

Supplementary Materials

**A highly sensitive method for simultaneous determination of the quaternary ammonium pesticides chlormequat and mepiquat in pear and potato by modified QuEChERS-High performance liquid chromatography-tandem mass spectrometry**

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## Chlormequat (CQ)

### Precursor (RC)

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.183730 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.192693                    |
| Thermal correction to Enthalpy=              | 0.193637                    |
| Thermal correction to Gibbs Free Energy=     | 0.149805                    |
| Sum of electronic and zero-point Energies=   | -712.899741                 |
| Sum of electronic and thermal Energies=      | -712.890778                 |
| Sum of electronic and thermal Enthalpies=    | -712.889834                 |
| Sum of electronic and thermal Free Energies= | -712.933666                 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | -1.30464000 | 0.03954800  | 0.00000800  |
| C  | -1.61577000 | -0.77641100 | -1.23196500 |
| H  | -1.35100100 | -0.19616000 | -2.11663300 |
| H  | -1.04857500 | -1.70567700 | -1.20748000 |
| H  | -2.68282500 | -1.00086600 | -1.24016900 |
| C  | -1.61646000 | -0.76955200 | 1.23631700  |
| H  | -1.04708700 | -1.69762900 | 1.21865900  |
| H  | -1.35478000 | -0.18327700 | 2.11792100  |
| H  | -2.68301800 | -0.99637500 | 1.24372700  |
| C  | -2.17456900 | 1.27680500  | -0.00364800 |
| H  | -1.95656900 | 1.86557200  | 0.88772000  |
| H  | -1.95761800 | 1.85962700  | -0.89917200 |
| H  | -3.22103500 | 0.97070100  | -0.00201600 |
| C  | 1.20401700  | -0.60813900 | 0.00005600  |
| H  | 1.15832500  | -1.23419900 | 0.89163200  |
| H  | 1.15871900  | -1.23506600 | -0.89092400 |
| C  | 0.15577200  | 0.50380500  | -0.00080700 |
| H  | 0.27739200  | 1.12972300  | -0.88733700 |
| H  | 0.27775600  | 1.13154300  | 0.88438500  |
| Cl | 2.81440400  | 0.19154100  | -0.00000500 |

### TS (Frequencies -- -535.1182)

|  |                             |
|--|-----------------------------|
| Zero-point correction=                     | 0.175446 (Hartree/Particle) |
| Thermal correction to Energy=              | 0.185558                    |
| Thermal correction to Enthalpy=            | 0.186502                    |
| Thermal correction to Gibbs Free Energy=   | 0.139350                    |
| Sum of electronic and zero-point Energies= | -712.801677                 |

|  |             |
|--|-------------|
| Sum of electronic and thermal Energies=      | -712.791565 |
| Sum of electronic and thermal Enthalpies=    | -712.790621 |
| Sum of electronic and thermal Free Energies= | -712.837773 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | 1.73477900  | -0.08472800 | -0.01172800 |
| C  | 1.51078600  | 1.29686700  | -0.30938500 |
| H  | 1.59718500  | 1.50142900  | -1.37845800 |
| H  | 0.45341900  | 1.60196400  | -0.01662300 |
| H  | 2.14230100  | 1.99955700  | 0.25350900  |
| C  | 2.16644000  | -0.32927200 | 1.36876400  |
| H  | 1.48324100  | 0.16122200  | 2.07004000  |
| H  | 2.16067900  | -1.40294700 | 1.57309000  |
| H  | 3.18071300  | 0.05424200  | 1.55930500  |
| C  | 2.53182100  | -0.81929200 | -1.00520700 |
| H  | 2.50222000  | -1.88693500 | -0.77393500 |
| H  | 2.11500700  | -0.67039600 | -2.00481000 |
| H  | 3.58399500  | -0.49697400 | -1.01469300 |
| C  | -1.32352500 | 1.01600800  | -0.00375600 |
| H  | -1.42924500 | 1.51724000  | 0.95297900  |
| H  | -1.49480800 | 1.58569800  | -0.91092900 |
| C  | -1.06029200 | -0.42121900 | -0.06630000 |
| H  | -0.76249100 | -0.85711700 | -1.01318900 |
| H  | -0.69820400 | -0.92591000 | 0.82159900  |
| Cl | -2.93699100 | -0.35567800 | 0.00350100  |

