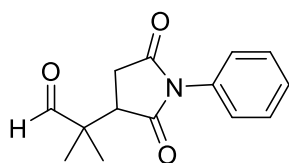


## **Supplementary Materials:**

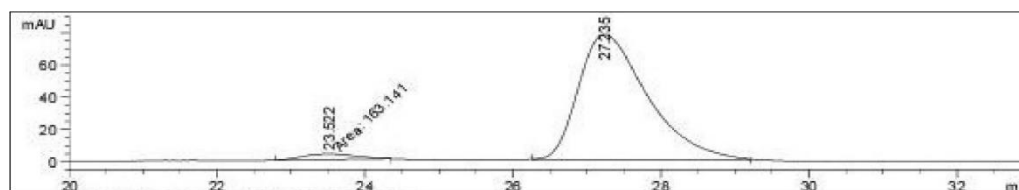
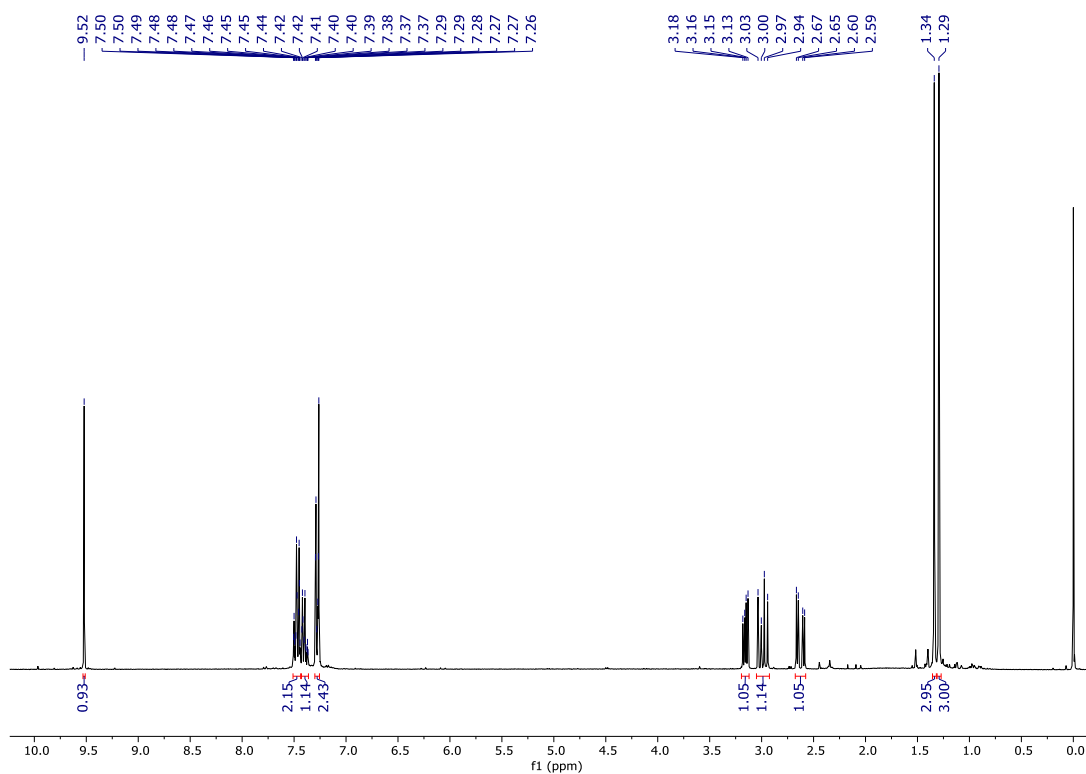
### **Enantioselective Michael addition of aldehydes to maleimides organocatalyzed by a chiral primary amine-salicylamide**

Alejandro Torregrosa-Chinillach, Adrien Moragues, Haritz Pérez-Furundarena, Rafael Chinchilla,\* Enrique Gómez-Bengoa,\* Gabriela Guillena\*

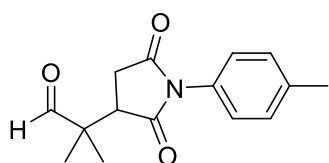
# <sup>1</sup>H NMR spectra and HPLC chromatograms



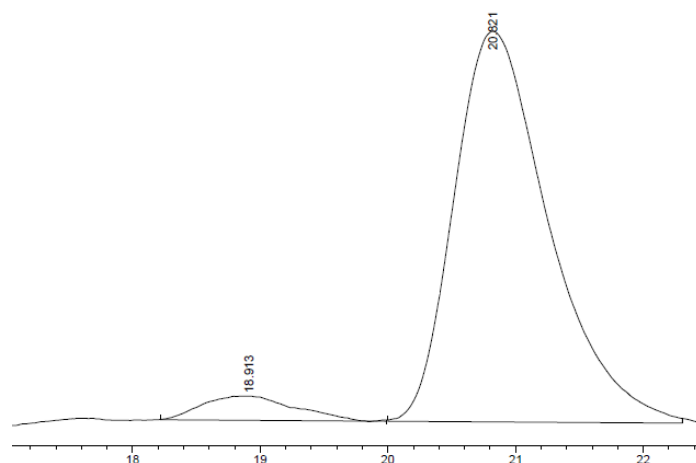
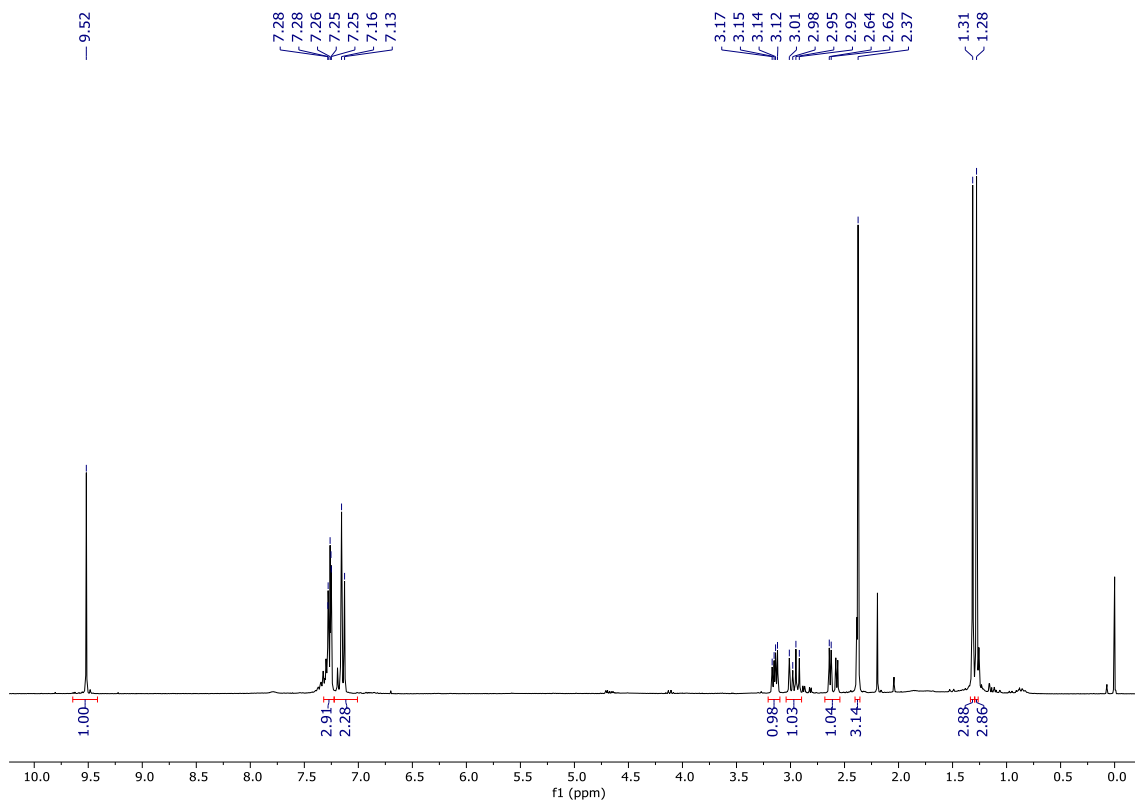
**18aa**



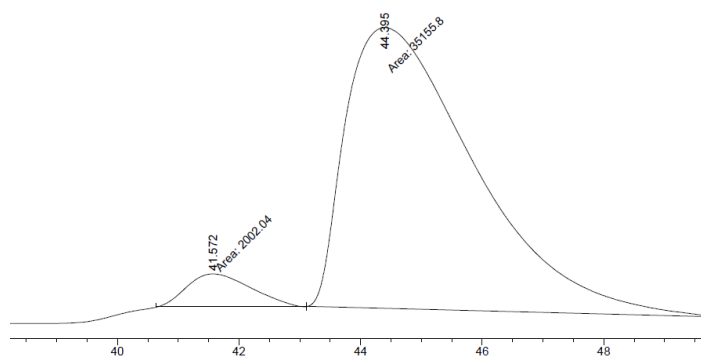
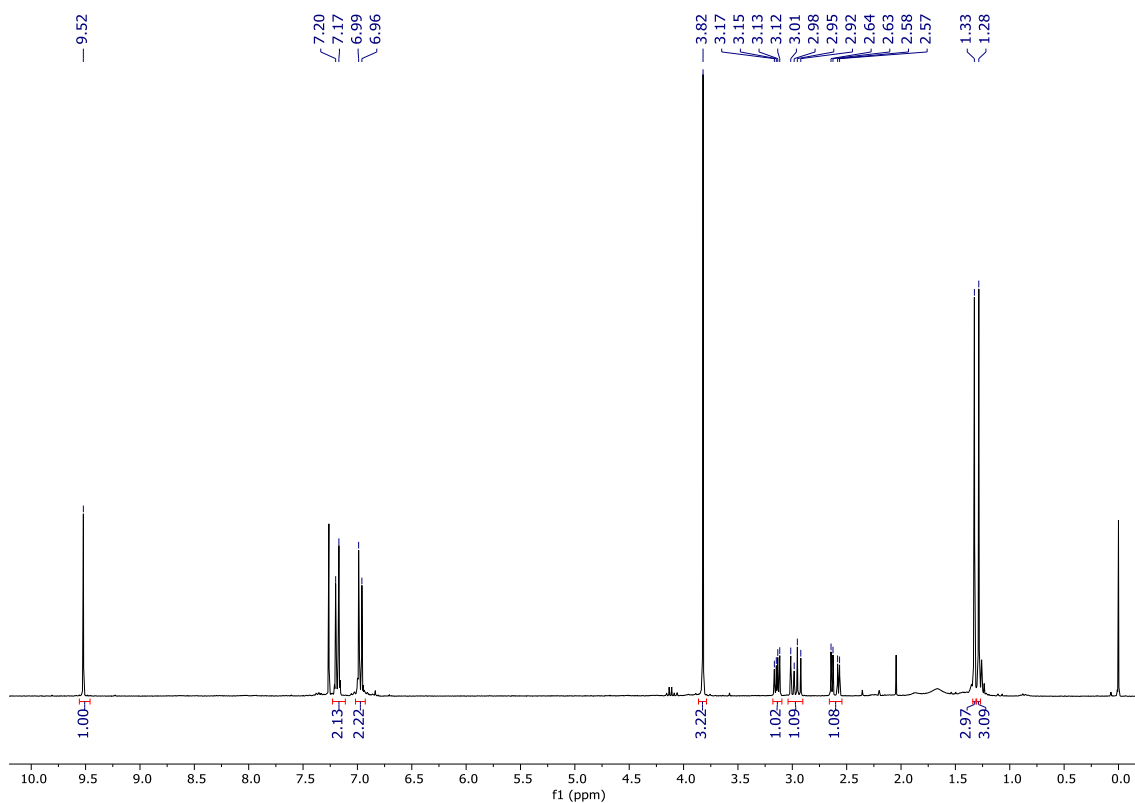
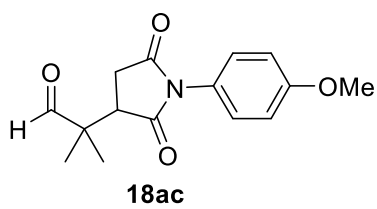
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|--------|
| 1      | 23.522        | MM   | 0.78        | 163.14       | 3.48         | 3.14   |
| 2      | 27.235        | BB   | 0.92        | 5028.85      | 77.73        | 96.86  |



