Supplementary Materials

Thiol- and Thioether-Based Bifunctional Chelates for the $\{M(CO)_3\}^+$ Core

(M = Tc, Re)

Neva Lazarova, John Babich, John Valliant, Paul Schaffer, Shelly James, and Jon Zubieta

1. CIF files for Re-1a and Re-2.
2. Table S1: Fractions from Sep-Pak Purification (1000 μL Fractions).
3. Supplementary Figure 5. Radiochromatogram of $[^{99m}Tc(CO)_3(L1)]^+$ (^{99m}Tc-1) before histidine challenge.
4. Supplementary Figure 6. Radiochromatogram of $[^{99m}Tc(CO)_3(L1)]^+$ (^{99m}Tc-1) after histidine challenge.
5. Supplementary Figure 7. Radiochromatogram of $[^{99m}Tc(CO)_3(L1)]^+$ (^{99m}Tc-1) and UV trace of $[Re(CO)_3(L1)]^+$ (Re-1).
6. Supplementary Figure 8. Radiochromatogram of $[^{99m}Tc(CO)_3(L2)]$ (^{99m}Tc-2) and UV trace of $[Re(CO)_3(L2)]$ (Re-2).

data_p21-c **Compound Re-2**

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'x, -y-1/2, z-1/2'

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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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used when they are defined by crystal symmetry. An approximate (isotropic)
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_diffrn_standards_number         ?
_diffrn_standards_interval_count  ?
_diffrn_standards_interval_time  ?
_diffrn_standards_decay_%        ?
_diffrn_reflns_number            25406
_diffrn_reflns_av_R_equivalents  0.0749
```

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_diffrn_reflns_av_sigmaI/netI     0.0656
_diffrn_reflns_limit_h_min        -14
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_diffrn_reflns_limit_k_min        -25
_diffrn_reflns_limit_k_max        25
_diffrn_reflns_limit_l_min        -15
_diffrn_reflns_limit_l_max        15
_diffrn_reflns_theta_min          1.84
_diffrn_reflns_theta_max          27.00
_reflns_number_total              5869
_reflns_number_gt                 5155
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        'Bruker SMART'
_computing_cell_refinement        'Bruker SMART'
_computing_data_reduction         'Bruker SAINT'
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     'Bruker SHELXTL'
_computing_publication_material   'Bruker SHELXTL'

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0372P)^2^+179.4181P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          5869
_refine_ls_number_parameters      326
_refine_ls_number_restraints      54
```

_refine_ls_R_factor_all 0.1091
_refine_ls_R_factor_gt 0.0961
_refine_ls_wR_factor_ref 0.1924
_refine_ls_wR_factor_gt 0.1873
_refine_ls_goodness_of_fit_ref 1.296
_refine_ls_restrained_S_all 1.292
_refine_ls_shift/su_max 0.001
_refine_ls_shift/su_mean 0.000

