Supplementary file

A simple and efficient approach to the synthesis of 4-aryl-2-dialkylphosphonomethyl-4-oxobutanenitrile

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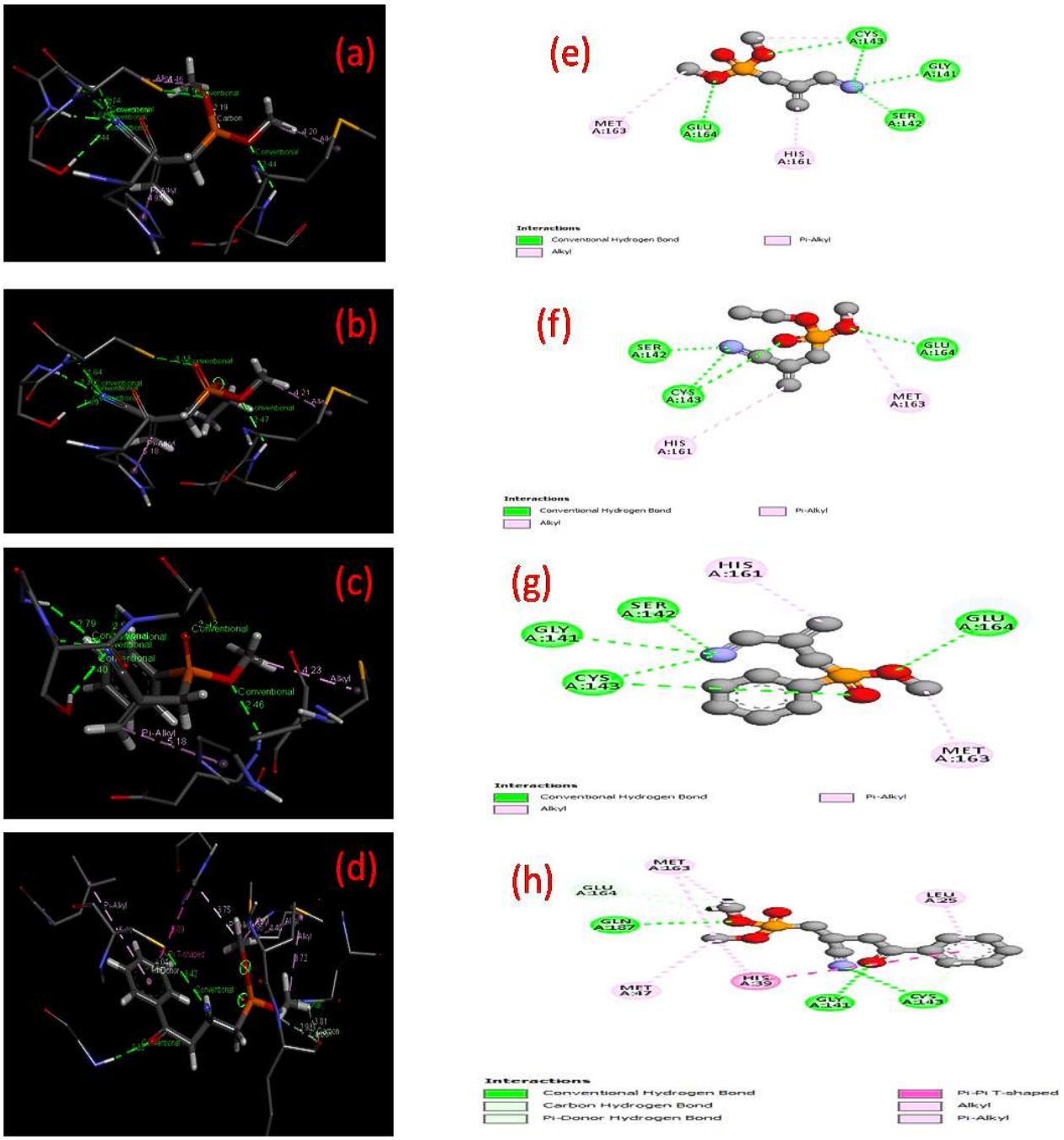

Figure S1. molecular docked model of compounds **3a-5a** with (1uk4) : (the target is presented as thin sticks; the ligands are drawn as ball-and-stick) where (a), (b), (c) and (d) represent the 3D docking styles for **1uk4** with compounds **3a, 3b, 3e** and **5a**, respectively, and (e), (f), (g),and (h) represent the 2D docking styles for **1uk4** with compounds **3a, 3b, 3e** and **5a**, respectively.

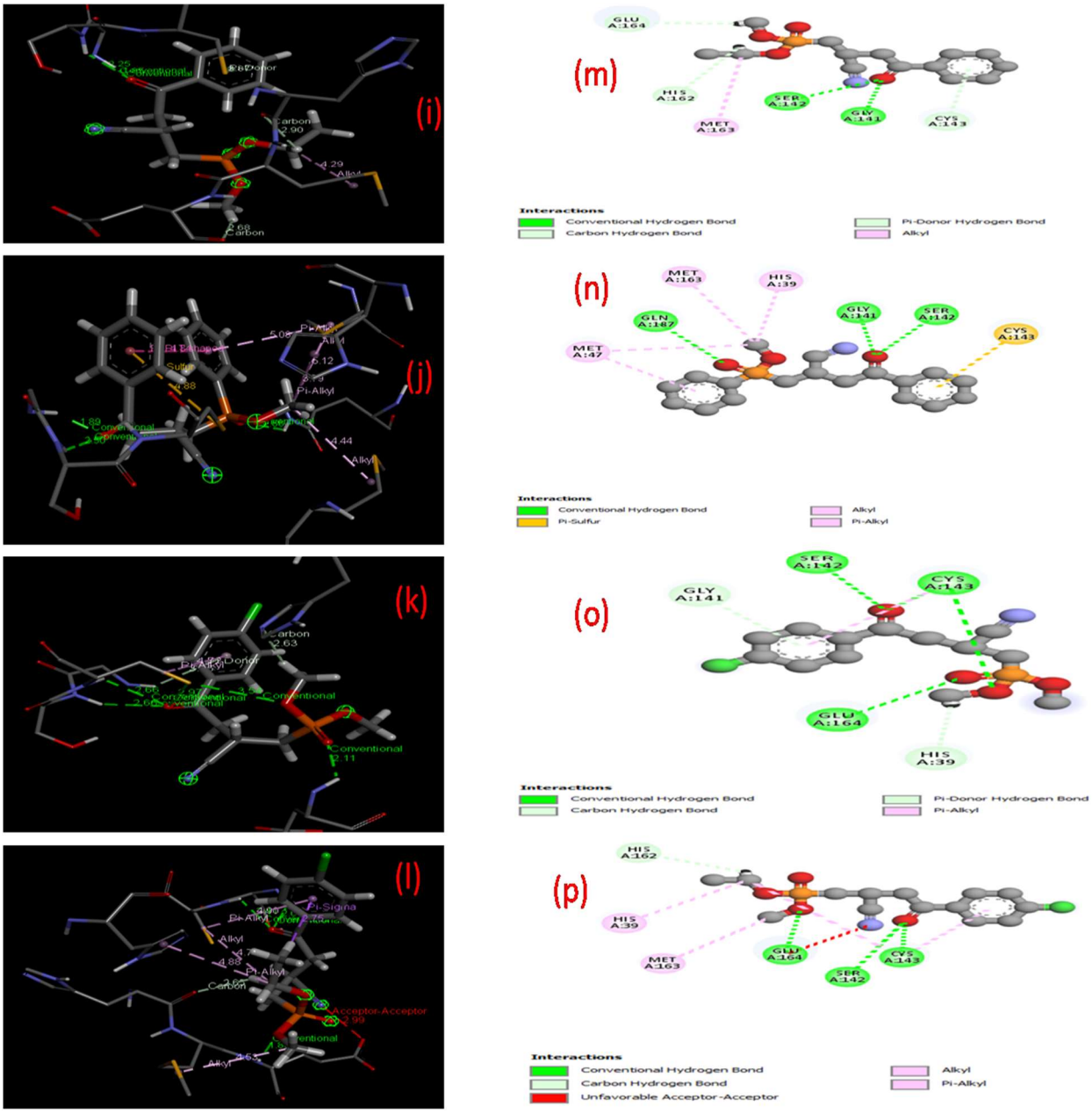

Figure S2. molecular docked model of compounds 5b-5e with (1uk4) : (the target is presented as thin sticks; the ligands are drawn as ball-and-stick) where (i), (j), (k)and(l) represent the 3D docking styles for **1uk4** with compounds **5b, 5c, 5d** and **5e**, respectively, and (m), (n), (o),and (p) represent the 2D docking styles for **1uk4** with compounds **5b, 5c, 5d** and **5e**, respectively.

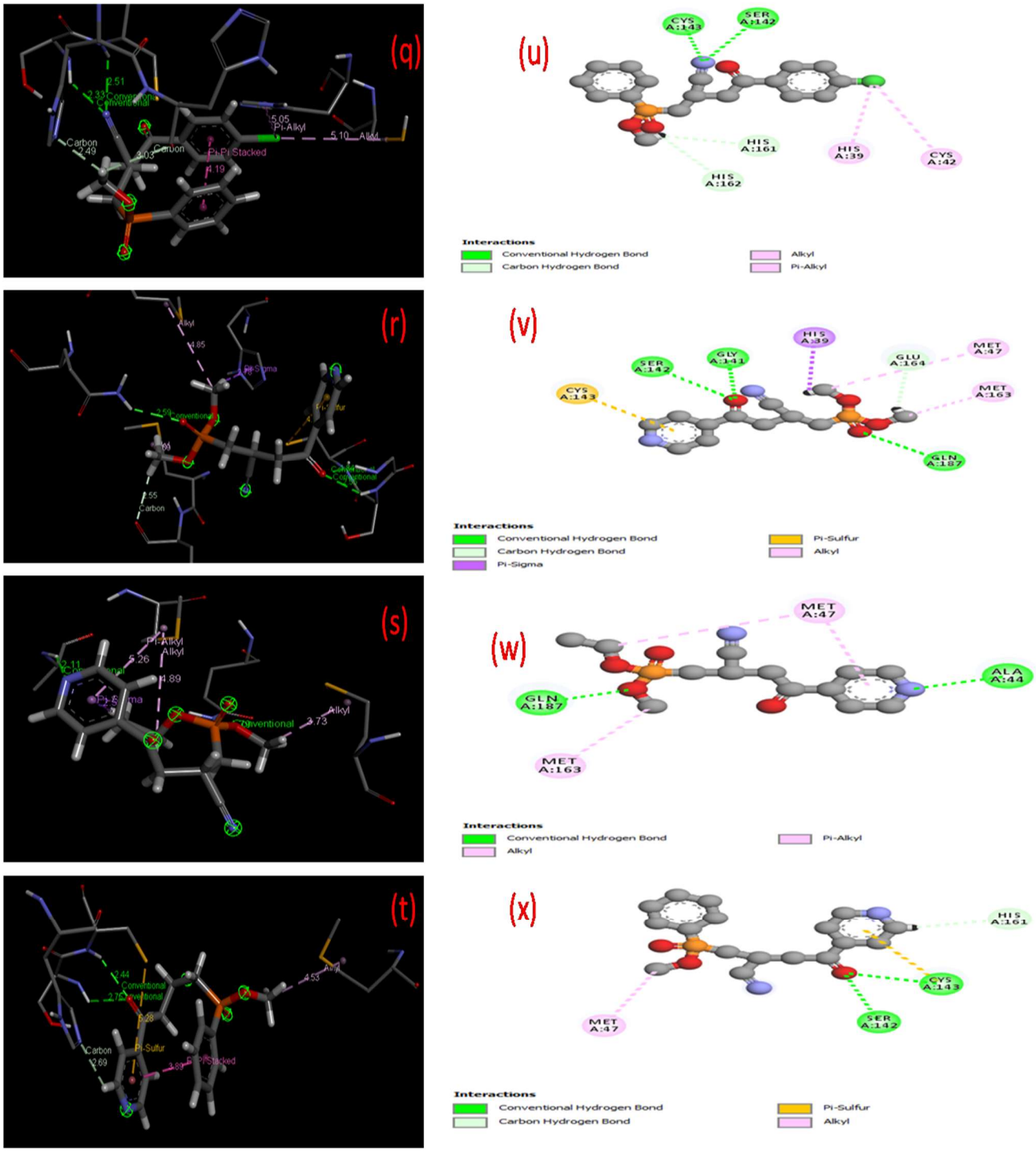

Figure S3. molecular docked model of compounds 5f-5i with (1uk4) : (the target is presented as thin sticks; the ligands are drawn as ball-and-stick) where (q), (r), (s)and(t) represent the 3D docking styles for **1uk4** with compounds **5f, 5g, 5h** and **5i**, respectively, and (u), (v), (w),and (x) represent the 2D docking styles for **1uk4** with compounds **5f, 5g, 5h** and **5i**, respectively.

