

Supplementary Information

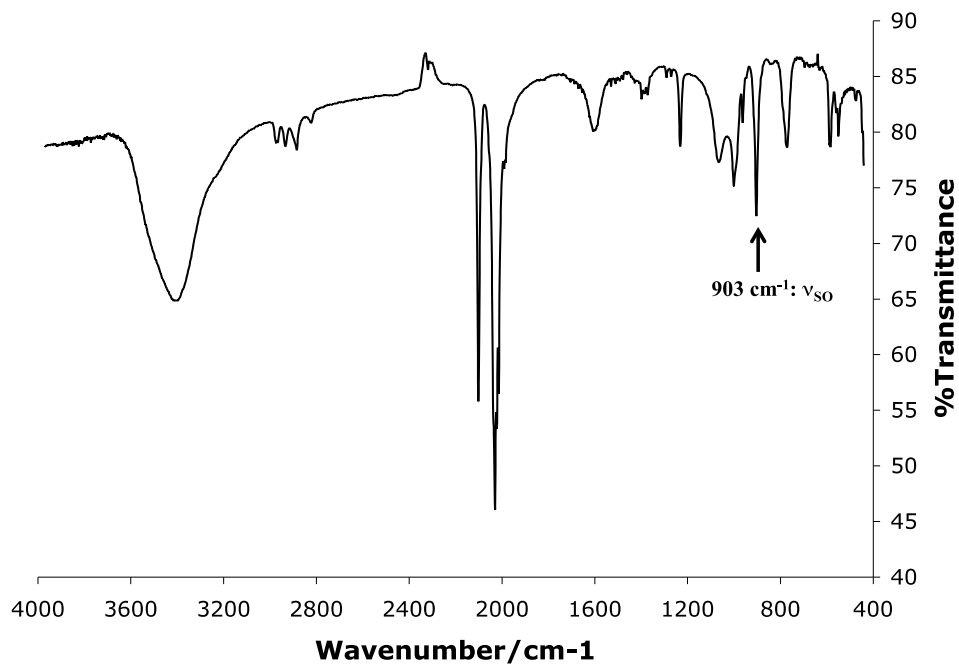
A contribution to the rational design of Ru(CO)₃Cl₂L complexes for in vivo delivery of CO