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Re1 Re 0.52095(6) 0.66829(3) 0.32096(6) 0.01021(17) Uani 1 1 d . . .
Re2 Re 0.94883(8) 0.92612(4) 0.27173(7) 0.0255(2) Uani 1 1 d . . .
Br1 Br 1.0326(2) 0.83949(13) 0.1429(2) 0.0409(6) Uani 1 1 d . . .
Br2 Br 0.7351(2) 0.88063(12) 0.1834(2) 0.0374(6) Uani 1 1 d . . .
S1 S 0.9552(5) 0.8359(3) 0.4214(5) 0.0293(12) Uani 1 1 d . . .
O1 O 0.5180(14) 0.7230(7) 0.5514(12) 0.027(3) Uani 1 1 d . . .
O2 O 0.4344(13) 0.8128(7) 0.2577(11) 0.025(3) Uani 1 1 d . . .
O3 O 0.2520(15) 0.6343(8) 0.3056(16) 0.044(4) Uani 1 1 d . . .
O4 O 1.1988(17) 0.9816(11) 0.3558(16) 0.056(5) Uani 1 1 d . . .
O5 O 0.8296(19) 1.0186(10) 0.4099(15) 0.052(5) Uani 1 1 d . . .
O6 O 0.9370(16) 1.0416(8) 0.1070(15) 0.040(4) Uani 1 1 d . . .
N1 N 0.5335(14) 0.6329(7) 0.1561(13) 0.017(3) Uani 1 1 d . . .
N2 N 0.7201(13) 0.6783(7) 0.3203(12) 0.014(3) Uani 1 1 d . . .
N3 N 0.5872(14) 0.5656(7) 0.3600(11) 0.012(3) Uani 1 1 d . . .
C1 C 0.5246(16) 0.6982(8) 0.4661(13) 0.011(3) Uani 1 1 d U . .
C2 C 0.4696(15) 0.7598(10) 0.2789(15) 0.016(4) Uani 1 1 d . . .
C3 C 0.3545(18) 0.6475(10) 0.3120(19) 0.026(5) Uani 1 1 d U . .
C4 C 0.4422(16) 0.6038(8) 0.0864(14) 0.013(3) Uani 1 1 d U . .
H4 H 0.3665 0.5968 0.1091 0.016 Uiso 1 1 calc R . .
C5 C 0.457(2) 0.5840(10) -0.0188(17) 0.027(5) Uani 1 1 d . . .
H5 H 0.3905 0.5675 -0.0696 0.033 Uiso 1 1 calc R . .
C6 C 0.570(2) 0.5887(9) -0.0486(16) 0.026(5) Uani 1 1 d . . .
H6 H 0.5829 0.5736 -0.1186 0.032 Uiso 1 1 calc R . .

C7 C 0.6667(18) 0.6163(9) 0.0268(15) 0.019(4) Uani 1 1 d . . .
H7 H 0.7460 0.6193 0.0100 0.023 Uiso 1 1 calc R . .
C8 C 0.6411(16) 0.6389(8) 0.1266(14) 0.012(3) Uani 1 1 d U . .
C9 C 0.7389(18) 0.6795(9) 0.2018(15) 0.018(4) Uani 1 1 d . . .
H9A H 0.8194 0.6603 0.1973 0.022 Uiso 1 1 calc R . .
H9B H 0.7375 0.7270 0.1760 0.022 Uiso 1 1 calc R . .
C10 C 0.7841(17) 0.6201(9) 0.3818(16) 0.018(4) Uani 1 1 d U . .
H10A H 0.8074 0.6326 0.4601 0.021 Uiso 1 1 calc R . .
H10B H 0.8590 0.6102 0.3527 0.021 Uiso 1 1 calc R . .
C11 C 0.7058(17) 0.5570(9) 0.3726(15) 0.017(4) Uani 1 1 d . . .
C12 C 0.758(2) 0.4924(9) 0.3899(17) 0.024(4) Uani 1 1 d . . .
H12 H 0.8437 0.4876 0.4007 0.029 Uiso 1 1 calc R . .
C13 C 0.688(2) 0.4370(10) 0.391(2) 0.033(5) Uani 1 1 d . . .
H13 H 0.7231 0.3931 0.4008 0.040 Uiso 1 1 calc R . .
C14 C 0.562(2) 0.4452(9) 0.3782(17) 0.024(4) Uani 1 1 d U . .
H14 H 0.5103 0.4073 0.3806 0.029 Uiso 1 1 calc R . .
C15 C 0.5141(17) 0.5116(9) 0.3613(13) 0.013(3) Uani 1 1 d U . .
H15 H 0.4289 0.5181 0.3506 0.016 Uiso 1 1 calc R . .
C16 C 0.7733(19) 0.7431(9) 0.3740(16) 0.021(4) Uani 1 1 d . . .
H16A H 0.7652 0.7426 0.4524 0.026 Uiso 1 1 calc R . .
H16B H 0.7266 0.7821 0.3388 0.026 Uiso 1 1 calc R . .
C17 C 0.9064(17) 0.7523(10) 0.365(2) 0.028(5) Uani 1 1 d U . .
H17A H 0.9169 0.7492 0.2877 0.034 Uiso 1 1 calc R . .
H17B H 0.9558 0.7163 0.4073 0.034 Uiso 1 1 calc R . .
C18 C 1.104(2) 0.8183(12) 0.492(3) 0.055(8) Uani 1 1 d U . .
H18A H 1.1402 0.8608 0.5258 0.066 Uiso 1 1 calc R . .
H18B H 1.0991 0.7860 0.5524 0.066 Uiso 1 1 calc R . .
C19 C 1.187(3) 0.7897(17) 0.422(3) 0.071(11) Uani 1 1 d . . .
H19A H 1.1558 0.7458 0.3931 0.107 Uiso 1 1 calc R . .
H19B H 1.2677 0.7836 0.4665 0.107 Uiso 1 1 calc R . .
H19C H 1.1920 0.8208 0.3616 0.107 Uiso 1 1 calc R . .
C20 C 1.1058(18) 0.9567(12) 0.3295(19) 0.030(5) Uani 1 1 d . . .
C21 C 0.875(2) 0.9877(10) 0.3589(19) 0.032(5) Uani 1 1 d . . .
C22 C 0.9378(18) 0.9981(10) 0.169(2) 0.027(5) Uani 1 1 d . . .