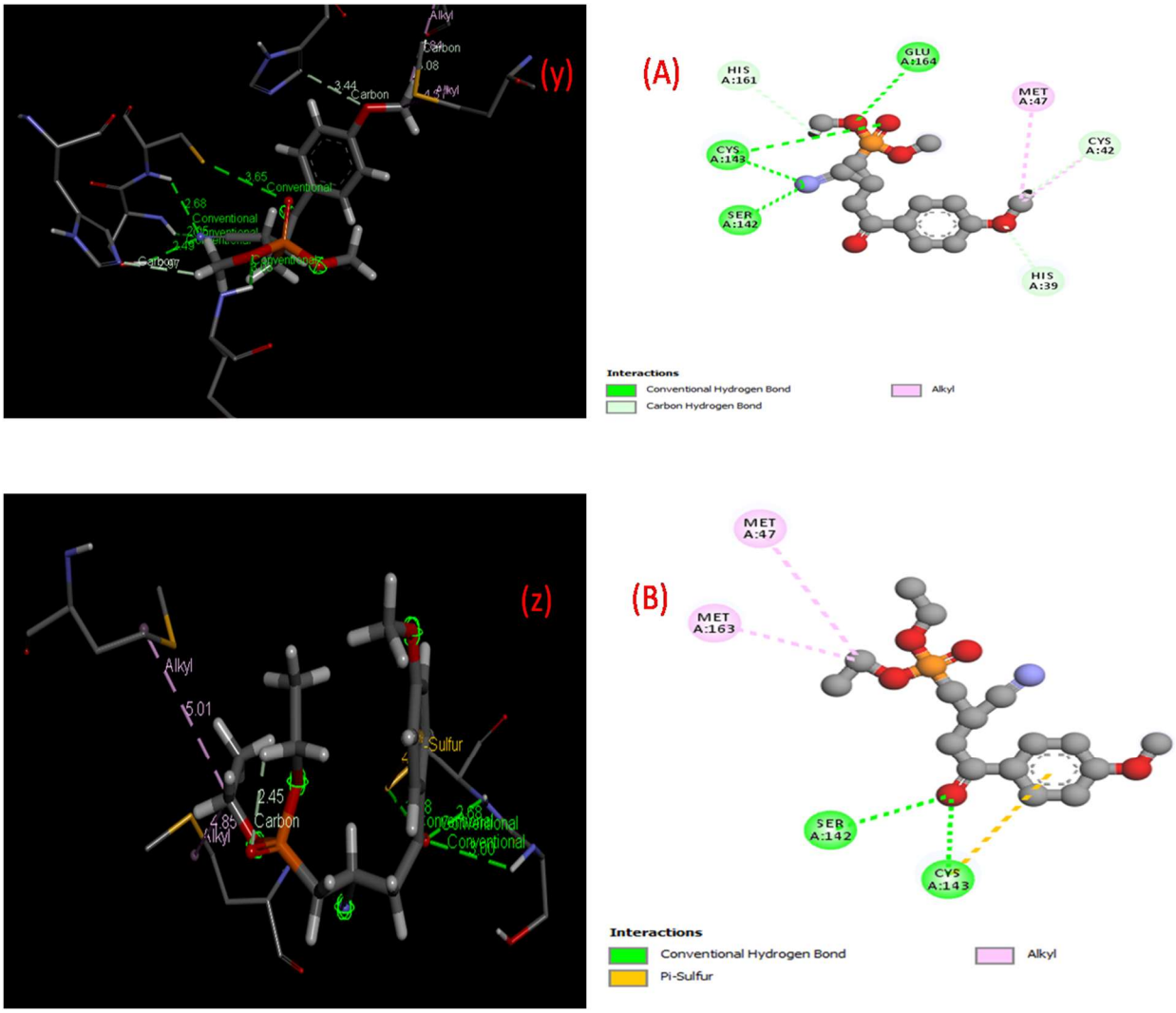

Figure S4. molecular docked model of compounds 5j and 5k with (1uk4) : (the target is presented as thin sticks; the ligands are drawn as ball-and-stick) where (y) and (z) represent the 3D docking styles for **1uk4** with compounds **5j** and **5k**, respectively, and (A) and (B) represent the 2D docking styles for **1uk4** with compounds **5j** and **5k**, respectively.

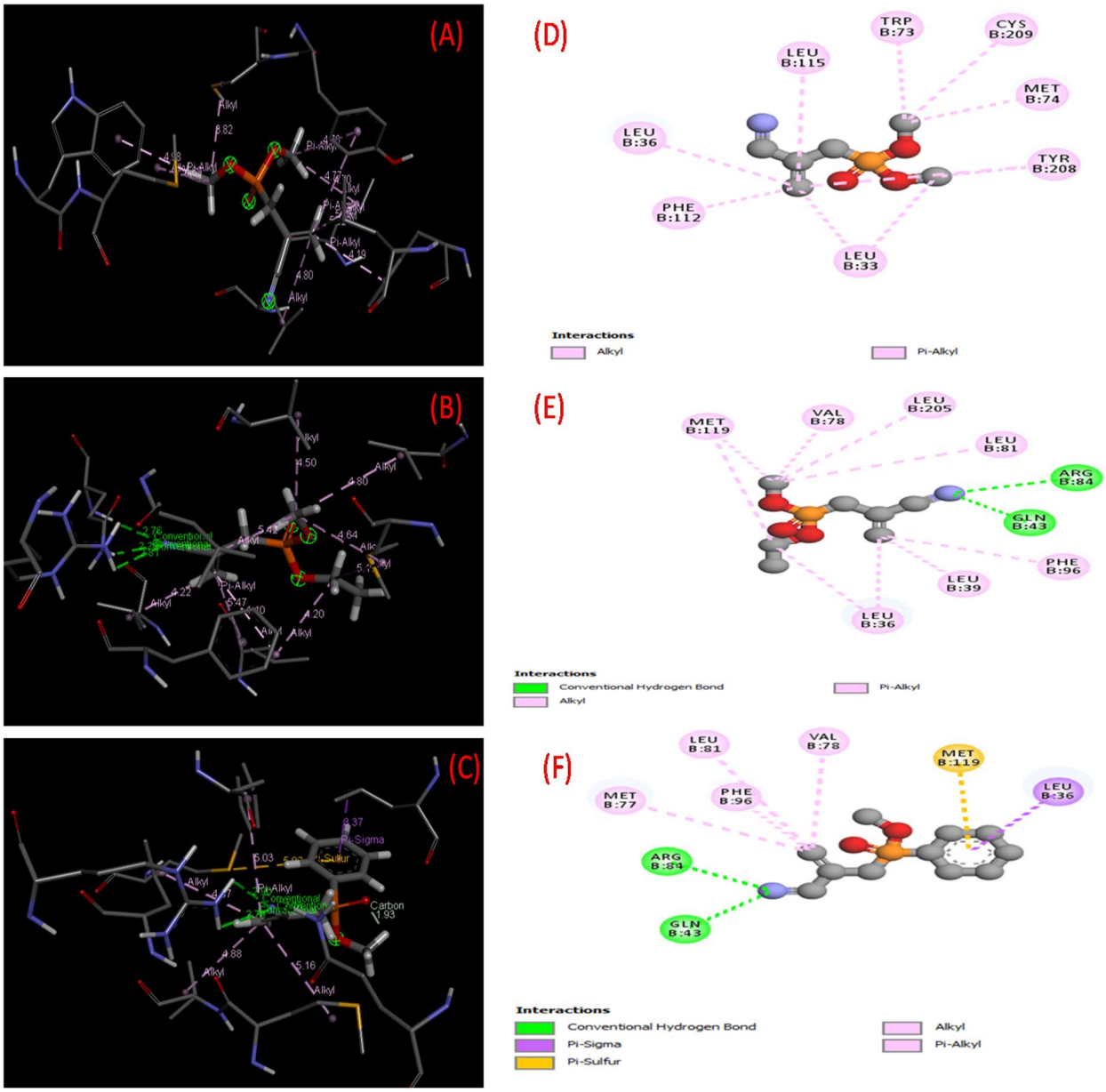

Figure S5. molecular docked model of compounds 3a-3e with (1e3k) : (the target is presented as thin sticks; the ligands are drawn as ball-and-stick) where (A), (B) and (C) represent the 3D docking styles for **1e3k** with compounds **3a, 3b** and **3e**, respectively, and (D), (E),and (F) represent the 2D docking styles for **1e3k** with compounds **3a, 3b** and **3e**, respectively.