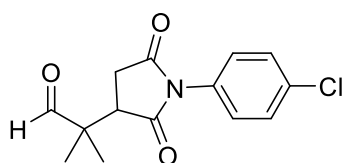
**18ab**



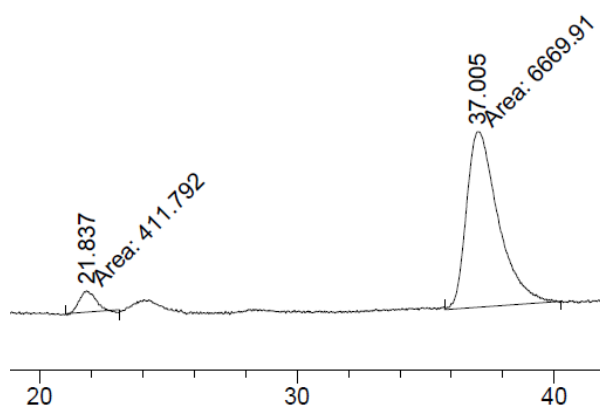
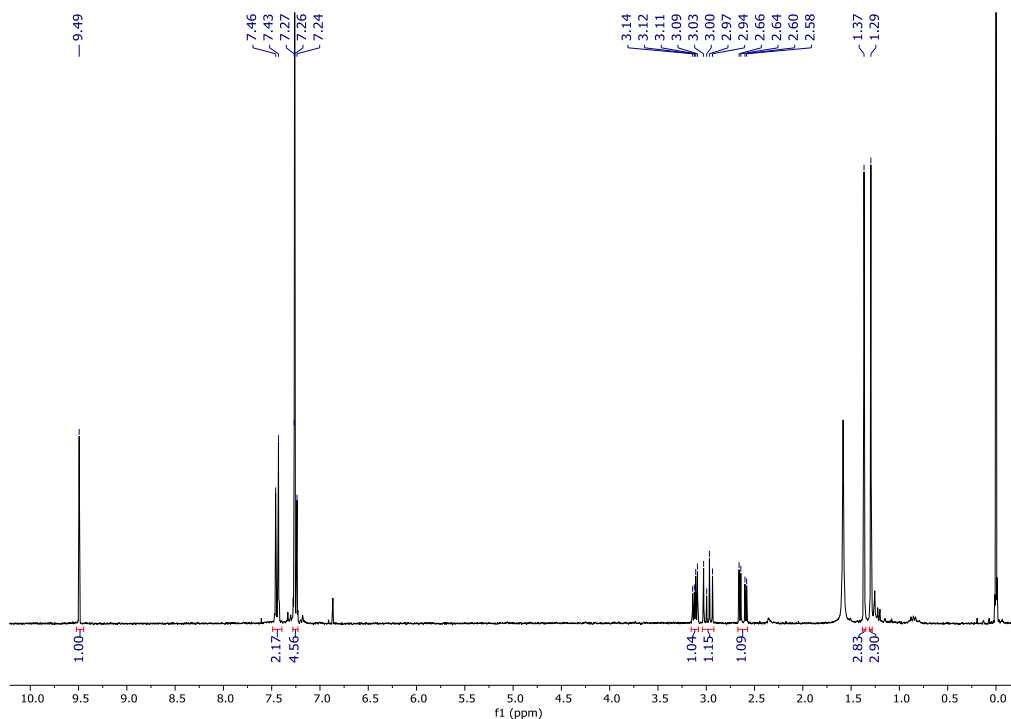
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area %  |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1      | 18.913        | BB   | 0.6072      | 196.51817    | 3.86466      | 5.8223  |
| 2      | 20.821        | BB   | 0.7592      | 3178.73779   | 61.68907     | 94.1777 |



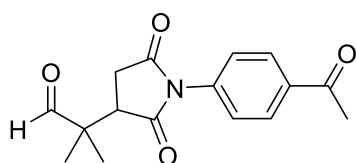
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area %  |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1      | 41.572        | MM   | 1.2081      | 2002.03589   | 27.62063     | 5.3879  |
| 2      | 44.395        | MM   | 2.4573      | 3.51558e4    | 238.44348    | 94.6121 |



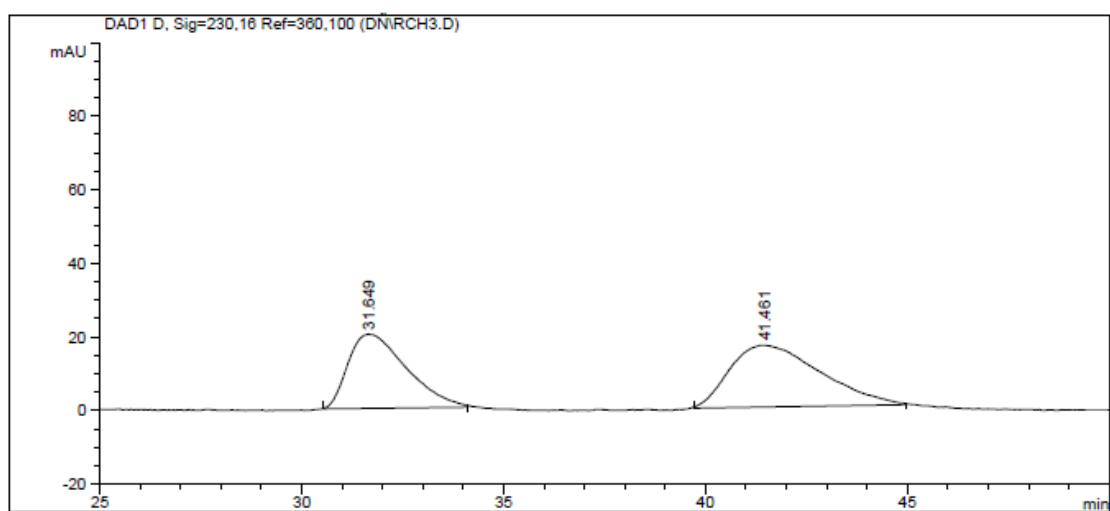
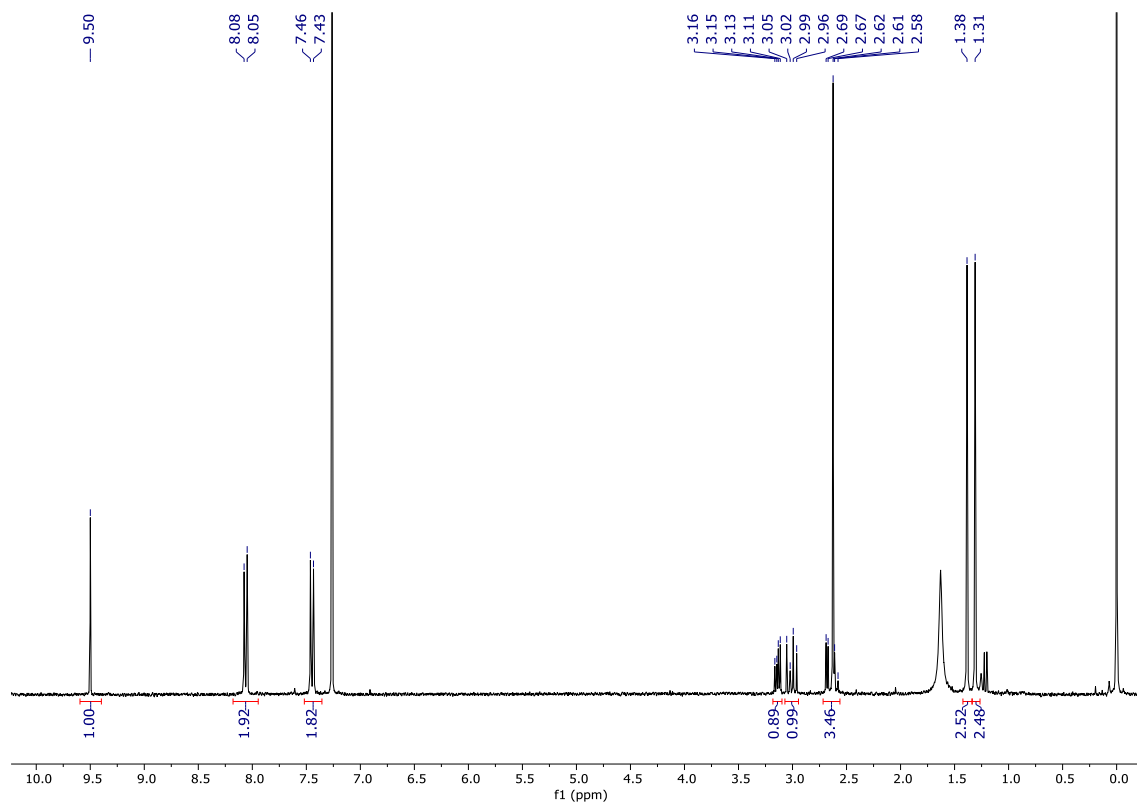
**18ad**



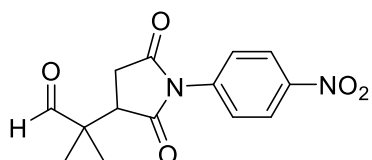
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area %  |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1      | 21.837        | MM   | 0.7213      | 411.79233    | 9.51546      | 5.8149  |
| 2      | 37.005        | MM   | 1.4320      | 6669.90967   | 77.62900     | 94.1851 |