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Re1 0.0126(3) 0.0059(3) 0.0127(3) 0.0015(3) 0.0037(2) -0.0010(3)
Re2 0.0193(4) 0.0204(4) 0.0356(5) -0.0008(3) 0.0017(3) -0.0024(3)
Br1 0.0409(14) 0.0376(13) 0.0440(14) -0.0048(11) 0.0067(11) 0.0044(11)

Br2 0.0214(11) 0.0403(13) 0.0454(14) 0.0178(11) -0.0087(10) -0.0112(9)
S1 0.024(3) 0.016(2) 0.045(3) -0.003(2) -0.003(2) -0.007(2)
O1 0.043(9) 0.016(7) 0.026(8) -0.003(6) 0.014(7) 0.000(6)
O2 0.027(8) 0.021(7) 0.026(7) 0.007(6) 0.008(6) 0.014(6)
O3 0.028(9) 0.032(9) 0.071(13) -0.012(9) 0.008(9) 0.000(7)
O4 0.038(11) 0.073(14) 0.052(12) 0.000(10) -0.004(9) -0.023(10)
O5 0.064(13) 0.053(12) 0.038(10) 0.016(9) 0.006(10) 0.015(10)
O6 0.041(10) 0.034(9) 0.050(11) 0.009(8) 0.019(8) 0.007(8)
N1 0.015(8) 0.011(7) 0.022(8) 0.004(6) -0.005(6) -0.002(6)
N2 0.013(7) 0.009(7) 0.019(8) -0.003(6) 0.003(6) 0.000(6)
N3 0.026(8) 0.005(6) 0.003(6) 0.001(5) -0.002(6) -0.002(6)
C1 0.015(5) 0.012(5) 0.007(5) 0.005(4) 0.003(4) -0.004(4)
C2 0.003(8) 0.025(10) 0.021(9) 0.003(8) 0.001(7) 0.007(7)
C3 0.012(9) 0.026(10) 0.043(11) -0.011(9) 0.013(8) 0.009(8)
C4 0.016(5) 0.007(5) 0.016(5) 0.003(4) 0.002(4) 0.005(4)
C5 0.034(12) 0.016(9) 0.026(11) 0.000(8) -0.010(9) -0.009(9)
C6 0.057(15) 0.006(8) 0.022(10) -0.006(7) 0.024(10) -0.008(9)
C7 0.024(10) 0.018(9) 0.017(9) 0.007(7) 0.008(8) 0.000(8)
C8 0.020(7) 0.007(6) 0.011(6) 0.007(5) 0.003(6) -0.001(6)
C9 0.028(10) 0.007(8) 0.021(9) -0.003(7) 0.006(8) -0.008(7)
C10 0.013(7) 0.013(7) 0.025(7) 0.004(6) -0.002(6) 0.008(6)
C11 0.015(9) 0.015(9) 0.018(9) -0.004(7) -0.003(7) -0.002(7)
C12 0.033(12) 0.009(8) 0.030(11) -0.004(8) 0.003(9) 0.006(8)
C13 0.041(13) 0.008(9) 0.047(14) -0.003(9) -0.003(11) 0.011(9)
C14 0.040(12) 0.002(8) 0.034(11) 0.000(7) 0.016(9) 0.006(8)
C15 0.022(7) 0.014(7) 0.002(6) -0.004(5) -0.001(5) 0.003(6)
C16 0.029(11) 0.013(9) 0.019(9) -0.006(7) -0.003(8) -0.002(8)
C17 0.010(9) 0.023(10) 0.046(13) -0.011(9) -0.011(9) -0.008(8)
C18 0.011(10) 0.028(12) 0.11(2) -0.001(14) -0.025(13) -0.010(9)
C19 0.038(17) 0.06(2) 0.12(3) -0.04(2) 0.012(18) -0.030(15)
C20 0.014(10) 0.039(12) 0.035(12) 0.000(10) 0.000(9) -0.020(9)
C21 0.052(15) 0.013(10) 0.036(12) 0.000(9) 0.023(11) 0.007(10)
C22 0.016(10) 0.015(9) 0.049(14) 0.002(9) 0.003(9) -0.001(8)