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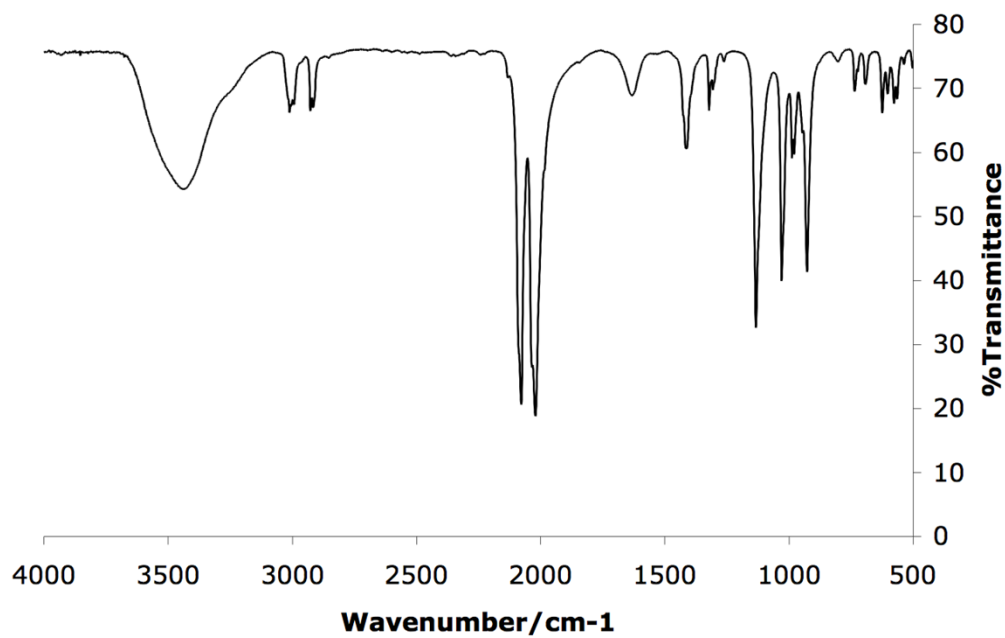
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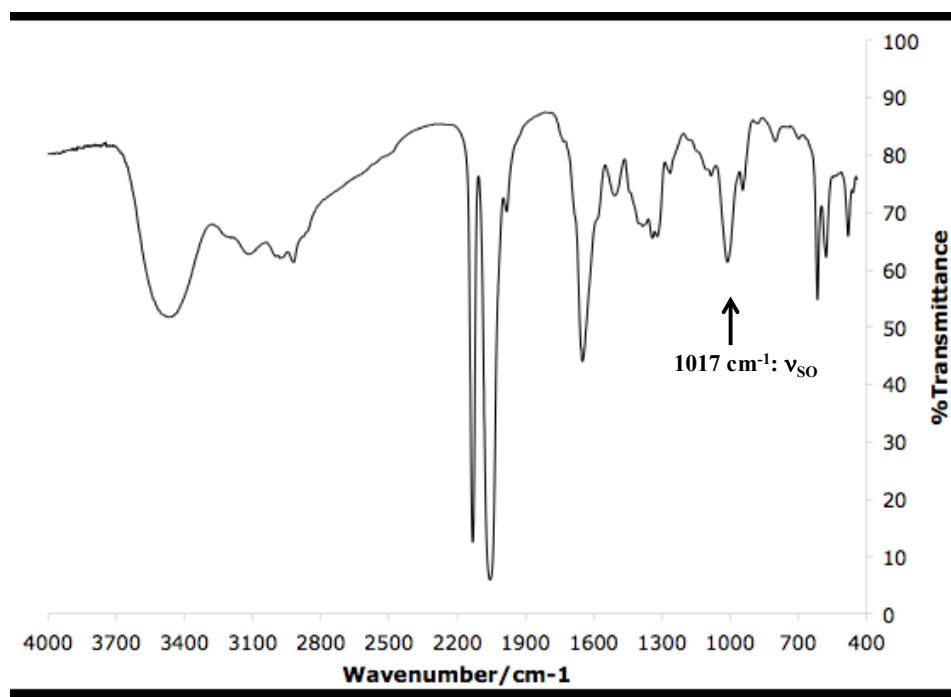
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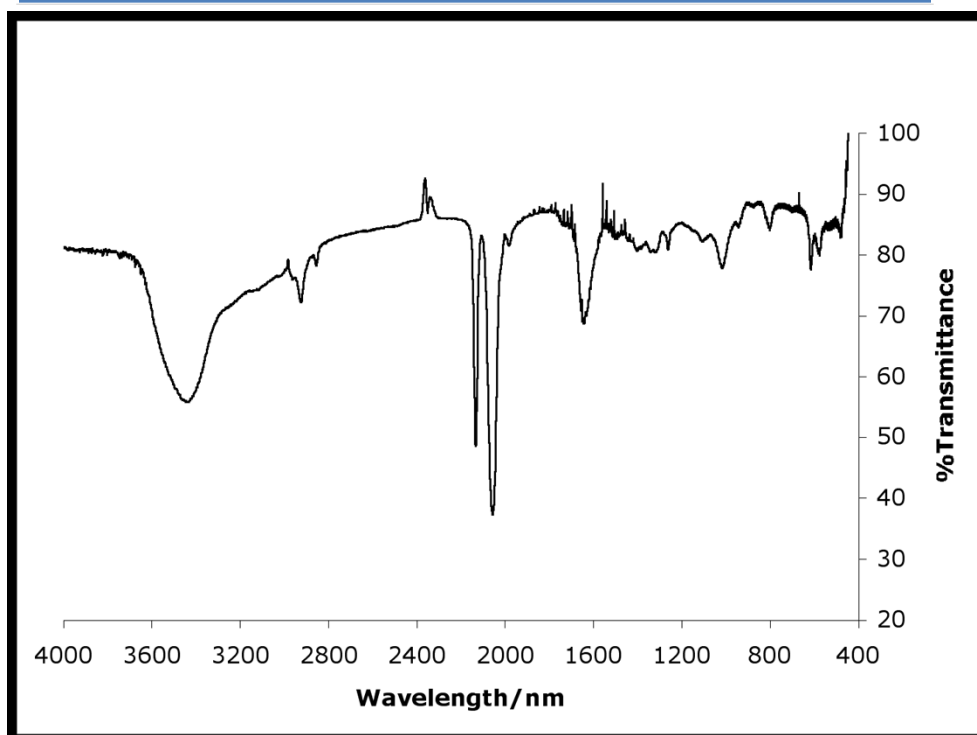
FTIR spectrum of $\text{RuCl}_2(\text{CO})_3(\text{DMSO})$ (**3**) in KBr pellet