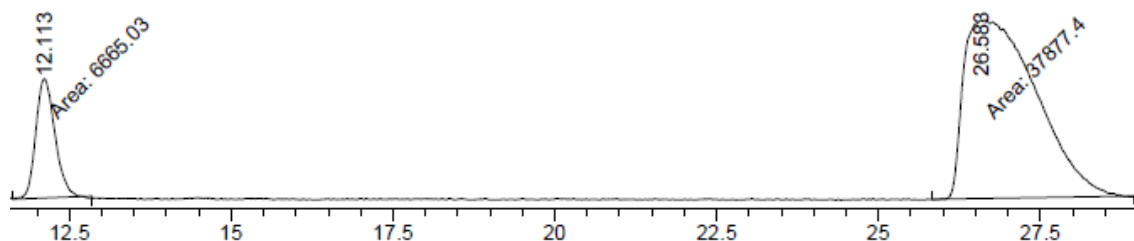
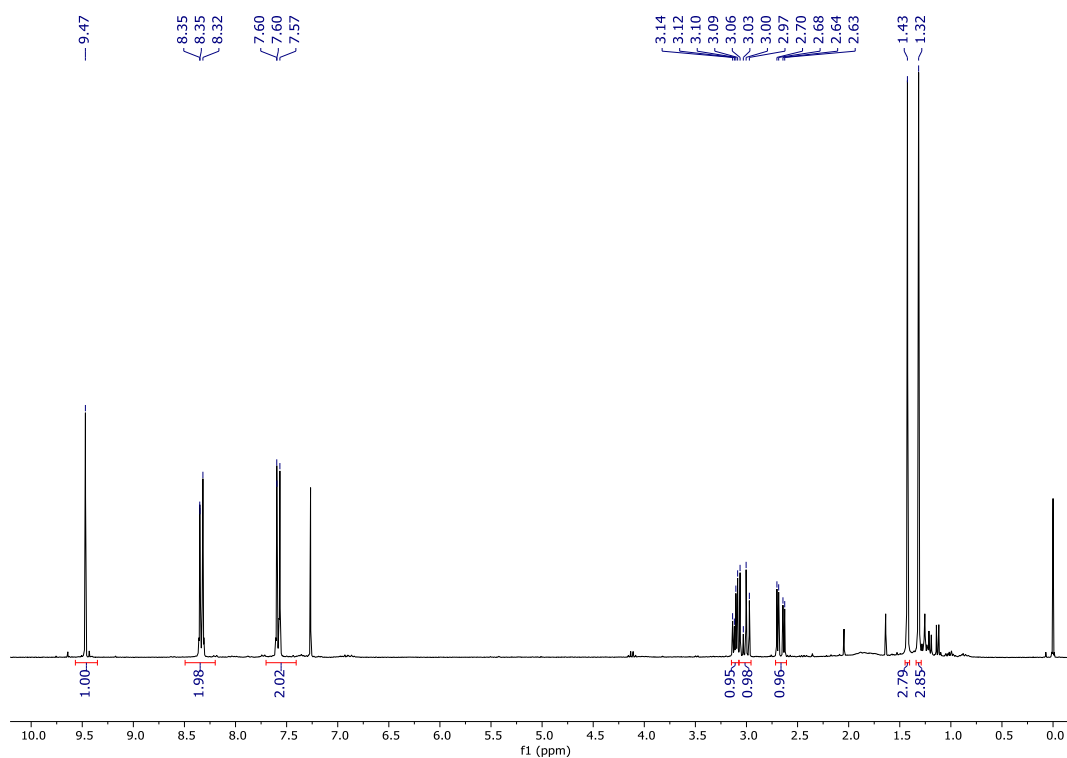
**18ae**



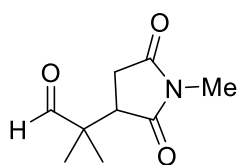
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area %  |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1      | 31.649        | BB   | 1.1917      | 2029.12036   | 20.23937     | 43.4919 |
| 2      | 41.461        | BB   | 1.8556      | 2636.38892   | 16.79266     | 56.5081 |



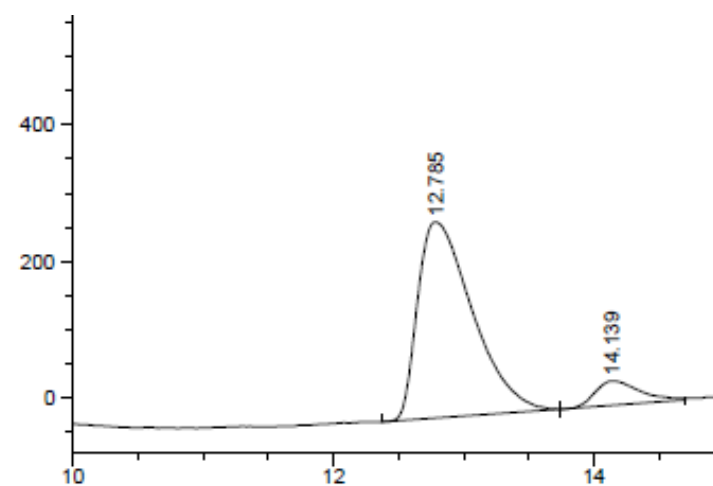
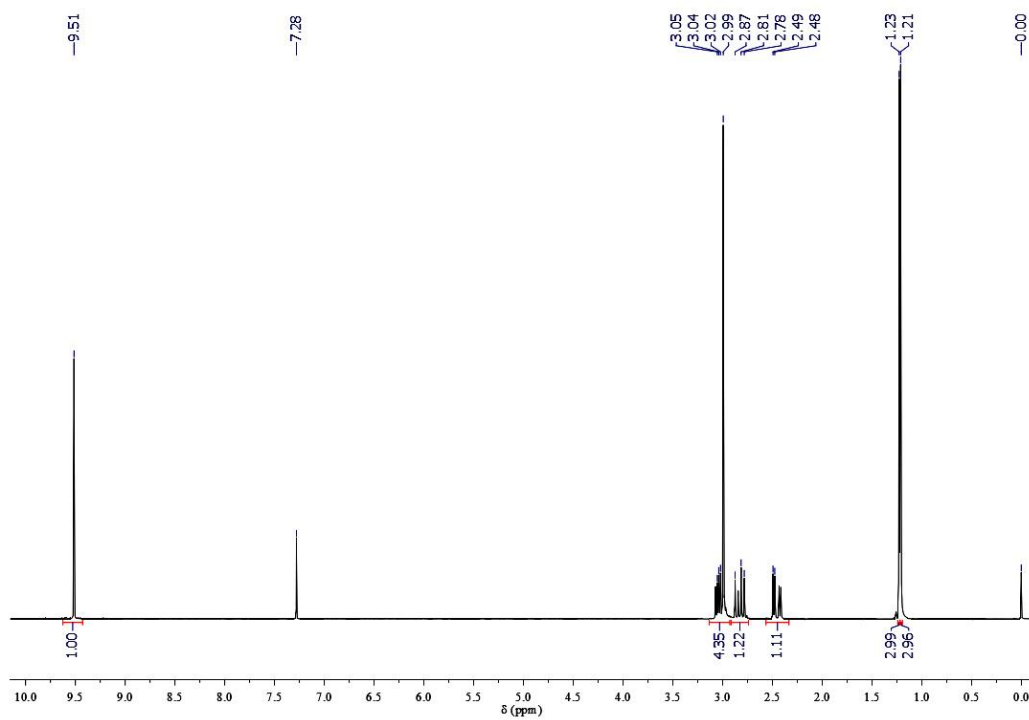
**18af**



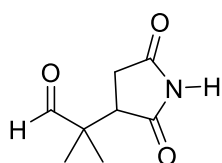
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area %  |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1      | 12.113        | MM   | 0.3436      | 6665.03223   | 323.28546    | 14.9633 |
| 2      | 26.583        | MM   | 1.3037      | 3.78774e4    | 484.23560    | 85.0367 |



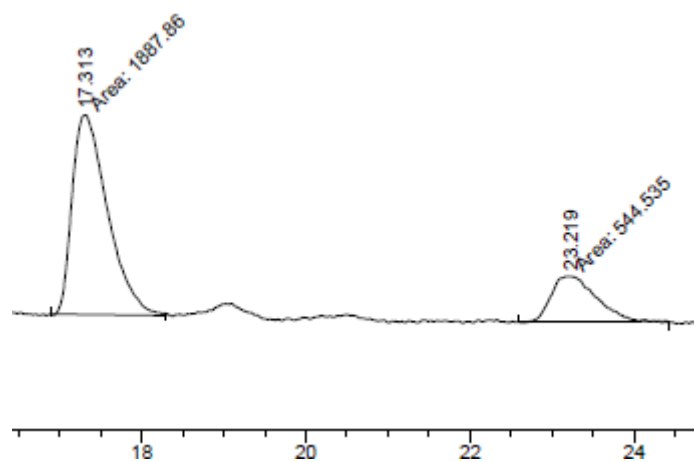
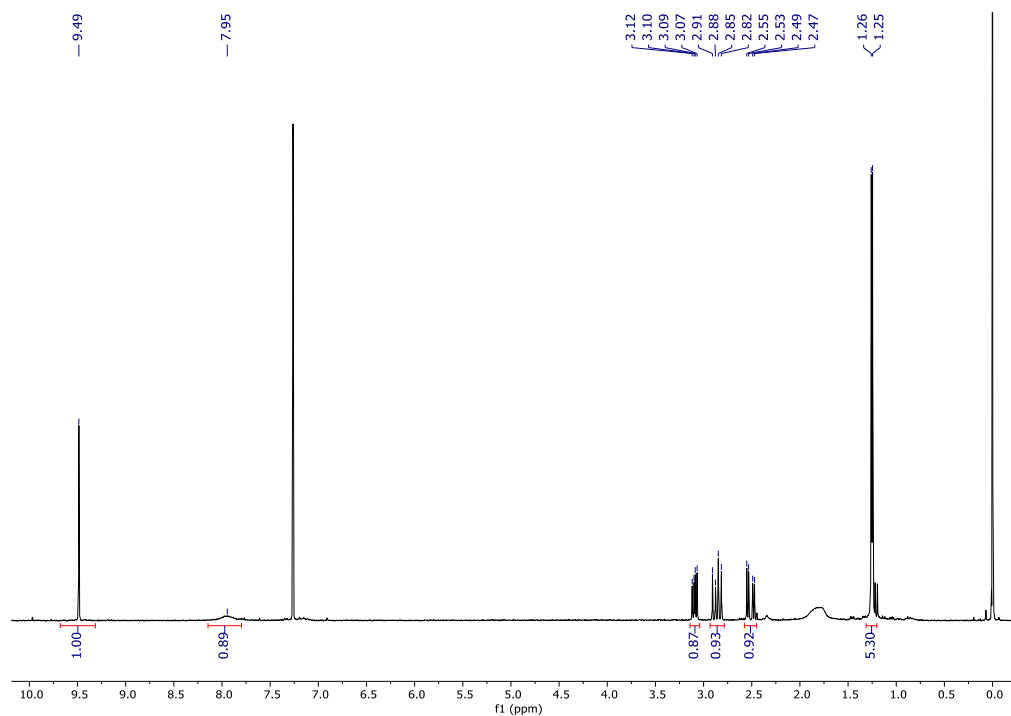
**18ag**