### Product (PC)

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.177910 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.189574                    |
| Thermal correction to Enthalpy=              | 0.190518                    |
| Thermal correction to Gibbs Free Energy=     | 0.134799                    |
| Sum of electronic and zero-point Energies=   | -712.906855                 |
| Sum of electronic and thermal Energies=      | -712.895191                 |
| Sum of electronic and thermal Enthalpies=    | -712.894247                 |
| Sum of electronic and thermal Free Energies= | -712.949966                 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 2.25051700  | 0.14805200  | 0.21213800  |
| C | 1.57774300  | 0.42565700  | 1.26650800  |
| H | 1.18322400  | 1.42609900  | 1.40973100  |
| H | -4.76025100 | 0.40420000  | 0.12235100  |
| H | 1.40614300  | -0.33938400 | 2.01658900  |
| C | 2.78789400  | -1.20508500 | -0.04182900 |
| H | 2.57375000  | -1.85323800 | 0.80664300  |
| H | 2.31416900  | -1.59928900 | -0.94427700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 3.86588000  | -1.13032700 | -0.19920000 |
| C  | 2.49063500  | 1.14441400  | -0.85307800 |
| H  | 2.00783200  | 0.79273200  | -1.76767300 |
| H  | 2.07663500  | 2.10781000  | -0.55897100 |
| H  | 3.56754600  | 1.22862500  | -1.01641800 |
| C  | -3.69216600 | 0.59571600  | 0.27985900  |
| H  | -3.45435600 | 1.56677900  | -0.16282300 |
| H  | -3.51192600 | 0.63924800  | 1.35673200  |
| C  | -2.91066800 | -0.52251300 | -0.37393100 |
| H  | -3.10768300 | -1.49957800 | 0.06699500  |
| H  | -3.04983300 | -0.56662700 | -1.45400700 |
| Cl | -1.08149300 | -0.28485600 | -0.16622400 |

## Mepiquat (MQ)

### Concerted pathway

#### Q-Precursor (Q-RC)

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.229936 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.238180                    |
| Thermal correction to Enthalpy=              | 0.239124                    |
| Thermal correction to Gibbs Free Energy=     | 0.198221                    |
| Sum of electronic and zero-point Energies=   | -330.706073                 |
| Sum of electronic and thermal Energies=      | -330.697828                 |
| Sum of electronic and thermal Enthalpies=    | -330.696884                 |
| Sum of electronic and thermal Free Energies= | -330.737787                 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.08764200 | -1.25027100 | -0.40641200 |
| C | 1.33139000  | -1.26262900 | 0.15851300  |
| C | 2.10908900  | -0.00005400 | -0.23746400 |
| C | 1.33151400  | 1.26260200  | 0.15849100  |
| C | -0.08769500 | 1.25044700  | -0.40604300 |
| H | 3.09341400  | -0.00007500 | 0.23869600  |
| H | 1.31279900  | -1.38206000 | 1.24776800  |
| H | 1.82073800  | -2.16020100 | -0.23399200 |
| H | -0.06462900 | -1.25226000 | -1.49999200 |
| H | -0.67648200 | -2.10834500 | -0.07282600 |
| H | 1.31323500  | 1.38218000  | 1.24773700  |
| H | 1.82084800  | 2.16008900  | -0.23423000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.67641200 | 2.10836100  | -0.07182700 |
| H | -0.06506200 | 1.25297700  | -1.49962900 |
| H | 2.28406900  | -0.00009900 | -1.32128800 |
| N | -0.88148500 | 0.00000000  | -0.01608600 |
| C | -1.19266800 | -0.00019600 | 1.45936300  |
| H | -1.77516400 | 0.89188900  | 1.69239000  |
| H | -1.77298700 | -0.89363100 | 1.69264200  |
| H | -0.27203500 | 0.00100900  | 2.03700000  |
| C | -2.18561300 | 0.00008000  | -0.77052500 |
| H | -2.75115200 | 0.89358200  | -0.50264700 |
| H | -1.97920100 | -0.00057900 | -1.84105100 |
| H | -2.75183400 | -0.89270100 | -0.50168400 |