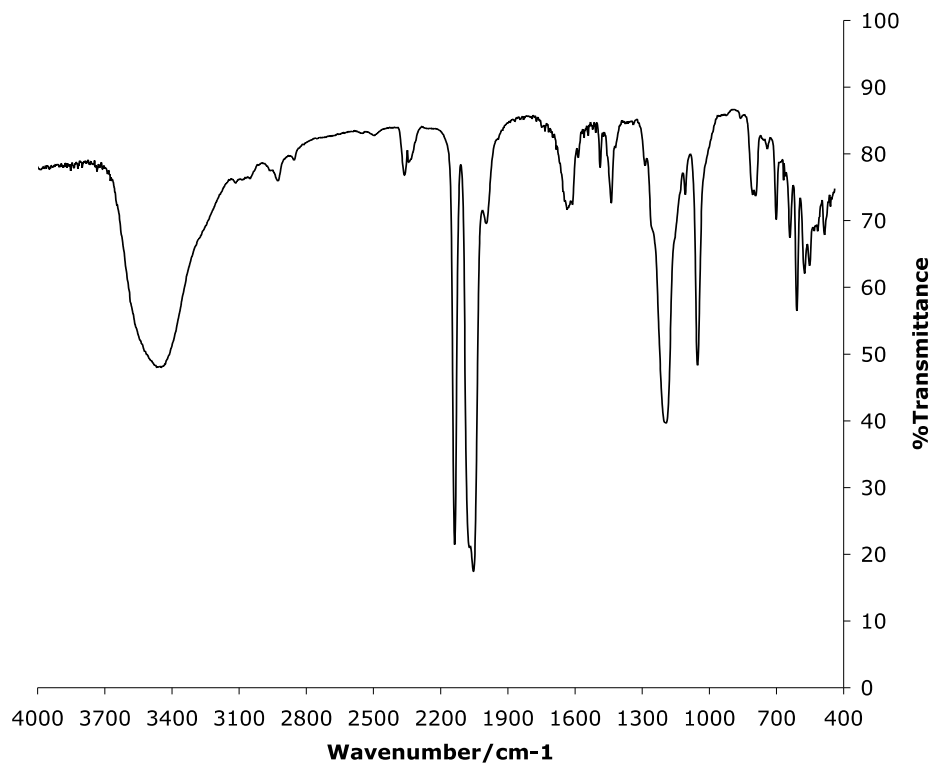
FTIR spectrum of $\text{RuCl}_2(\text{CO})_2(\text{DMSO})_2$ (**4a + 4b**) in KBr pellet



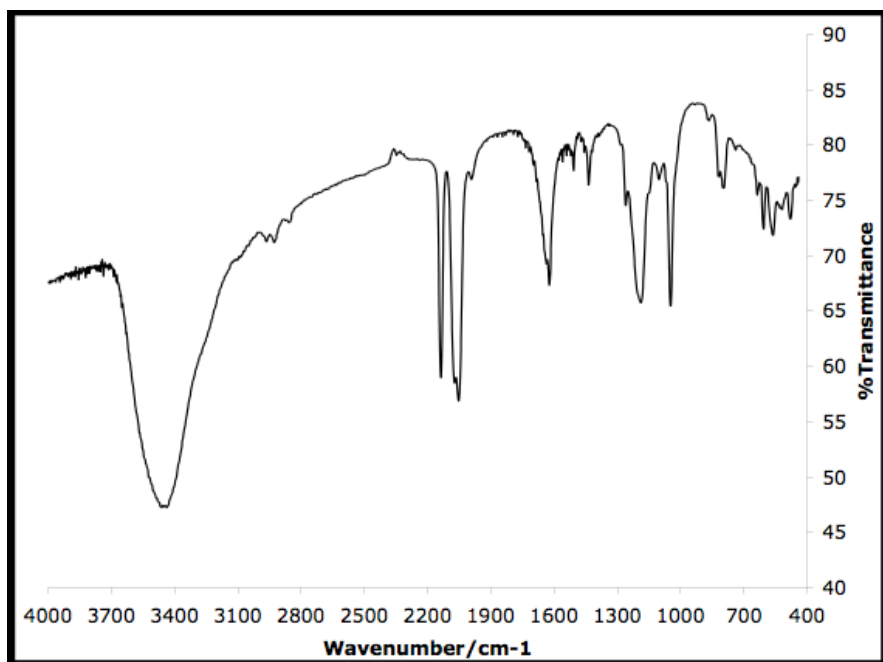
FTIR spectrum of $\text{RuCl}_2(\text{CO})_3(\text{L}-(\text{CH}_3\text{SO}(\text{CH}_2)_2\text{CH}(\text{NH}_2)\text{CO}_2\text{H}))$ (**6a**) in KBr pellet.