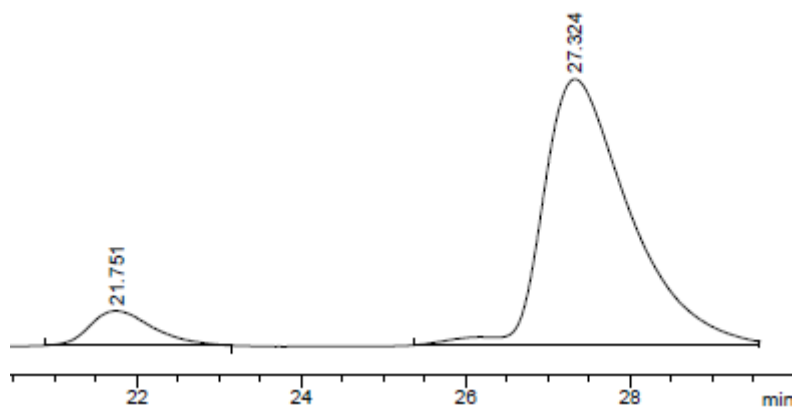
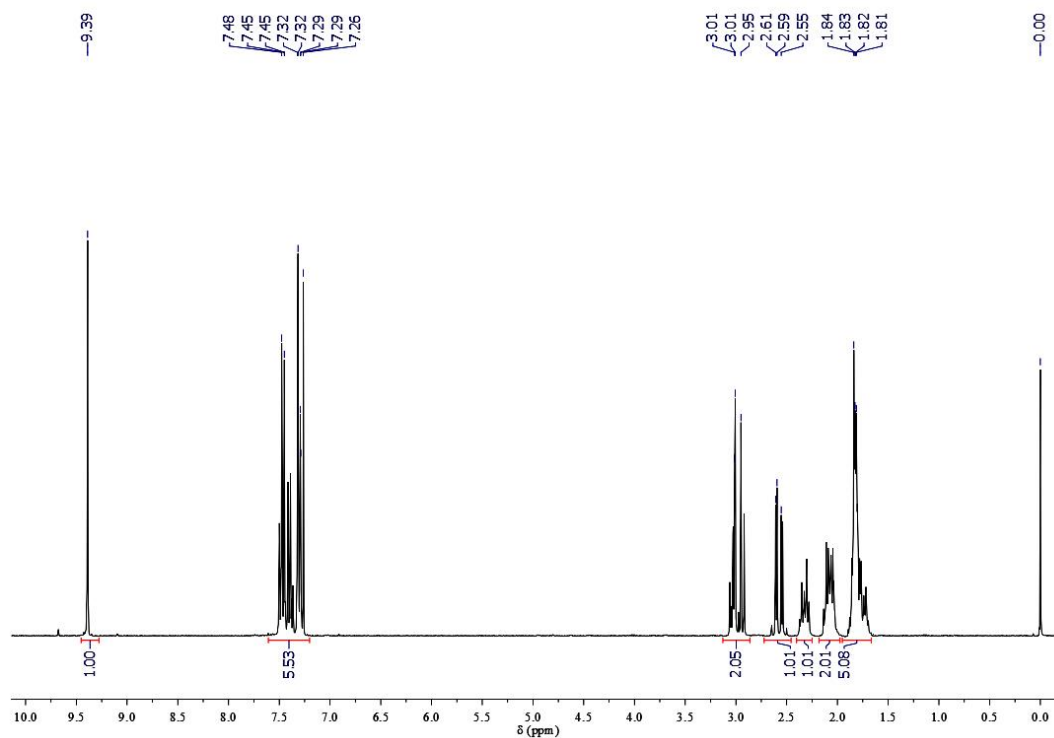
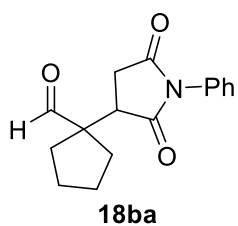
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area %  |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1      | 12.785        | PP   | 0.4493      | 8396.49512   | 287.05466    | 90.7502 |
| 2      | 14.139        | BV   | 0.3608      | 855.82037    | 35.55899     | 9.2498  |



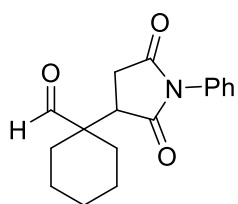
18ah



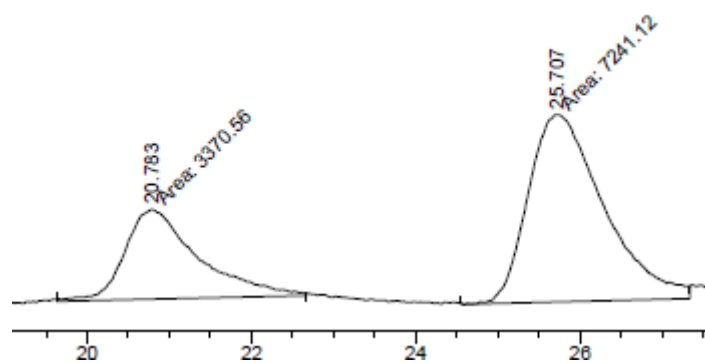
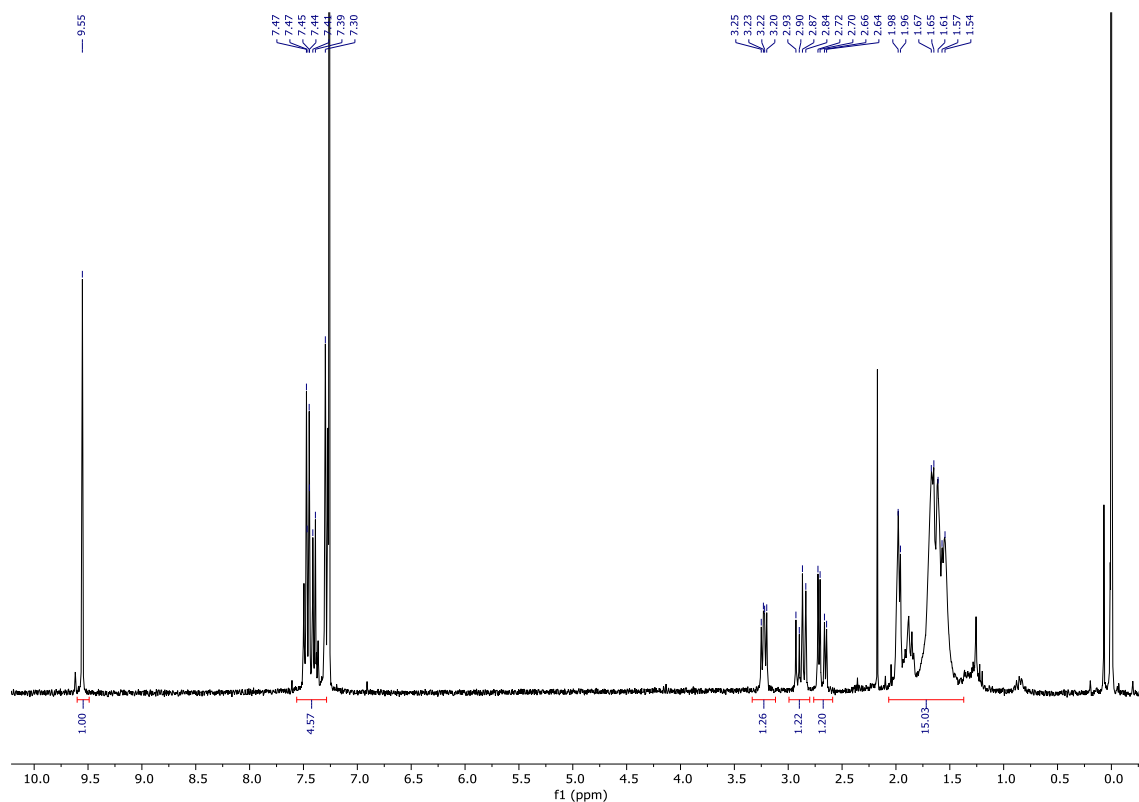
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area %  |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1      | 17.313        | MM   | 0.4993      | 1887.86304   | 63.02269     | 77.6132 |
| 2      | 23.219        | MM   | 0.6300      | 544.53534    | 14.40677     | 22.3868 |



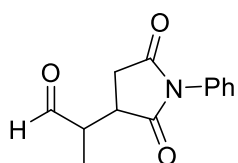
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area %  |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1      | 21.751        | BB   | 0.6458      | 1327.12219   | 24.50738     | 8.8007  |
| 2      | 27.324        | BBA  | 1.0545      | 1.37525e4    | 186.90102    | 91.1993 |



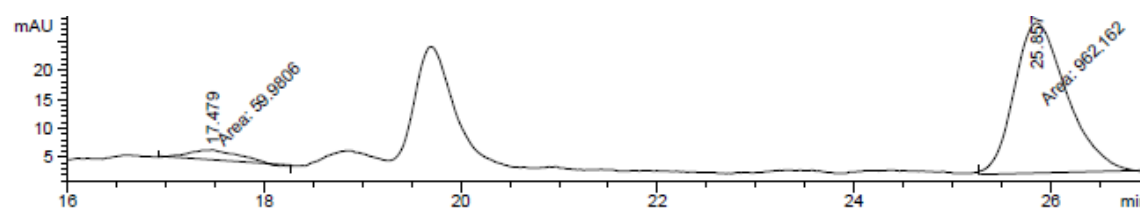
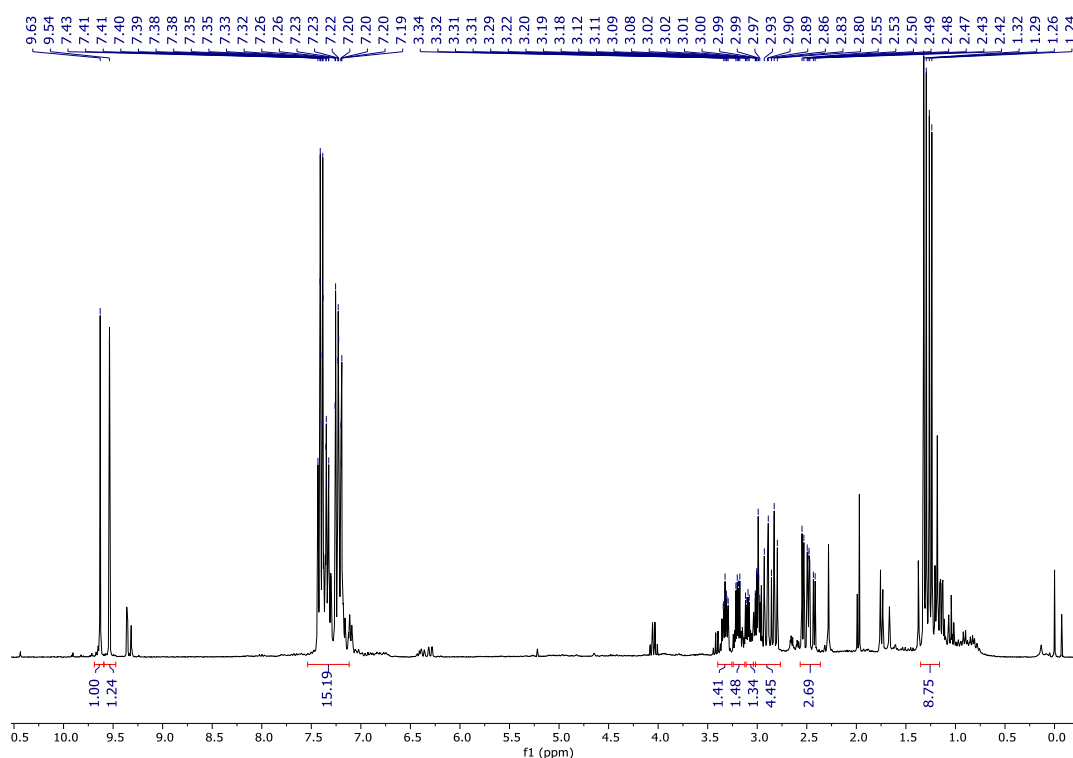
**18ca**