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;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
;

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Re1 C1 1.884(16) . ?
Re1 C3 1.90(2) . ?
Re1 C2 1.939(18) . ?
Re1 N3 2.184(14) . ?
Re1 N1 2.184(16) . ?
Re1 N2 2.245(15) . ?
Re2 C20 1.882(19) . ?
Re2 C22 1.90(2) . ?
Re2 C21 1.90(2) . ?
Re2 S1 2.561(6) . ?
Re2 Br2 2.616(2) . ?
Re2 Br1 2.621(3) . ?
S1 C18 1.78(2) . ?
S1 C17 1.84(2) . ?
O1 C1 1.18(2) . ?
O2 C2 1.13(2) . ?
O3 C3 1.17(2) . ?
O4 C20 1.15(3) . ?
O5 C21 1.07(3) . ?
O6 C22 1.15(3) . ?
N1 C8 1.33(2) . ?
N1 C4 1.35(2) . ?
N2 C10 1.49(2) . ?
N2 C16 1.51(2) . ?
N2 C9 1.52(2) . ?
N3 C11 1.32(2) . ?
N3 C15 1.35(2) . ?
C4 C5 1.40(3) . ?
C5 C6 1.38(3) . ?
C6 C7 1.41(3) . ?
C7 C8 1.39(2) . ?
C8 C9 1.54(2) . ?
C10 C11 1.52(3) . ?
C11 C12 1.40(3) . ?
C12 C13 1.35(3) . ?
C13 C14 1.40(3) . ?
C14 C15 1.42(2) . ?
C16 C17 1.53(3) . ?
C18 C19 1.48(4) . ?