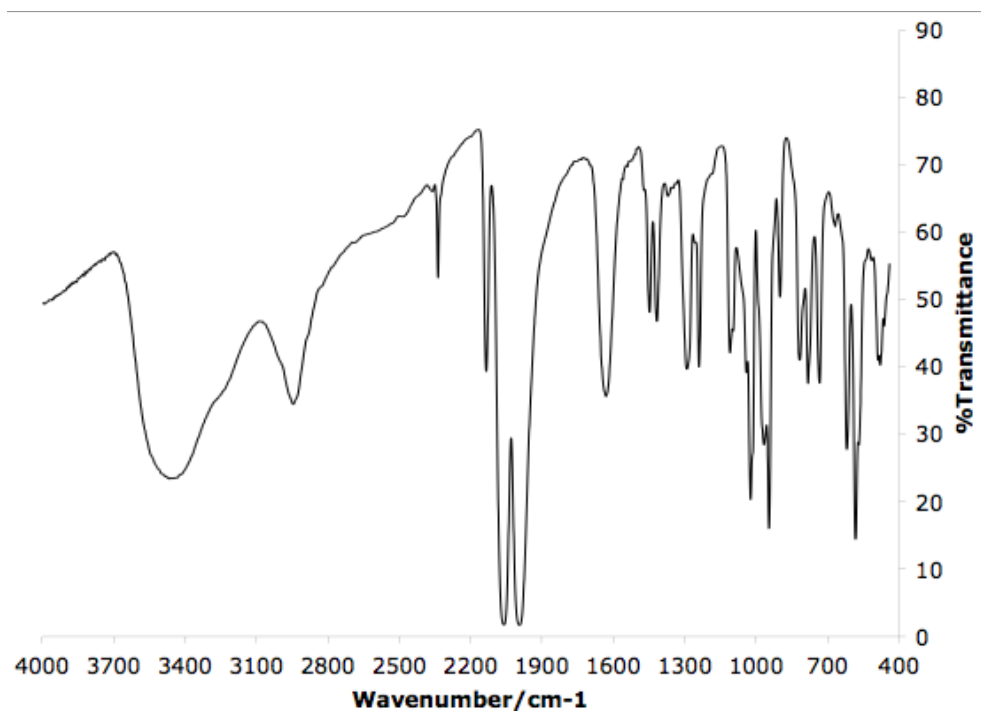
FTIR spectrum of $\text{RuCl}_2(\text{CO})_3(\text{D,L}-(\text{CH}_3\text{SO}(\text{CH}_2)_2\text{CH}(\text{NH}_2)\text{CO}_2\text{H}))$ (**6b**) in KBr pellet.