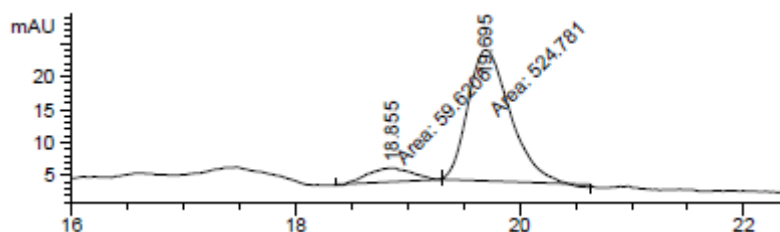
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area %  |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1      | 20.783        | MM   | 1.0307      | 3370.56055   | 54.50221     | 31.7628 |
| 2      | 25.707        | MM   | 1.0623      | 7241.11621   | 113.60856    | 68.2372 |



18da



| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area %  |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1      | 17.479        | MM   | 0.5795      | 59.98059     | 1.72519      | 5.8681  |
| 2      | 25.857        | MM   | 0.6208      | 962.16193    | 25.83209     | 94.1319 |



| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area %  |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1      | 18.855        | MM   | 0.4686      | 59.62057     | 2.12067      | 10.2020 |
| 2      | 19.695        | MM   | 0.4402      | 524.78149    | 19.86934     | 89.7980 |

## Cartesian coordinates of the computed structures

### Maleimide **17a**

E(SCRF) (M06-2X/def2tzvpp): -590,377082 Hartrees

Correction to Enthalpy: 0.160012

Correction to Gibbs Free Energy: 0.112975

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.994112                | 0.652767  | -0.138004 |
| 2                | 6                | 0              | -1.362907               | 1.074336  | 0.564592  |
| 3                | 6                | 0              | -2.756733               | -1.071343 | -0.553363 |
| 4                | 6                | 0              | -1.362905               | -1.074353 | -0.564592 |
| 5                | 6                | 0              | -0.666283               | -0.000014 | 0.000013  |
| 6                | 6                | 0              | 2.994128                | -0.652736 | 0.137941  |
| 7                | 6                | 0              | -3.458752               | -0.000006 | -0.000008 |
| 8                | 6                | 0              | 1.575728                | -1.129335 | 0.236030  |
| 9                | 6                | 0              | -2.756735               | 1.071331  | 0.553348  |
| 10               | 6                | 0              | 1.575701                | 1.129356  | -0.235967 |
| 11               | 7                | 0              | 0.761961                | -0.000003 | 0.000014  |
| 12               | 8                | 0              | 1.195607                | -2.256339 | 0.468559  |
| 13               | 8                | 0              | 1.195544                | 2.256339  | -0.468541 |
| 14               | 1                | 0              | 3.826734                | 1.328209  | -0.282364 |
| 15               | 1                | 0              | -3.293213               | 1.910254  | 0.986219  |
| 16               | 1                | 0              | -4.544477               | -0.000004 | -0.000015 |
| 17               | 1                | 0              | -3.293211               | -1.910261 | -0.986246 |
| 18               | 1                | 0              | -0.818827               | -1.906676 | -0.992196 |
| 19               | 1                | 0              | -0.818830               | 1.906664  | 0.992189  |
| 20               | 1                | 0              | 3.826768                | -1.328172 | 0.282226  |

### Enamine of catalyst **15**

E(SCRF) (M06-2X/def2tzvpp): -922,208385 Hartrees

Correction to Enthalpy: 0.411283

Correction to Gibbs Free Energy: 0.338581

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 4.280546                | -1.907720 | 0.198236  |
| 2                | 6                | 0              | 4.836793                | -0.563285 | -0.292479 |
| 3                | 6                | 0              | 3.943761                | 0.606649  | 0.145119  |
| 4                | 1                | 0              | 4.902695                | -0.578242 | -1.389505 |
| 5                | 1                | 0              | 5.858162                | -0.417148 | 0.077695  |
| 6                | 6                | 0              | 2.483963                | 0.427240  | -0.310864 |
| 7                | 1                | 0              | 3.960677                | 0.697008  | 1.240898  |
| 8                | 6                | 0              | 1.937796                | -0.928750 | 0.217145  |
| 9                | 6                | 0              | 2.820584                | -2.103319 | -0.234859 |
| 10               | 1                | 0              | 2.774686                | -2.188061 | -1.331898 |
| 11               | 1                | 0              | 2.415887                | -3.036822 | 0.171975  |
| 12               | 1                | 0              | 4.336702                | -1.946314 | 1.295180  |
| 13               | 1                | 0              | 4.893129                | -2.736199 | -0.173820 |
| 14               | 7                | 0              | 0.547836                | -1.159956 | -0.165703 |
| 15               | 1                | 0              | 1.936967                | -0.883616 | 1.310734  |
| 16               | 1                | 0              | 4.316285                | 1.556626  | -0.249900 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 17 | 6 | 0 | -0.503376 | -0.806674 | 0.617015  |
| 18 | 1 | 0 | 0.363461  | -1.420696 | -1.122636 |
| 19 | 8 | 0 | -0.314615 | -0.262681 | 1.728736  |
| 20 | 6 | 0 | -1.876238 | -1.083926 | 0.123684  |
| 21 | 6 | 0 | -2.969493 | -0.492904 | 0.810243  |
| 22 | 6 | 0 | -4.277162 | -0.690852 | 0.334508  |
| 23 | 6 | 0 | -2.145950 | -1.902489 | -0.989905 |
| 24 | 6 | 0 | -3.439236 | -2.107162 | -1.444690 |
| 25 | 6 | 0 | -4.505934 | -1.485156 | -0.778447 |
| 26 | 1 | 0 | -5.090228 | -0.216133 | 0.871606  |
| 27 | 1 | 0 | -1.330348 | -2.415195 | -1.492776 |
| 28 | 1 | 0 | -3.622968 | -2.748229 | -2.300807 |
| 29 | 1 | 0 | -5.523301 | -1.635816 | -1.128285 |
| 30 | 8 | 0 | -2.808901 | 0.262919  | 1.908681  |
| 31 | 1 | 0 | -1.840554 | 0.217718  | 2.131020  |
| 32 | 1 | 0 | 2.474474  | 0.388736  | -1.409799 |
| 33 | 1 | 0 | -1.719463 | 2.660677  | 1.158991  |
| 34 | 1 | 0 | -0.043823 | 2.953187  | 1.634930  |
| 35 | 6 | 0 | -0.797983 | 3.186745  | 0.877405  |
| 36 | 1 | 0 | -2.264368 | 3.008553  | -1.544376 |
| 37 | 6 | 0 | -0.361373 | 2.836395  | -0.523850 |
| 38 | 6 | 0 | -1.228664 | 3.367758  | -1.635892 |
| 39 | 1 | 0 | -1.009459 | 4.261638  | 0.957281  |
| 40 | 1 | 0 | 1.317311  | 1.479681  | 1.033016  |
| 41 | 7 | 0 | 1.665066  | 1.566612  | 0.084545  |
| 42 | 6 | 0 | 0.727585  | 2.097928  | -0.808485 |
| 43 | 1 | 0 | -0.860749 | 3.067075  | -2.621340 |
| 44 | 1 | 0 | -1.281595 | 4.465601  | -1.620125 |
| 45 | 1 | 0 | 0.980532  | 1.914608  | -1.852602 |

Enamine of catalyst **19**

E(SCRF) (M06-2X/def2tzvpp): -846,964216 Hartrees

Correction to Enthalpy: 0.405793

Correction to Gibbs Free Energy: 0.334758

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.479144                | -3.513553 | 0.300648  |
| 2                | 6                | 0              | 3.525840                | -2.564607 | -0.298413 |
| 3                | 6                | 0              | 3.216690                | -1.104600 | 0.060018  |
| 4                | 1                | 0              | 3.534895                | -2.675961 | -1.392214 |
| 5                | 1                | 0              | 4.529183                | -2.837024 | 0.047468  |
| 6                | 6                | 0              | 1.796482                | -0.689530 | -0.385082 |
| 7                | 1                | 0              | 3.296542                | -0.959766 | 1.146228  |
| 8                | 6                | 0              | 0.760232                | -1.636632 | 0.263703  |
| 9                | 6                | 0              | 1.053047                | -3.102882 | -0.096214 |
| 10               | 1                | 0              | 0.921662                | -3.239990 | -1.180049 |
| 11               | 1                | 0              | 0.313842                | -3.744105 | 0.395183  |
| 12               | 1                | 0              | 2.563153                | -3.500959 | 1.396098  |
| 13               | 1                | 0              | 2.669060                | -4.546168 | -0.013856 |
| 14               | 7                | 0              | -0.617793               | -1.294275 | -0.070355 |
| 15               | 1                | 0              | 0.830508                | -1.513756 | 1.349582  |
| 16               | 1                | 0              | 3.946541                | -0.426648 | -0.398055 |
| 17               | 6                | 0              | -1.351319               | -0.428151 | 0.694565  |
| 18               | 1                | 0              | -0.921371               | -1.458052 | -1.020092 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 19 | 8 | 0 | -0.912777 | 0.068295  | 1.733489  |
| 20 | 6 | 0 | -2.740041 | -0.126523 | 0.209049  |
| 21 | 6 | 0 | -3.340846 | 1.054078  | 0.664735  |
| 22 | 6 | 0 | -4.625813 | 1.395713  | 0.251545  |
| 23 | 6 | 0 | -3.457562 | -0.973911 | -0.646735 |
| 24 | 6 | 0 | -4.747236 | -0.634432 | -1.055659 |
| 25 | 6 | 0 | -5.330678 | 0.553580  | -0.611999 |
| 26 | 1 | 0 | -5.079899 | 2.318183  | 0.602905  |
| 27 | 1 | 0 | -3.028654 | -1.918029 | -0.969539 |
| 28 | 1 | 0 | -5.298505 | -1.300947 | -1.711403 |
| 29 | 1 | 0 | -6.333600 | 0.818507  | -0.932372 |
| 30 | 1 | 0 | 1.737146  | -0.821643 | -1.479734 |
| 31 | 1 | 0 | 1.132648  | 4.085653  | 1.110886  |
| 32 | 1 | 0 | 1.762526  | 2.591518  | 1.809541  |
| 33 | 6 | 0 | 2.007995  | 3.419977  | 1.137672  |
| 34 | 1 | 0 | 2.425792  | 4.855276  | -1.301878 |
| 35 | 6 | 0 | 2.411761  | 2.961265  | -0.239361 |
| 36 | 6 | 0 | 3.080050  | 3.990666  | -1.113935 |
| 37 | 1 | 0 | 2.818048  | 3.991629  | 1.609738  |
| 38 | 1 | 0 | 1.105681  | 0.861163  | 0.833666  |
| 39 | 7 | 0 | 1.456548  | 0.695867  | -0.101600 |
| 40 | 6 | 0 | 2.167262  | 1.723359  | -0.711647 |
| 41 | 1 | 0 | 3.361858  | 3.577098  | -2.088192 |
| 42 | 1 | 0 | 3.988816  | 4.391560  | -0.643422 |
| 43 | 1 | 0 | 2.504138  | 1.466218  | -1.716970 |
| 44 | 1 | 0 | -2.779127 | 1.685839  | 1.344913  |