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C1 Re1 C3 89.0(8) . . ?
C1 Re1 C2 85.4(7) . . ?
C3 Re1 C2 86.7(8) . . ?
C1 Re1 N3 97.5(6) . . ?
C3 Re1 N3 96.1(7) . . ?
C2 Re1 N3 176.0(7) . . ?
C1 Re1 N1 175.1(7) . . ?
C3 Re1 N1 95.7(8) . . ?
C2 Re1 N1 96.4(7) . . ?
N3 Re1 N1 80.5(5) . . ?
C1 Re1 N2 96.8(6) . . ?
C3 Re1 N2 171.7(7) . . ?
C2 Re1 N2 99.6(6) . . ?
N3 Re1 N2 77.4(5) . . ?
N1 Re1 N2 78.4(6) . . ?
C20 Re2 C22 87.9(9) . . ?
C20 Re2 C21 92.8(11) . . ?
C22 Re2 C21 85.4(9) . . ?
C20 Re2 S1 92.4(7) . . ?
C22 Re2 S1 175.1(7) . . ?
C21 Re2 S1 89.7(7) . . ?
C20 Re2 Br2 177.1(8) . . ?
C22 Re2 Br2 91.6(6) . . ?
C21 Re2 Br2 90.0(8) . . ?
S1 Re2 Br2 88.39(13) . . ?
C20 Re2 Br1 91.7(8) . . ?
C22 Re2 Br1 93.9(7) . . ?
C21 Re2 Br1 175.4(8) . . ?
S1 Re2 Br1 91.05(14) . . ?
Br2 Re2 Br1 85.51(9) . . ?
C18 S1 C17 101.8(11) . . ?
C18 S1 Re2 113.3(10) . . ?
C17 S1 Re2 112.5(8) . . ?
C8 N1 C4 119.3(16) . . ?
C8 N1 Re1 116.0(12) . . ?
C4 N1 Re1 124.7(13) . . ?
C10 N2 C16 108.0(14) . . ?
C10 N2 C9 111.7(14) . . ?
C16 N2 C9 107.5(13) . . ?
C10 N2 Re1 108.8(11) . . ?
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C16 N2 Re1 112.9(11) . . ?
C9 N2 Re1 108.1(11) . . ?
C11 N3 C15 120.0(15) . . ?
C11 N3 Re1 116.2(11) . . ?
C15 N3 Re1 123.5(12) . . ?
O1 C1 Re1 172.1(15) . . ?
O2 C2 Re1 176.0(16) . . ?
O3 C3 Re1 179(2) . . ?
N1 C4 C5 120.8(18) . . ?
C6 C5 C4 119.7(18) . . ?
C5 C6 C7 118.8(17) . . ?
C8 C7 C6 117.4(18) . . ?
N1 C8 C7 123.7(17) . . ?
N1 C8 C9 117.9(15) . . ?
C7 C8 C9 118.0(16) . . ?
N2 C9 C8 111.9(14) . . ?
N2 C10 C11 111.9(15) . . ?
N3 C11 C12 121.4(17) . . ?
N3 C11 C10 117.4(15) . . ?
C12 C11 C10 120.8(17) . . ?
C13 C12 C11 120(2) . . ?
C12 C13 C14 119.0(18) . . ?
C13 C14 C15 118.1(18) . . ?
N3 C15 C14 121.1(18) . . ?
N2 C16 C17 112.7(16) . . ?
C16 C17 S1 108.2(14) . . ?
C19 C18 S1 115(2) . . ?
O4 C20 Re2 172(2) . . ?
O5 C21 Re2 175(2) . . ?
O6 C22 Re2 176.7(19) . . ?

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C20 Re2 S1 C18 -16.9(13) . . . . ?
C22 Re2 S1 C18 -110(7) . . . . ?
C21 Re2 S1 C18 -109.7(14) . . . . ?
Br2 Re2 S1 C18 160.3(11) . . . . ?
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Br1 Re2 S1 C18 74.8(11) . . . . ?
C20 Re2 S1 C17 -131.7(11) . . . . ?
C22 Re2 S1 C17 135(7) . . . . ?
C21 Re2 S1 C17 135.5(11) . . . . ?
Br2 Re2 S1 C17 45.5(7) . . . . ?
Br1 Re2 S1 C17 -40.0(7) . . . . ?
C1 Re1 N1 C8 -20(8) . . . . ?
C3 Re1 N1 C8 179.6(13) . . . . ?
C2 Re1 N1 C8 92.3(13) . . . . ?
N3 Re1 N1 C8 -85.1(12) . . . . ?
N2 Re1 N1 C8 -6.2(12) . . . . ?
C1 Re1 N1 C4 158(7) . . . . ?
C3 Re1 N1 C4 -2.9(15) . . . . ?
C2 Re1 N1 C4 -90.2(14) . . . . ?
N3 Re1 N1 C4 92.3(14) . . . . ?
N2 Re1 N1 C4 171.3(14) . . . . ?
C1 Re1 N2 C10 77.0(12) . . . . ?
C3 Re1 N2 C10 -57(6) . . . . ?
C2 Re1 N2 C10 163.5(12) . . . . ?
N3 Re1 N2 C10 -19.2(11) . . . . ?
N1 Re1 N2 C10 -101.9(11) . . . . ?
C1 Re1 N2 C16 -42.8(13) . . . . ?
C3 Re1 N2 C16 -177(5) . . . . ?
C2 Re1 N2 C16 43.7(13) . . . . ?
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N1 Re1 N2 C16 138.3(12) . . . . ?
C1 Re1 N2 C9 -161.6(11) . . . . ?
C3 Re1 N2 C9 64(6) . . . . ?
C2 Re1 N2 C9 -75.1(11) . . . . ?
N3 Re1 N2 C9 102.3(10) . . . . ?
N1 Re1 N2 C9 19.6(10) . . . . ?
C1 Re1 N3 C11 -91.0(13) . . . . ?
C3 Re1 N3 C11 179.3(13) . . . . ?
C2 Re1 N3 C11 45(10) . . . . ?
N1 Re1 N3 C11 84.5(13) . . . . ?
N2 Re1 N3 C11 4.4(12) . . . . ?
C1 Re1 N3 C15 95.4(13) . . . . ?
C3 Re1 N3 C15 5.6(14) . . . . ?
C2 Re1 N3 C15 -128(9) . . . . ?
N1 Re1 N3 C15 -89.1(13) . . . . ?
N2 Re1 N3 C15 -169.3(13) . . . . ?
C3 Re1 C1 O1 -67(11) . . . . ?
C2 Re1 C1 O1 20(11) . . . . ?
N3 Re1 C1 O1 -163(11) . . . . ?
N1 Re1 C1 O1 132(10) . . . . ?
N2 Re1 C1 O1 119(11) . . . . ?