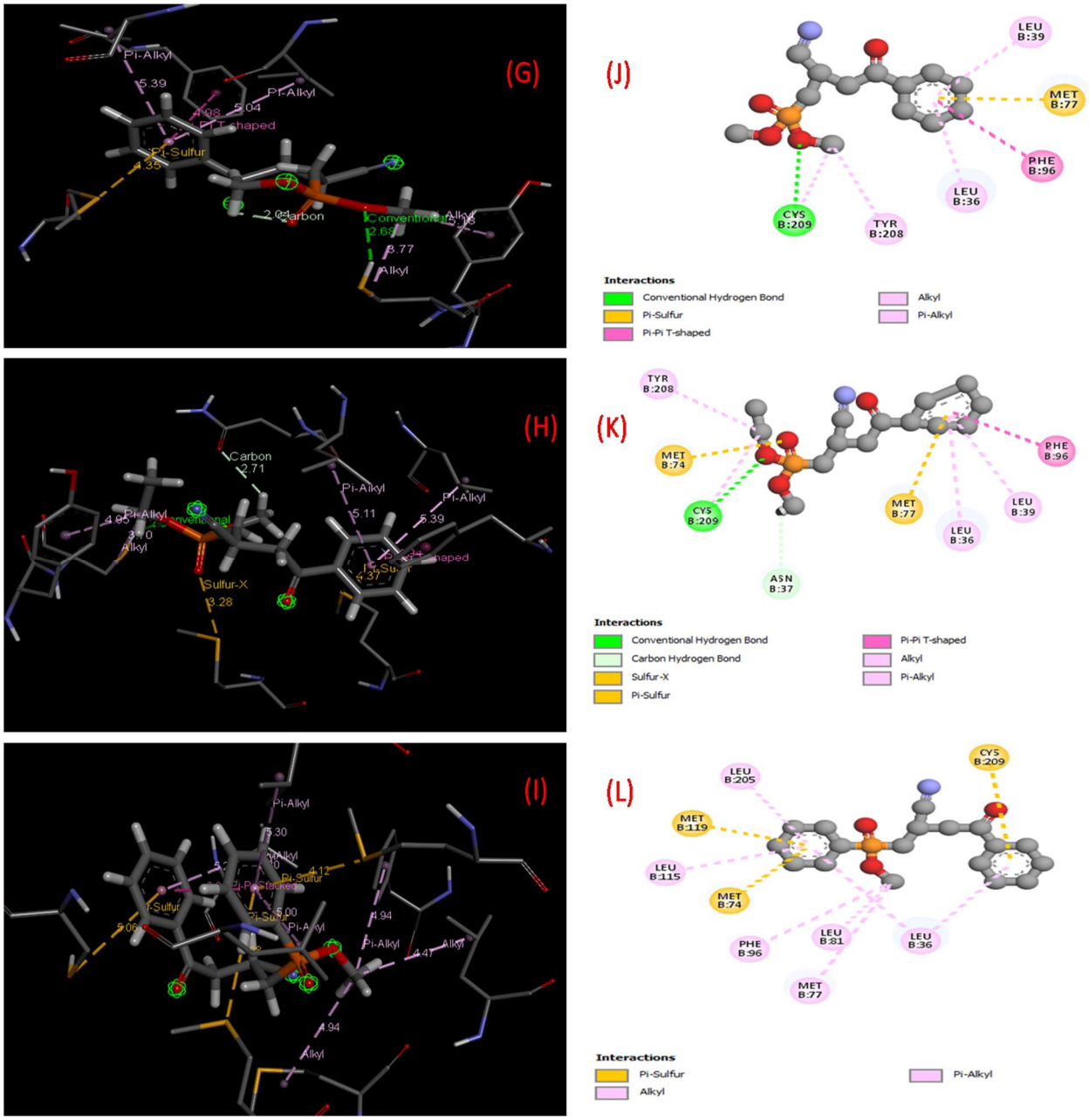

Figure S6. molecular docked model of compounds 5a-5c with (1e3k) : (the target is presented as thin sticks; the ligands are drawn as ball-and-stick) where (G), (H) and (I) represent the 3D docking styles for **1e3k** with compounds **5a, 5b** and **5c**, respectively, and (J), (K),and (L) represent the 2D docking styles for **1e3k** with compounds **5a, 5b** and **5c**, respectively.

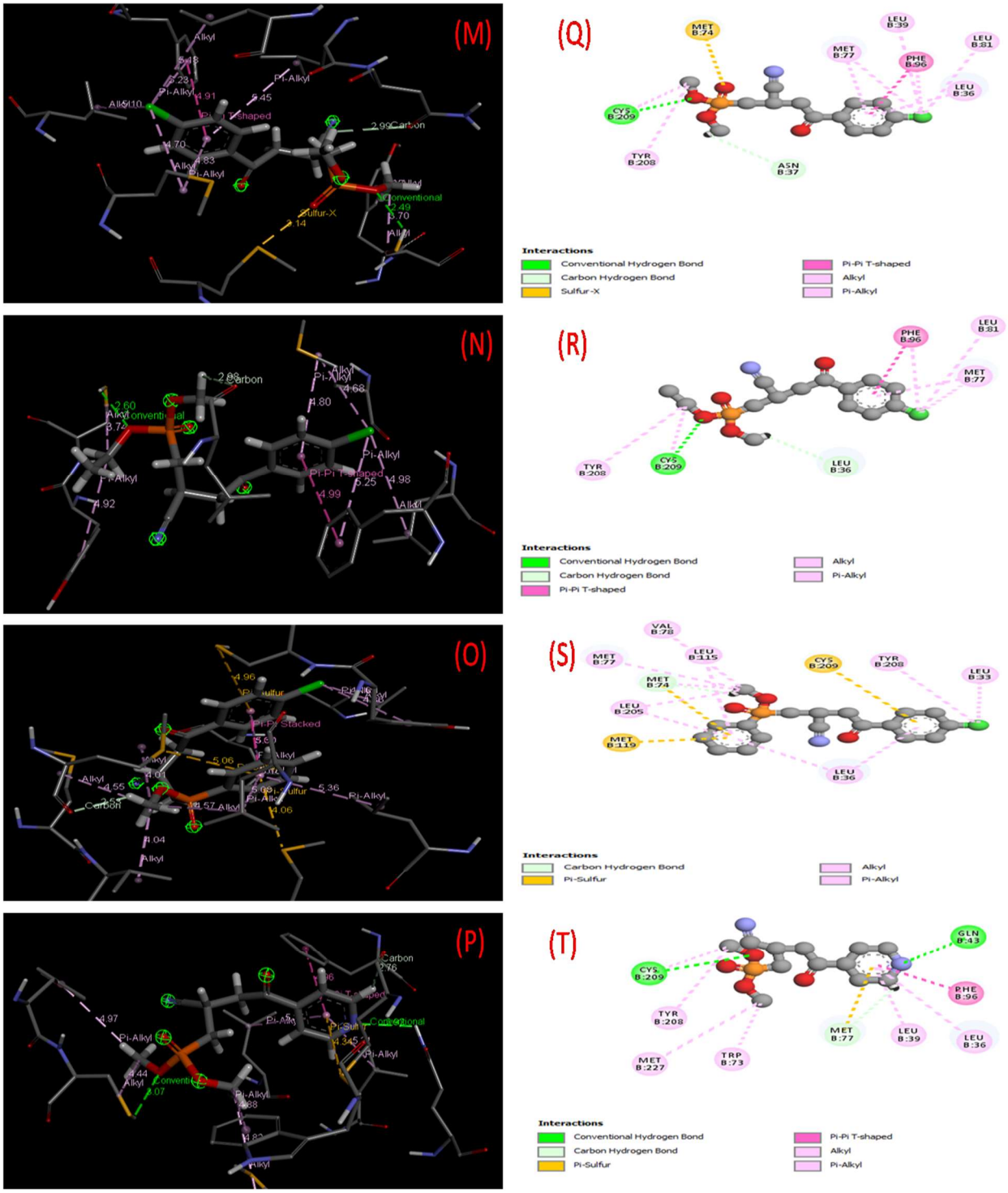

Figure S7. molecular docked model of compounds 5d-5g with (1e3k) : (the target is presented as thin sticks; the ligands are drawn as ball-and-stick) where (M), (N), (O) and (P) represent the 3D docking styles for **1e3k** with compounds **5d, 5e, 5f** and **5g**, respectively, and (Q), (R), (S) and (T) represent the 2D docking styles for **1e3k** with compounds **5d, 5e, 5f** and **5g**, respectively.

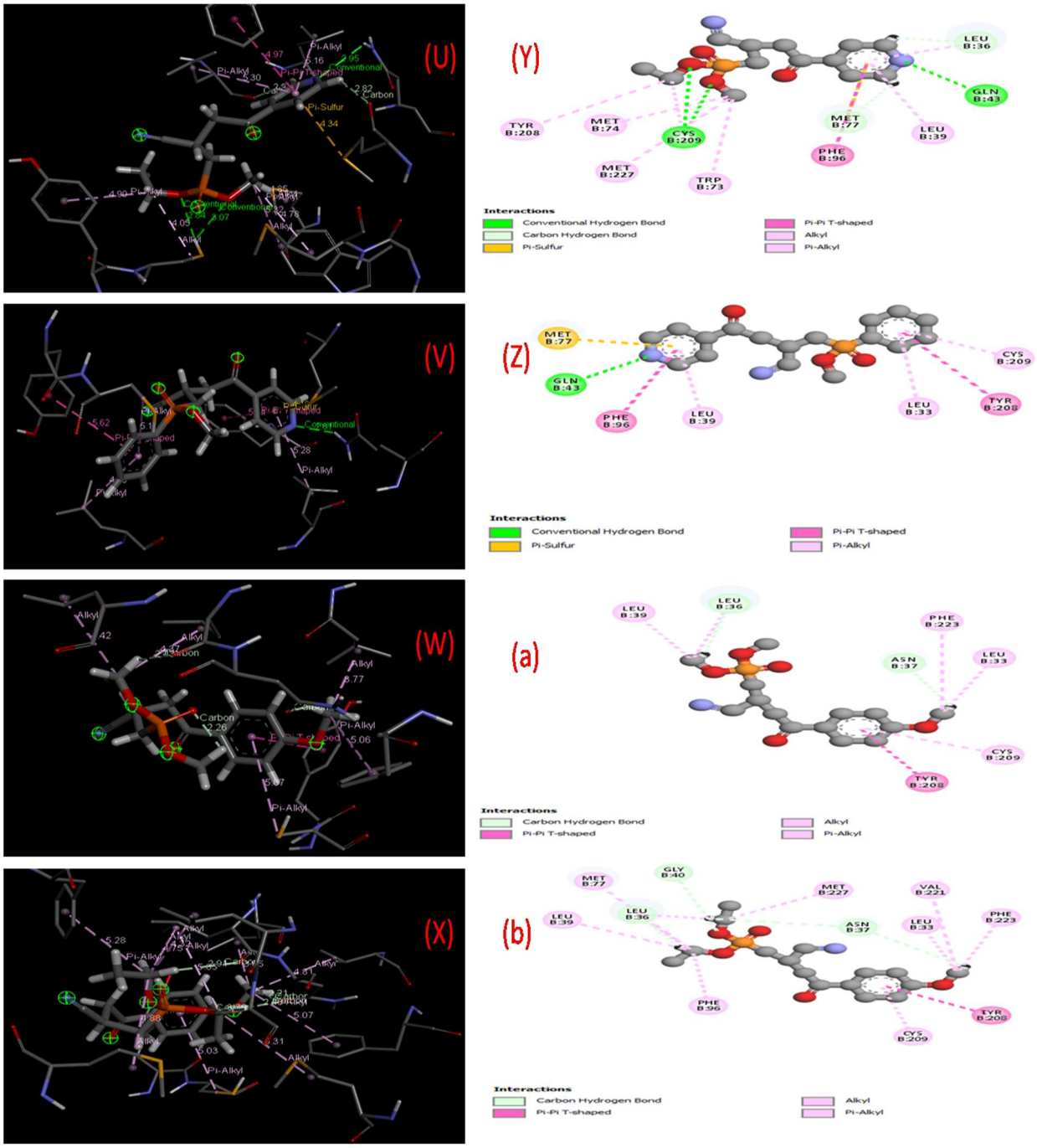

Figure S8. molecular docked model of compounds 5h-5k with (1e3k) : (the target is presented as thin sticks; the ligands are drawn as ball-and-stick) where (U), (V), (W) and (X) represent the 3D docking styles for **1e3k** with compounds **5h, 5i, 5j** and **5k**, respectively, and (Y), (Z), (a) and (b) represent the 2D docking styles for **1e3k** with compounds **5h, 5i, 5j** and **5k**, respectively.