Complex Enamine (**15**):Maleimide

E(SCRF) (M06-2X/def2tzvpp): -1512.705464 Hartrees

Correction to Enthalpy: 0.573784

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |          |           |
|------------------|------------------|----------------|-------------------------|----------|-----------|
|                  |                  |                | X                       | Y        | Z         |
| 1                | 6                | 0              | -1.091052               | 1.394007 | 3.945049  |
| 2                | 6                | 0              | -0.587004               | 3.646996 | -0.363951 |
| 3                | 6                | 0              | 1.405964                | 2.135954 | -0.651951 |
| 4                | 7                | 0              | 1.937935                | 0.775942 | -0.604951 |
| 5                | 1                | 0              | 1.205965                | 2.185958 | -2.803951 |
| 6                | 1                | 0              | -0.670968               | 5.339998 | -1.715951 |
| 7                | 1                | 0              | 0.367955                | 1.725976 | 1.669049  |
| 8                | 1                | 0              | -3.746075               | 0.293063 | 3.540049  |
| 9                | 1                | 0              | -0.643047               | 1.603997 | -1.072951 |
| 10               | 1                | 0              | -0.071992               | 4.212985 | 0.426049  |
| 11               | 1                | 0              | 1.952976                | 2.702942 | 0.111049  |
| 12               | 1                | 0              | -3.795038               | 2.030065 | 3.851049  |
| 13               | 1                | 0              | 1.739022                | 4.857947 | -1.388951 |
| 14               | 1                | 0              | -0.034052               | 1.368984 | 3.662049  |
| 15               | 1                | 0              | -1.267070               | 0.533011 | 4.601049  |
| 16               | 1                | 0              | 2.761977                | 2.756925 | -2.202951 |
| 17               | 1                | 0              | -0.911001               | 3.784003 | -2.497951 |
| 18               | 6                | 0              | 3.204930                | 0.532916 | -0.191951 |
| 19               | 6                | 0              | -3.502054               | 1.274058 | 3.110049  |
| 20               | 6                | 0              | -2.037052               | 1.382027 | 2.770049  |
| 21               | 7                | 0              | -0.348049               | 1.530991 | 0.980049  |
| 22               | 6                | 0              | -0.322990               | 4.300991 | -1.726951 |
| 23               | 6                | 0              | -0.097035               | 2.182986 | -0.311951 |
| 24               | 6                | 0              | 1.682978                | 2.791948 | -2.020951 |
| 25               | 6                | 0              | 1.166009                | 4.233959 | -2.088951 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 26 | 6 | 0 | -1.646050 | 1.494019  | 1.482049  |
| 27 | 1 | 0 | -4.134051 | 1.412072  | 2.228049  |
| 28 | 1 | 0 | -1.655003 | 3.678019  | -0.121951 |
| 29 | 1 | 0 | -2.405050 | 1.489035  | 0.702049  |
| 30 | 1 | 0 | 1.339018  | 4.646955  | -3.088951 |
| 31 | 1 | 0 | -1.245033 | 2.289010  | 4.563049  |
| 32 | 6 | 0 | -0.091115 | -1.570014 | 1.201049  |
| 33 | 6 | 0 | -1.003120 | -1.822995 | 2.147049  |
| 34 | 1 | 0 | 1.341919  | 0.027955  | -0.946951 |
| 35 | 6 | 0 | -2.357120 | -1.825966 | 1.527049  |
| 36 | 6 | 0 | 3.736900  | -0.856096 | -0.241951 |
| 37 | 6 | 0 | 3.046878  | -1.934081 | -0.832951 |
| 38 | 6 | 0 | 5.019895  | -1.101123 | 0.325049  |
| 39 | 6 | 0 | 3.581850  | -3.214092 | -0.849951 |
| 40 | 1 | 0 | 2.076881  | -1.773060 | -1.290951 |
| 41 | 6 | 0 | 5.547868  | -2.404134 | 0.307049  |
| 42 | 6 | 0 | 4.837845  | -3.444119 | -0.270951 |
| 43 | 1 | 0 | 3.032833  | -4.027081 | -1.314951 |
| 44 | 1 | 0 | 6.524864  | -2.559155 | 0.752049  |
| 45 | 1 | 0 | 5.264824  | -4.443128 | -0.280951 |
| 46 | 8 | 0 | 3.914950  | 1.470900  | 0.244049  |
| 47 | 8 | 0 | 5.758916  | -0.135139 | 0.886049  |
| 48 | 1 | 0 | 5.235934  | 0.707872  | 0.760049  |
| 49 | 6 | 0 | -0.792111 | -1.382999 | -0.101951 |
| 50 | 8 | 0 | -0.290105 | -1.130010 | -1.190951 |
| 51 | 8 | 0 | -3.425125 | -2.034943 | 2.061049  |
| 52 | 1 | 0 | 0.983887  | -1.502037 | 1.282049  |
| 53 | 1 | 0 | -0.863124 | -2.014998 | 3.202049  |
| 54 | 1 | 0 | -4.591092 | -0.520919 | 0.500049  |
| 55 | 1 | 0 | -6.385089 | -0.367880 | -1.195951 |
| 56 | 6 | 0 | -4.422100 | -0.888922 | -0.503951 |
| 57 | 6 | 0 | -5.431099 | -0.814901 | -1.461951 |
| 58 | 6 | 0 | -3.194113 | -1.472948 | -0.836951 |
| 59 | 6 | 0 | -5.222109 | -1.302905 | -2.751951 |
| 60 | 1 | 0 | -6.010108 | -1.236888 | -3.496951 |
| 61 | 6 | 0 | -2.981123 | -1.975953 | -2.125951 |
| 62 | 6 | 0 | -3.994121 | -1.878931 | -3.077951 |
| 63 | 1 | 0 | -3.821130 | -2.265935 | -4.077951 |
| 64 | 7 | 0 | -2.158114 | -1.557970 | 0.142049  |
| 65 | 1 | 0 | -2.029133 | -2.422973 | -2.380951 |

Complex Enamine(**19**):Maleimide

E(SCRF) (M06-2X/def2tzvpp): -1437.460085 Hartrees

Correction to Enthalpy: 0.568314

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |          |           |
|------------------|------------------|----------------|-------------------------|----------|-----------|
|                  |                  |                | X                       | Y        | Z         |
| 1                | 6                | 0              | -1.000959               | 1.438060 | 3.931063  |
| 2                | 6                | 0              | -0.366844               | 3.651027 | -0.386937 |
| 3                | 6                | 0              | 1.626077                | 2.123924 | -0.596937 |
| 4                | 7                | 0              | 2.148006                | 0.764897 | -0.514937 |
| 5                | 1                | 0              | 1.495078                | 2.153931 | -2.754937 |
| 6                | 1                | 0              | -0.399756               | 5.329029 | -1.758937 |
| 7                | 1                | 0              | 0.523056                | 1.727981 | 1.689063  |
| 8                | 1                | 0              | -3.654015               | 0.350199 | 3.462063  |
| 9                | 1                | 0              | -0.411950               | 1.601030 | -1.076937 |
| 10               | 1                | 0              | 0.126186                | 4.222002 | 0.412063  |
| 11               | 1                | 0              | 2.155107                | 2.695896 | 0.175063  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 12 | 1 | 0 | -3.696925 | 2.090201  | 3.763063  |
| 13 | 1 | 0 | 1.997218  | 4.837904  | -1.350937 |
| 14 | 1 | 0 | 0.062039  | 1.403005  | 3.676063  |
| 15 | 1 | 0 | -1.202003 | 0.585071  | 4.591063  |
| 16 | 1 | 0 | 3.034108  | 2.722851  | -2.106937 |
| 17 | 1 | 0 | -0.621838 | 3.765041  | -2.531937 |
| 18 | 6 | 0 | 3.417994  | 0.533831  | -0.070937 |
| 19 | 6 | 0 | -3.389965 | 1.328185  | 3.034063  |
| 20 | 6 | 0 | -1.916960 | 1.423108  | 2.732063  |
| 21 | 7 | 0 | -0.181953 | 1.548018  | 0.985063  |
| 22 | 6 | 0 | -0.055810 | 4.288011  | -1.747937 |
| 23 | 6 | 0 | 0.114080  | 2.184002  | -0.305937 |
| 24 | 6 | 0 | 1.950110  | 2.764907  | -1.962937 |
| 25 | 6 | 0 | 1.443185  | 4.208933  | -2.061937 |
| 26 | 6 | 0 | -1.490954 | 1.525086  | 1.454063  |
| 27 | 1 | 0 | -3.997957 | 1.466216  | 2.135063  |
| 28 | 1 | 0 | -1.441842 | 3.690083  | -0.179937 |
| 29 | 1 | 0 | -2.229954 | 1.523124  | 0.655063  |
| 30 | 1 | 0 | 1.650206  | 4.611923  | -3.059937 |
| 31 | 1 | 0 | -1.163912 | 2.341069  | 4.537063  |
| 32 | 6 | 0 | 0.059887  | -1.533995 | 1.247063  |
| 33 | 6 | 0 | -0.878126 | -1.765946 | 2.173063  |
| 34 | 1 | 0 | 1.562967  | 0.013927  | -0.865937 |
| 35 | 6 | 0 | -2.215126 | -1.781876 | 1.518063  |
| 36 | 6 | 0 | 3.919920  | -0.888196 | -0.097937 |
| 37 | 6 | 0 | 3.272865  | -1.948162 | -0.752937 |
| 38 | 6 | 0 | 5.130907  | -1.135259 | 0.564063  |
| 39 | 6 | 0 | 3.827798  | -3.229191 | -0.732937 |
| 40 | 1 | 0 | 2.340873  | -1.793113 | -1.284937 |
| 41 | 6 | 0 | 5.679841  | -2.415287 | 0.585063  |
| 42 | 6 | 0 | 5.028786  | -3.466253 | -0.063937 |
| 43 | 1 | 0 | 3.320756  | -4.040164 | -1.245937 |
| 44 | 1 | 0 | 6.617832  | -2.592336 | 1.105063  |
| 45 | 1 | 0 | 5.456734  | -4.464276 | -0.050937 |
| 46 | 8 | 0 | 4.132042  | 1.443793  | 0.359063  |
| 47 | 6 | 0 | -0.605105 | -1.378960 | -0.078937 |
| 48 | 8 | 0 | -0.074094 | -1.156988 | -1.159937 |
| 49 | 8 | 0 | -3.297137 | -1.980820 | 2.028063  |
| 50 | 1 | 0 | 1.131890  | -1.461050 | 1.354063  |
| 51 | 1 | 0 | -0.766134 | -1.931952 | 3.236063  |
| 52 | 1 | 0 | -4.420060 | -0.502762 | 0.408063  |
| 53 | 1 | 0 | -6.169054 | -0.383671 | -1.336937 |
| 54 | 6 | 0 | -4.225080 | -0.890772 | -0.583937 |
| 55 | 6 | 0 | -5.209077 | -0.835721 | -1.569937 |
| 56 | 6 | 0 | -2.988111 | -1.479836 | -0.872937 |
| 57 | 6 | 0 | -4.967104 | -1.348733 | -2.843937 |
| 58 | 1 | 0 | -5.735101 | -1.297693 | -3.609937 |
| 59 | 6 | 0 | -2.742138 | -2.006849 | -2.146937 |
| 60 | 6 | 0 | -3.731134 | -1.930797 | -3.126937 |
| 61 | 1 | 0 | -3.531155 | -2.335808 | -4.113937 |
| 62 | 7 | 0 | -1.979114 | -1.543889 | 0.134063  |
| 63 | 1 | 0 | -1.784162 | -2.457899 | -2.367937 |
| 64 | 1 | 0 | 5.622951  | -0.300284 | 1.049063  |