C1 Re1 C2 O2 -54(25) . . . . ?
C3 Re1 C2 O2 35(25) . . . . ?
N3 Re1 C2 O2 169(19) . . . . ?
N1 Re1 C2 O2 130(25) . . . . ?
N2 Re1 C2 O2 -150(25) . . . . ?
C1 Re1 C3 O3 -161(100) . . . . ?
C2 Re1 C3 O3 114(100) . . . . ?
N3 Re1 C3 O3 -63(100) . . . . ?
N1 Re1 C3 O3 18(100) . . . . ?
N2 Re1 C3 O3 -26(100) . . . . ?
C8 N1 C4 C5 -4(2) . . . . ?
Re1 N1 C4 C5 178.5(13) . . . . ?
N1 C4 C5 C6 6(3) . . . . ?
C4 C5 C6 C7 -3(3) . . . . ?
C5 C6 C7 C8 -2(3) . . . . ?
C4 N1 C8 C7 -1(3) . . . . ?
Re1 N1 C8 C7 177.1(13) . . . . ?
C4 N1 C8 C9 173.0(15) . . . . ?
Re1 N1 C8 C9 -9.4(19) . . . . ?
C6 C7 C8 N1 3(3) . . . . ?
C6 C7 C8 C9 -170.2(16) . . . . ?
C10 N2 C9 C8 89.9(18) . . . . ?
C16 N2 C9 C8 -151.8(15) . . . . ?
Re1 N2 C9 C8 -29.7(16) . . . . ?
N1 C8 C9 N2 27(2) . . . . ?
C7 C8 C9 N2 -158.8(15) . . . . ?
C16 N2 C10 C11 153.5(16) . . . . ?
C9 N2 C10 C11 -88.5(18) . . . . ?
Re1 N2 C10 C11 30.7(18) . . . . ?
C15 N3 C11 C12 -1(3) . . . . ?
Re1 N3 C11 C12 -175.3(14) . . . . ?
C15 N3 C11 C10 -174.0(15) . . . . ?
Re1 N3 C11 C10 12(2) . . . . ?
N2 C10 C11 N3 -30(2) . . . . ?
N2 C10 C11 C12 157.7(17) . . . . ?
N3 C11 C12 C13 2(3) . . . . ?
C10 C11 C12 C13 174(2) . . . . ?
C11 C12 C13 C14 -2(3) . . . . ?
C12 C13 C14 C15 2(3) . . . . ?
C11 N3 C15 C14 1(2) . . . . ?
Re1 N3 C15 C14 174.7(13) . . . . ?
C13 C14 C15 N3 -1(3) . . . . ?
C10 N2 C16 C17 64(2) . . . . ?
C9 N2 C16 C17 -56(2) . . . . ?
Re1 N2 C16 C17 -175.5(13) . . . . ?
N2 C16 C17 S1 174.6(13) . . . . ?