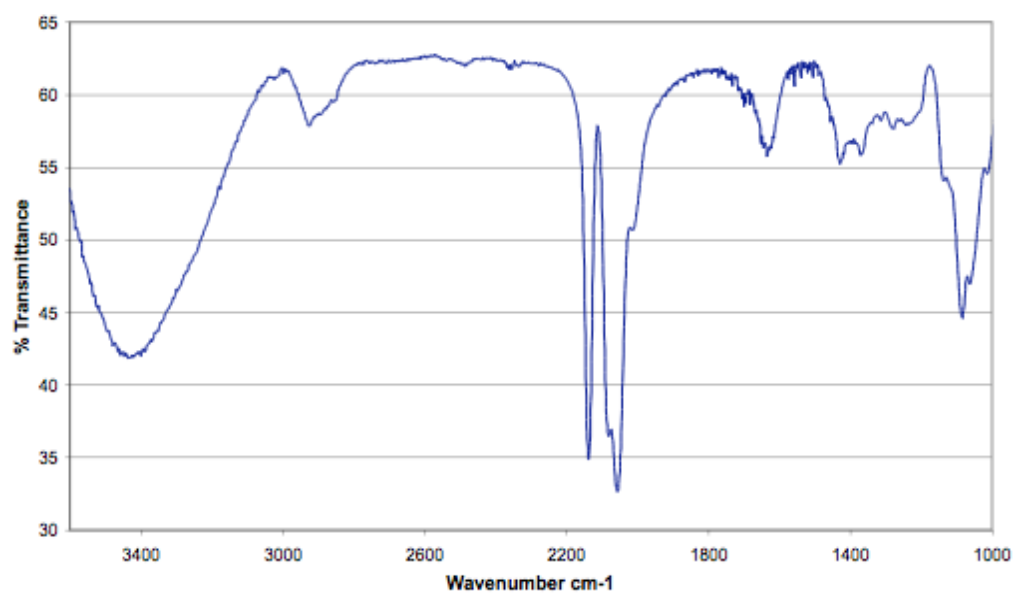
FTIR spectrum of $\text{RuCl}_2(\text{CO})_3(3\text{-NC}_5\text{H}_4(\text{CH}_2)_2\text{SO}_3\text{Na})$ (**7**) in KBr pellet



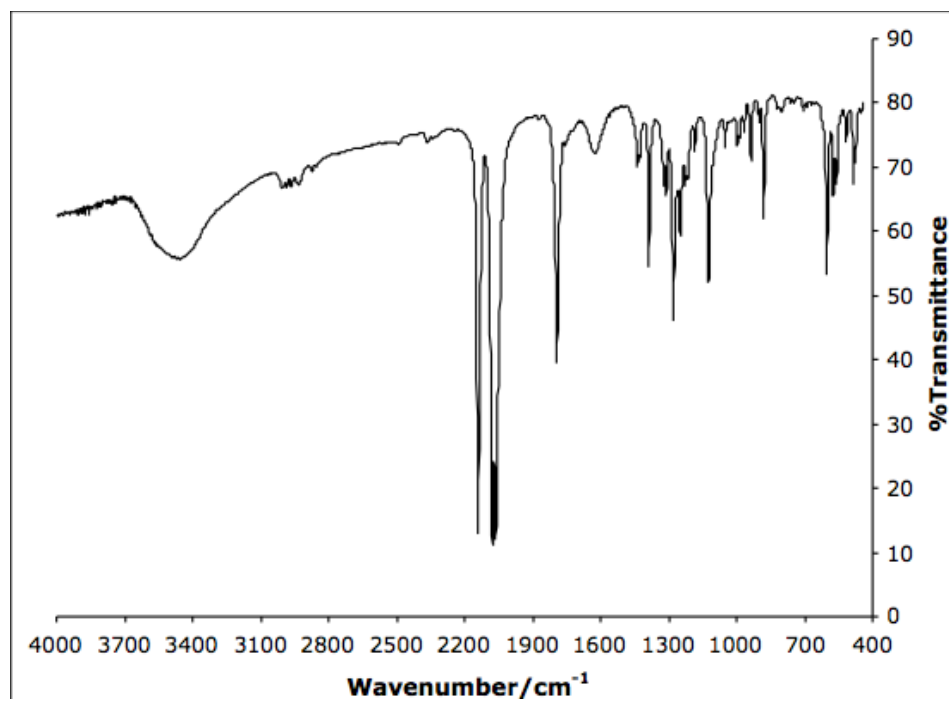
FTIR spectrum of $\text{RuCl}_2(\text{CO})_3(4\text{-NC}_5\text{H}_4(\text{CH}_2)_2\text{SO}_3\text{Na})$ (**8**) in KBr pellet



