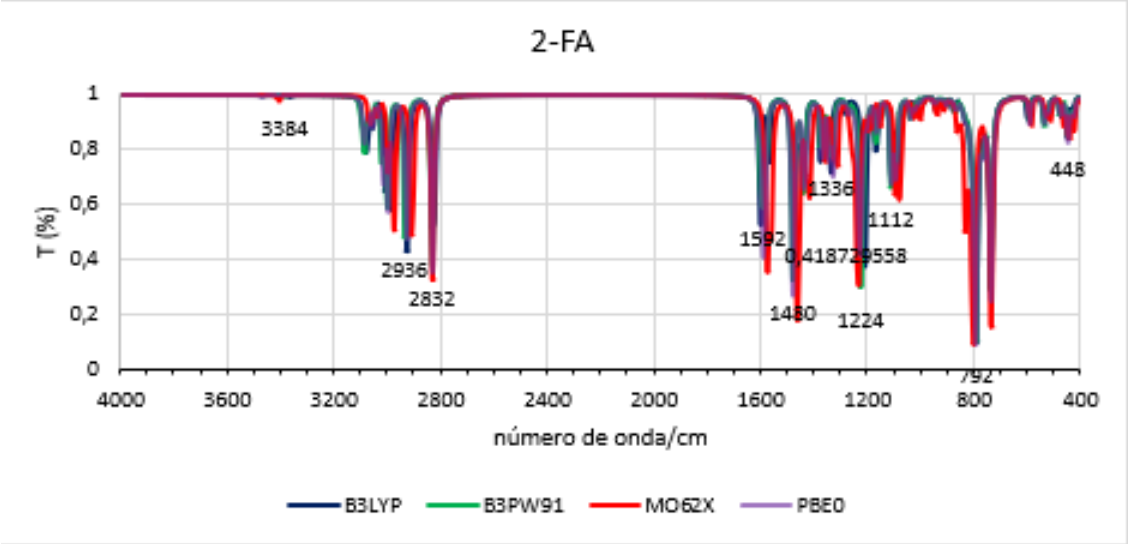


Figure S5. Infrared Theoretical Spectra for 2-FMA:

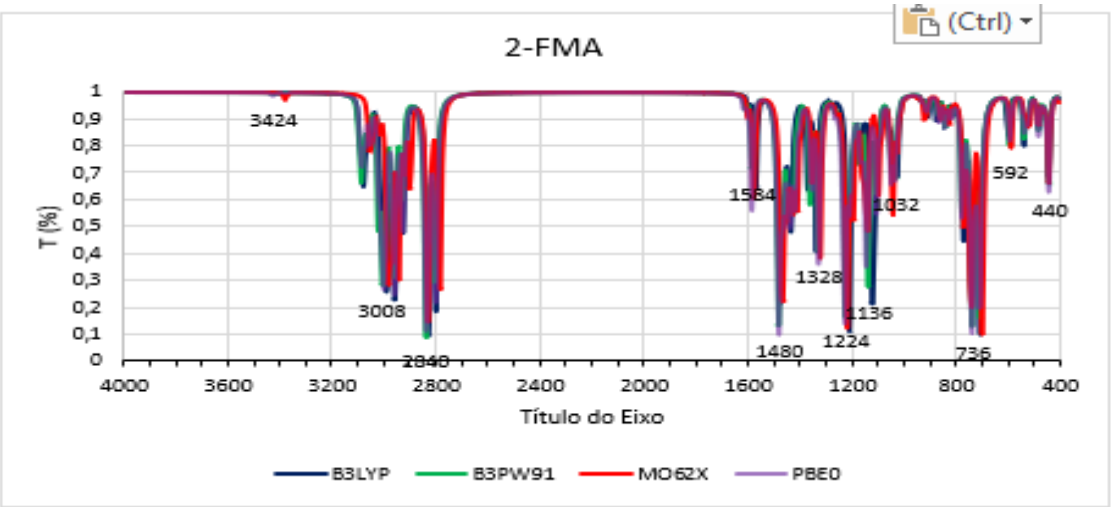


Figure S6. Infrared Theoretical Spectra for 3-FA:

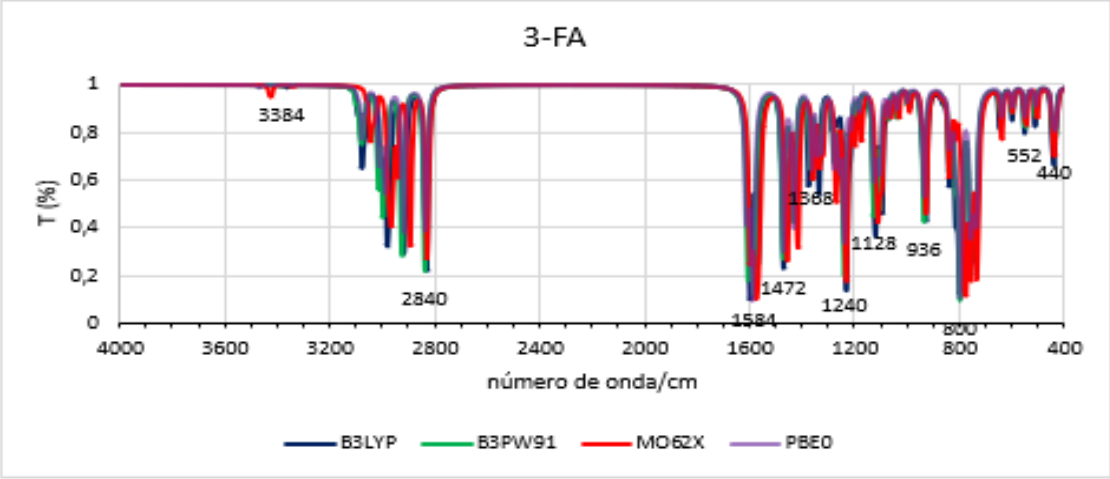


Figure S7. Infrared Theoretical Spectra for 3-FMA:

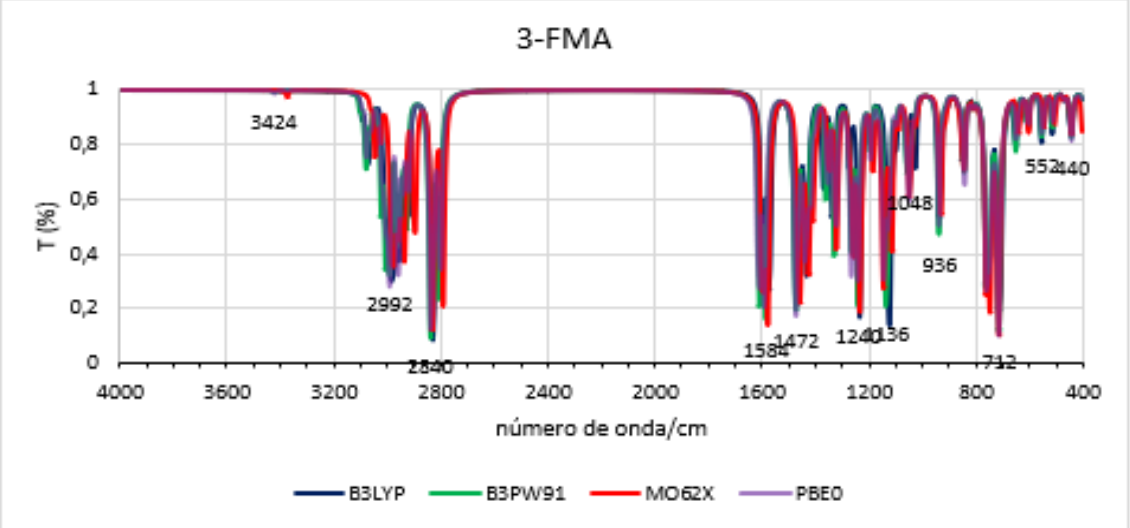


Figure S8. Infrared Theoretical Spectra for 4-FA:

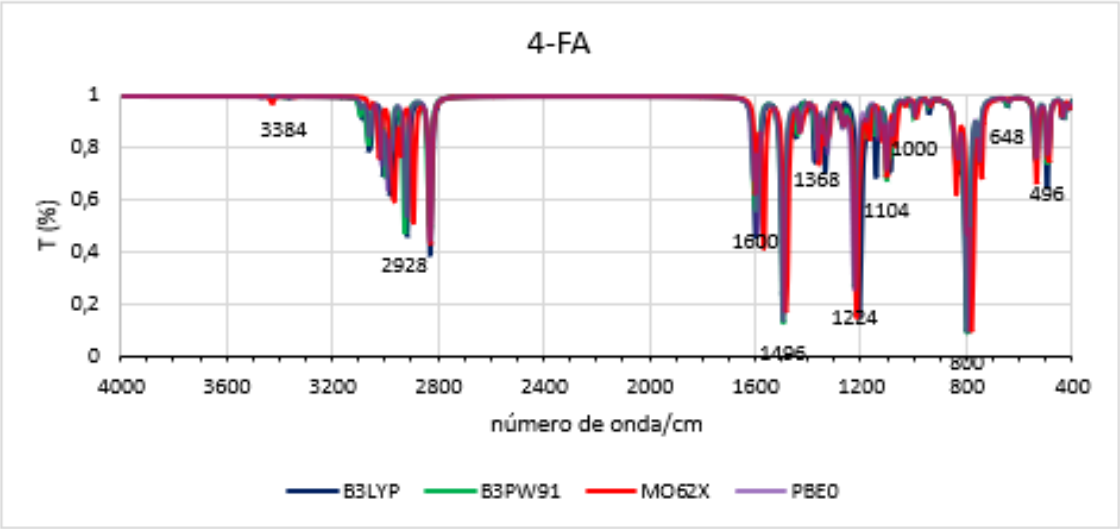


Figure S9. Infrared Theoretical Spectra for 4-FMA:

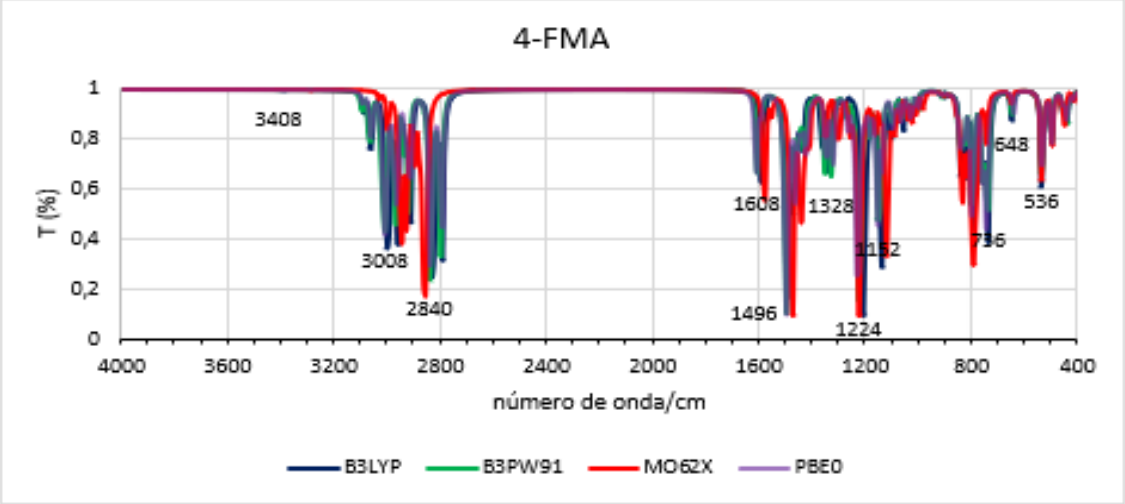


Figure S10. Infrared Theoretical Spectra for 4-MA:

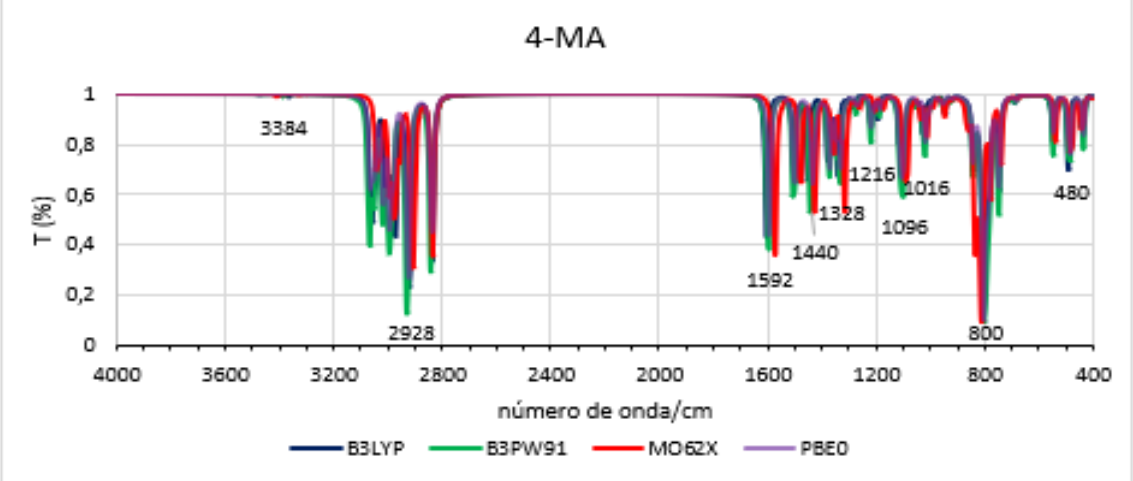


Figure S11. Infrared Theoretical Spectra for 25-DMA:

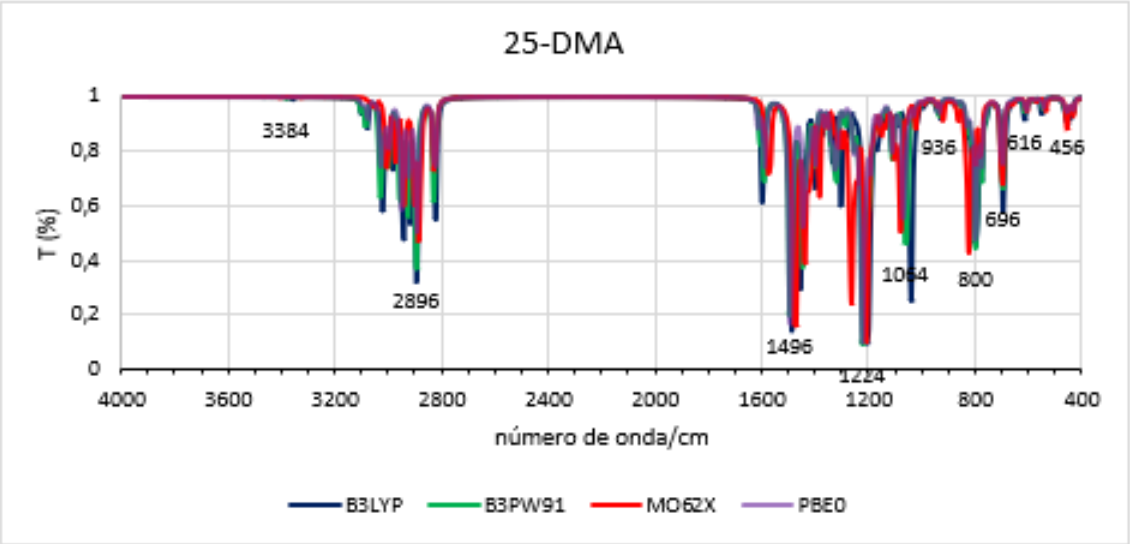


Figure S12. Infrared Theoretical Spectra for 34-MDA:

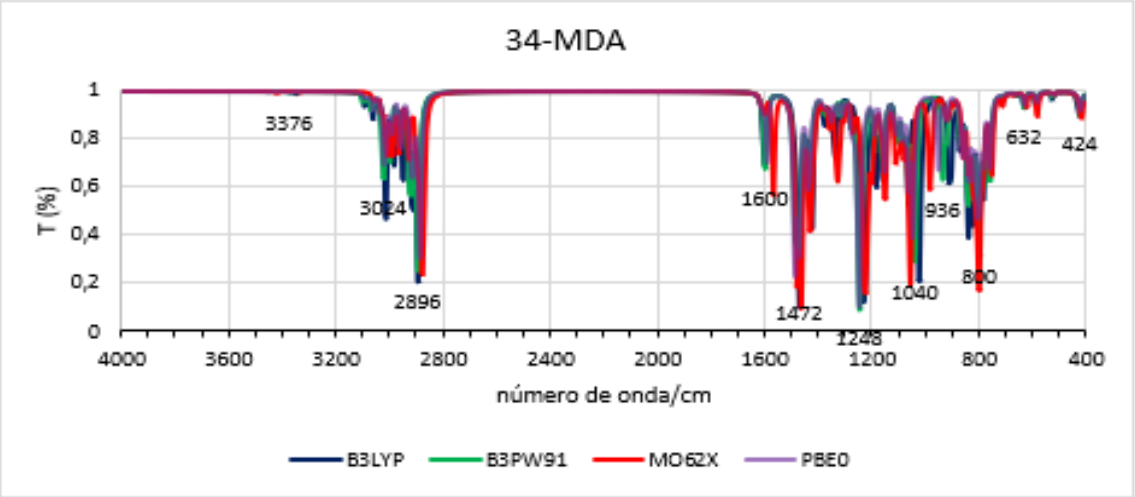


Figure S13. Infrared Theoretical Spectra for amphetamine:

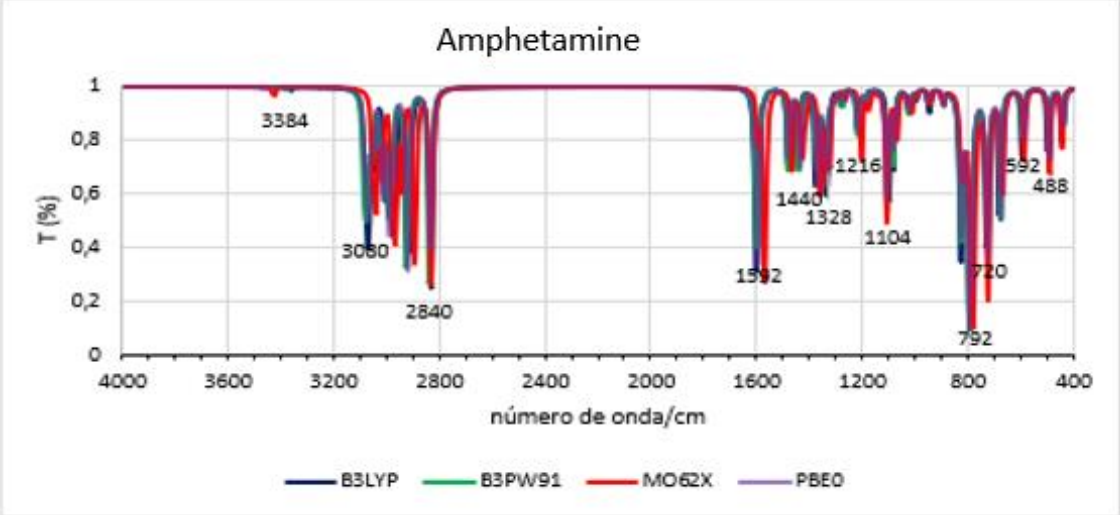


Figure S14. Infrared Theoretical Spectra for DMA:

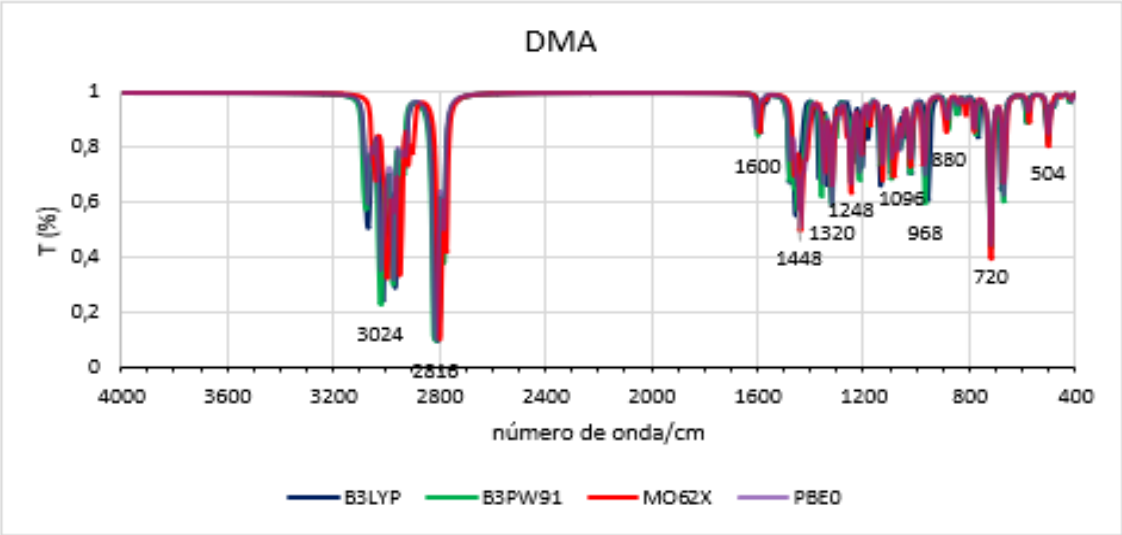


Figure S15. Infrared Theoretical Spectra for MDMA:

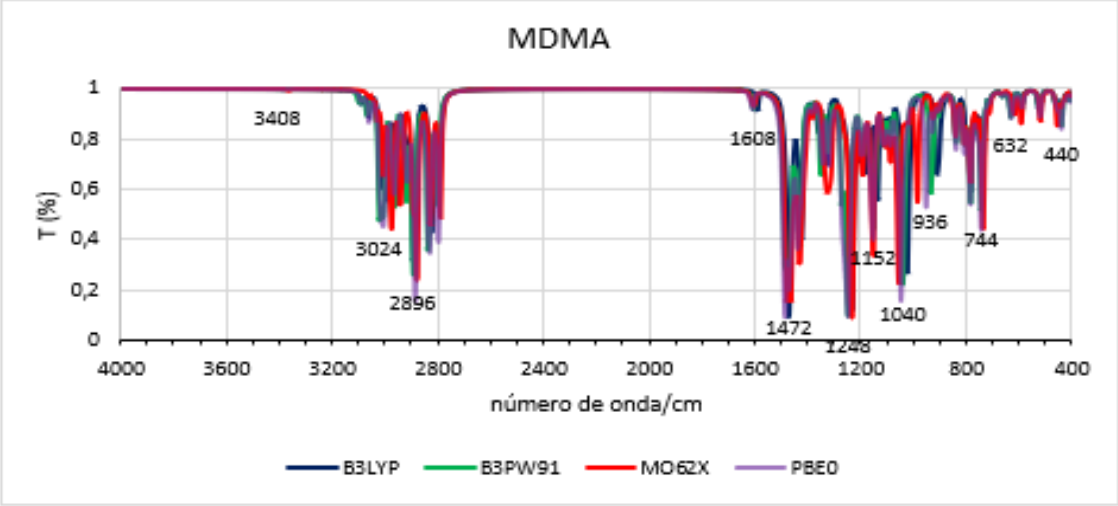


Figure S16. Infrared Theoretical Spectra for methamphetamine:

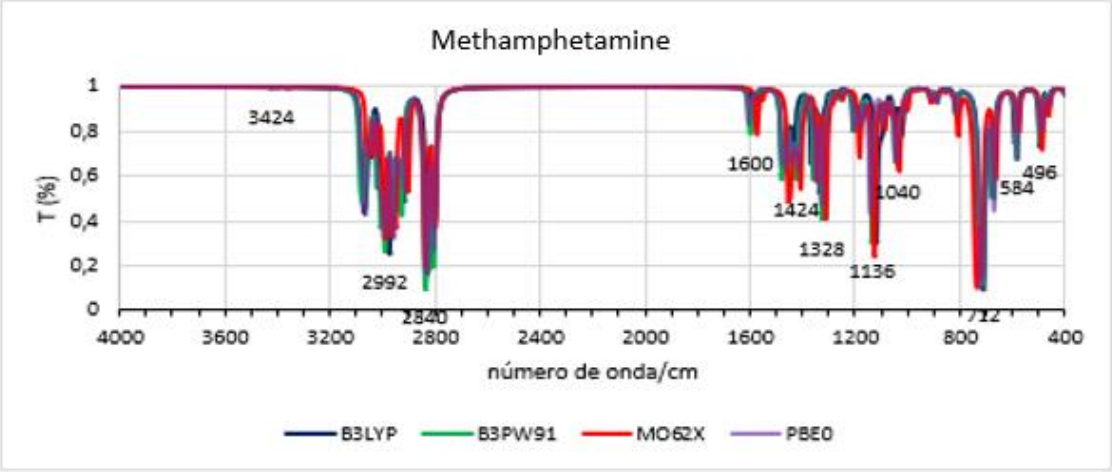


Figure S17. Infrared Theoretical Spectra for PMA:

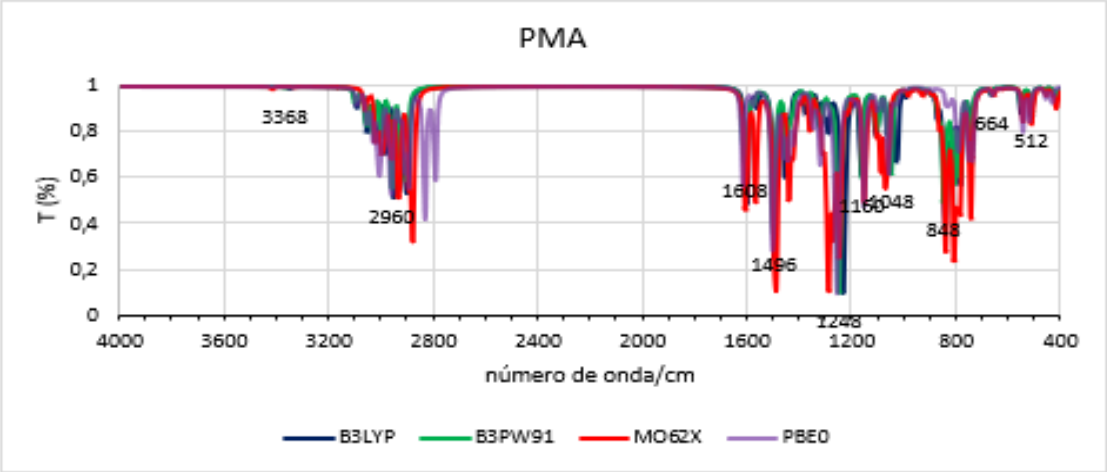


Figure S18. Infrared Theoretical Spectra for PMMA:

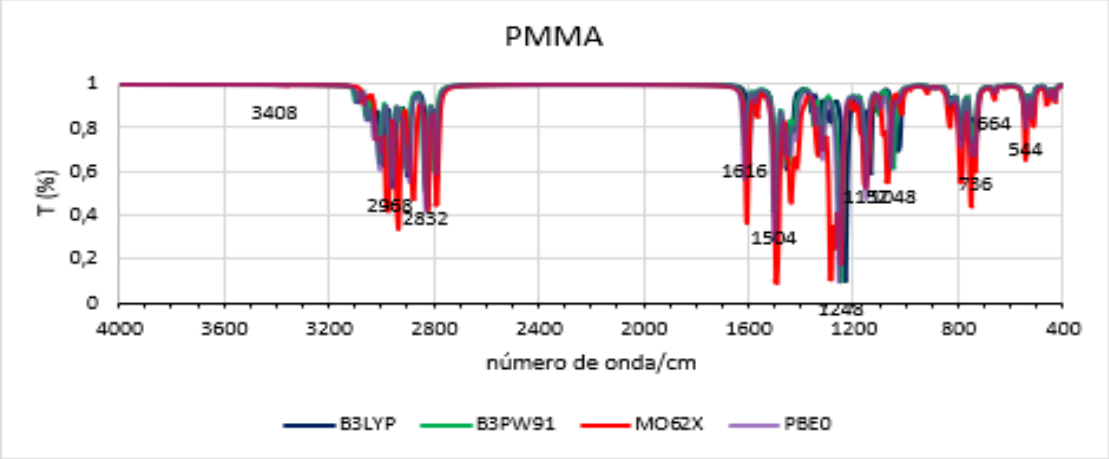


Figure S19. Infrared Theoretical Spectra for Adinazolam:

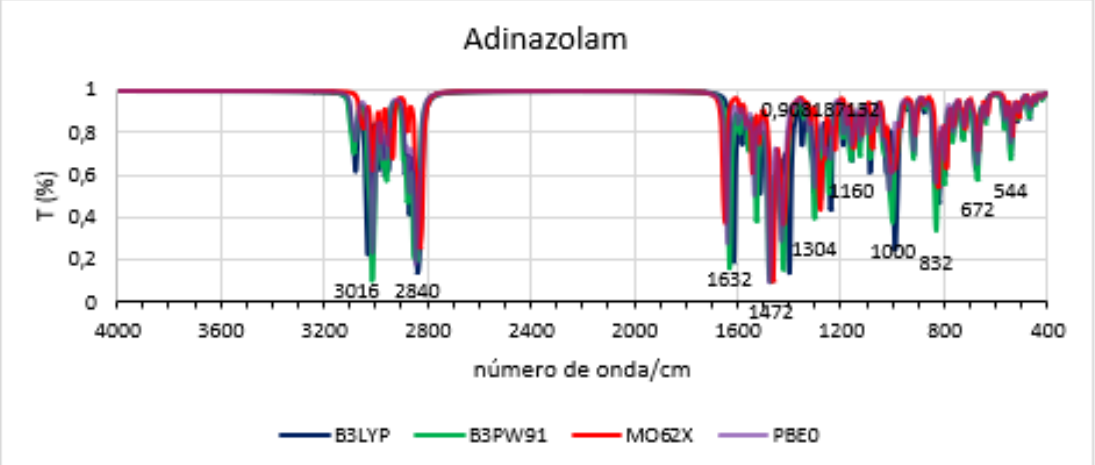


Figure S20. Infrared Theoretical Spectra for Alprazolam:

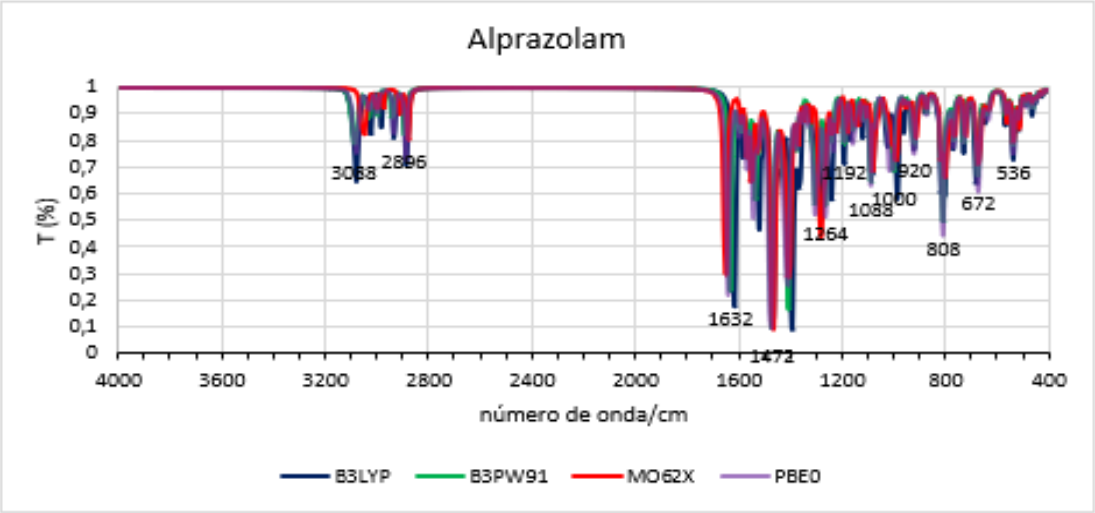


Figure S21. Infrared Theoretical Spectra for Bromazolam:

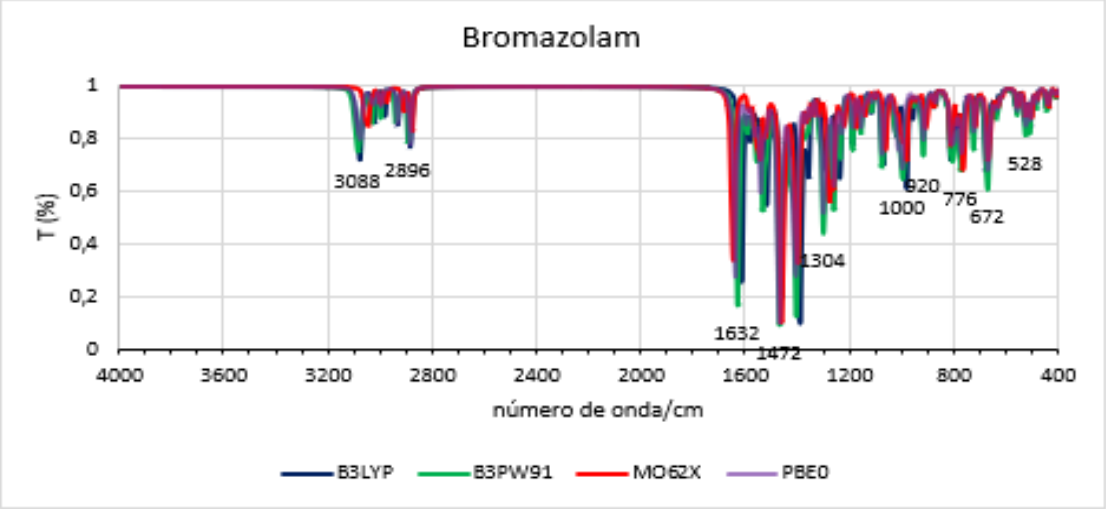


Figure S22. Infrared Theoretical Spectra for Clonazolam:

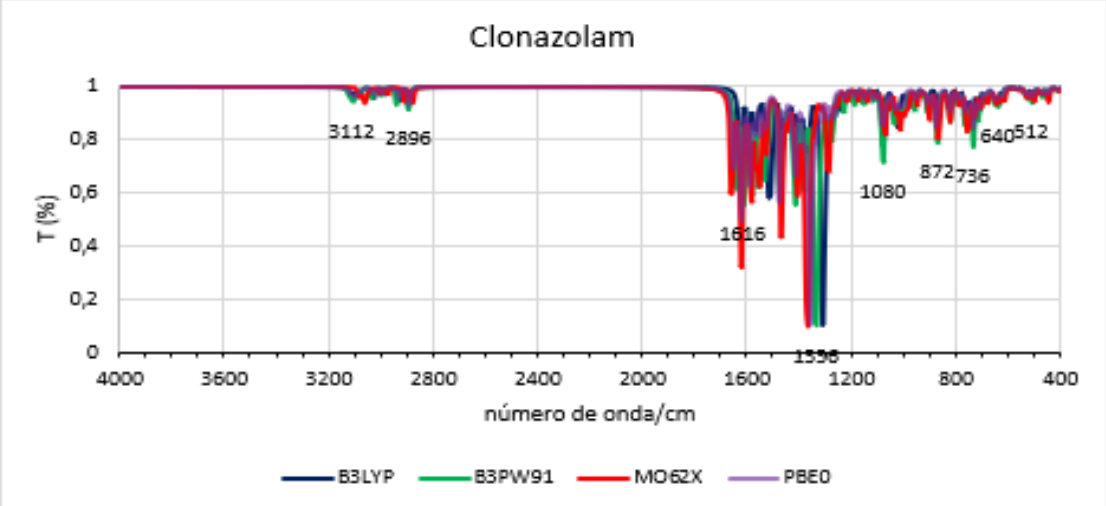


Figure S23. Infrared Theoretical Spectra for Diazepam:

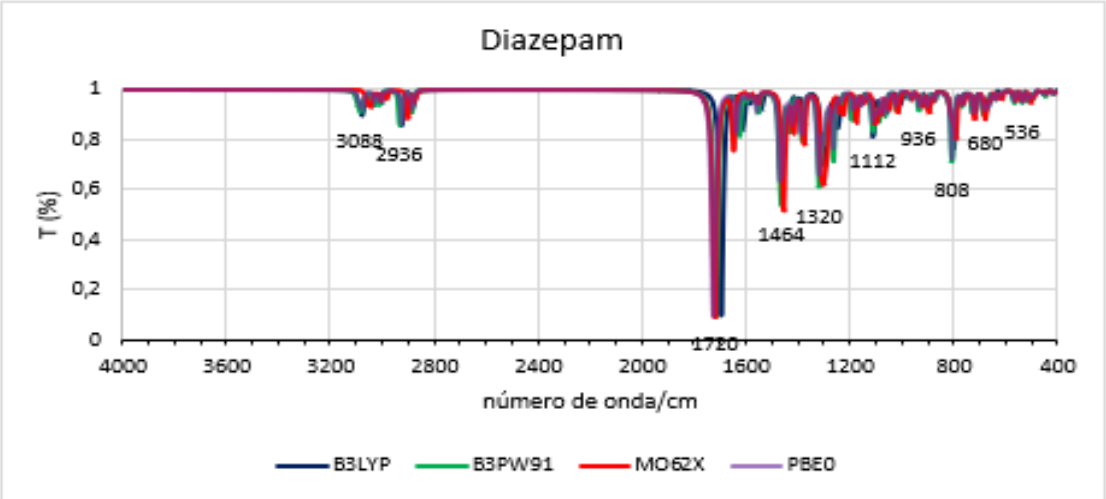


Figure S24. Infrared Theoretical Spectra for Diclazepam:

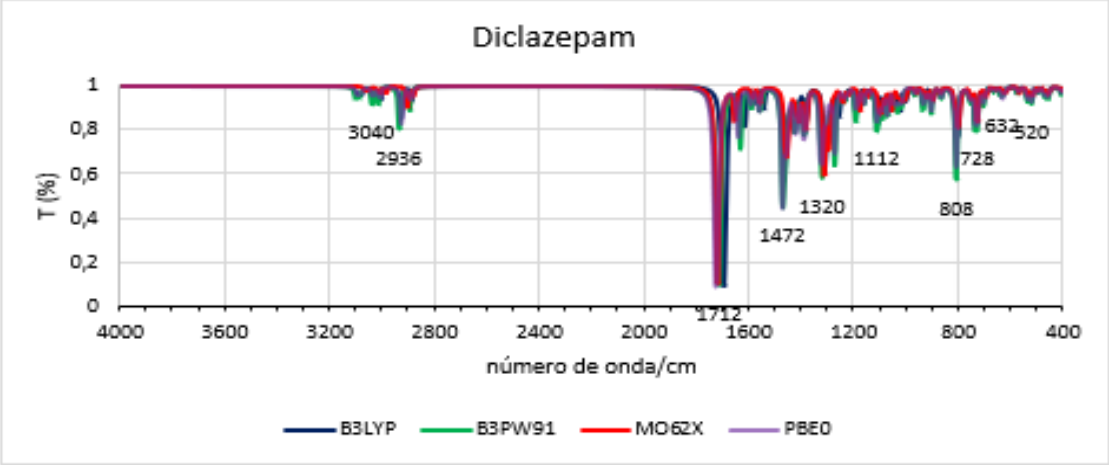


Figure S25. Infrared Theoretical Spectra for Flualprazolam:

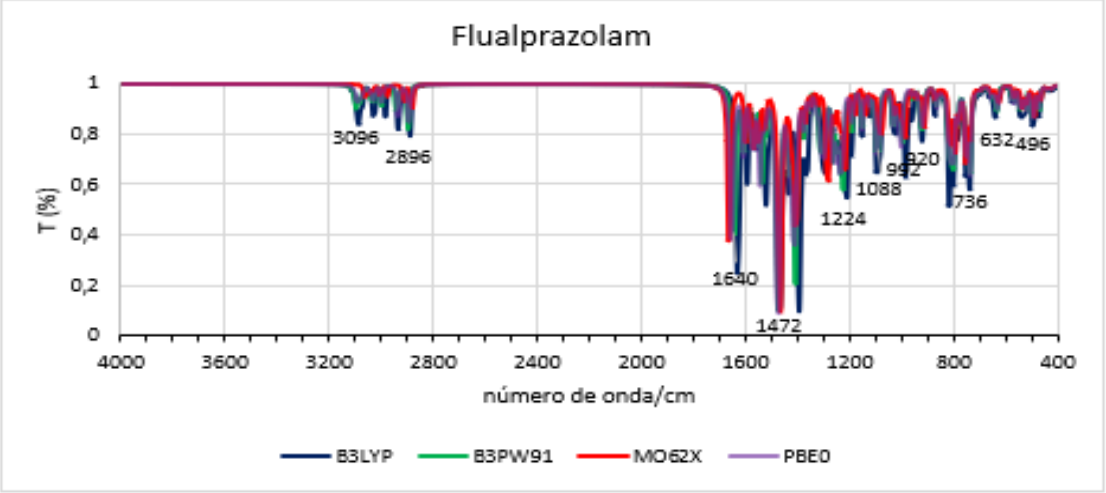


Figure S26. Infrared Theoretical Spectra for Flubromazepam:

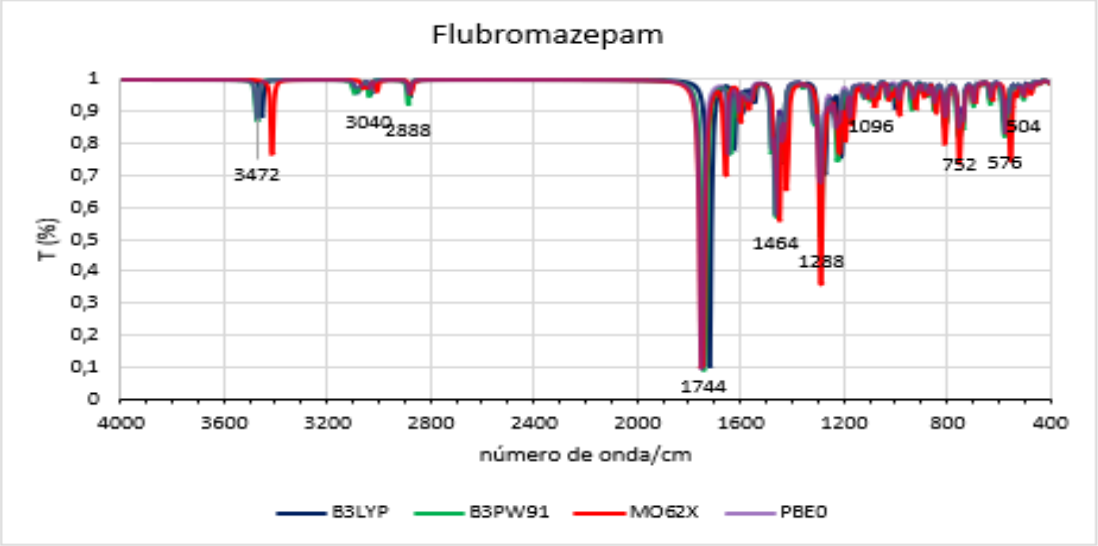


Figure S27. Infrared Theoretical Spectra for Flubromazolam:

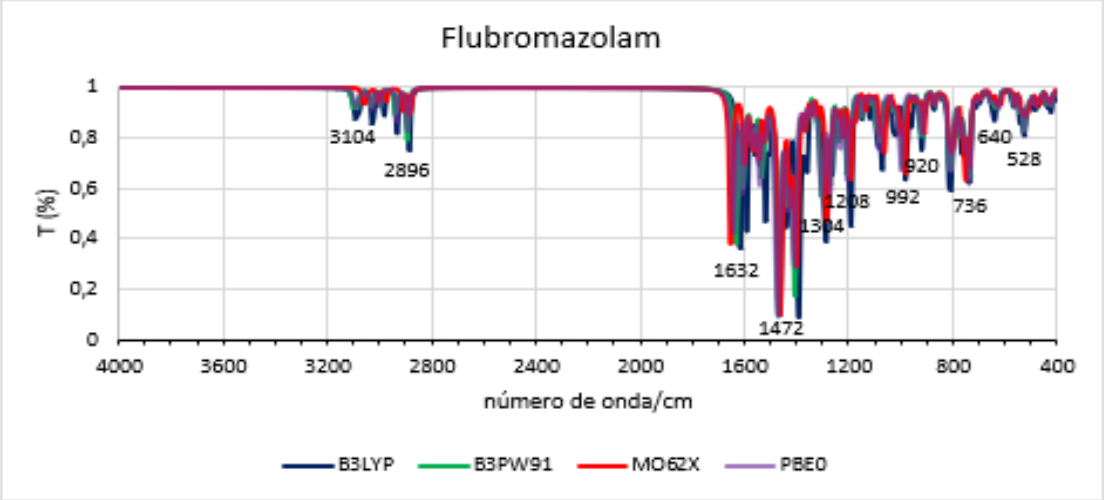


Figure S28. Infrared Theoretical Spectra for Flunitrazepam:

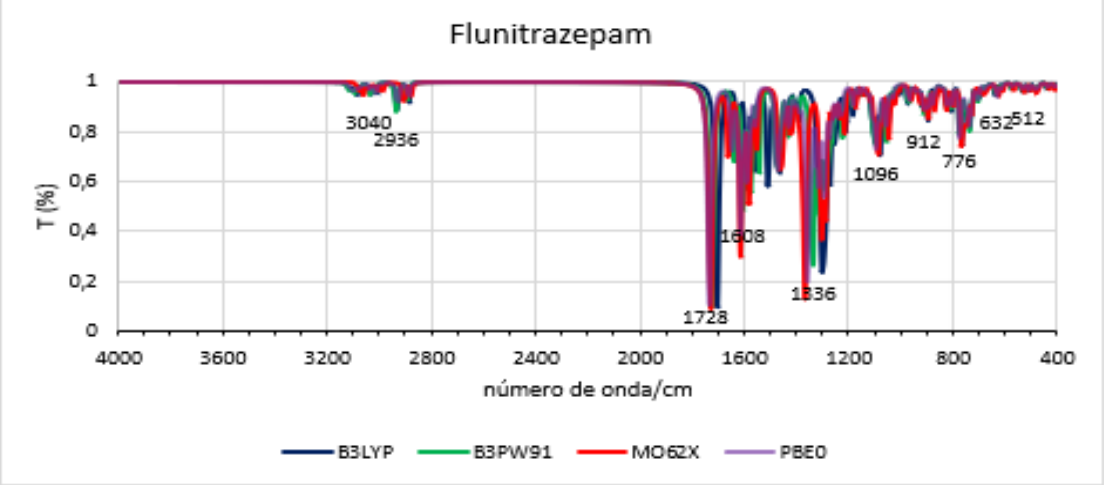


Figure S29. Infrared Theoretical Spectra for Flunitrazolam:

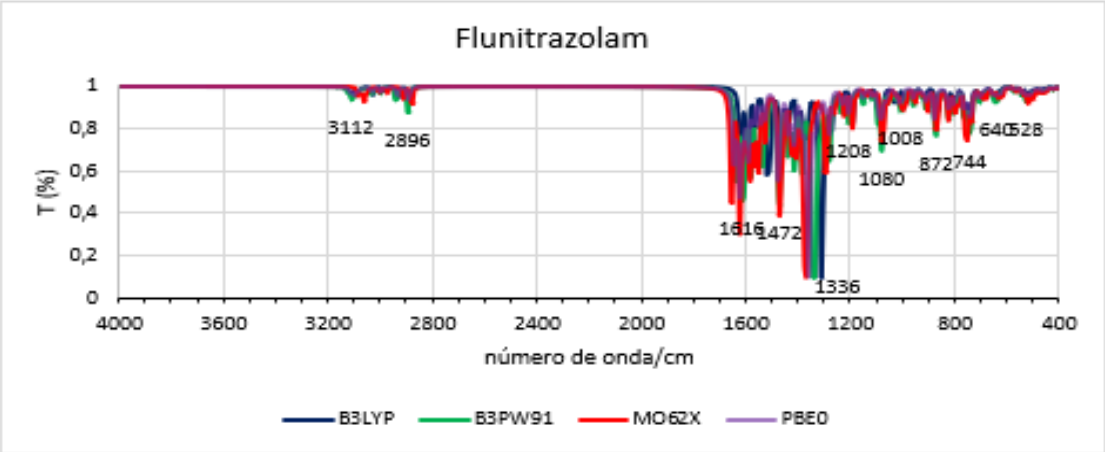


Figure S30. Infrared Theoretical Spectra for Midazolam:

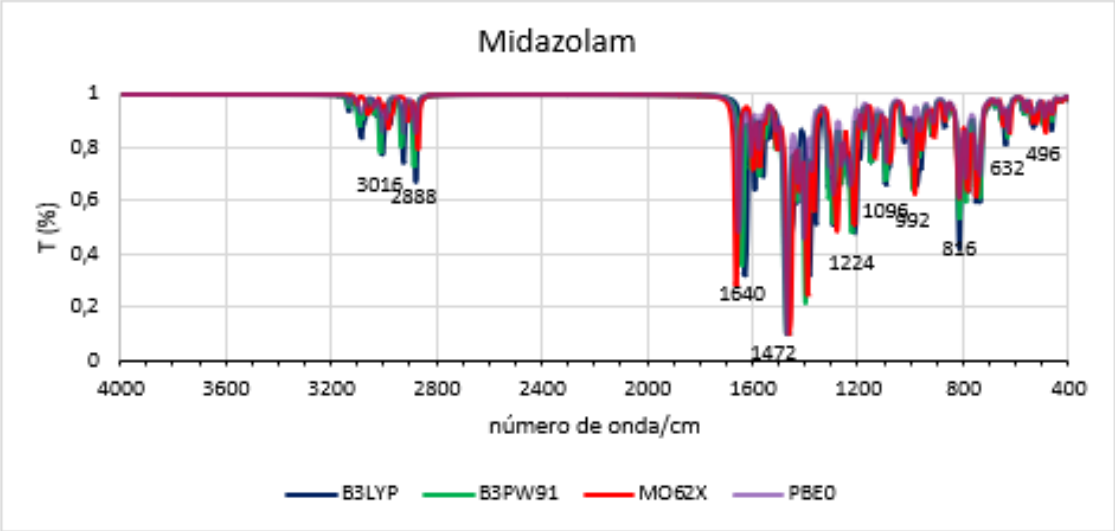


Figure S31. Infrared Theoretical Spectra for Oxazepam:

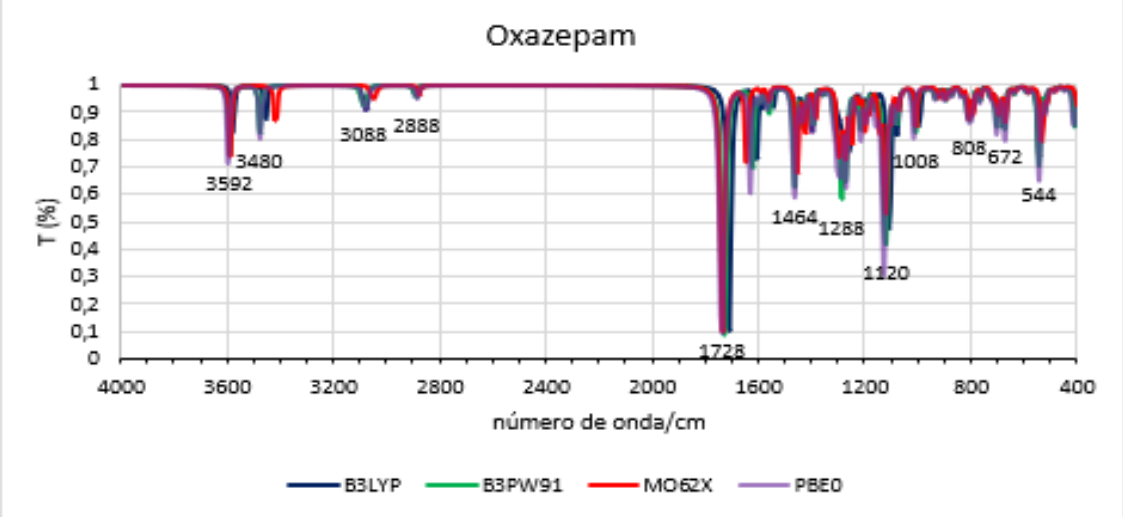


Figure S32. Infrared Theoretical Spectra for AM-1220:

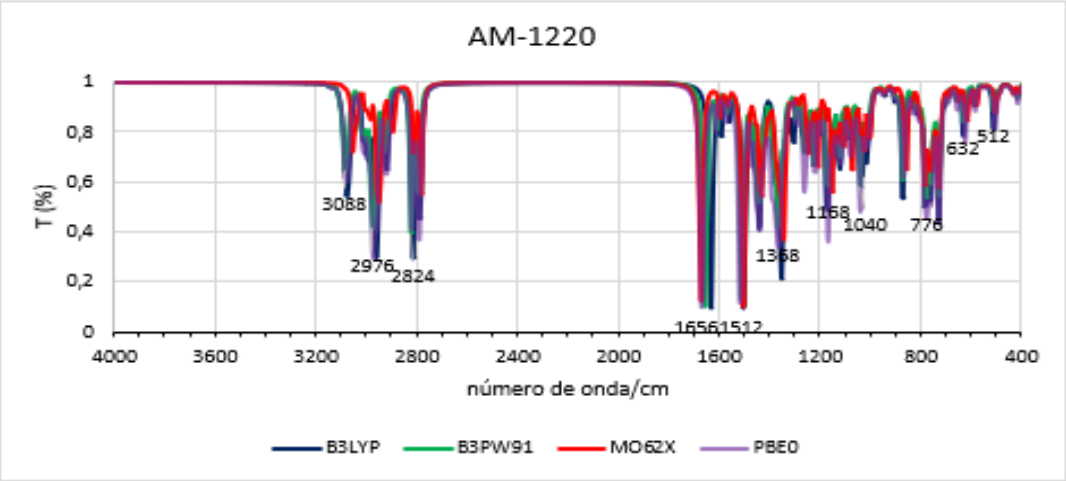


Figure S33. Infrared Theoretical Spectra for AM-1248:

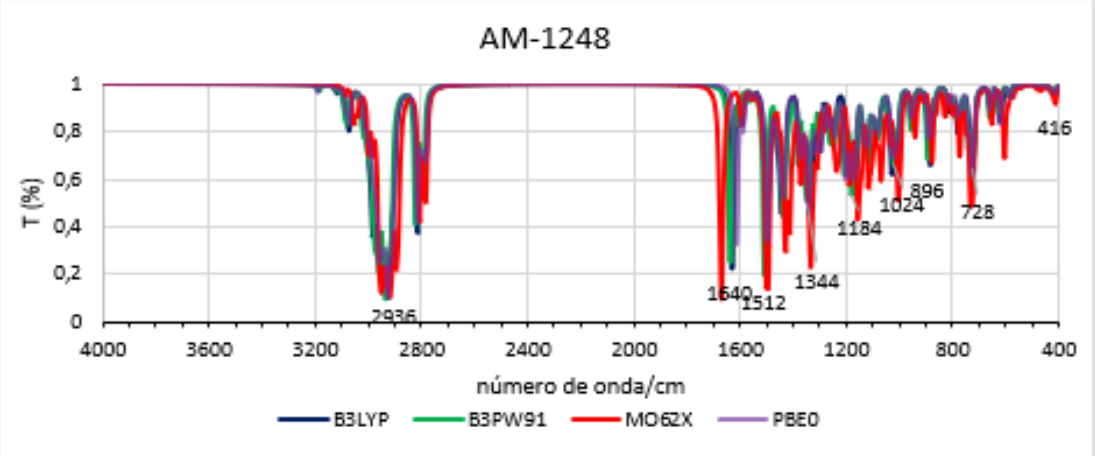


Figure S34. Infrared Theoretical Spectra for Cannabidiol:

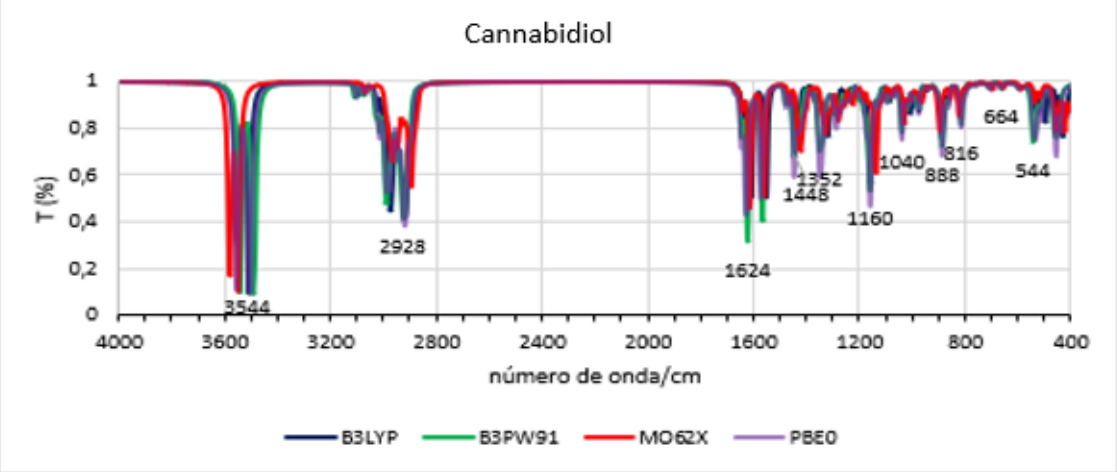


Figure S35. Infrared Theoretical Spectra for Cannabinol:

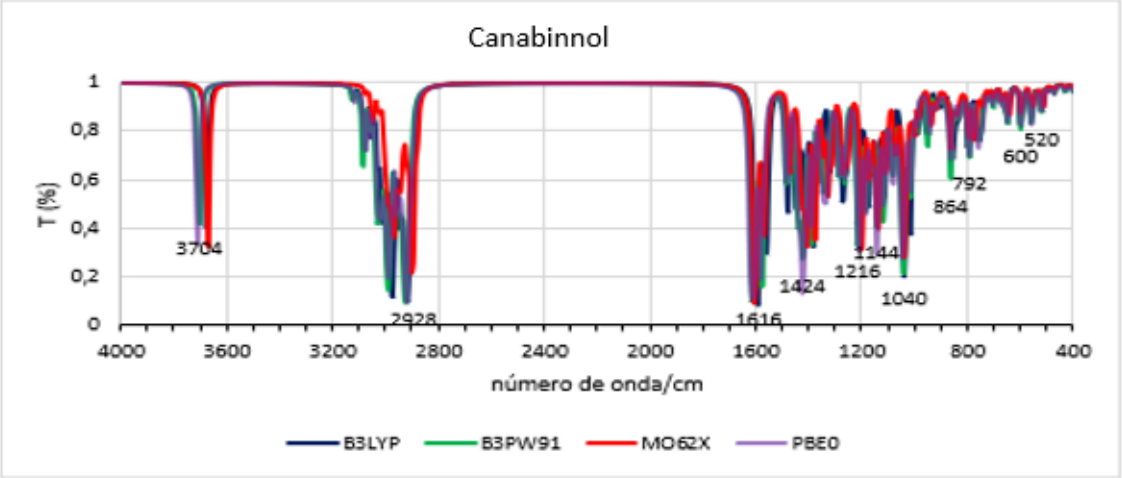


Figure S36. Infrared Theoretical Spectra for Δ9-THC:

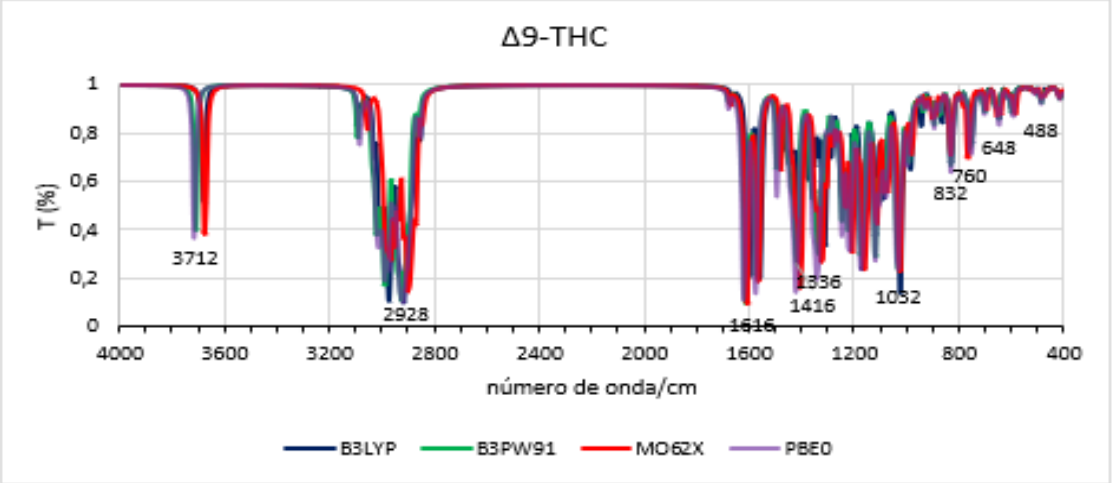


Figure S37. Infrared Theoretical Spectra for JWH-018:

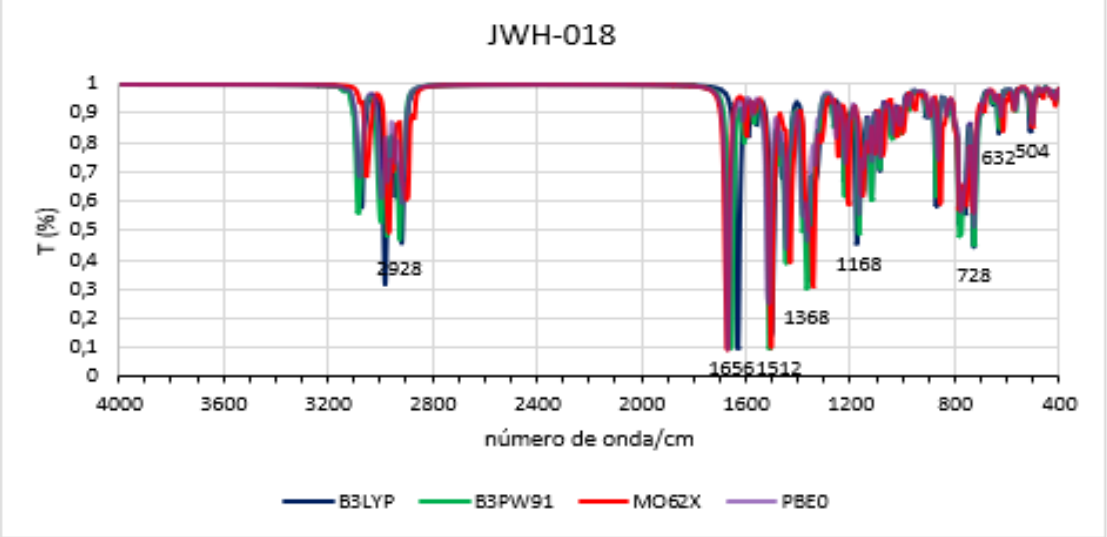


Figure S38. Infrared Theoretical Spectra for JWH-019:

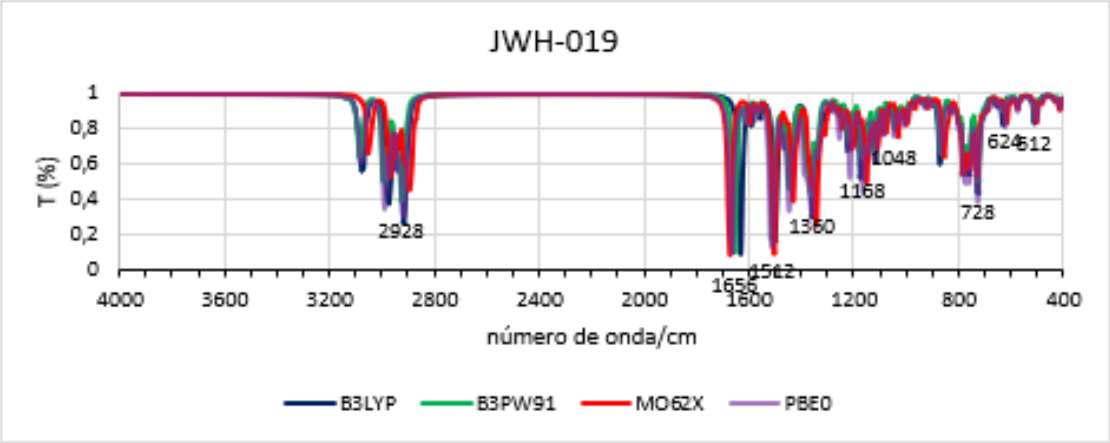


Figure S39. Infrared Theoretical Spectra for JWH-022:

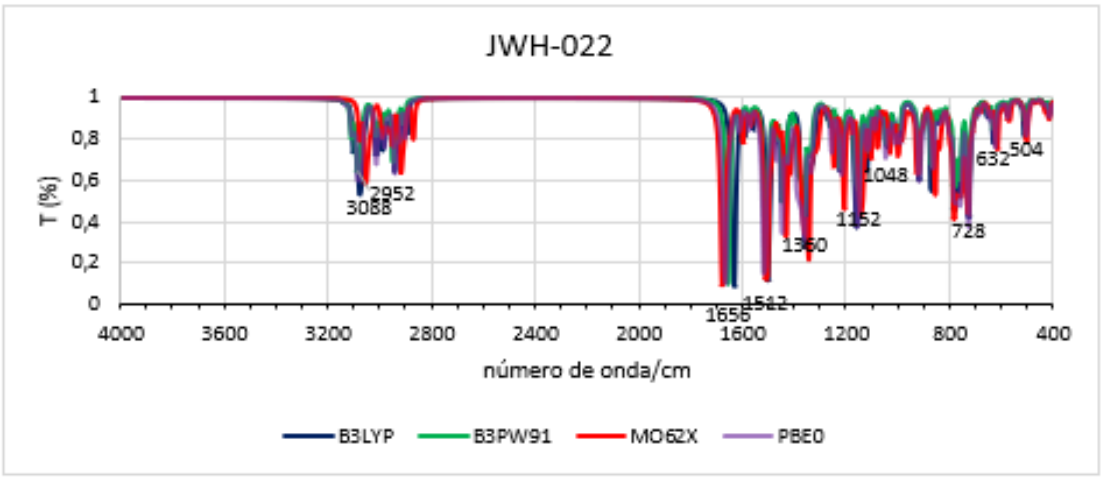


Figure S40. Infrared Theoretical Spectra for JWH-073:

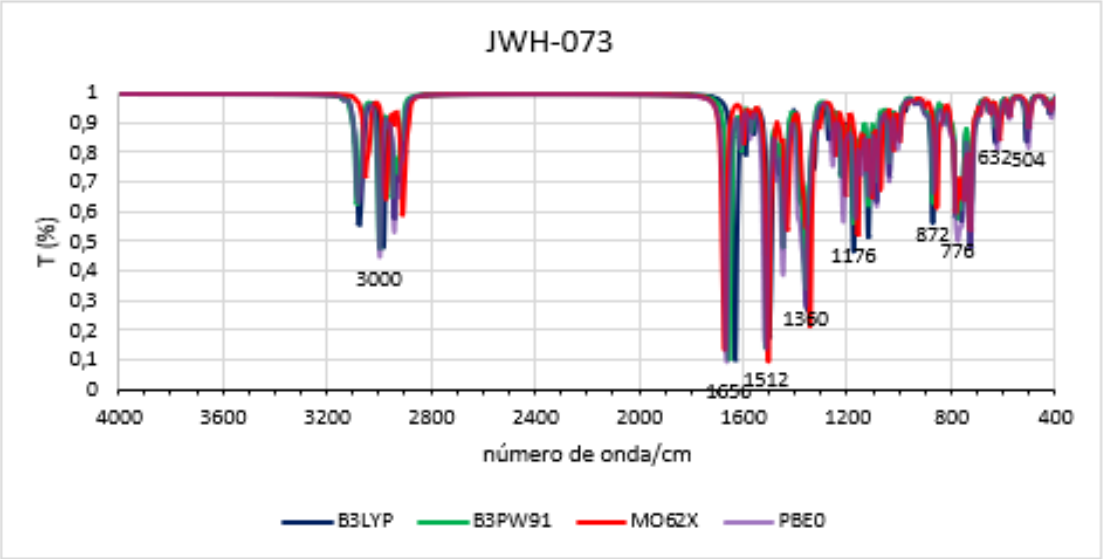


Figure S41. Infrared Theoretical Spectra for JWH-081:

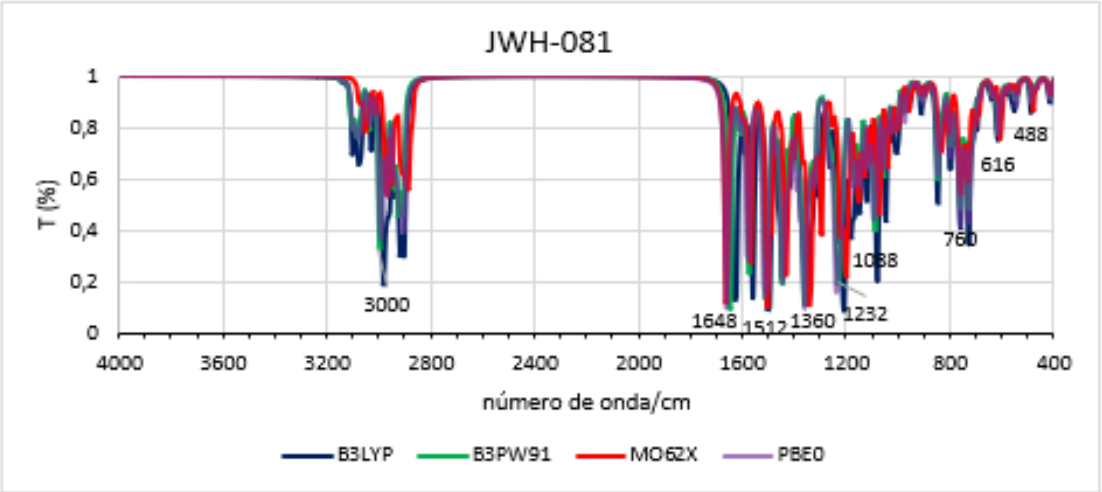


Figure S42. Infrared Theoretical Spectra for JWH-122:

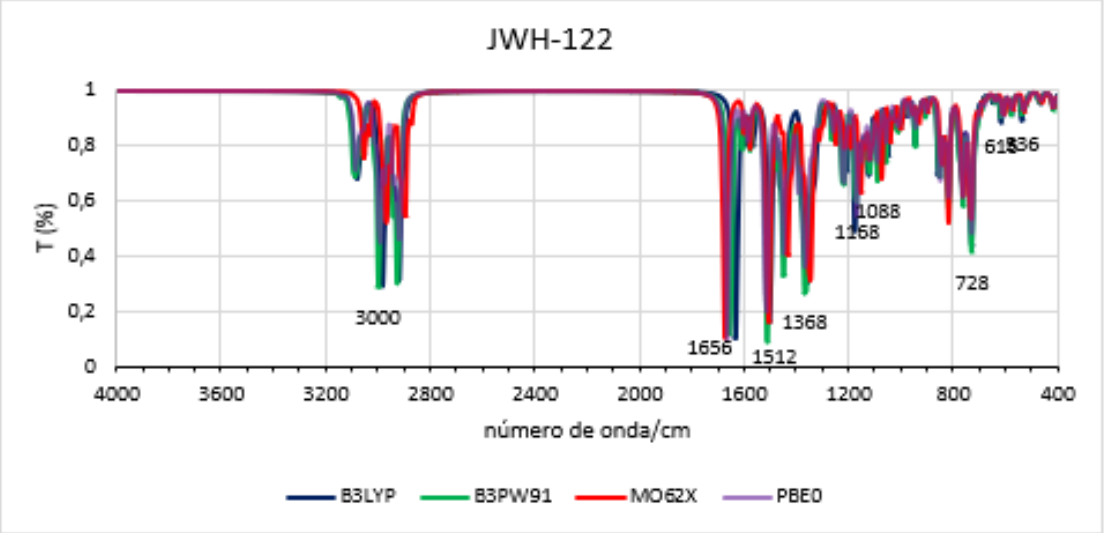


Figure S43. Infrared Theoretical Spectra for JWH-203:

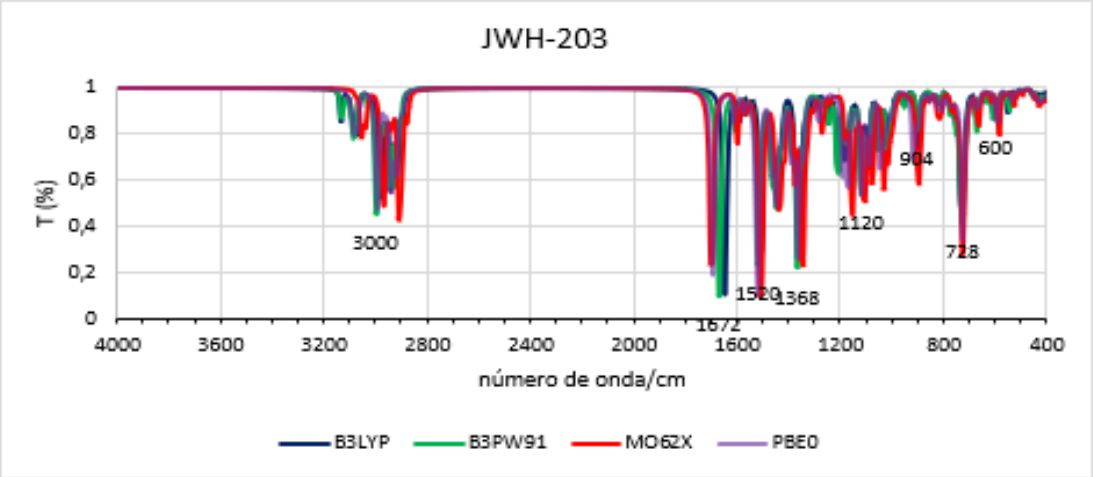


Figure S44. Infrared Theoretical Spectra for JWH-210:

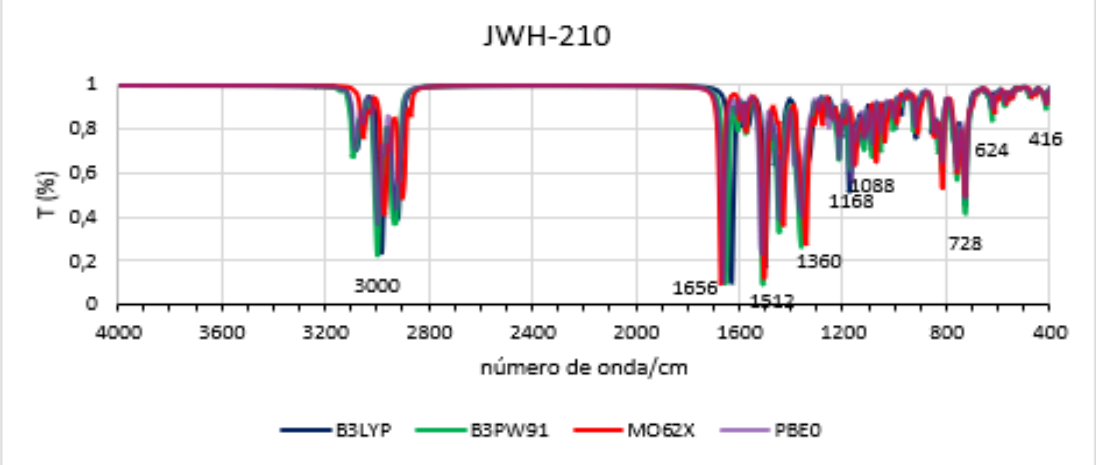


Figure S45. Infrared Theoretical Spectra for JWH-250:

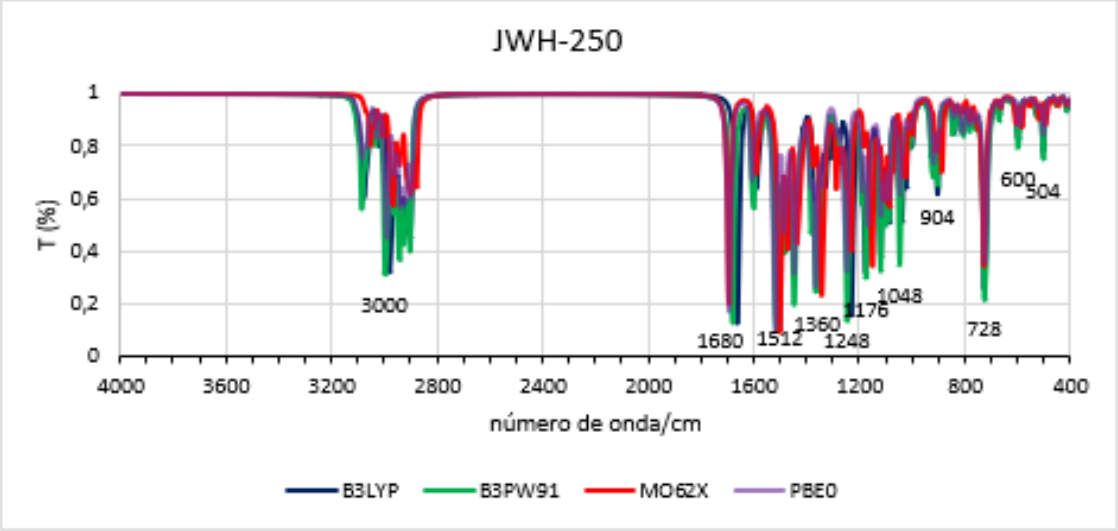


Figure S46. Infrared Theoretical Spectra for JWH-307:

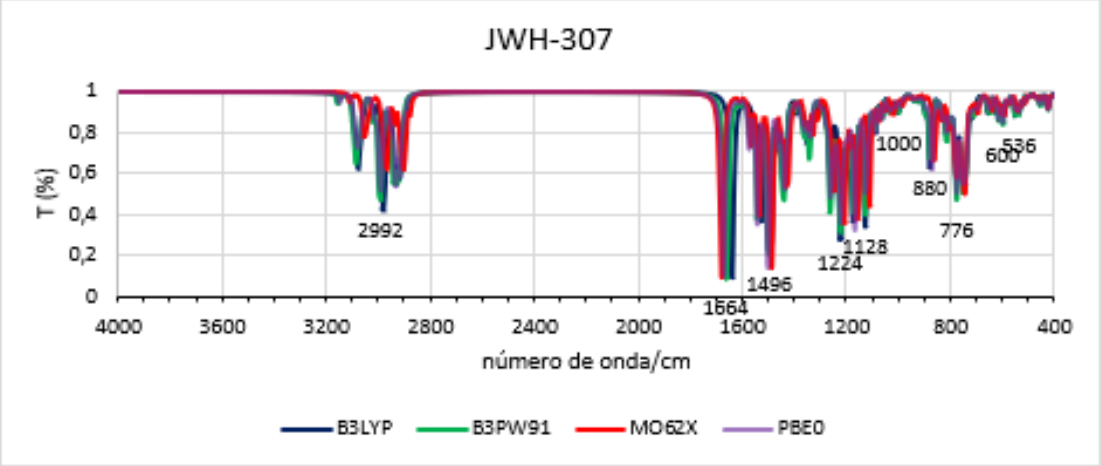


Figure S47. Infrared Theoretical Spectra for 2-FEC:

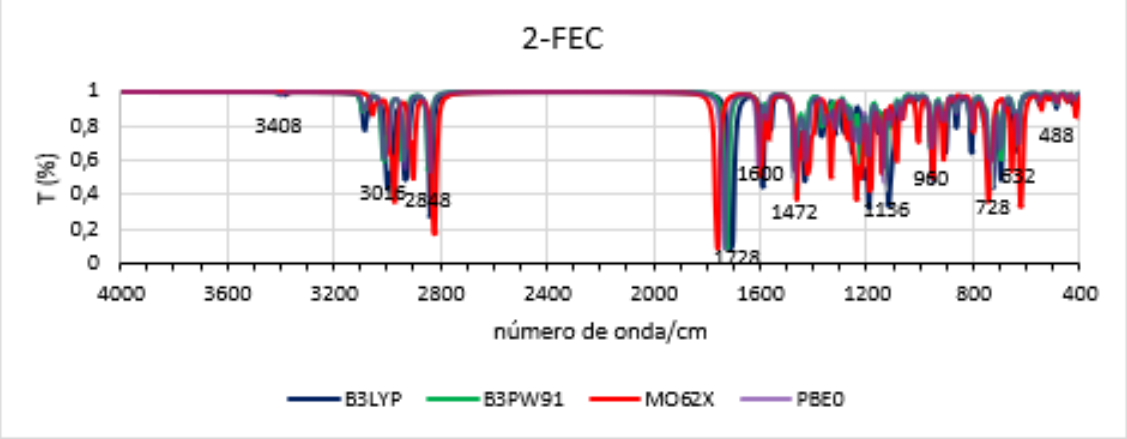


Figure S48. Infrared Theoretical Spectra for 2-FMC:

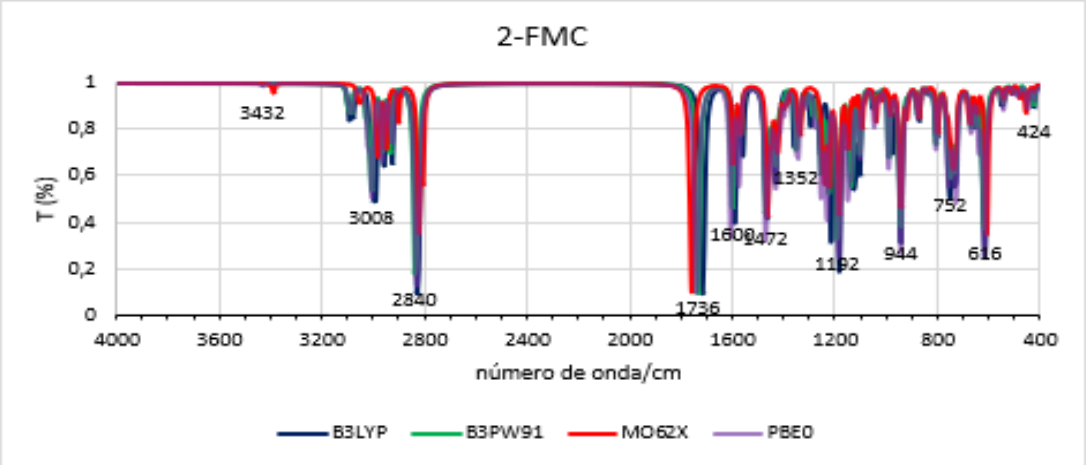


Figure S49. Infrared Theoretical Spectra for 2-MEC:

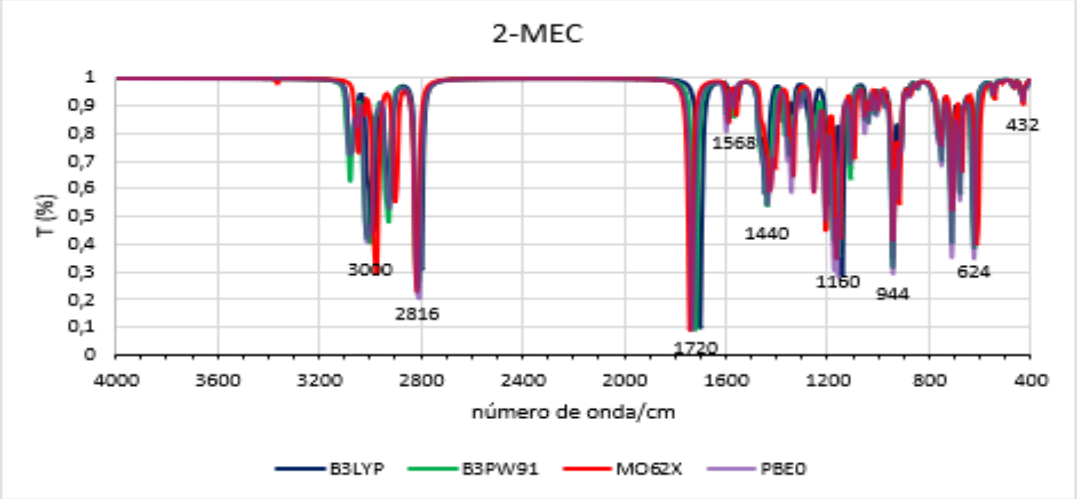


Figure S50. Infrared Theoretical Spectra for 2-FEC:

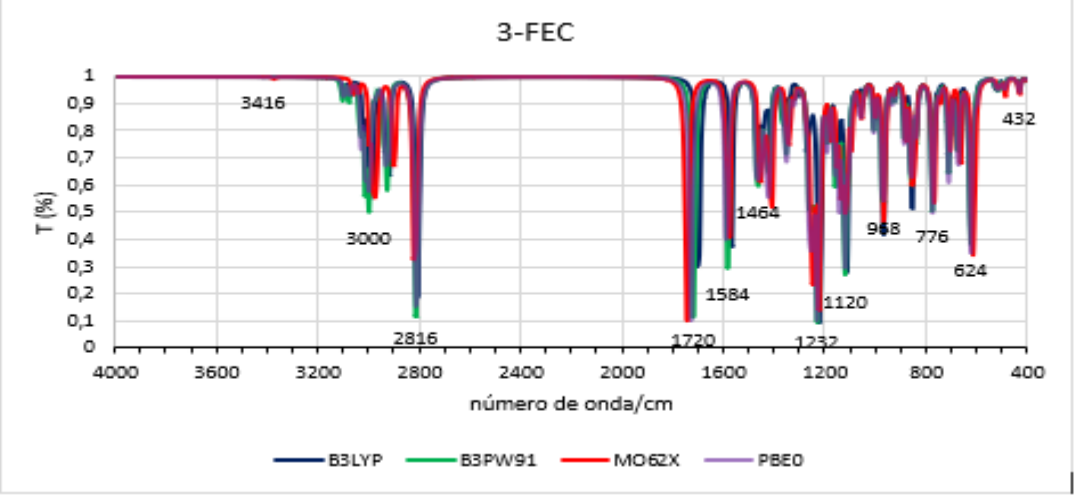


Figure S51. Infrared Theoretical Spectra for 3-FMC:

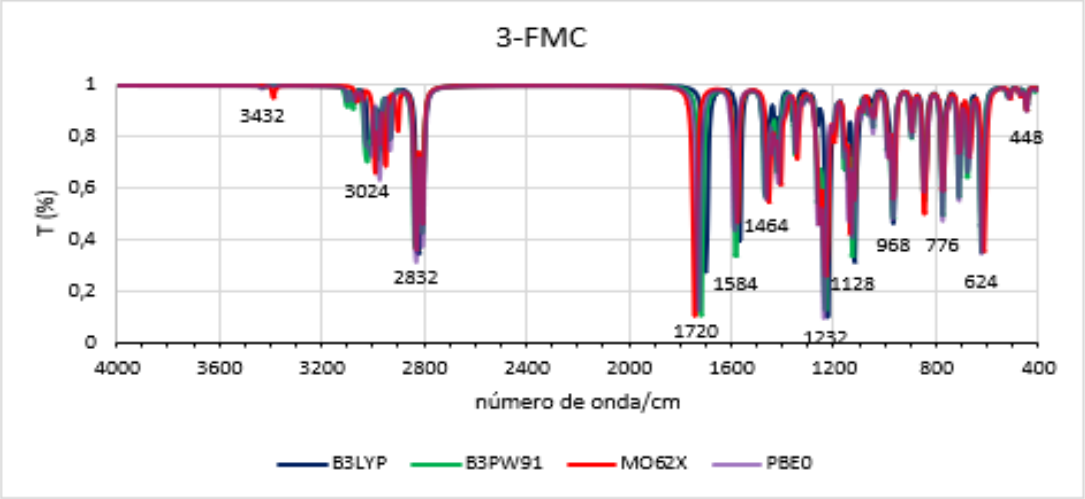


Figure S52. Infrared Theoretical Spectra for 3-MEC:

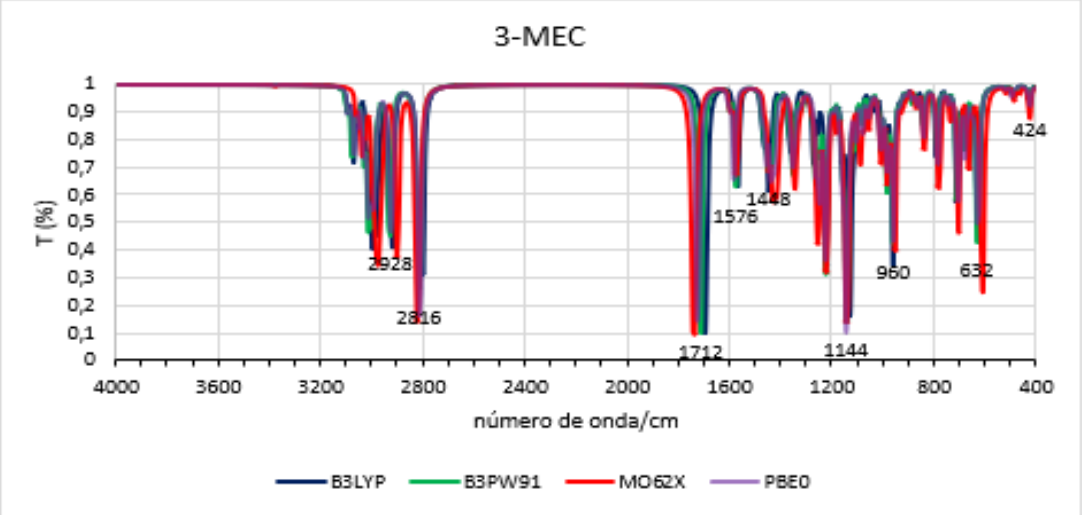


Figure S53. Infrared Theoretical Spectra for 4-FEC:

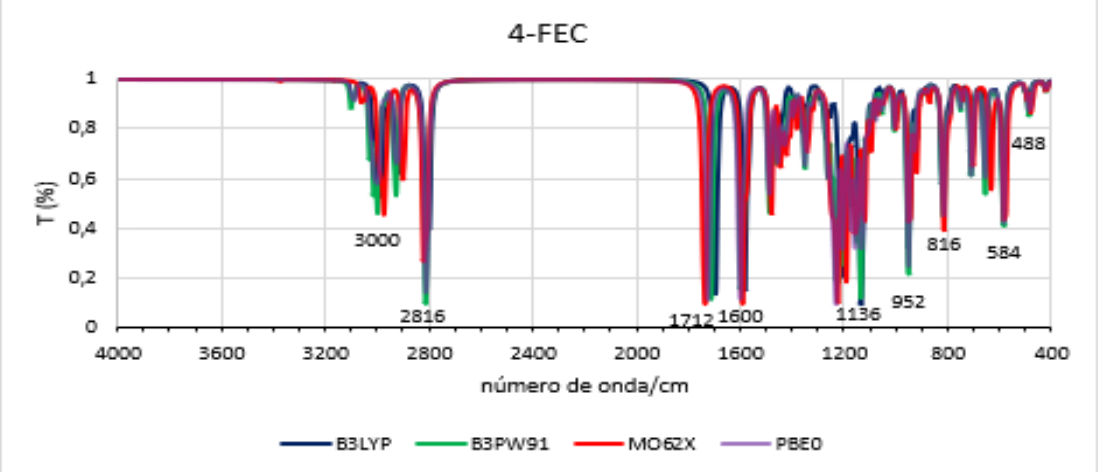


Figure S54. Infrared Theoretical Spectra for 4-FMC:

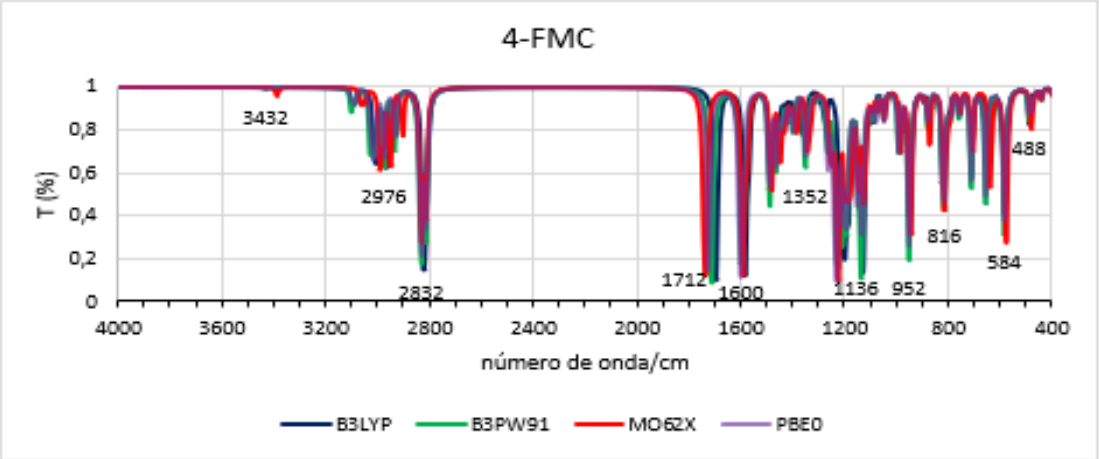


Figure S55. Infrared Theoretical Spectra for 4-MEC:

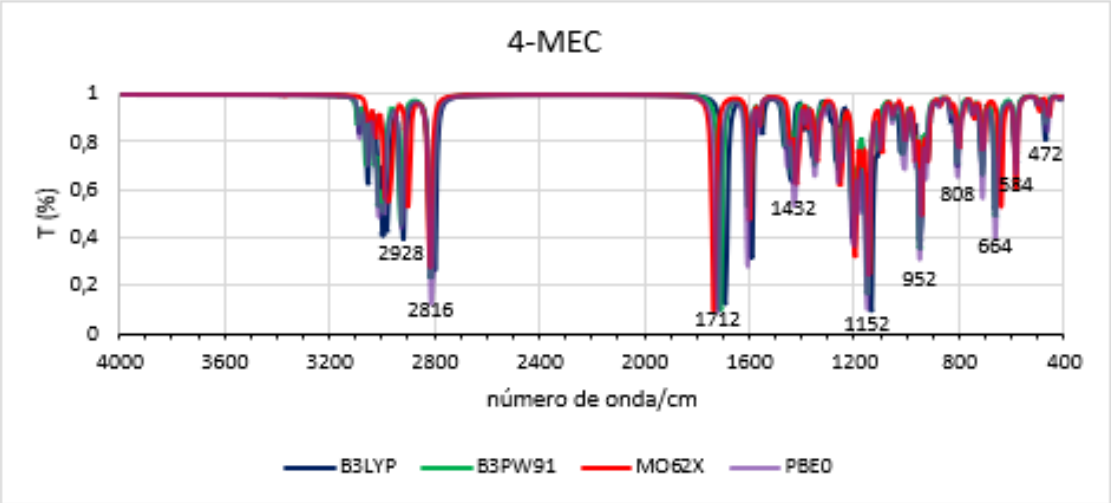


Figure S56. Infrared Theoretical Spectra for 23-DMMC:

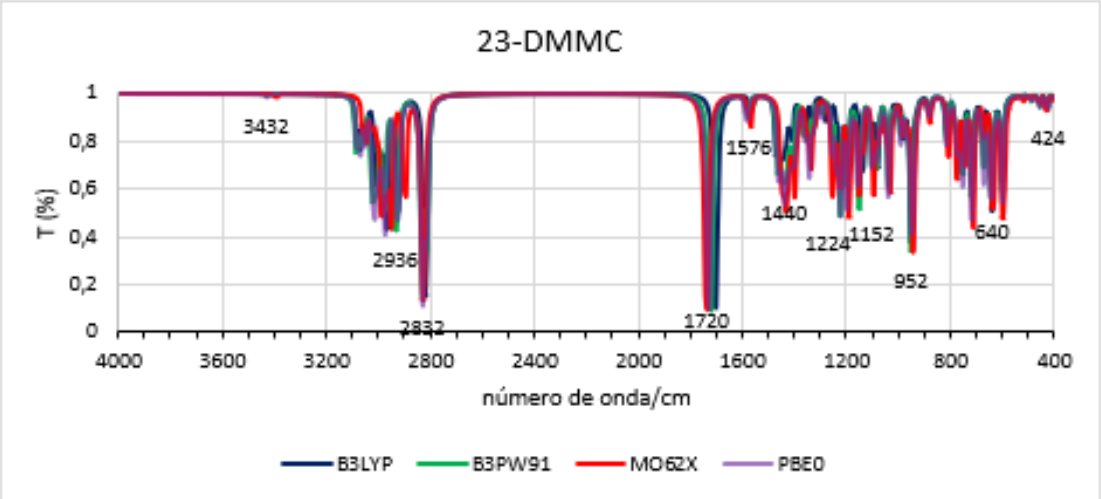


Figure S57. Infrared Theoretical Spectra for 24-DMMC:

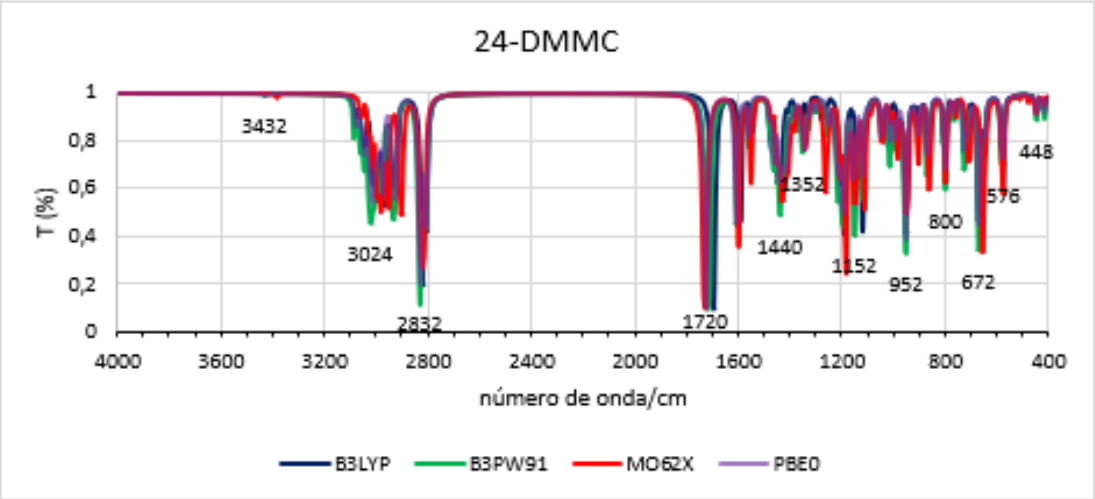


Figure S58. Infrared Theoretical Spectra for 25-DMMC:

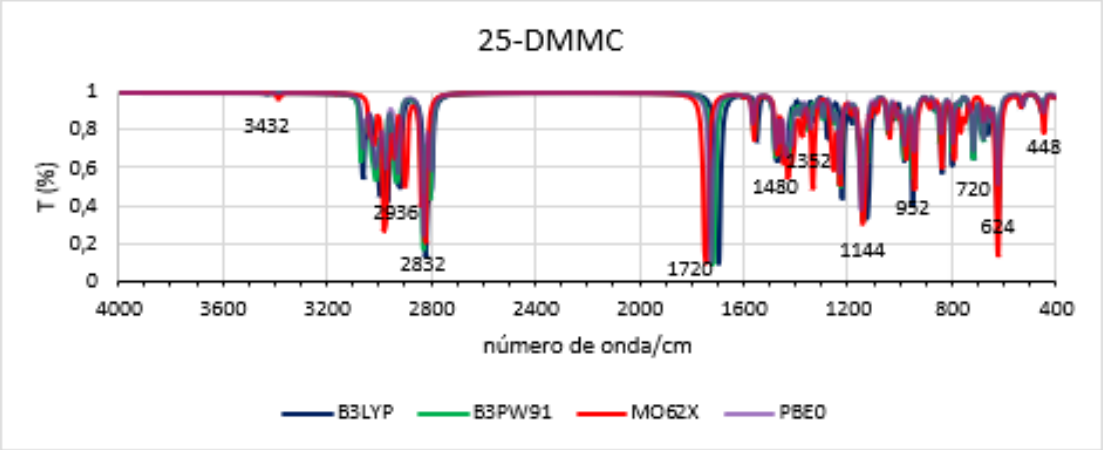


Figure S59. Infrared Theoretical Spectra for 34-DMMC:

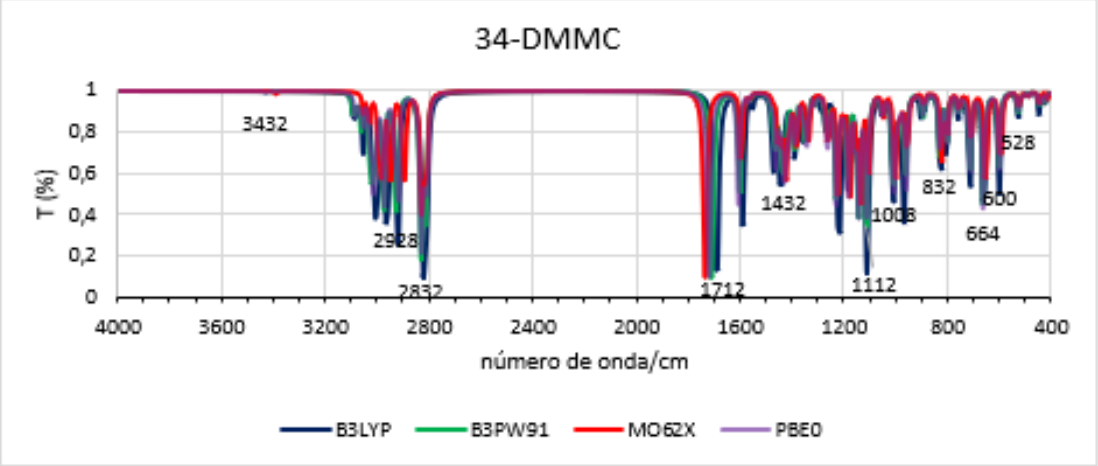


Figure S60. Infrared Theoretical Spectra for Cathinone:

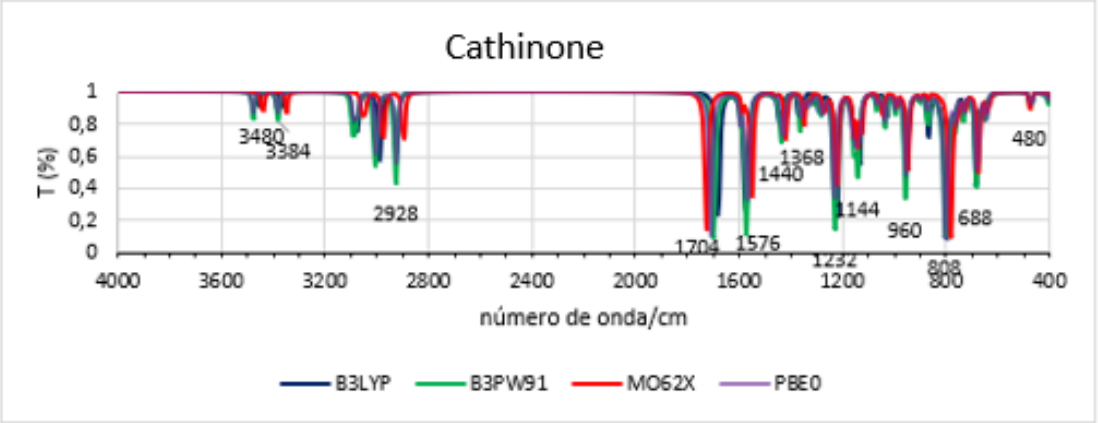


Figure S61. Infrared Theoretical Spectra for Diethylcathinone:

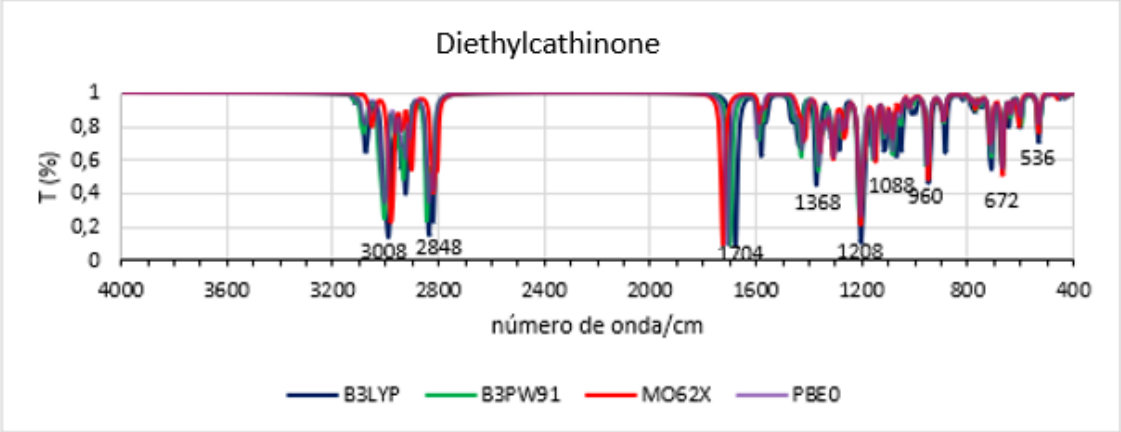


Figure S62. Infrared Theoretical Spectra for Methcathinone:

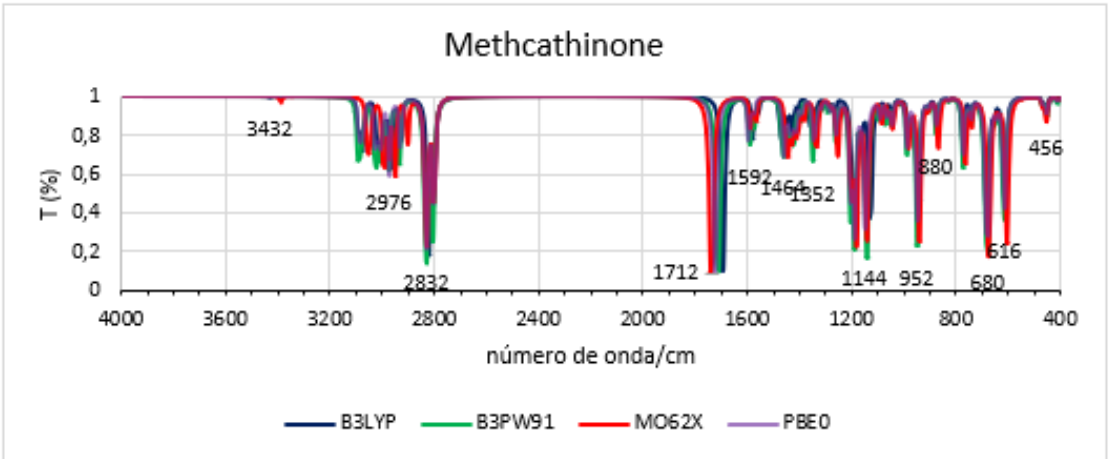


Figure S63. Infrared Theoretical Spectra for 2-Furanylbenzyl:

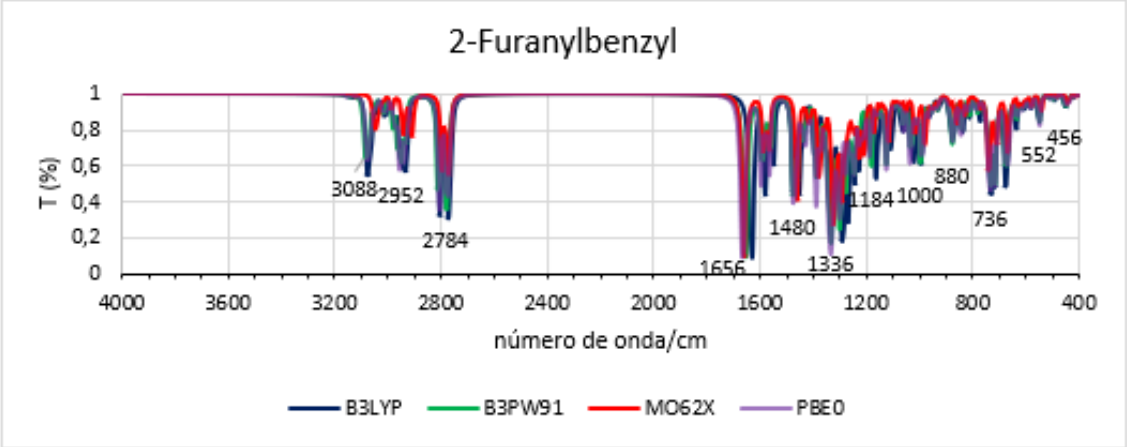


Figure S64. Infrared Theoretical Spectra for 2-Thiophenoyl:

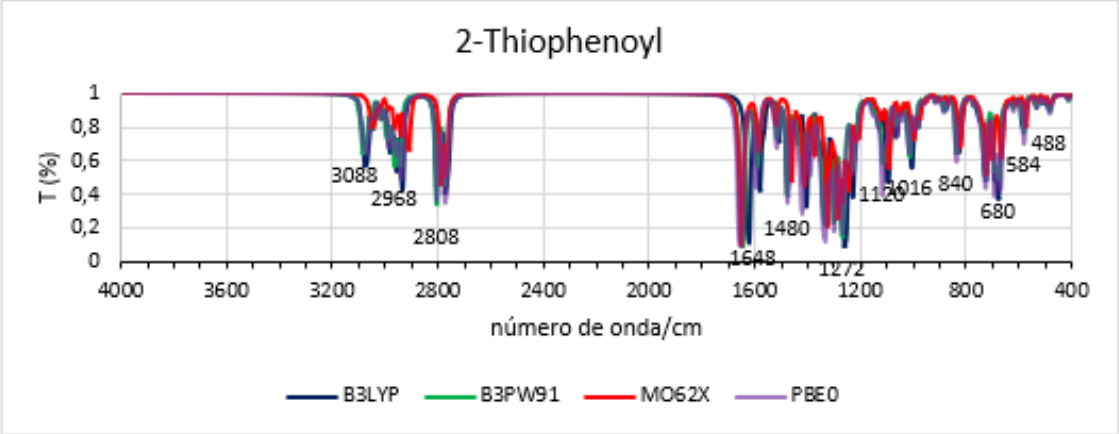


Figure S65. Infrared Theoretical Spectra for 3-Furanyl:

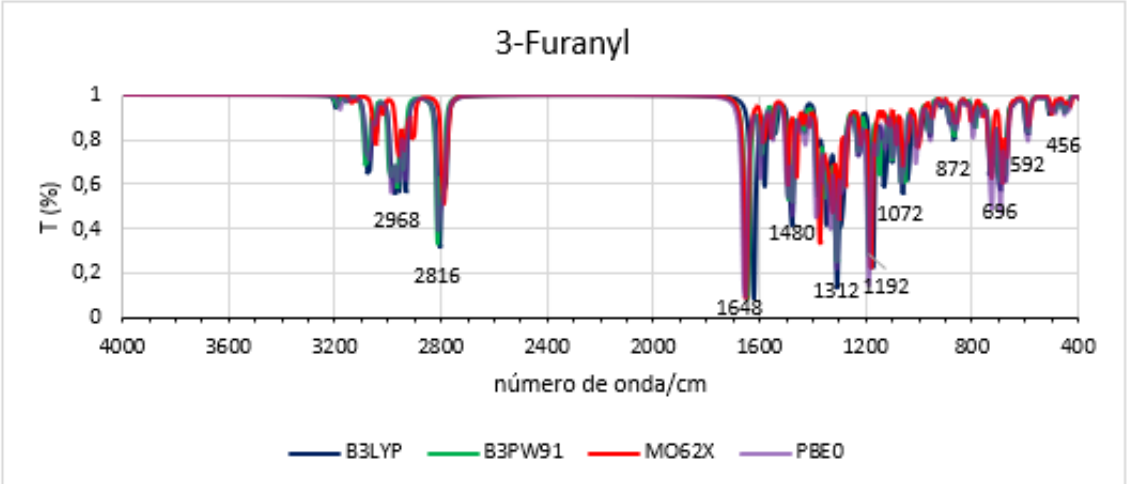


Figure S66. Infrared Theoretical Spectra for Acetilfen:

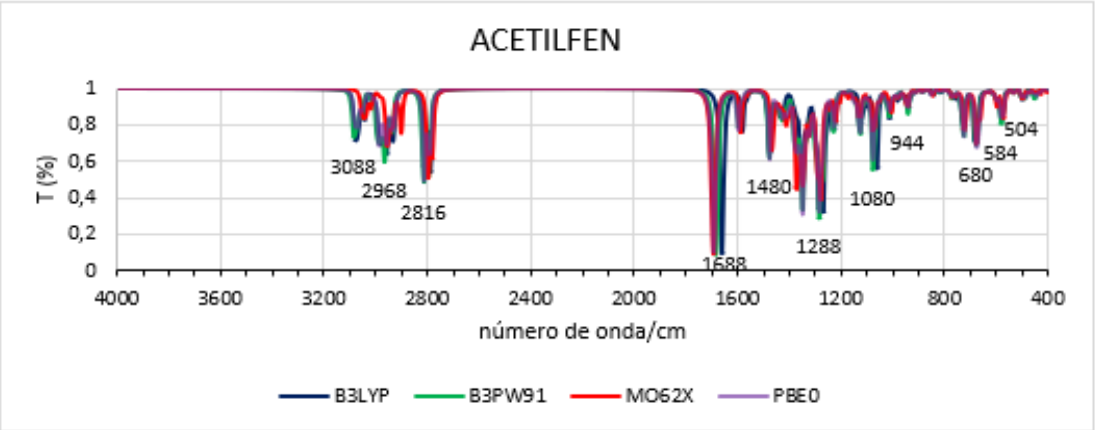


Figure S67. Infrared Theoretical Spectra for Benzoylbenzyl:

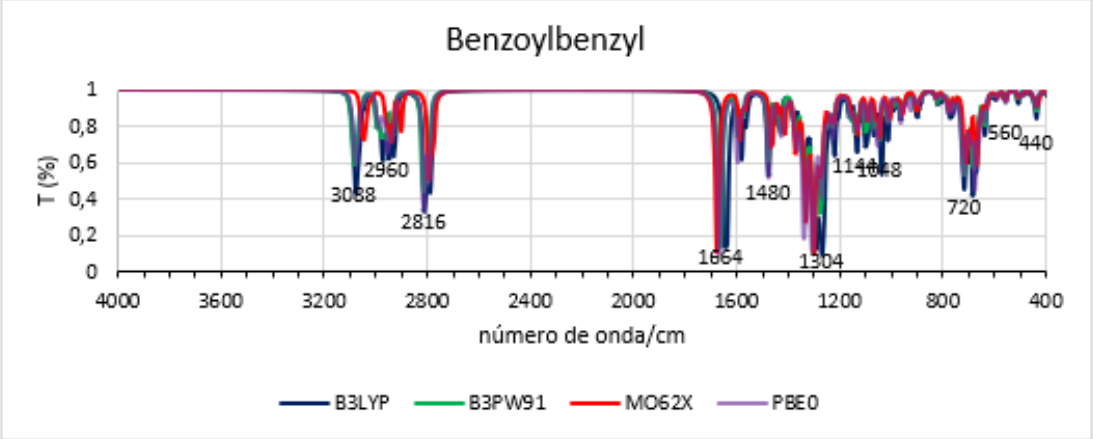


Figure S68. Infrared Theoretical Spectra for Butyryl:

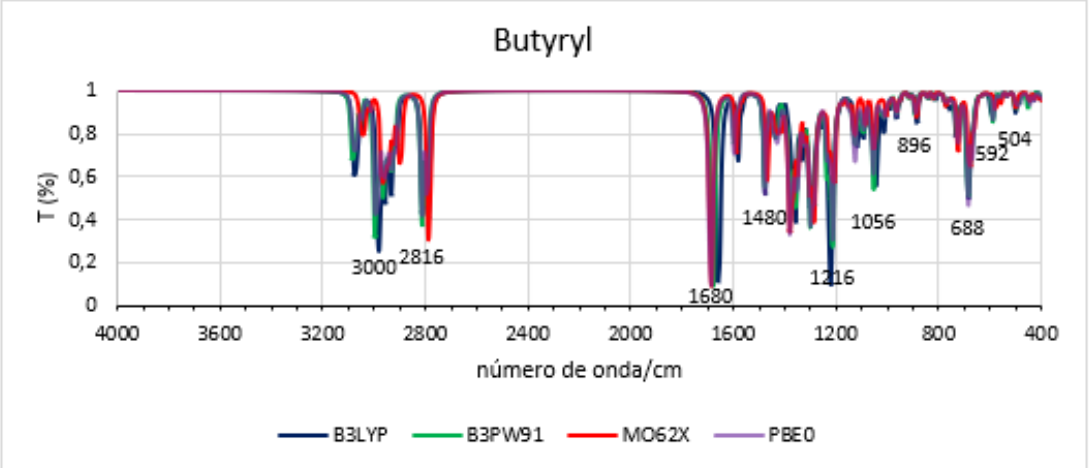


Figure S69. Infrared Theoretical Spectra for Crotonyl-fentanyl:

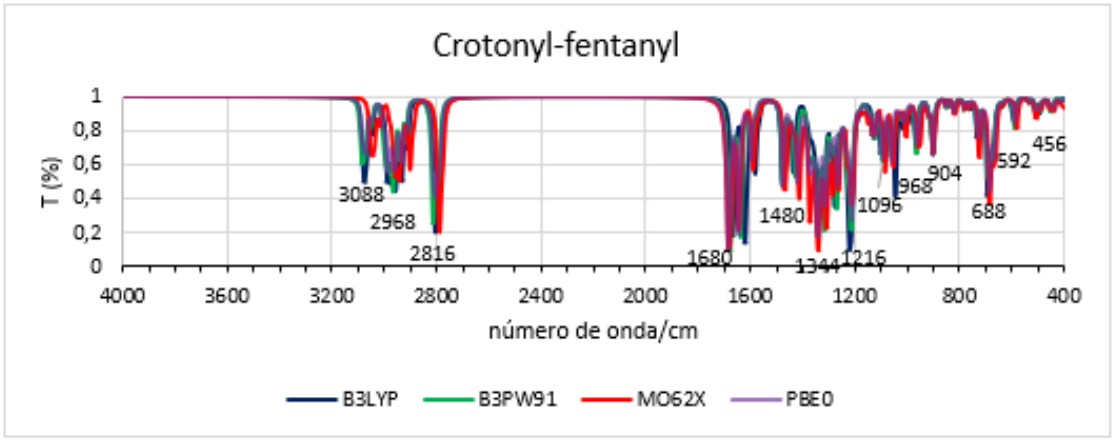


Figure S70. Infrared Theoretical Spectra for Cyclopentanoyl:

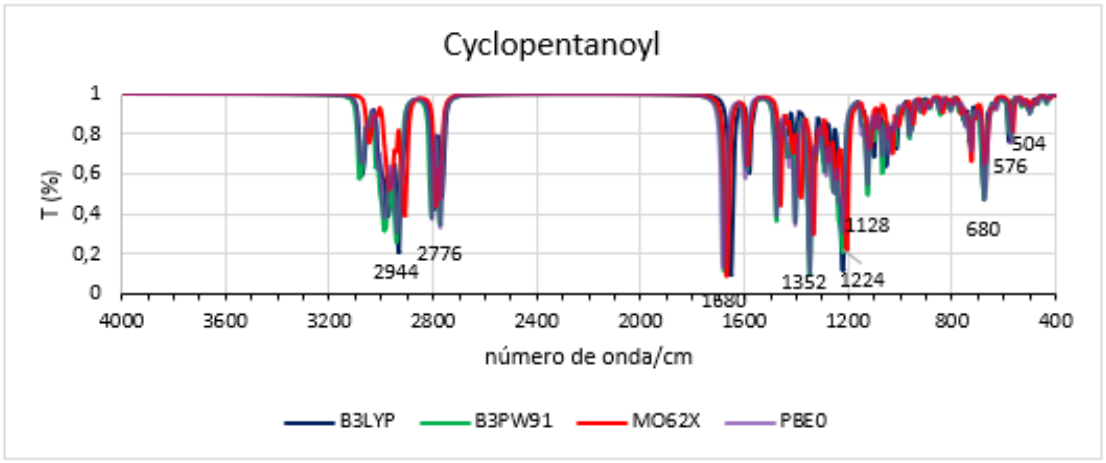


Figure S71. Infrared Theoretical Spectra for Cyclopropyl:

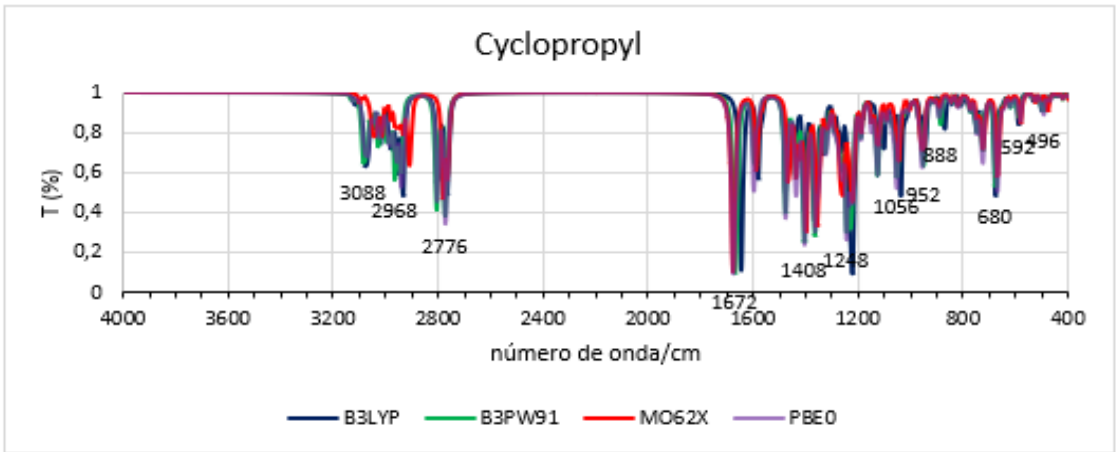


Figure S72. Infrared Theoretical Spectra for Fentanyl:

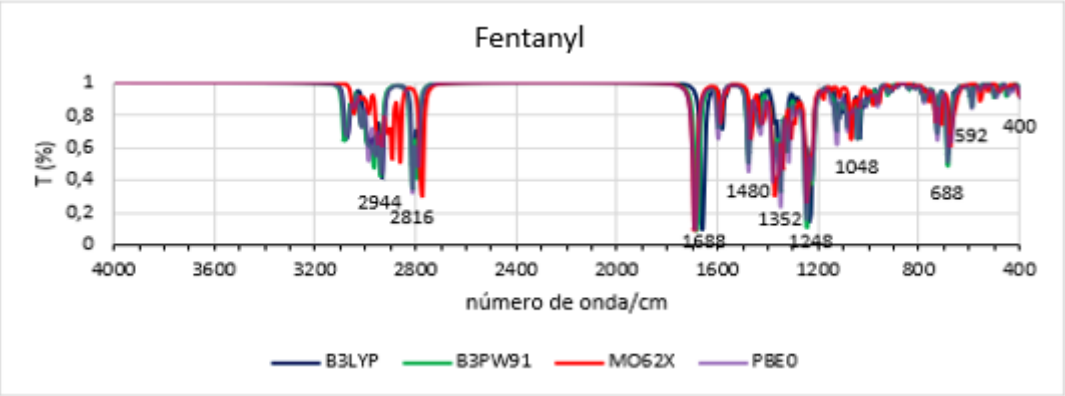


Figure S73. Infrared Theoretical Spectra for Furanylfentanyl:

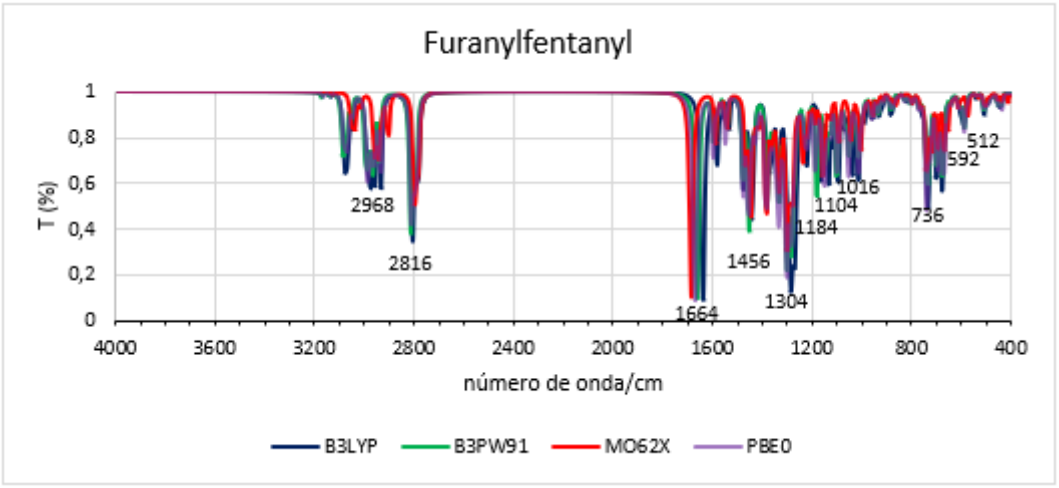


Figure S74. Infrared Theoretical Spectra for Isobutyryl-fentanyl:

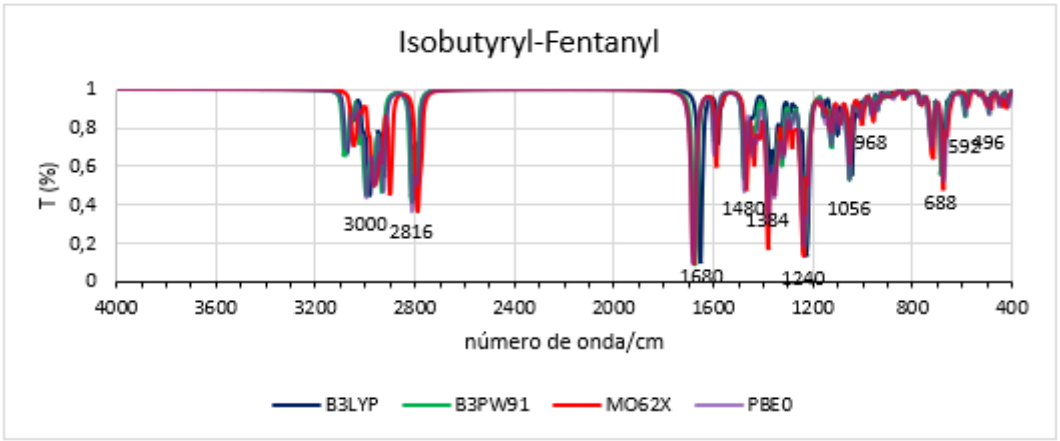


Figure S75. Infrared Theoretical Spectra for P-F-ACETILFEN:

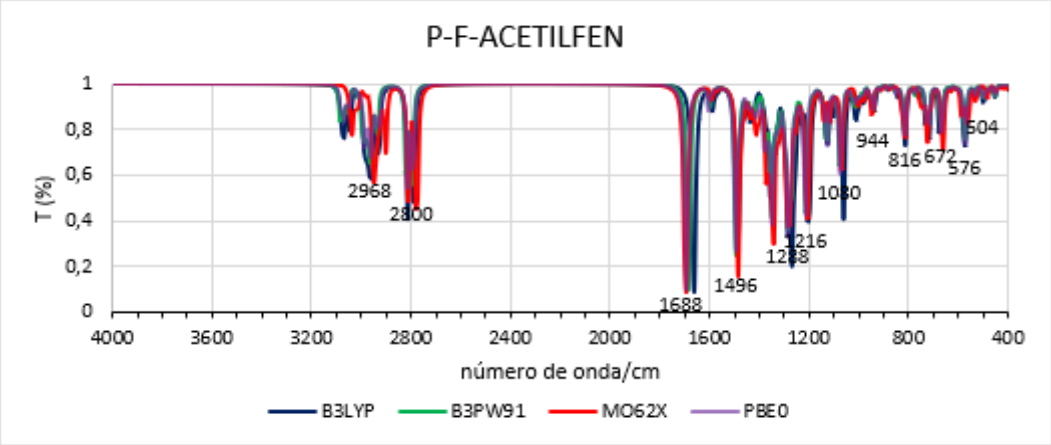


Figure S76. Infrared Theoretical Spectra for Tetrahydrofuranfentanyl:

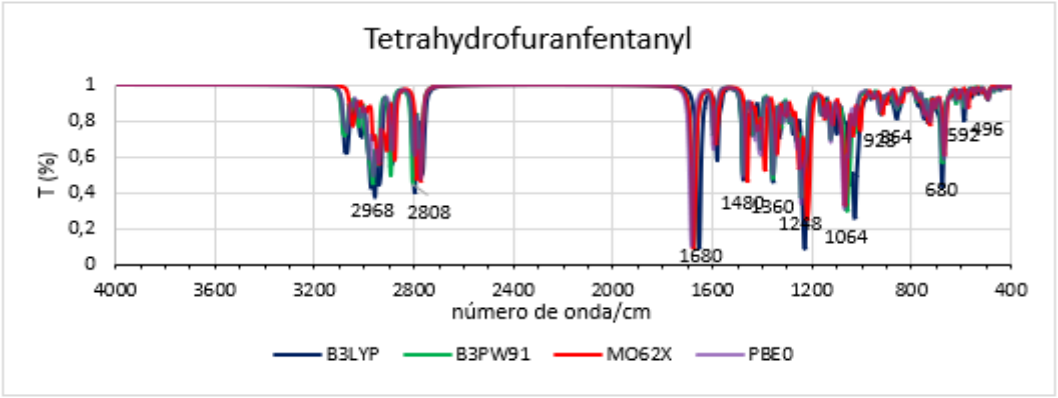
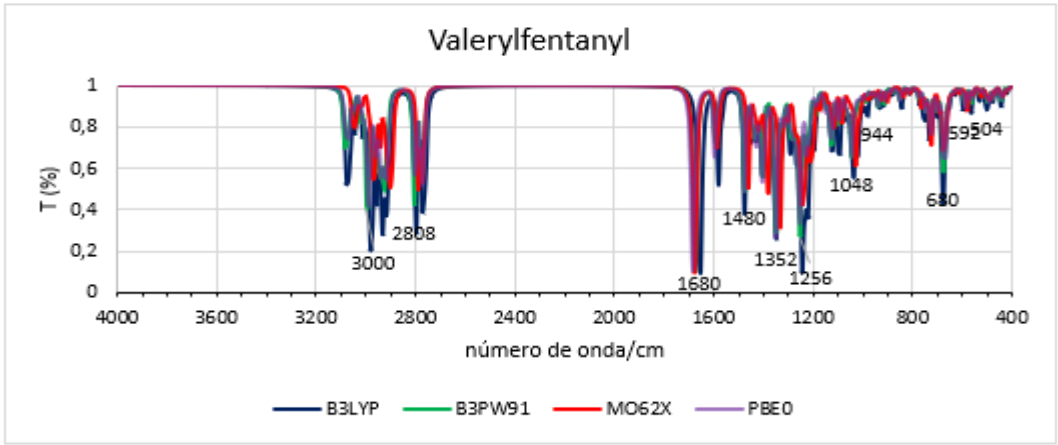


Figure S77. Infrared Theoretical Spectra for Valerylfentanyl:



1. PubChem CID 3007 Available online: https://pubchem.ncbi.nlm.nih.gov/compound/3007#section=3D-Conformer (accessed on 10 June 2020).

2. PubChem CID 121531 Available online: https://pubchem.ncbi.nlm.nih.gov/compound/121531#section=3D-Conformer (accessed on 10 June 2020).

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