C18 S1 C17 C16 141.3(18) . . . . ?
Re2 S1 C17 C16 -97.1(15) . . . . ?
C17 S1 C18 C19 58(2) . . . . ?
Re2 S1 C18 C19 -63(2) . . . . ?
C22 Re2 C20 O4 3(16) . . . . ?
C21 Re2 C20 O4 -82(16) . . . . ?
S1 Re2 C20 O4 -172(16) . . . . ?
Br2 Re2 C20 O4 82(24) . . . . ?
Br1 Re2 C20 O4 97(16) . . . . ?
C20 Re2 C21 O5 -132(28) . . . . ?
C22 Re2 C21 O5 141(28) . . . . ?
S1 Re2 C21 O5 -39(28) . . . . ?
Br2 Re2 C21 O5 49(28) . . . . ?
Br1 Re2 C21 O5 60(33) . . . . ?
C20 Re2 C22 O6 24(36) . . . . ?
C21 Re2 C22 O6 117(36) . . . . ?
S1 Re2 C22 O6 117(34) . . . . ?
Br2 Re2 C22 O6 -153(36) . . . . ?
Br1 Re2 C22 O6 -67(36) . . . . ?

_diffrn_measured_fraction_theta_max 0.997
_diffrn_reflns_theta_full 27.00
_diffrn_measured_fraction_theta_full 0.997
_refine_diff_density_max 3.996
_refine_diff_density_min -4.004
_refine_diff_density_rms 0.399

Table S1. Fractions from Sep-Pak Purification (1000 μL Fractions).

Fraction(s) (Elution Solv.)	Activity (μCi)
1 (10 mM HCl)	0.02
2 (10 mM HCl)	3.58
3 (10 mM HCl)	0.97
4 (10 mM HCl)	0
5 (10 mM HCl)	0
6 (10 mM HCl)	0
7 (10 mM HCl)	0
8 (10 mM HCl/ACN; 80:20) *	3.28
9 (10 mM HCl/ACN; 80:20) *	1.88
10 (10 mM HCl/ACN; 80:20)	0
11 (30 mL AIR)	0
12 (ACN)*	0
13 (ACN)*	0
14 (ACN)	0
15 (ACN)	0

* Indicates fractions containing pure product (> 95%).

Figure 5.

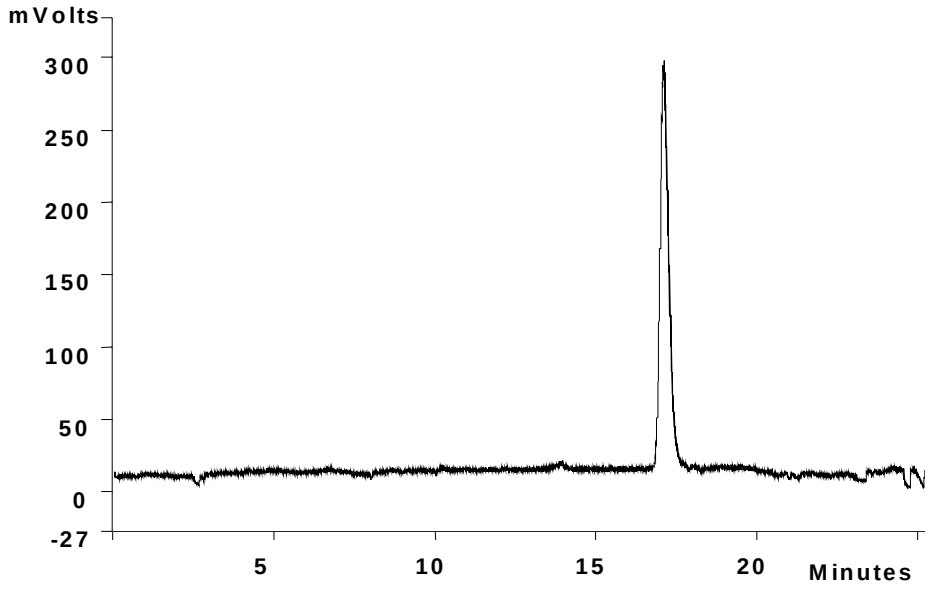

Figure 6.