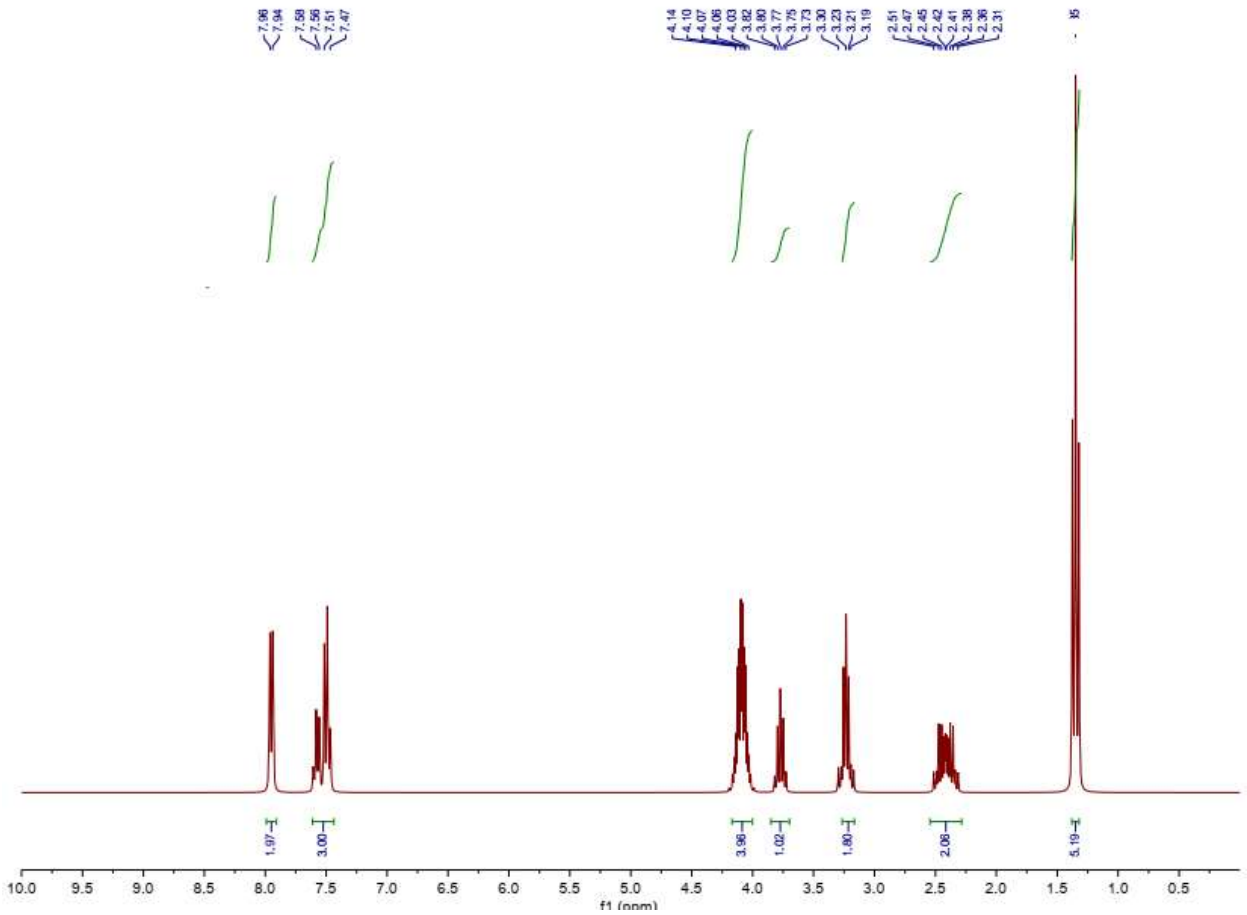

Figure S9. ^{1}H-NMR spectra of diethyl (2-cyano-4-oxo-4-phenylbutyl)phosphonate **5b**

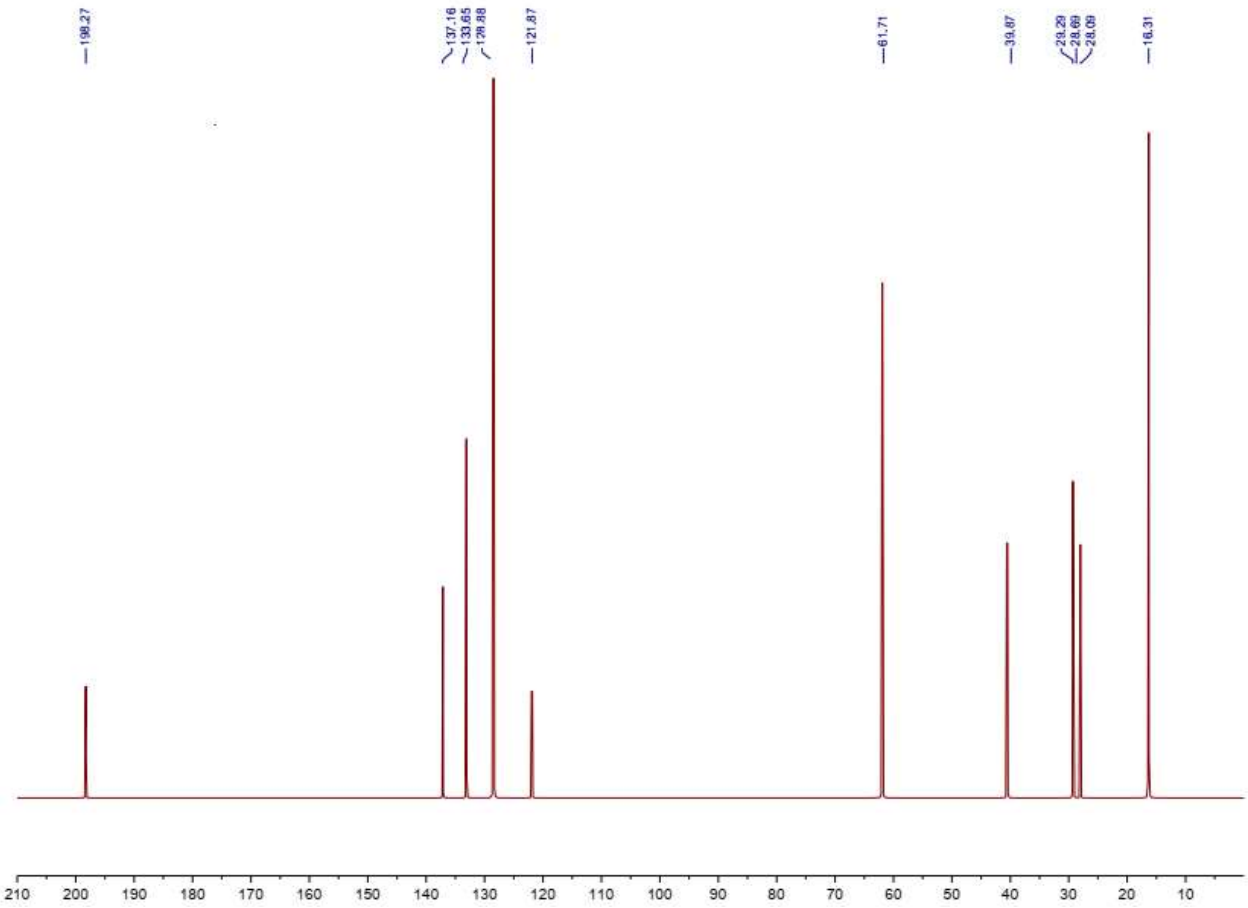

Figure S10. ^{13}C-NMR spectra of diethyl (2-cyano-4-oxo-4-phenylbutyl)phosphonate **5b**

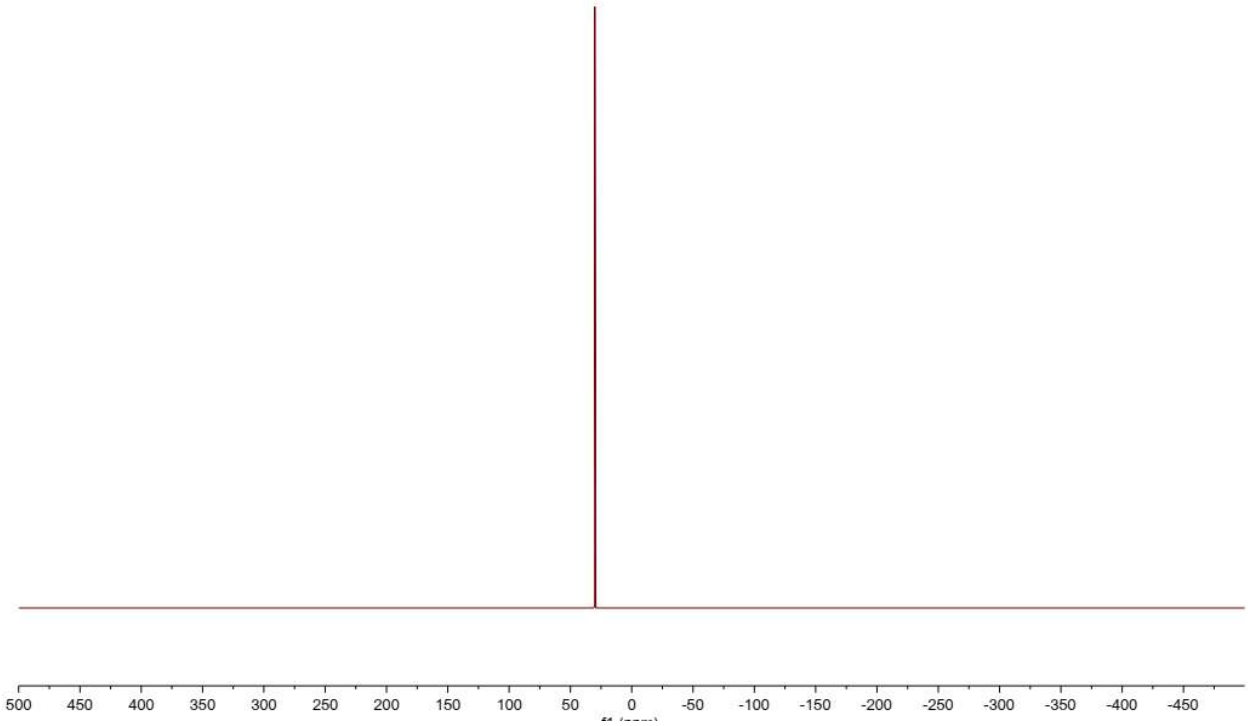

Figure S11. ^{31}P-NMR spectra of diethyl (2-cyano-4-oxo-4-phenylbutyl)phosphonate **5b**

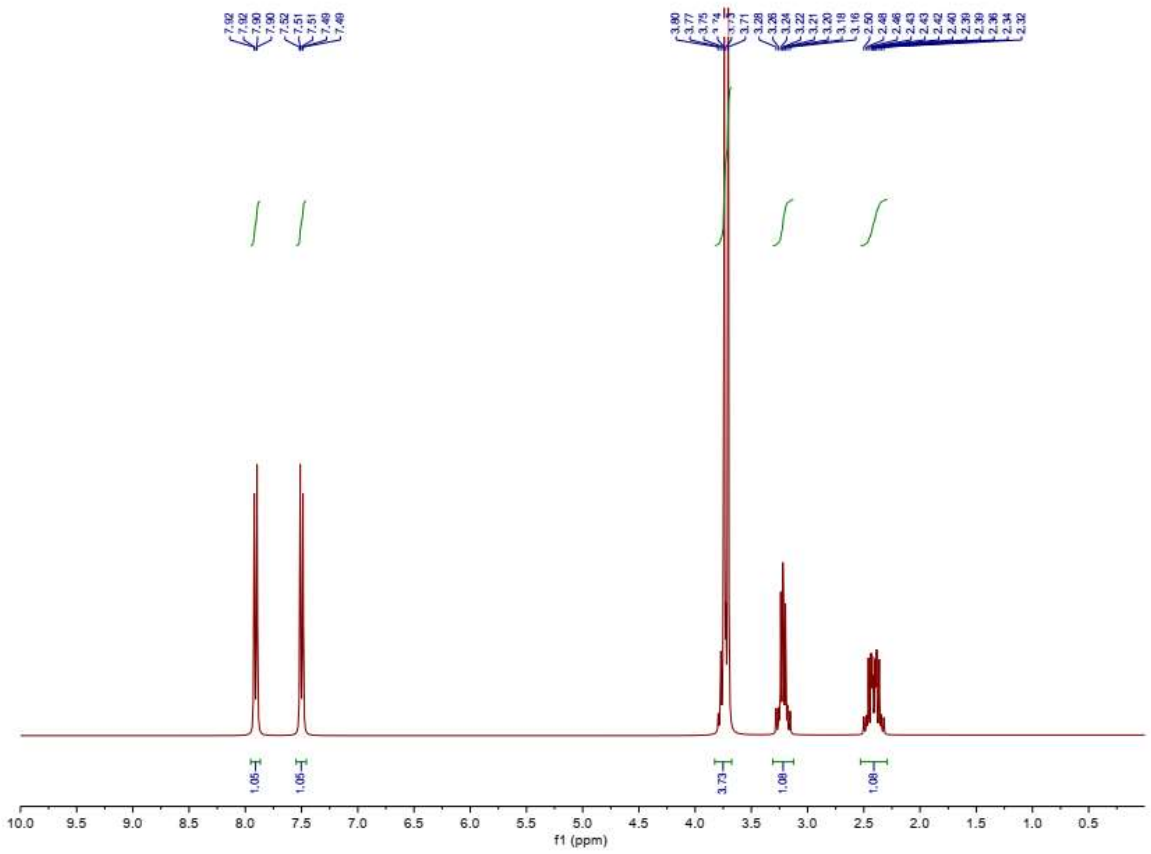

Figure S12. ^{1}H-NMR spectra of dimethyl (4-(4-chlorophenyl)-2-cyano-4-oxobutyl)phosphonate **5d**