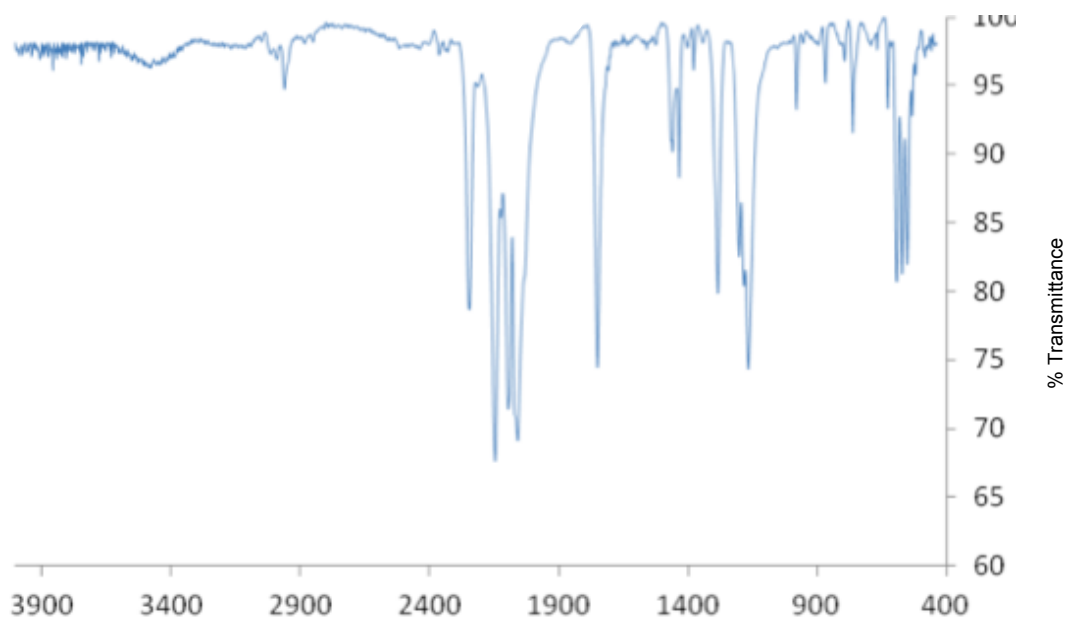
FTIR spectrum of $\text{RuCl}_2(\text{CO})_3(\text{PTA})$ (9) in KBr pellet.



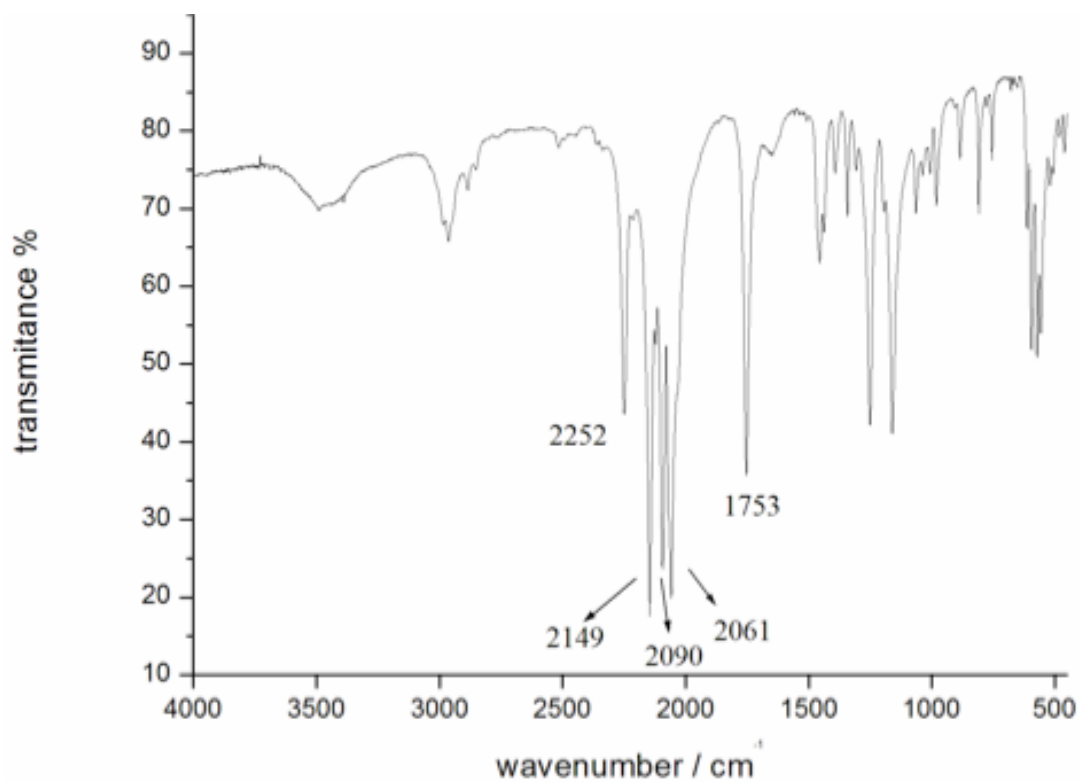
FTIR spectrum of $\text{RuCl}_2(\text{CO})_3(\text{DAPTA})$ (10) in KBr pellet.