### Q-TS (Frequencies -- -1220.0951)

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.220721 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.229797                    |
| Thermal correction to Enthalpy=              | 0.230741                    |
| Thermal correction to Gibbs Free Energy=     | 0.187505                    |
| Sum of electronic and zero-point Energies=   | -330.558241                 |
| Sum of electronic and thermal Energies=      | -330.549165                 |
| Sum of electronic and thermal Enthalpies=    | -330.548221                 |
| Sum of electronic and thermal Free Energies= | -330.591457                 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.02501500  | 1.16631800  | -0.48022500 |
| C | -1.29178400 | 1.34968000  | 0.29958500  |
| C | -2.28470500 | 0.22498500  | -0.02667600 |
| C | -1.63669200 | -1.15008100 | 0.18955400  |
| C | -0.31777900 | -1.25030400 | -0.60265800 |
| H | -3.18354500 | 0.32372500  | 0.59019400  |
| H | -1.09842200 | 1.37611600  | 1.38032700  |
| H | -1.70560800 | 2.33127700  | 0.04279400  |
| H | -0.16159400 | 1.27325100  | -1.55468300 |
| H | 0.74824900  | 1.94074000  | -0.19501100 |
| H | -1.45526100 | -1.31909900 | 1.25973100  |
| H | -2.29893900 | -1.95798100 | -0.13973500 |
| H | 0.17757400  | -2.21292700 | -0.43783600 |
| H | -0.52963000 | -1.17188100 | -1.67538100 |
| H | -2.60837800 | 0.31379600  | -1.07249700 |
| N | 0.64269000  | -0.16928300 | -0.28629900 |
| C | 1.27109700  | -0.33388600 | 1.03345100  |
| H | 1.61074300  | -1.35802700 | 1.19032900  |
| H | 2.18307000  | 0.35985100  | 1.05705700  |
| H | 0.71478700  | 0.00457700  | 1.92774800  |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 3.13252300 | 0.13510200  | -0.28646200 |
| H | 3.00139500 | -0.81877000 | -0.78045900 |
| H | 2.80993800 | 1.02422400  | -0.81667000 |
| H | 3.91074500 | 0.22522500  | 0.46877500  |

### Q-Product (Q-PC)

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.222705 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.234297                    |
| Thermal correction to Enthalpy=              | 0.235241                    |
| Thermal correction to Gibbs Free Energy=     | 0.180749                    |
| Sum of electronic and zero-point Energies=   | -330.698694                 |
| Sum of electronic and thermal Energies=      | -330.687102                 |
| Sum of electronic and thermal Enthalpies=    | -330.686158                 |
| Sum of electronic and thermal Free Energies= | -330.740650                 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.20698300 | -1.35556300 | 0.31967000  |
| C | -2.24457500 | -0.68212900 | -0.58920200 |
| C | -2.46089700 | 0.78683500  | -0.20082500 |
| C | -1.12938300 | 1.55051400  | -0.18609300 |
| C | -0.09757200 | 0.86304800  | 0.71911200  |
| H | -3.15122600 | 1.25900300  | -0.90559600 |
| H | -1.91340100 | -0.75921500 | -1.63198500 |
| H | -3.17454400 | -1.25322700 | -0.50688000 |
| H | -1.55223300 | -1.37774100 | 1.35919200  |
| H | -0.96938400 | -2.37343000 | 0.00548600  |
| H | -0.72082300 | 1.62992600  | -1.20086500 |
| H | -1.26367600 | 2.57156800  | 0.18435000  |
| H | 0.88503100  | 1.33561700  | 0.67215900  |
| H | -0.43564500 | 0.85248900  | 1.76117400  |
| H | -2.93394900 | 0.84444200  | 0.78808600  |
| N | 0.05823600  | -0.56595200 | 0.32142700  |
| C | 1.18381300  | -1.06644800 | -0.02508900 |
| H | 2.08025000  | -0.45175200 | -0.02176400 |
| H | 4.74709100  | -0.73717000 | -0.54306800 |
| H | 1.24132500  | -2.11072400 | -0.31951100 |
| C | 4.71872500  | 0.32004200  | -0.26561300 |
| H | 4.08398000  | 0.87749300  | -0.96107700 |
| H | 4.35938500  | 0.43294100  | 0.76173700  |
| H | 5.73140300  | 0.72365200  | -0.32318400 |