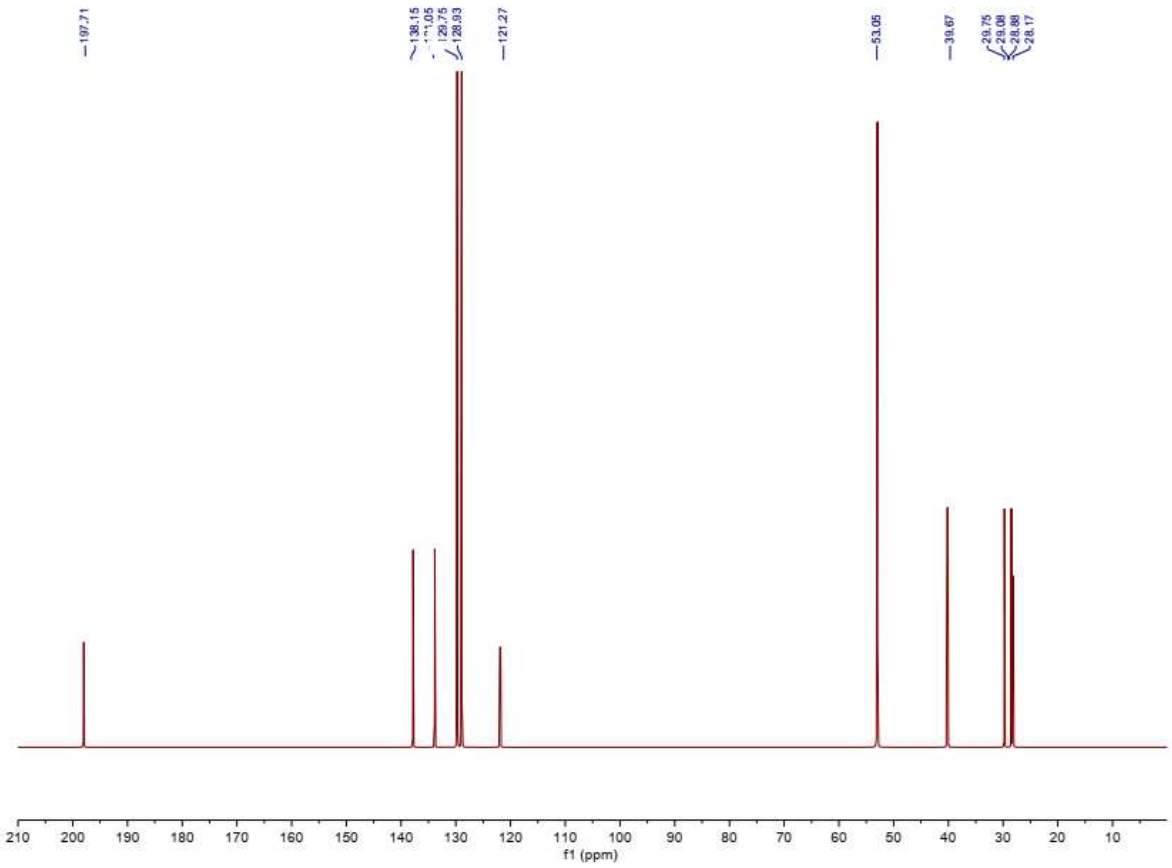

Figure S13. ^{13}C-NMR spectra of dimethyl (4-(4-chlorophenyl)-2-cyano-4-oxobutyl)phosphonate **5d**

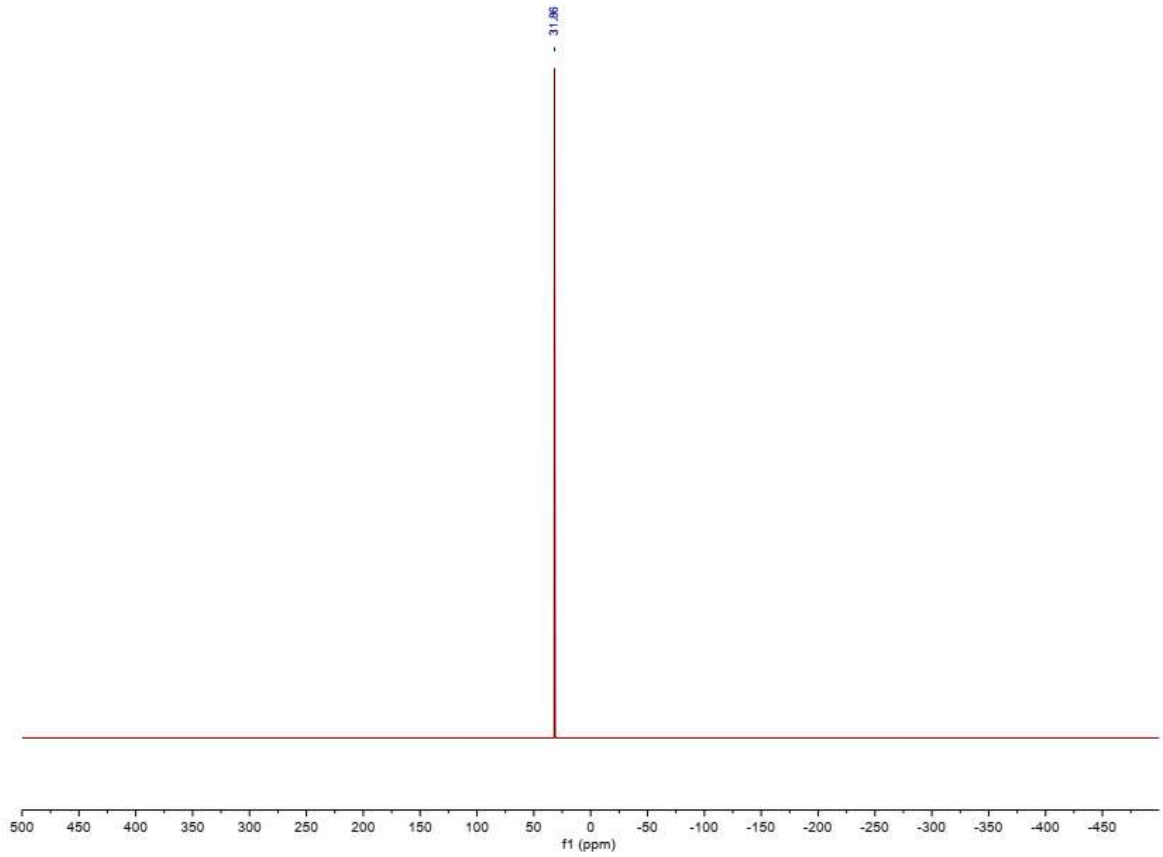

Figure S14. ^{31}P-NMR spectra of dimethyl (4-(4-chlorophenyl)-2-cyano-4-oxobutyl)phosphonate **5d**

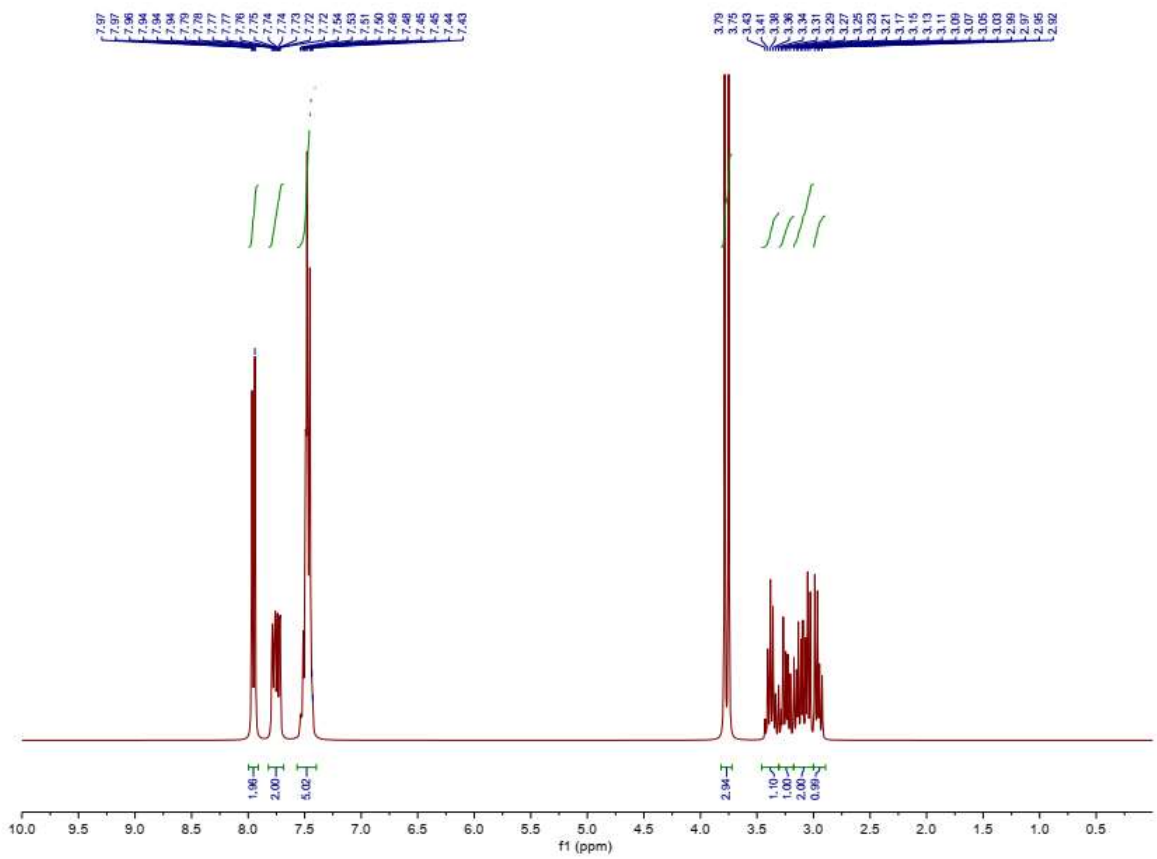

Figure S15. ^{1}H-NMR spectra of methyl phenyl (4-(4-chlorophenyl)-2-cyano-4-oxobutyl)phosphonate **5f**