# **TS-1R**

E(SCRF) (M06-2X/def2tzvpp): -1512,6899 Hatrees

Correction to Enthalpy: 0.573192

Correction to Gibbs Free Energy: 0.480294

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.165957               | -2.983569 | -2.536312 |
| 2                | 6                | 0              | 1.329964                | 2.057505  | -2.336587 |
| 3                | 6                | 0              | -0.888016               | 1.810768  | -1.135496 |
| 4                | 7                | 0              | -1.659990               | 0.967982  | -0.225276 |
| 5                | 1                | 0              | -0.329020               | 3.287144  | 0.340129  |
| 6                | 1                | 0              | 1.974927                | 4.103446  | -2.616105 |
| 7                | 1                | 0              | -0.507981               | -0.605316 | -1.498900 |
| 8                | 1                | 0              | 2.301063                | -4.241536 | -2.564031 |
| 9                | 1                | 0              | 1.036004                | 1.230992  | -0.361377 |
| 10               | 1                | 0              | 0.842952                | 2.002252  | -3.318567 |
| 11               | 1                | 0              | -1.418028               | 1.794521  | -2.093485 |
| 12               | 1                | 0              | 2.288027                | -3.093870 | -3.905317 |
| 13               | 1                | 0              | -0.502074               | 4.198412  | -2.589096 |
| 14               | 1                | 0              | -0.989956               | -2.553439 | -1.961408 |
| 15               | 1                | 0              | -0.188937               | -4.064528 | -2.370042 |
| 16               | 1                | 0              | -1.803038               | 3.665898  | -0.551946 |
| 17               | 1                | 0              | 2.007958                | 3.563863  | -0.941971 |
| 18               | 6                | 0              | -3.010990               | 0.841923  | -0.374227 |
| 19               | 6                | 0              | 2.350043                | -3.177598 | -2.814297 |
| 20               | 6                | 0              | 1.203040                | -2.425450 | -2.146469 |
| 21               | 7                | 0              | 0.386009                | -0.190363 | -1.746015 |
| 22               | 6                | 0              | 1.422947                | 3.519622  | -1.870952 |
| 23               | 6                | 0              | 0.522991                | 1.220742  | -1.333368 |
| 24               | 6                | 0              | -0.788033               | 3.269889  | -0.656861 |
| 25               | 6                | 0              | 0.032940                | 4.124659  | -1.632084 |
| 26               | 6                | 0              | 1.351016                | -1.000446 | -2.140826 |
| 27               | 1                | 0              | 3.324041                | -2.811499 | -2.481401 |
| 28               | 1                | 0              | 2.337969                | 1.645492  | -2.452498 |
| 29               | 1                | 0              | 2.334008                | -0.559464 | -2.274948 |
| 30               | 1                | 0              | 0.125929                | 5.146756  | -1.248340 |
| 31               | 1                | 0              | -0.361973               | -2.805837 | -3.599354 |
| 32               | 6                | 0              | 0.238069                | -2.151819 | 0.449476  |
| 33               | 6                | 0              | 1.278070                | -2.779988 | -0.295382 |
| 34               | 1                | 0              | -1.192974               | 0.663203  | 0.632794  |
| 35               | 6                | 0              | 2.567065                | -2.126849 | 0.178439  |
| 36               | 6                | 0              | -3.782964               | 0.071161  | 0.629975  |
| 37               | 6                | 0              | -3.199940               | -0.516546 | 1.771114  |
| 38               | 6                | 0              | -5.183965               | -0.078913 | 0.425031  |
| 39               | 6                | 0              | -3.964916               | -1.231332 | 2.681302  |
| 40               | 1                | 0              | -2.133939               | -0.419483 | 1.956076  |
| 41               | 6                | 0              | -5.946941               | -0.805694 | 1.356222  |
| 42               | 6                | 0              | -5.342917               | -1.372407 | 2.467355  |
| 43               | 1                | 0              | -3.494898               | -1.674107 | 3.553406  |
| 44               | 1                | 0              | -7.010941               | -0.901757 | 1.172260  |
| 45               | 1                | 0              | -5.947898               | -1.930240 | 3.177502  |
| 46               | 8                | 0              | -3.575012               | 1.356666  | -1.368348 |
| 47               | 8                | 0              | -5.823987               | 0.444814  | -0.630091 |
| 48               | 1                | 0              | -5.126002               | 0.918693  | -1.161218 |
| 49               | 6                | 0              | 0.746060                | -1.016644 | 1.120186  |
| 50               | 8                | 0              | 0.176053                | -0.106496 | 1.750967  |
| 51               | 8                | 0              | 3.707068                | -2.477893 | -0.072489 |
| 52               | 1                | 0              | -0.800925               | -2.442823 | 0.502562  |
| 53               | 1                | 0              | 1.336086                | -3.863013 | -0.401113 |
| 54               | 1                | 0              | 4.487029                | -0.164895 | -0.133075 |
| 55               | 1                | 0              | 6.055016                | 1.463377  | 0.859499  |
| 56               | 6                | 0              | 4.261035                | 0.287339  | 0.822815  |
| 57               | 6                | 0              | 5.148027                | 1.197496  | 1.395577  |
| 58               | 6                | 0              | 3.092050                | -0.076509 | 1.507921  |

|    |   |   |          |           |          |
|----|---|---|----------|-----------|----------|
| 59 | 6 | 0 | 4.878035 | 1.762802  | 2.642440 |
| 60 | 1 | 0 | 5.571029 | 2.473923  | 3.083254 |
| 61 | 6 | 0 | 2.824057 | 0.480800  | 2.766786 |
| 62 | 6 | 0 | 3.714049 | 1.400952  | 3.319545 |
| 63 | 1 | 0 | 3.494055 | 1.829191  | 4.292442 |
| 64 | 7 | 0 | 2.187057 | -1.007670 | 0.922165 |
| 65 | 1 | 0 | 1.919068 | 0.206915  | 3.289866 |

# **TS-1S**

E(SCRF) (M06-2X/def2tzvpp): -1512,67939 Hartrees

Correction to Enthalpy: 0.572736

Correction to Gibbs Free Energy: 0.477886

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 1                | 0              | 0.003978                | -3.610992 | -2.914984 |
| 2                | 1                | 0              | -1.688026               | -3.212008 | -2.506984 |
| 3                | 6                | 0              | -0.723023               | -3.520999 | -2.099984 |
| 4                | 1                | 0              | -0.861014               | -4.518000 | -1.671984 |
| 5                | 1                | 0              | -1.645072               | 1.569992  | 0.311016  |
| 6                | 1                | 0              | 3.541955                | -1.204958 | 1.655016  |
| 7                | 6                | 0              | -0.220033               | -2.553994 | -1.028984 |
| 8                | 8                | 0              | 2.428944                | -0.066969 | 1.186016  |
| 9                | 7                | 0              | 0.199945                | -0.199990 | -0.670984 |
| 10               | 8                | 0              | 4.452958                | -1.583949 | 1.555016  |
| 11               | 1                | 0              | 1.882972                | -3.059974 | -1.196984 |
| 12               | 1                | 0              | 0.855926                | 1.812016  | 0.947016  |
| 13               | 6                | 0              | -1.362074               | 1.762995  | -0.729984 |
| 14               | 1                | 0              | -0.743095               | 3.957001  | 0.892016  |
| 15               | 6                | 0              | 1.106972                | -3.023981 | -0.422984 |
| 16               | 1                | 0              | 0.994982                | -4.034982 | -0.018984 |
| 17               | 1                | 0              | -2.065068               | 1.202988  | -1.354984 |
| 18               | 6                | 0              | -0.288046               | -1.174995 | -1.417984 |
| 19               | 1                | 0              | -2.482091               | 3.604984  | -0.834984 |
| 20               | 6                | 0              | 0.065931                | 1.240009  | -0.965984 |
| 21               | 6                | 0              | -1.459088               | 3.264994  | -1.024984 |
| 22               | 6                | 0              | 1.080924                | 2.024018  | -0.103984 |
| 23               | 6                | 0              | -0.465096               | 4.053004  | -0.164984 |
| 24               | 6                | 0              | 3.091937                | 0.640038  | 0.386016  |
| 25               | 6                | 0              | 5.137950                | -0.723943 | 0.789016  |
| 26               | 1                | 0              | 1.466966                | -2.383978 | 0.384016  |
| 27               | 7                | 0              | 2.466928                | 1.604032  | -0.334984 |
| 28               | 6                | 0              | 0.965909                | 3.536017  | -0.360984 |
| 29               | 1                | 0              | -0.902049               | -0.872000 | -2.262984 |
| 30               | 1                | 0              | -0.503106               | 5.122003  | -0.404984 |
| 31               | 6                | 0              | 4.542939                | 0.423052  | 0.195016  |
| 32               | 1                | 0              | 6.924961                | -1.874926 | 1.029016  |
| 33               | 1                | 0              | 1.664904                | 4.057024  | 0.302016  |
| 34               | 6                | 0              | 6.502953                | -0.985930 | 0.573016  |
| 35               | 1                | 0              | 0.333930                | 1.378011  | -2.023984 |
| 36               | 1                | 0              | -1.257090               | 3.454996  | -2.088984 |
| 37               | 1                | 0              | 2.989923                | 2.100037  | -1.039984 |
| 38               | 1                | 0              | 1.287907                | 3.745020  | -1.392984 |
| 39               | 6                | 0              | 5.361931                | 1.293059  | -0.552984 |
| 40               | 6                | 0              | 7.272944                | -0.120922 | -0.185984 |
| 41               | 6                | 0              | 6.708933                | 1.035072  | -0.747984 |
| 42               | 1                | 0              | 4.947922                | 2.208055  | -0.968984 |
| 43               | 1                | 0              | 8.326946                | -0.334912 | -0.334984 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 44 | 1 | 0 | 7.319927  | 1.722078  | -1.322984 |
| 45 | 8 | 0 | -1.981060 | 0.278989  | 2.343016  |
| 46 | 1 | 0 | -4.381050 | -0.687034 | -1.662984 |
| 47 | 6 | 0 | -1.025040 | -1.782002 | 1.508016  |
| 48 | 6 | 0 | -4.784056 | -0.115038 | -0.838984 |
| 49 | 1 | 0 | -6.401064 | 0.692947  | -1.992984 |
| 50 | 6 | 0 | -5.932063 | 0.655951  | -1.013984 |
| 51 | 6 | 0 | -1.366032 | -2.638005 | 0.421016  |
| 52 | 7 | 0 | -2.998048 | -0.969020 | 0.604016  |
| 53 | 6 | 0 | -4.170055 | -0.187032 | 0.423016  |
| 54 | 6 | 0 | -2.732036 | -2.160018 | -0.057984 |
| 55 | 6 | 0 | -6.479070 | 1.370946  | 0.052016  |
| 56 | 6 | 0 | -4.724062 | 0.524963  | 1.499016  |
| 57 | 1 | 0 | -7.373076 | 1.970938  | -0.088984 |
| 58 | 6 | 0 | -5.867069 | 1.299952  | 1.304016  |
| 59 | 8 | 0 | -3.444031 | -2.712025 | -0.884984 |
| 60 | 1 | 0 | -4.245061 | 0.479968  | 2.467016  |
| 61 | 1 | 0 | -6.283075 | 1.845948  | 2.146016  |
| 62 | 6 | 0 | -1.952050 | -0.712011 | 1.614016  |
| 63 | 1 | 0 | -0.204039 | -1.895994 | 2.202016  |
| 64 | 1 | 0 | -1.306021 | -3.723004 | 0.522016  |
| 65 | 1 | 0 | 0.717947  | -0.435985 | 0.177016  |