## Stepwise pathway

### C-Precursor (C-RC)

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.229935 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.238180                    |
| Thermal correction to Enthalpy=              | 0.239124                    |
| Thermal correction to Gibbs Free Energy=     | 0.198221                    |
| Sum of electronic and zero-point Energies=   | -330.706073                 |
| Sum of electronic and thermal Energies=      | -330.697828                 |
| Sum of electronic and thermal Enthalpies=    | -330.696884                 |
| Sum of electronic and thermal Free Energies= | -330.737788                 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.08766900 | -1.25036600 | -0.40621000 |
| C | 1.33145700  | -1.26261300 | 0.15850800  |
| C | 2.10908700  | -0.00000300 | -0.23747800 |
| C | 1.33146500  | 1.26261000  | 0.15851700  |
| C | -0.08766000 | 1.25036800  | -0.40620400 |
| H | 3.09342500  | -0.00001000 | 0.23865300  |
| H | 1.31302500  | -1.38210000 | 1.24776000  |
| H | 1.82079300  | -2.16014700 | -0.23409900 |
| H | -0.06485800 | -1.25265400 | -1.49979300 |
| H | -0.67644100 | -2.10835300 | -0.07227900 |
| H | 1.31303300  | 1.38209600  | 1.24776900  |
| H | 1.82080900  | 2.16014100  | -0.23408800 |
| H | -0.67643300 | 2.10835200  | -0.07227300 |
| H | -0.06484100 | 1.25265800  | -1.49978800 |
| H | 2.28403300  | 0.00000300  | -1.32130700 |
| N | -0.88148100 | 0.00000000  | -0.01608600 |
| C | -1.19271000 | -0.00000500 | 1.45935500  |
| H | -1.77405400 | 0.89279600  | 1.69250900  |
| H | -1.77419300 | -0.89272600 | 1.69247400  |
| H | -0.27208900 | -0.00009000 | 2.03701400  |
| C | -2.18559300 | 0.00000900  | -0.77056200 |
| H | -2.75147900 | 0.89314300  | -0.50219700 |
| H | -1.97914800 | 0.00002600  | -1.84108000 |
| H | -2.75147500 | -0.89313800 | -0.50222700 |

### C-TS1 (Frequencies -- -768.9744)

|  |                             |
|--|-----------------------------|
| Zero-point correction=                   | 0.219975 (Hartree/Particle) |
| Thermal correction to Energy=            | 0.229682                    |
| Thermal correction to Enthalpy=          | 0.230626                    |
| Thermal correction to Gibbs Free Energy= | 0.185948                    |