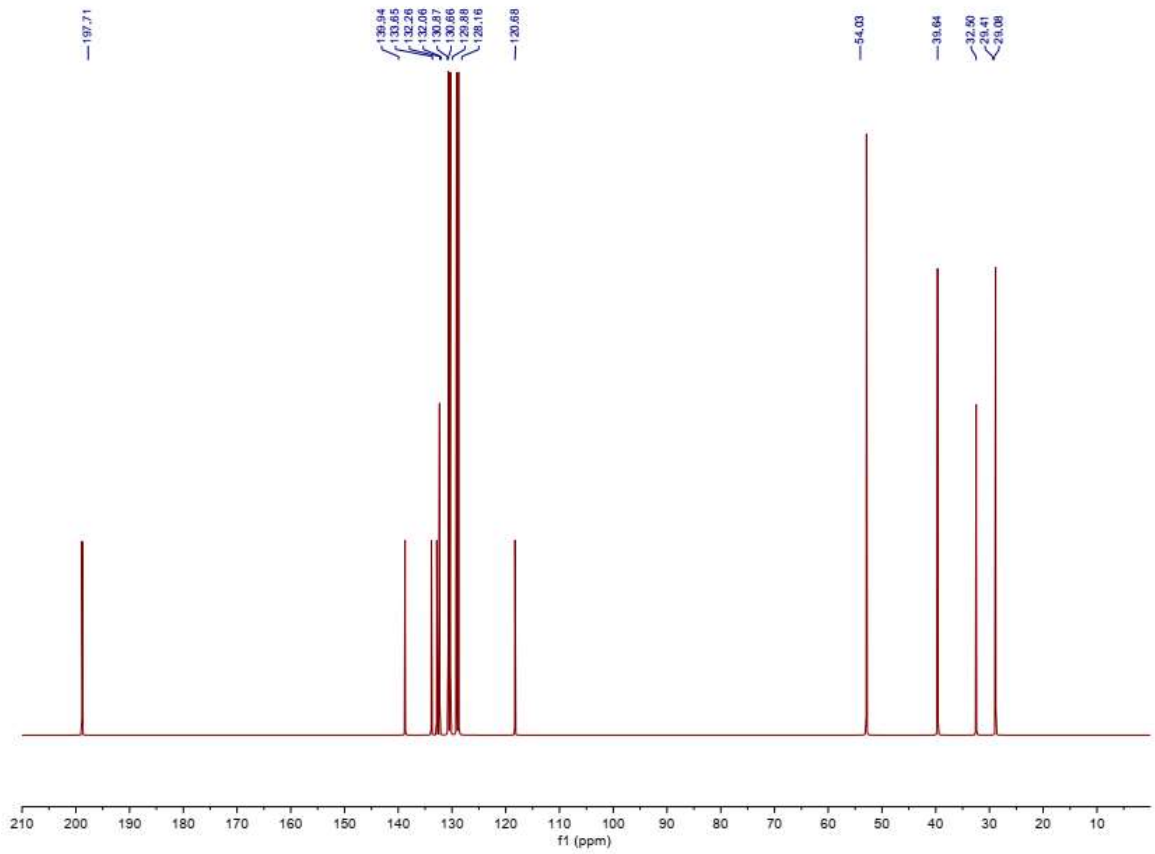

Figure S16. ^{13}C-NMR spectra of methyl phenyl (4-(4-chlorophenyl)-2-cyano-4-oxobutyl)phosphonate **5f**

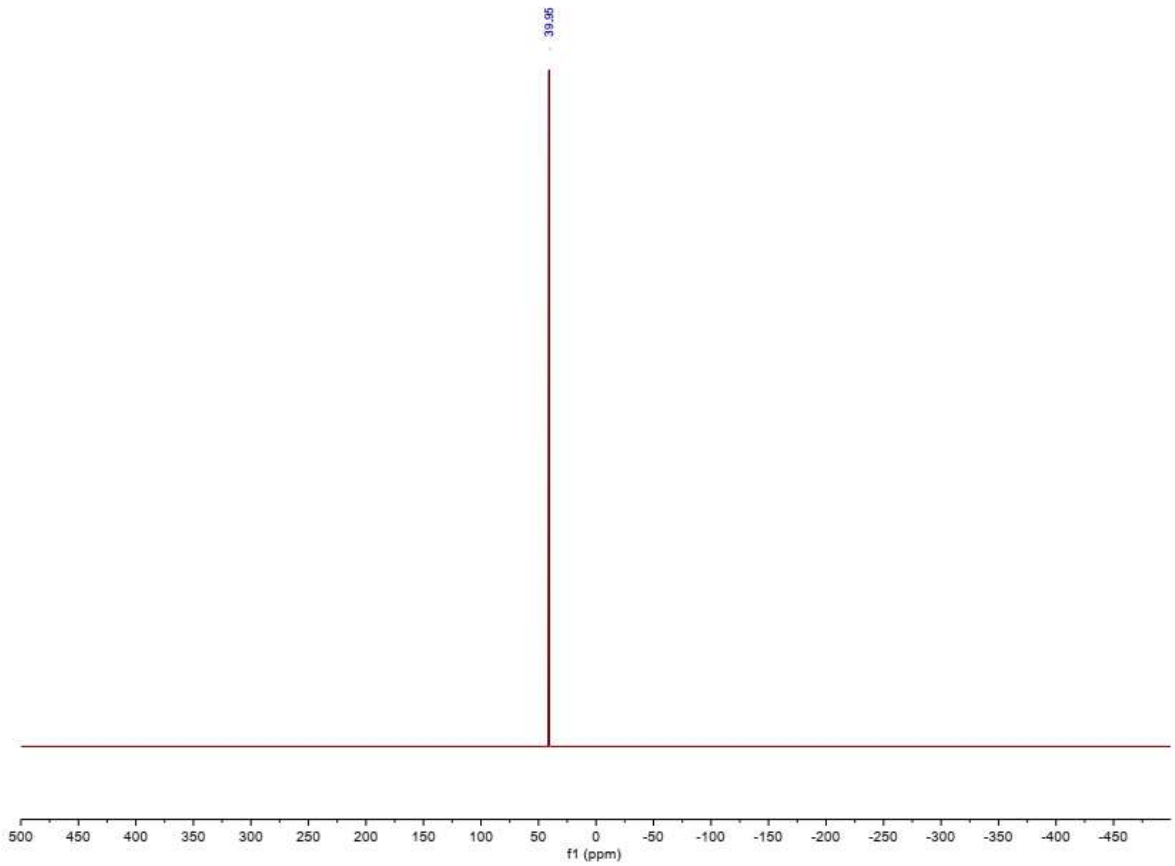

Figure S17. ^{31}P-NMR spectra of methyl phenyl (4-(4-chlorophenyl)-2-cyano-4-oxobutyl)phosphonate **5f**

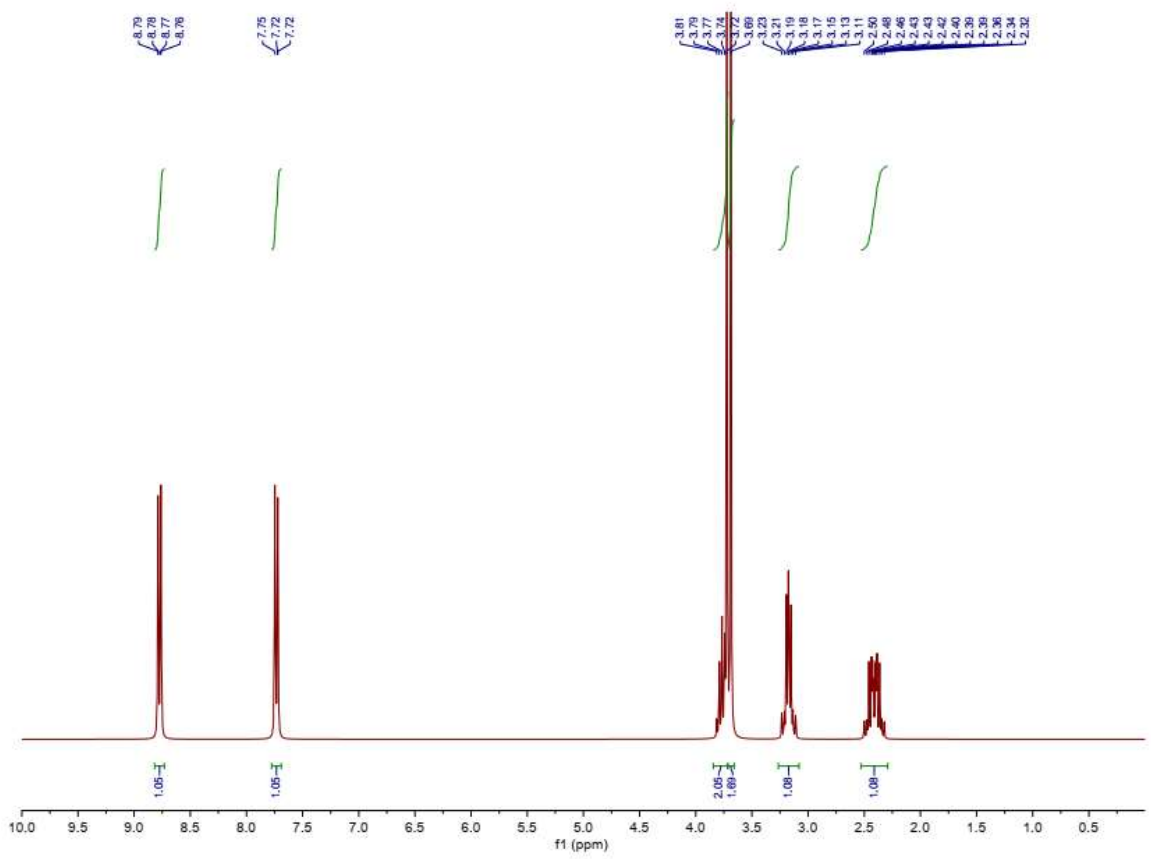

Figure S18. [1]H-NMR spectra of dimethyl (2-cyano-4-oxo-4-(pyridin-4-yl)butyl)phosphonate **5g**

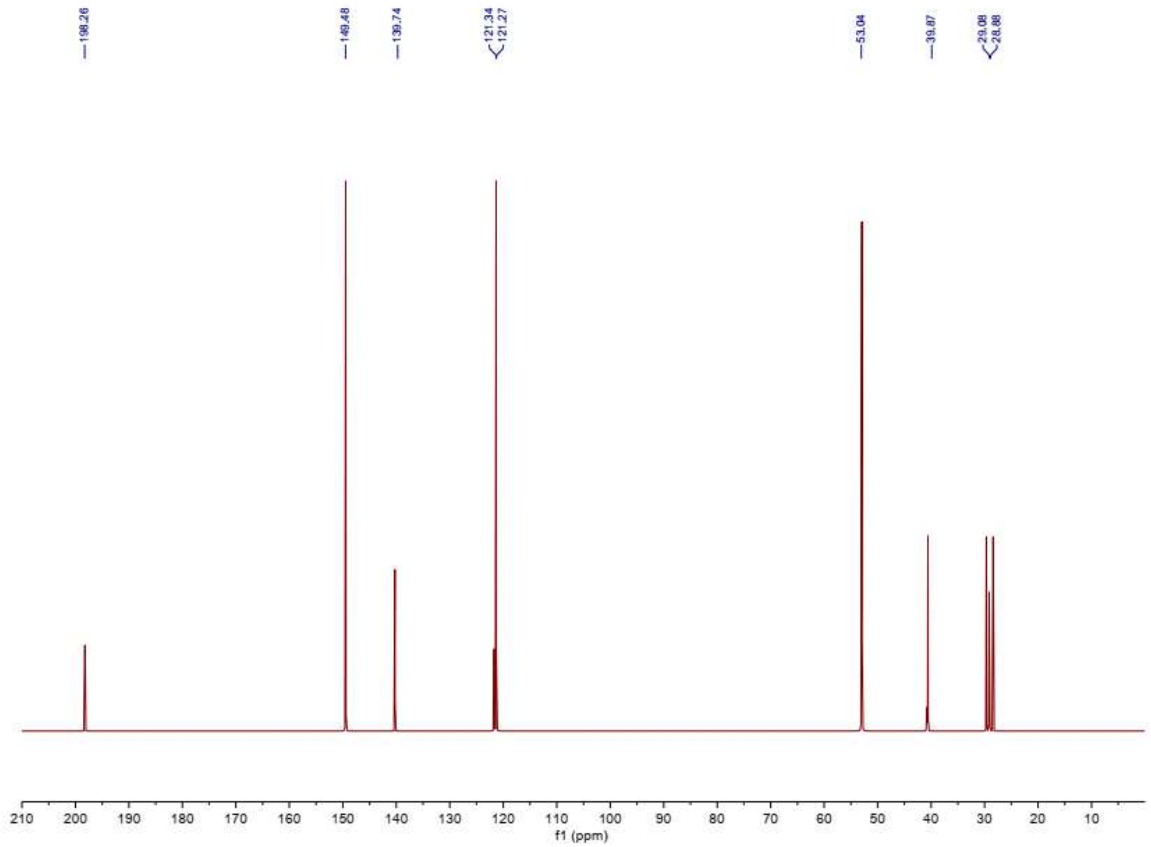

Figure S19. ^{13}C-NMR spectra of dimethyl (2-cyano-4-oxo-4-(pyridin-4-yl)butyl)phosphonate **5g**