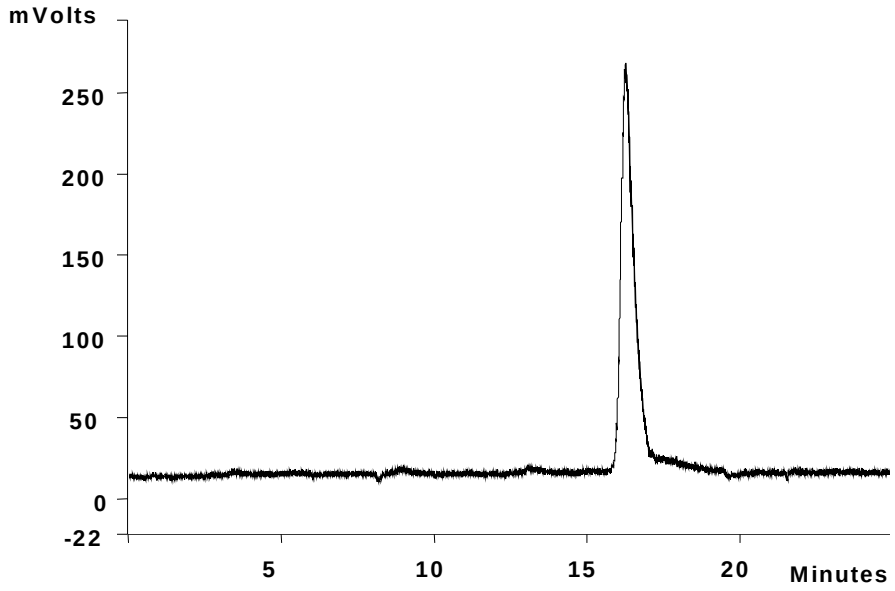

Figure 7.

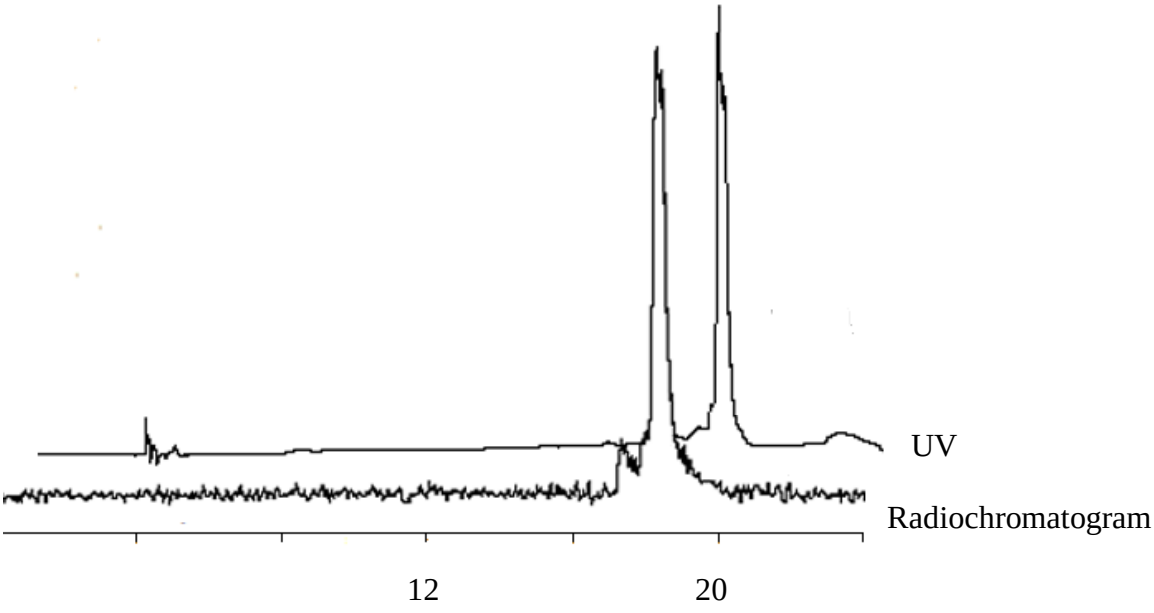

Figure 8.