|  |             |
|--|-------------|
| Sum of electronic and zero-point Energies=   | -330.607384 |
| Sum of electronic and thermal Energies=      | -330.597677 |
| Sum of electronic and thermal Enthalpies=    | -330.596733 |
| Sum of electronic and thermal Free Energies= | -330.641411 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.05734500 | 1.76356600  | -0.23001100 |
| C | -1.80735000 | 0.74604800  | 0.34829800  |
| C | -2.03540600 | -0.57065400 | -0.30234600 |
| C | -0.85773000 | -1.50774500 | 0.13526500  |
| C | 0.51676200  | -1.16487000 | -0.46318700 |
| H | -2.98597700 | -1.00407800 | 0.01751300  |
| H | -2.13415100 | 0.88655700  | 1.38011900  |
| H | -2.33733600 | 1.87058900  | -0.30081500 |
| H | -0.70959400 | 1.67371300  | -1.25337200 |
| H | -0.74461500 | 2.62703000  | 0.35197400  |
| H | -0.81830200 | -1.57551500 | 1.22743400  |
| H | -1.13597700 | -2.50704600 | -0.21477800 |
| H | 1.20273800  | -2.00234700 | -0.24350000 |
| H | 0.42145500  | -1.12356300 | -1.55477800 |
| H | -2.03304800 | -0.47833300 | -1.39331200 |
| N | 1.10063000  | 0.11704400  | -0.01755200 |
| C | 1.50876100  | 0.07285600  | 1.39273000  |
| H | 2.24274000  | -0.72653200 | 1.58972800  |
| H | 1.96003200  | 1.02804000  | 1.67317000  |
| H | 0.64760200  | -0.09643300 | 2.04682900  |
| C | 2.24640900  | 0.47470200  | -0.86811600 |
| H | 3.05198900  | -0.27656600 | -0.82225700 |
| H | 1.92597900  | 0.56658800  | -1.91037100 |
| H | 2.65744500  | 1.43517000  | -0.54652300 |

## C-IM

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.228648 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.237401                    |
| Thermal correction to Enthalpy=              | 0.238345                    |
| Thermal correction to Gibbs Free Energy=     | 0.195086                    |
| Sum of electronic and zero-point Energies=   | -330.703210                 |
| Sum of electronic and thermal Energies=      | -330.694457                 |
| Sum of electronic and thermal Enthalpies=    | -330.693513                 |
| Sum of electronic and thermal Free Energies= | -330.736772                 |

|   |             |            |             |
|---|-------------|------------|-------------|
| C | -1.07030500 | 1.96014700 | -0.08847400 |
| C | -0.03474500 | 0.90115500 | -0.43433500 |
| C | 1.36524900  | 1.08862100 | 0.14424000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.03563800  | -0.26495000 | -0.11788800 |
| C | 0.93825100  | -1.28464900 | 0.20501100  |
| H | 1.87872400  | 1.91975500  | -0.34524700 |
| H | 0.04739500  | 0.82032300  | -1.52300500 |
| H | -0.74572100 | 2.89947800  | -0.54570200 |
| H | -1.15492300 | 2.13367000  | 0.98700400  |
| H | -2.06056800 | 1.73476400  | -0.49552900 |
| H | 2.34347000  | -0.34161800 | -1.16545600 |
| H | 2.92045800  | -0.43616300 | 0.49905700  |
| H | 0.94745400  | -2.17093800 | -0.42994900 |
| H | 0.97680400  | -1.60533700 | 1.24653300  |
| H | 1.31987200  | 1.31681100  | 1.21607800  |
| N | -0.41538300 | -0.55591300 | 0.00594000  |
| C | -1.23588500 | -1.22379900 | -1.06294200 |
| H | -1.51299100 | -2.22442700 | -0.72829800 |
| H | -2.13575300 | -0.63419100 | -1.24342100 |
| H | -0.64580900 | -1.28857100 | -1.97742800 |
| C | -1.19019300 | -0.58304200 | 1.29658300  |
| H | -1.32003300 | -1.62403900 | 1.59519000  |
| H | -0.63346600 | -0.04824300 | 2.06575700  |
| H | -2.16529700 | -0.12078300 | 1.14965900  |