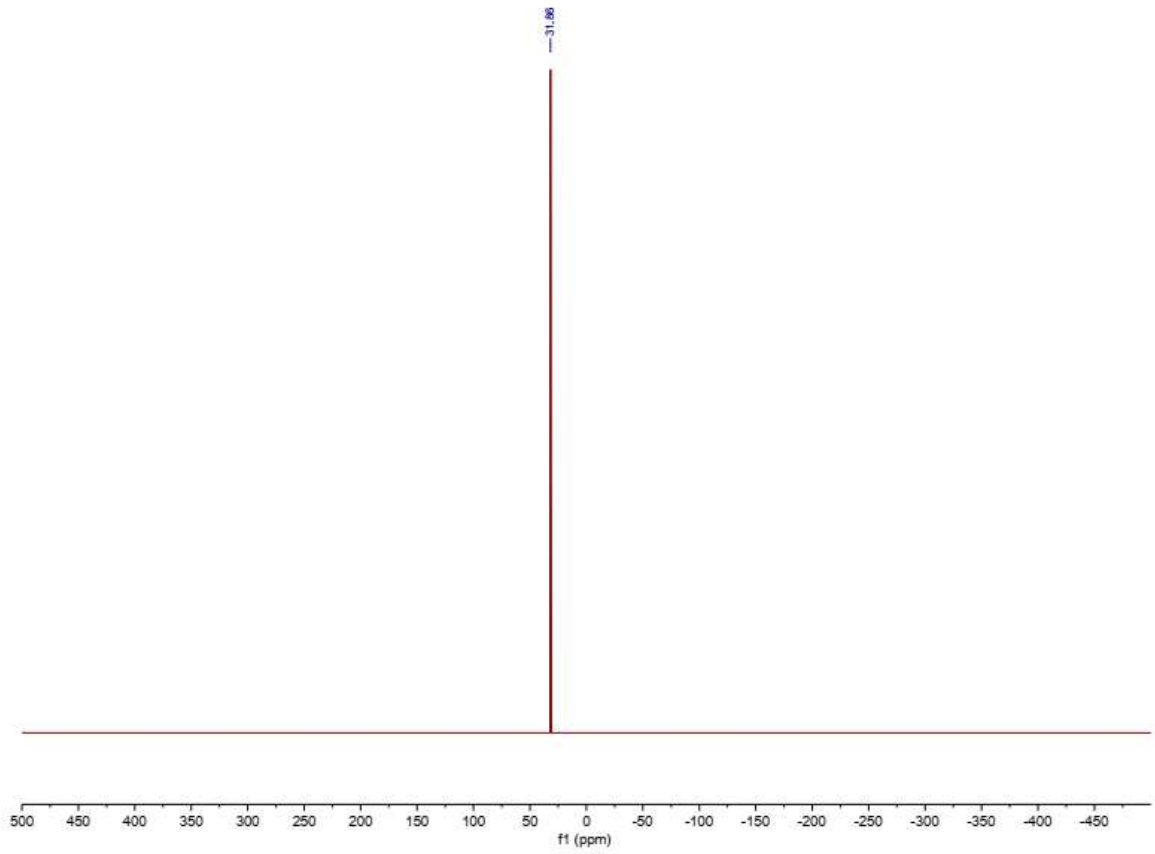

Figure S20. ^{31}P-NMR spectra of dimethyl (2-cyano-4-oxo-4-(pyridin-4-yl)butyl)phosphonate **5g**

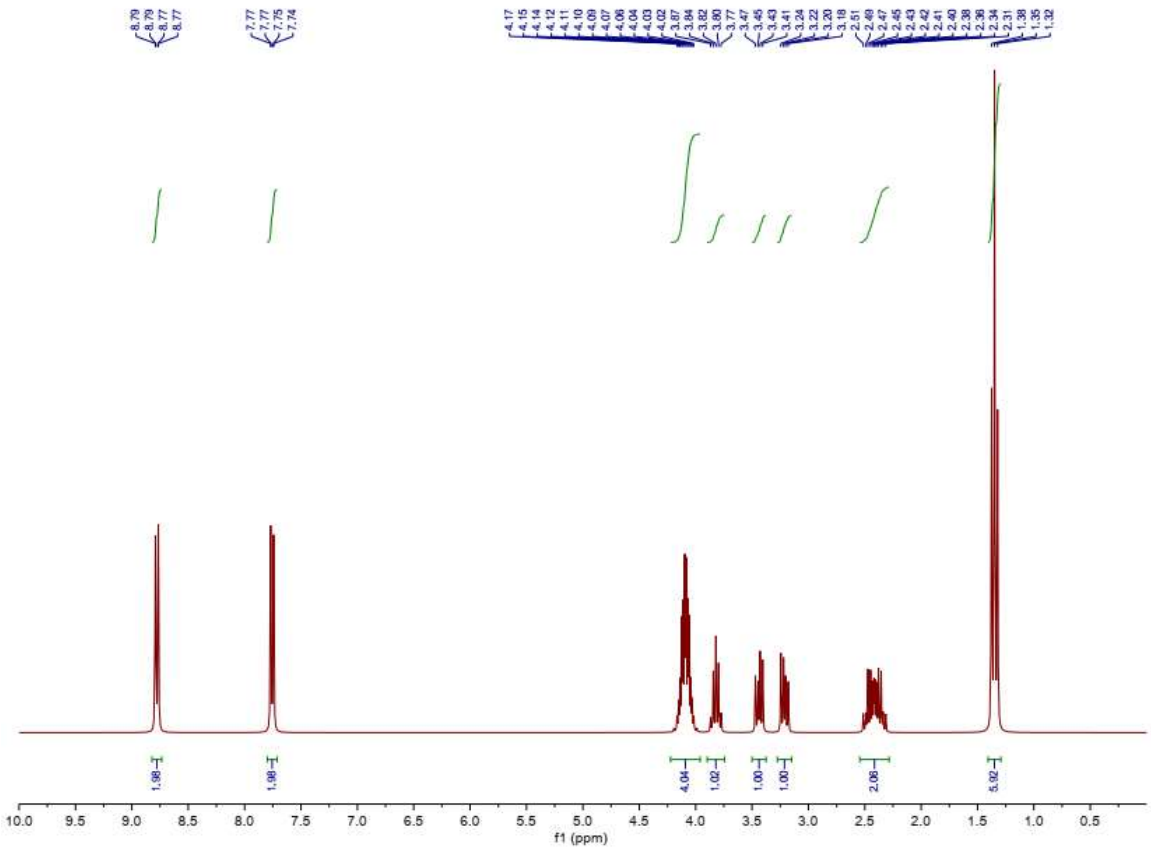

Figure S21. ^{1}H-NMR spectra of diethyl (2-cyano-4-oxo-4-(pyridin-4-yl)butyl)phosphonate **5h**

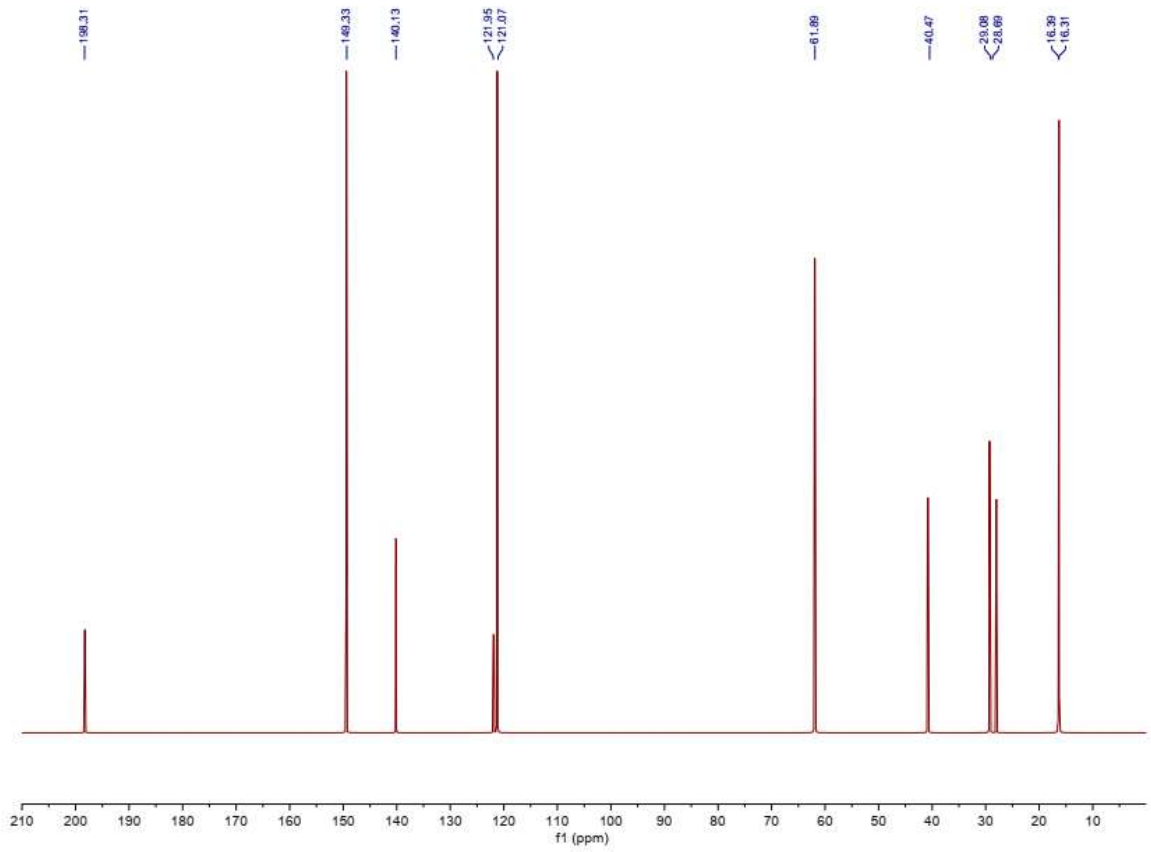

Figure S22. ^{13}C-NMR spectra of diethyl (2-cyano-4-oxo-4-(pyridin-4-yl)butyl)phosphonate **5h**