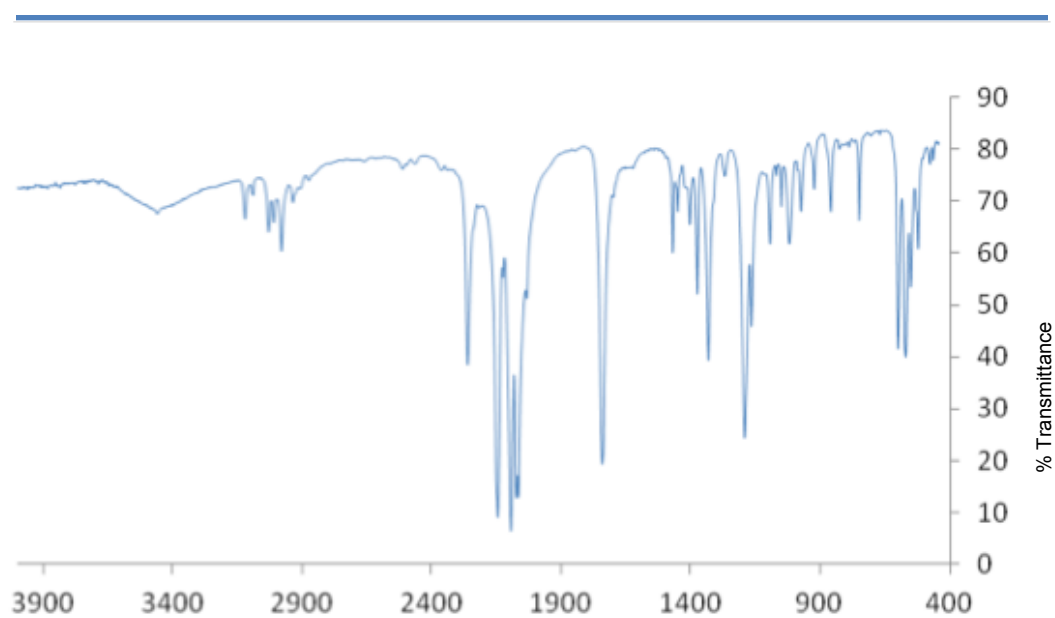
FTIR spectrum of $\text{RuCl}_2(\text{CO})_3(\text{CH}_3\text{S}(\text{CH}_2)_2\text{CH}(\text{OH})\text{CO}_2\text{H})$ (**11**) in KBr pellet.



FTIR spectrum of $\text{Ru}(\text{CO})_3\text{Cl}_2(\text{CNCMe}_2\text{CO}_2\text{Me})$ (**12**) in KBr pellet.



FTIR spectrum of Ru(CO)₃Cl₂(CNCMeEtCO₂Me) (**13**) in KBr pellet.



FTIR spectrum of Ru(CO)₃Cl₂(CNC(CH₂CH₂)CO₂Me) (**14**) in KBr pellet.