### C-TS2 (Frequencies -- -190.4457)

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.220633 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.230912                    |
| Thermal correction to Enthalpy=              | 0.231856                    |
| Thermal correction to Gibbs Free Energy=     | 0.185115                    |
| Sum of electronic and zero-point Energies=   | -330.605908                 |
| Sum of electronic and thermal Energies=      | -330.595630                 |
| Sum of electronic and thermal Enthalpies=    | -330.594685                 |
| Sum of electronic and thermal Free Energies= | -330.641427                 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.07869500  | 1.42392900  | 0.60528500  |
| C | 1.68622000  | 0.30316000  | -0.32107500 |
| C | 2.31458800  | -0.94123900 | -0.31776900 |
| C | 0.60395800  | -0.91044500 | 0.40869700  |
| C | -0.70674600 | -1.08192800 | -0.46015300 |
| H | 2.23814400  | -1.61528900 | -1.16656300 |
| H | 1.16823200  | 0.59058500  | -1.23272800 |
| H | 2.79334300  | 2.05991500  | 0.07035400  |
| H | 2.56233500  | 1.06078900  | 1.51576600  |
| H | 1.22152700  | 2.04674500  | 0.87017300  |
| H | 0.95602500  | -1.92153400 | 0.66633900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.50163700  | -0.41669800 | 1.37615500  |
| H | -0.41670500 | -1.13320500 | -1.51713500 |
| H | -1.10357200 | -2.06616500 | -0.18895900 |
| H | 3.02521400  | -1.20647400 | 0.46154700  |
| N | -1.74386000 | -0.11971700 | -0.28409600 |
| C | -1.56746900 | 1.19844600  | -0.87211000 |
| H | -2.53833500 | 1.69800100  | -0.92989300 |
| H | -0.89611300 | 1.86149500  | -0.29649500 |
| H | -1.18401100 | 1.10575300  | -1.89395900 |
| C | -2.44067300 | -0.12921100 | 0.99904900  |
| H | -3.39848700 | 0.38635100  | 0.88948300  |
| H | -2.64775200 | -1.15989000 | 1.30129800  |
| H | -1.88589800 | 0.37137000  | 1.81174600  |

### C-Product (C-PC)

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.220859 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.232875                    |
| Thermal correction to Enthalpy=              | 0.233819                    |
| Thermal correction to Gibbs Free Energy=     | 0.180271                    |
| Sum of electronic and zero-point Energies=   | -330.649094                 |
| Sum of electronic and thermal Energies=      | -330.637078                 |
| Sum of electronic and thermal Enthalpies=    | -330.636134                 |
| Sum of electronic and thermal Free Energies= | -330.689683                 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.38873900  | 1.51024000  | 0.47154100  |
| C | 1.89989600  | 0.37130200  | -0.38838800 |
| C | 3.25145200  | -0.22526300 | -0.10610800 |
| C | 2.01122400  | -1.04559500 | 0.17280800  |
| C | -1.10653000 | -1.17301300 | -0.35407400 |
| H | 3.87478200  | -0.51853900 | -0.94458100 |
| H | 1.64372000  | 0.44657000  | -1.44507800 |
| H | 1.79236500  | 2.46950800  | 0.13069800  |
| H | 1.68840900  | 1.38024200  | 1.51705200  |
| H | 0.29273400  | 1.59176000  | 0.44876400  |
| H | 1.82877300  | -1.89821000 | -0.47700900 |
| H | 1.75409900  | -1.20872300 | 1.21731000  |
| H | -0.71532100 | -1.26883900 | -1.36093600 |
| H | -0.76876000 | -1.84589200 | 0.42612700  |
| H | 3.80030200  | 0.15717200  | 0.74966600  |
| N | -1.97978900 | -0.27252800 | -0.08973600 |
| C | -2.47708800 | 0.66849100  | -1.11619100 |
| H | -3.56137900 | 0.55944400  | -1.19202900 |
| H | -2.23640400 | 1.68636000  | -0.80077900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.00930800 | 0.45221000  | -2.07547000 |
| C | -2.54534000 | -0.09797600 | 1.26547300  |
| H | -3.62973300 | -0.21684000 | 1.20805400  |
| H | -2.12102600 | -0.83778400 | 1.94255100  |
| H | -2.30884500 | 0.91013700  | 1.61345700  |