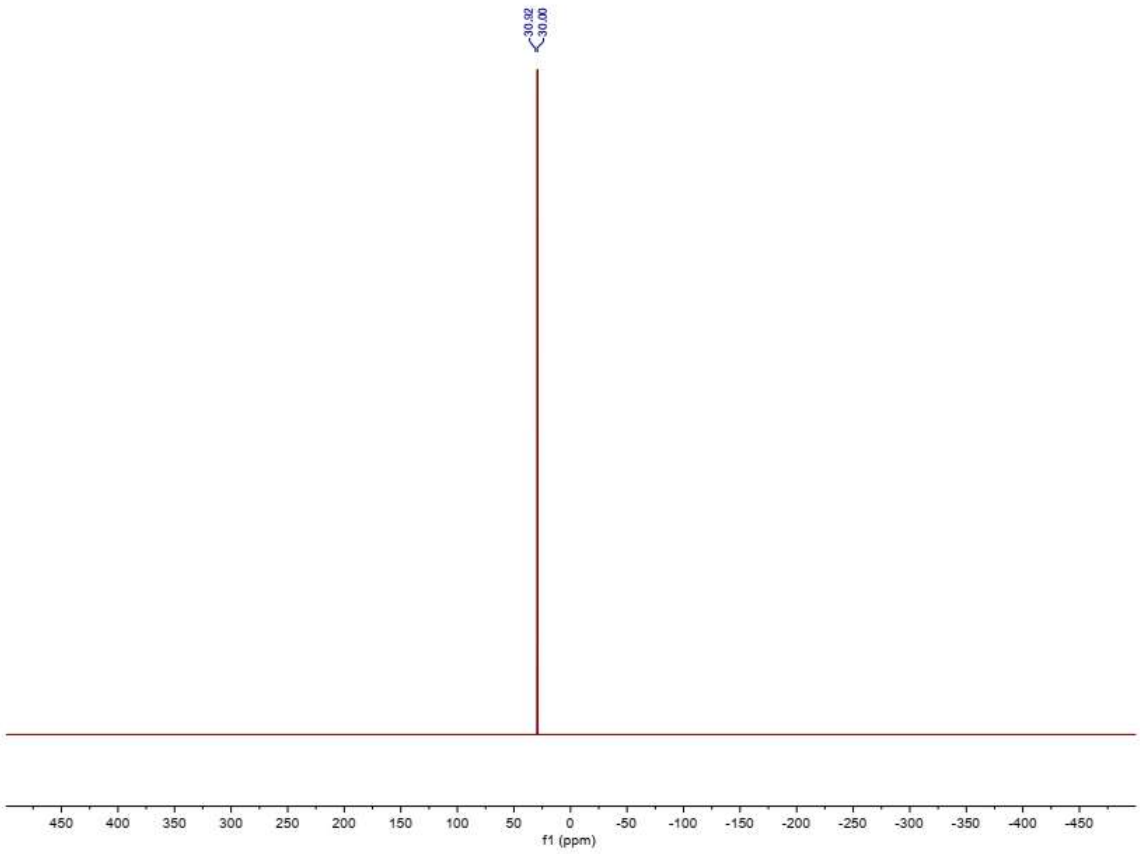

Figure S23. ^{31}P-NMR spectra of diethyl (2-cyano-4-oxo-4-(pyridin-4-yl)butyl)phosphonate **5h**

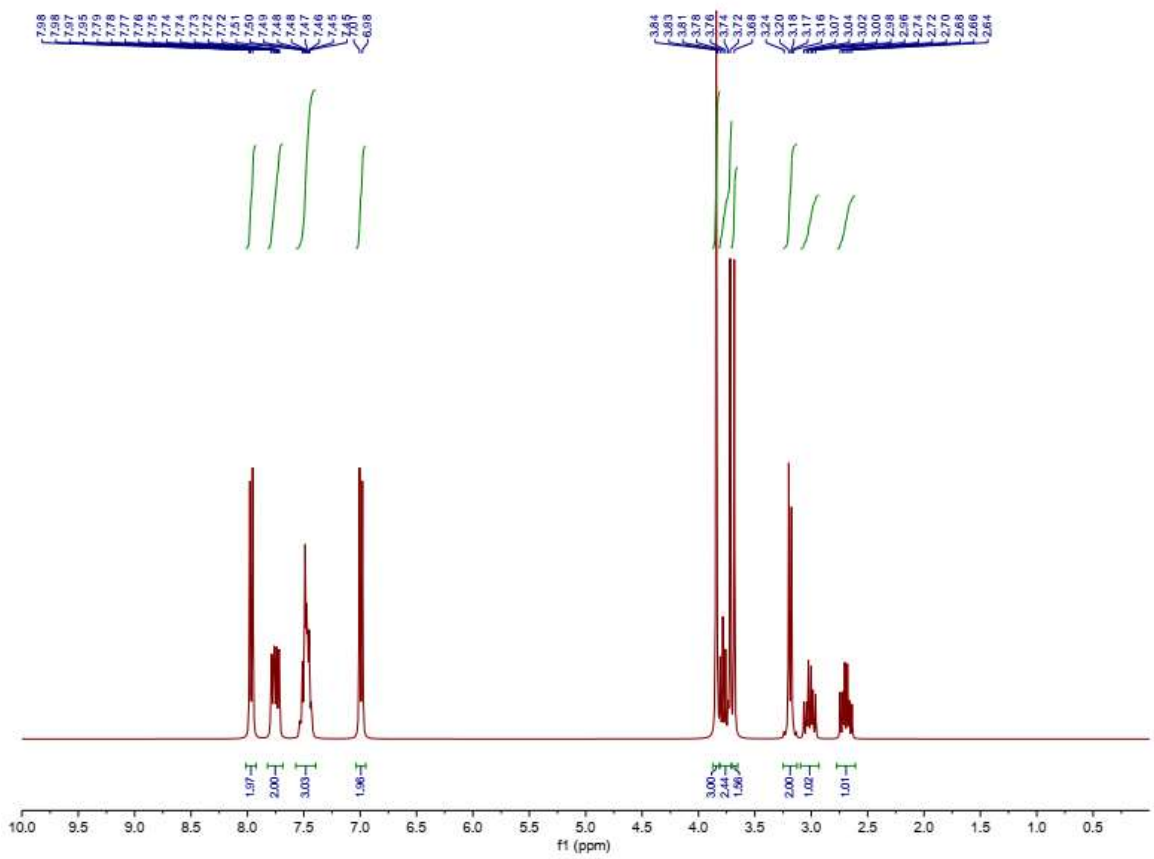

Figure S24. ^{1}H-NMR spectra of methyl phenyl (2-cyano-4-(4-methoxyphenyl)-4-oxobutyl)phosphonate **5l**

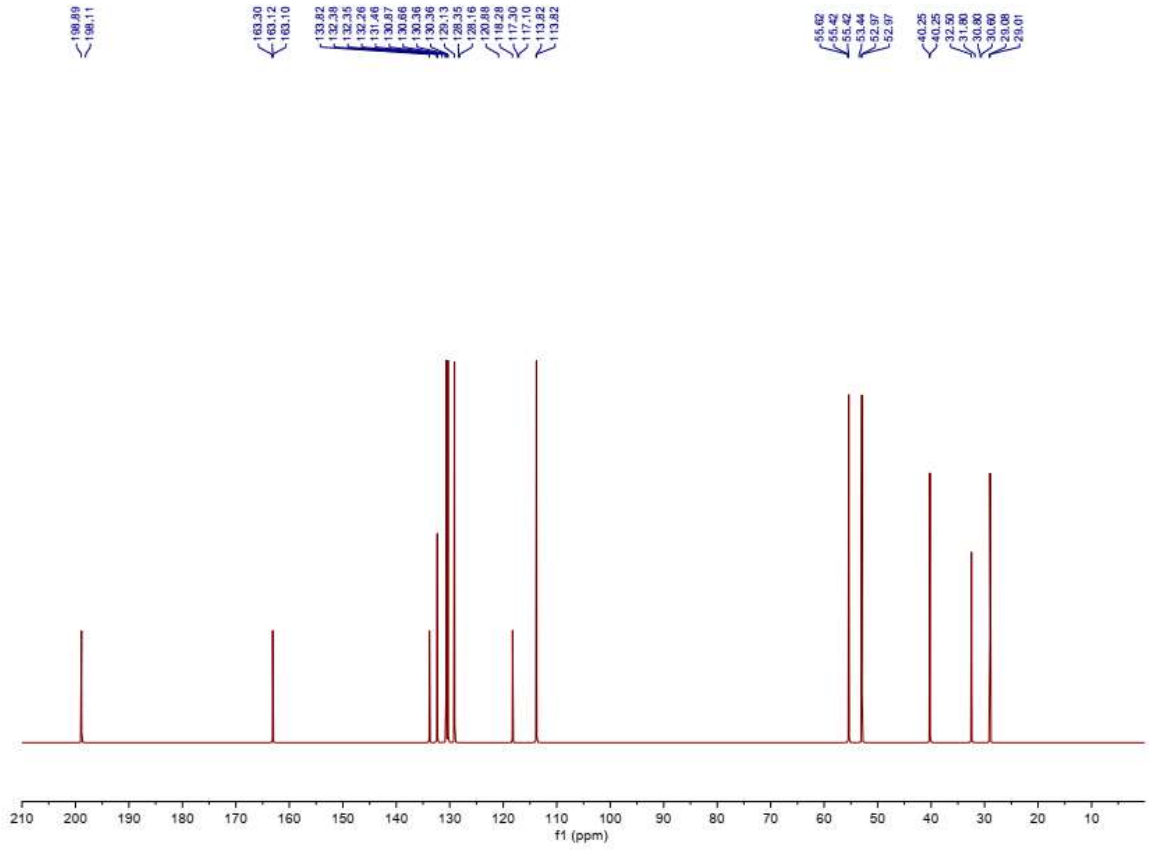

Figure S25. ^{13}C-NMR spectra of methyl phenyl (2-cyano-4-(4-methoxyphenyl)-4-oxobutyl)phosphonate **5l**

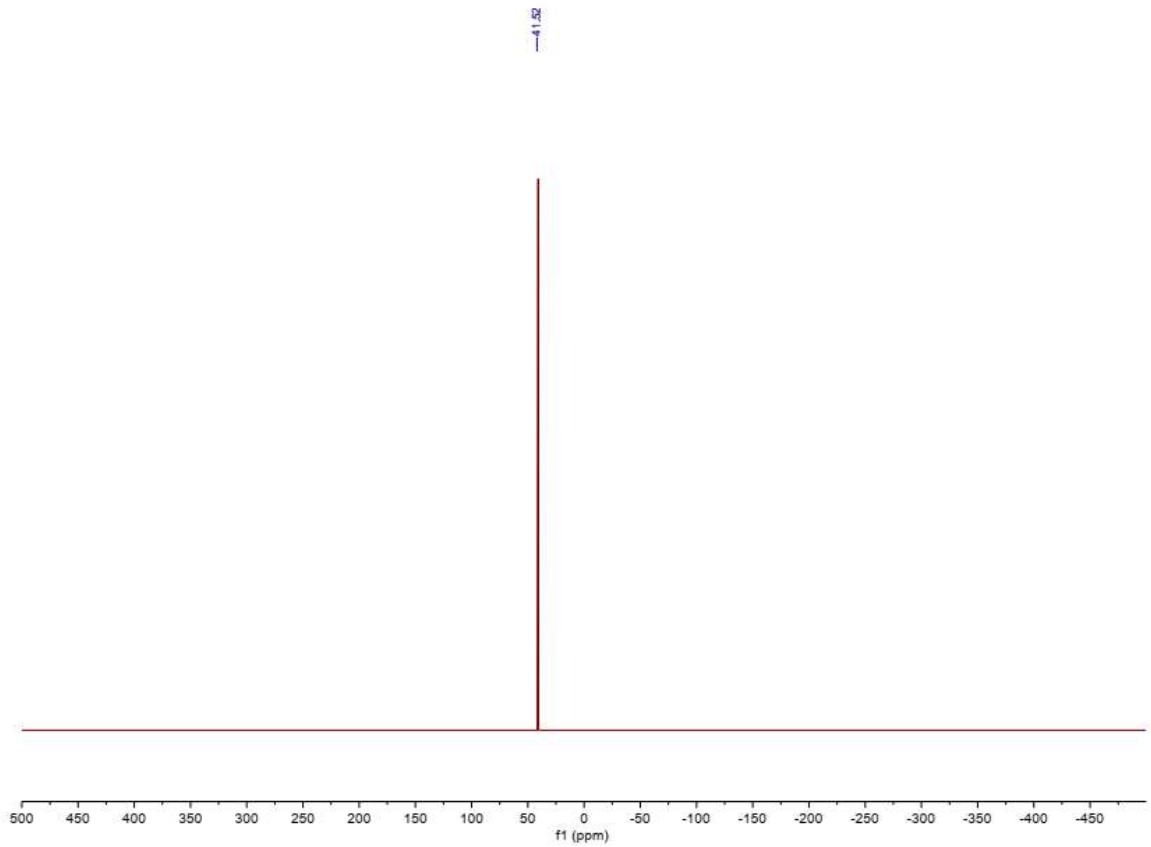

Figure S26. ^{31}P-NMR spectra of methyl phenyl (2-cyano-4-(4-methoxyphenyl)-4-oxobutyl)phosphonate **5l**