# **TS-2R**

E(SCRF) (M06-2X/def2tzvpp): -1437,436523 Hartrees

Correction to Enthalpy: 0.567603

Correction to Gibbs Free Energy: 0.476041

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 1                | 0              | -0.902025               | 4.444003  | 2.348029  |
| 2                | 1                | 0              | -2.378020               | 3.604995  | 1.801029  |
| 3                | 6                | 0              | -1.424023               | 4.026000  | 1.479029  |
| 4                | 1                | 0              | -1.652027               | 4.854999  | 0.802029  |
| 5                | 1                | 0              | -1.728995               | -0.887001 | 0.944029  |
| 6                | 6                | 0              | -0.550017               | 2.992005  | 0.770029  |
| 7                | 8                | 0              | 2.562996                | 0.787023  | -0.626971 |
| 8                | 7                | 0              | 0.327996                | 0.764010  | 1.053029  |
| 9                | 1                | 0              | 1.367978                | 3.920016  | 1.178029  |
| 10               | 1                | 0              | 0.685007                | -1.212988 | -0.543971 |
| 11               | 6                | 0              | -1.093994               | -1.149998 | 1.793029  |
| 12               | 1                | 0              | -1.114982               | -3.145998 | -0.094971 |
| 13               | 6                | 0              | 0.778980                | 3.599013  | 0.310029  |
| 14               | 1                | 0              | 0.587975                | 4.485012  | -0.303971 |
| 15               | 1                | 0              | -1.495996               | -0.631000 | 2.670029  |
| 16               | 6                | 0              | -0.483010               | 1.726006  | 1.448029  |
| 17               | 1                | 0              | -2.215984               | -2.949004 | 2.150029  |
| 18               | 6                | 0              | 0.335004                | -0.645990 | 1.513029  |
| 19               | 6                | 0              | -1.167985               | -2.664998 | 2.011029  |
| 20               | 6                | 0              | 1.086008                | -1.484986 | 0.440029  |
| 21               | 6                | 0              | -0.559981               | -3.401995 | 0.816029  |
| 22               | 6                | 0              | 3.171001                | -0.198974 | -0.186971 |
| 23               | 6                | 0              | 5.379995                | 0.899038  | -0.445971 |
| 24               | 1                | 0              | 1.389984                | 2.913016  | -0.279971 |
| 25               | 7                | 0              | 2.538007                | -1.223977 | 0.443029  |
| 26               | 6                | 0              | 0.906017                | -2.997987 | 0.649029  |
| 27               | 1                | 0              | -1.252008               | 1.465001  | 2.168029  |
| 28               | 1                | 0              | -0.629975               | -4.486995 | 0.950029  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 29 | 6 | 0 | 4.663002  | -0.295966 | -0.300971 |
| 30 | 1 | 0 | 7.316990  | 1.808049  | -0.658971 |
| 31 | 1 | 0 | 1.363020  | -3.514984 | -0.201971 |
| 32 | 6 | 0 | 6.767995  | 0.877046  | -0.554971 |
| 33 | 1 | 0 | 0.924004  | -0.698986 | 2.442029  |
| 34 | 1 | 0 | -0.637984 | -2.946995 | 2.932029  |
| 35 | 1 | 0 | 3.115011  | -1.923974 | 0.884029  |
| 36 | 1 | 0 | 1.464018  | -3.304983 | 1.549029  |
| 37 | 6 | 0 | 5.354008  | -1.515962 | -0.296971 |
| 38 | 6 | 0 | 7.453002  | -0.339950 | -0.535971 |
| 39 | 6 | 0 | 6.744009  | -1.536954 | -0.412971 |
| 40 | 1 | 0 | 4.813014  | -2.455965 | -0.243971 |
| 41 | 1 | 0 | 8.535002  | -0.357944 | -0.624971 |
| 42 | 1 | 0 | 7.270014  | -2.485951 | -0.419971 |
| 43 | 8 | 0 | -1.131995 | -0.828998 | -1.930971 |
| 44 | 1 | 0 | -4.514003 | 0.604983  | 1.075029  |
| 45 | 6 | 0 | -0.679009 | 1.526005  | -1.580971 |
| 46 | 6 | 0 | -4.645999 | -0.194018 | 0.358029  |
| 47 | 1 | 0 | -6.382994 | -0.989027 | 1.333029  |
| 48 | 6 | 0 | -5.704994 | -1.090024 | 0.489029  |
| 49 | 6 | 0 | -1.356014 | 2.539001  | -0.836971 |
| 50 | 7 | 0 | -2.685003 | 0.610993  | -0.869971 |
| 51 | 6 | 0 | -3.765998 | -0.299013 | -0.731971 |
| 52 | 6 | 0 | -2.725011 | 1.953993  | -0.512971 |
| 53 | 6 | 0 | -5.898988 | -2.105025 | -0.447971 |
| 54 | 6 | 0 | -3.964993 | -1.315014 | -1.680971 |
| 55 | 1 | 0 | -6.724984 | -2.802029 | -0.339971 |
| 56 | 6 | 0 | -5.021988 | -2.210020 | -1.527971 |
| 57 | 8 | 0 | -3.671014 | 2.545988  | -0.014971 |
| 58 | 1 | 0 | -3.280992 | -1.403010 | -2.513971 |
| 59 | 1 | 0 | -5.162983 | -2.992020 | -2.268971 |
| 60 | 6 | 0 | -1.405002 | 0.312001  | -1.541971 |
| 61 | 1 | 0 | 0.275991  | 1.606010  | -2.078971 |
| 62 | 1 | 0 | -1.410020 | 3.565001  | -1.204971 |
| 63 | 1 | 0 | 1.047995  | 0.976014  | 0.347029  |
| 64 | 1 | 0 | 4.828990  | 1.833035  | -0.471971 |

# TS-2S

E(SCRF) (M06-2X/def2tzvpp): -1437,444912 Hatrees

Correction to Enthalpy: 0.567739

Correction to Gibbs Free Energy: 0.476092

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.332924               | -3.047025 | -2.471021 |
| 2                | 6                | 0              | 1.235013                | 1.975995  | -2.394021 |
| 3                | 6                | 0              | -1.019985               | 1.797966  | -1.249021 |
| 4                | 7                | 0              | -1.829975               | 0.994956  | -0.340021 |
| 5                | 1                | 0              | -0.485004               | 3.319973  | 0.189979  |
| 6                | 1                | 0              | 1.913987                | 4.003003  | -2.724021 |
| 7                | 1                | 0              | -0.668954               | -0.626029 | -1.514021 |
| 8                | 1                | 0              | 2.117093                | -4.334994 | -2.409021 |
| 9                | 1                | 0              | 0.873022                | 1.221990  | -0.401021 |
| 10               | 1                | 0              | 0.776014                | 1.892989  | -3.387021 |
| 11               | 1                | 0              | -1.524984               | 1.756960  | -2.221021 |
| 12               | 1                | 0              | 2.150079                | -3.228994 | -3.784021 |
| 13               | 1                | 0              | -0.561014               | 4.128972  | -2.773021 |
| 14               | 1                | 0              | -1.161929               | -2.587036 | -1.926021 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 15 | 1 | 0 | -0.374910 | -4.122026 | -2.271021 |
| 16 | 1 | 0 | -1.928009 | 3.682955  | -0.759021 |
| 17 | 1 | 0 | 1.891993  | 3.522003  | -1.033021 |
| 18 | 6 | 0 | -3.187974 | 0.897939  | -0.534021 |
| 19 | 6 | 0 | 2.186079  | -3.279993 | -2.689021 |
| 20 | 6 | 0 | 1.034069  | -2.494008 | -2.071021 |
| 21 | 7 | 0 | 0.240041  | -0.237018 | -1.754021 |
| 22 | 6 | 0 | 1.333994  | 3.452996  | -1.976021 |
| 23 | 6 | 0 | 0.388023  | 1.185984  | -1.387021 |
| 24 | 6 | 0 | -0.915004 | 3.272967  | -0.819021 |
| 25 | 6 | 0 | -0.055014 | 4.082978  | -1.799021 |
| 26 | 6 | 0 | 1.201051  | -1.072006 | -2.101021 |
| 27 | 1 | 0 | 3.156075  | -2.915981 | -2.345021 |
| 28 | 1 | 0 | 2.241018  | 1.548007  | -2.466021 |
| 29 | 1 | 0 | 2.193046  | -0.648993 | -2.226021 |
| 30 | 1 | 0 | 0.040973  | 5.115980  | -1.449021 |
| 31 | 1 | 0 | -0.506926 | -2.900027 | -3.543021 |
| 32 | 6 | 0 | 0.015065  | -2.143021 | 0.499979  |
| 33 | 6 | 0 | 1.066073  | -2.797008 | -0.202021 |
| 34 | 1 | 0 | -1.402971 | 0.730961  | 0.549979  |
| 35 | 6 | 0 | 2.348065  | -2.136991 | 0.279979  |
| 36 | 6 | 0 | -3.989964 | 0.166929  | 0.508979  |
| 37 | 6 | 0 | -3.445957 | -0.403065 | 1.669979  |
| 38 | 6 | 0 | -5.368963 | 0.064911  | 0.274979  |
| 39 | 6 | 0 | -4.277949 | -1.063075 | 2.576979  |
| 40 | 1 | 0 | -2.382958 | -0.346051 | 1.886979  |
| 41 | 6 | 0 | -6.193955 | -0.594099 | 1.181979  |
| 42 | 6 | 0 | -5.648948 | -1.160092 | 2.336979  |
| 43 | 1 | 0 | -3.848943 | -1.500070 | 3.473979  |
| 44 | 1 | 0 | -7.259954 | -0.666113 | 0.989979  |
| 45 | 1 | 0 | -6.290941 | -1.675101 | 3.046979  |
| 46 | 8 | 0 | -3.725979 | 1.368932  | -1.537021 |
| 47 | 6 | 0 | 0.514050  | -0.992015 | 1.152979  |
| 48 | 8 | 0 | -0.063961 | -0.066022 | 1.750979  |
| 49 | 8 | 0 | 3.492069  | -2.501977 | 0.062979  |
| 50 | 1 | 0 | -1.027932 | -2.424034 | 0.533979  |
| 51 | 1 | 0 | 1.120087  | -3.882007 | -0.280021 |
| 52 | 1 | 0 | 4.293040  | -0.204967 | -0.037021 |
| 53 | 1 | 0 | 5.849020  | 1.441053  | 0.945979  |
| 54 | 6 | 0 | 4.048034  | 0.278030  | 0.899979  |
| 55 | 6 | 0 | 4.928023  | 1.199041  | 1.466979  |
| 56 | 6 | 0 | 2.859039  | -0.055985 | 1.565979  |
| 57 | 6 | 0 | 4.632015  | 1.804038  | 2.688979  |
| 58 | 1 | 0 | 5.319006  | 2.523046  | 3.124979  |
| 59 | 6 | 0 | 2.565031  | 0.541011  | 2.799979  |
| 60 | 6 | 0 | 3.448019  | 1.470023  | 3.346979  |
| 61 | 1 | 0 | 3.208013  | 1.930020  | 4.301979  |
| 62 | 7 | 0 | 1.961050  | -0.997996 | 0.986979  |
| 63 | 1 | 0 | 1.644034  | 0.290000  | 3.308979  |
| 64 | 1 | 0 | -5.765969 | 0.512906  | -0.628021 |