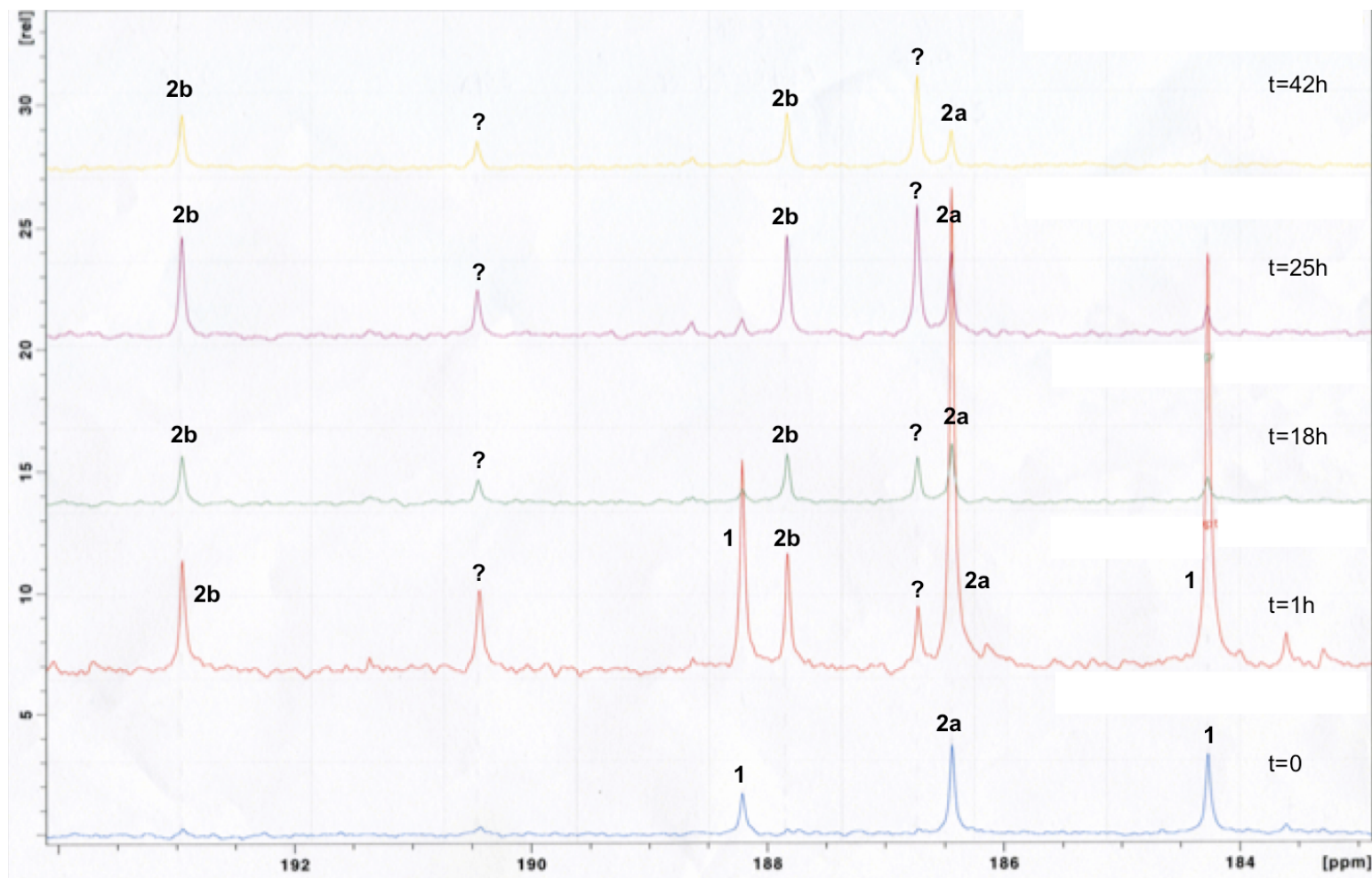


Figure S1. Time evolution of ^{13}C NMR spectrum of **CORM-2** in $\text{d}^6\text{-DMSO}$, at room temperature, in the carbonyl region at $t=0$; $t=1\text{h}$; $t=18\text{h}$; $t=25\text{h}$; $t=42\text{h}$. Each spectrum was acquired over 29min, except $t=1\text{h}$ that was acquired over 3h. At the time of dissolution 3 resonances are observed, two at δ 184.3 and 188.3 ppm from the tricarbonyl *fac*- $\text{RuCl}_2(\text{DMSO})(\text{CO})_3$ (**1**) and one peak at δ 186.5 ppm from $\text{RuCl}_2(\text{DMSO})_2(\text{CO})_2$ (**2a**). After 1h three isomers of dicarbonyl species are observed and an unknown peak is observed at δ 190.5 ppm. Later in time, after 18h, species **1** and **2a** concentrations' decreased and **2b** isomer increased in solution. This tendency results in the formation of dicarbonyl isomers with the *cis,trans,cis*- $\text{RuCl}_2(\text{DMSO})_2(\text{CO})_2$ as the main species after 42h.

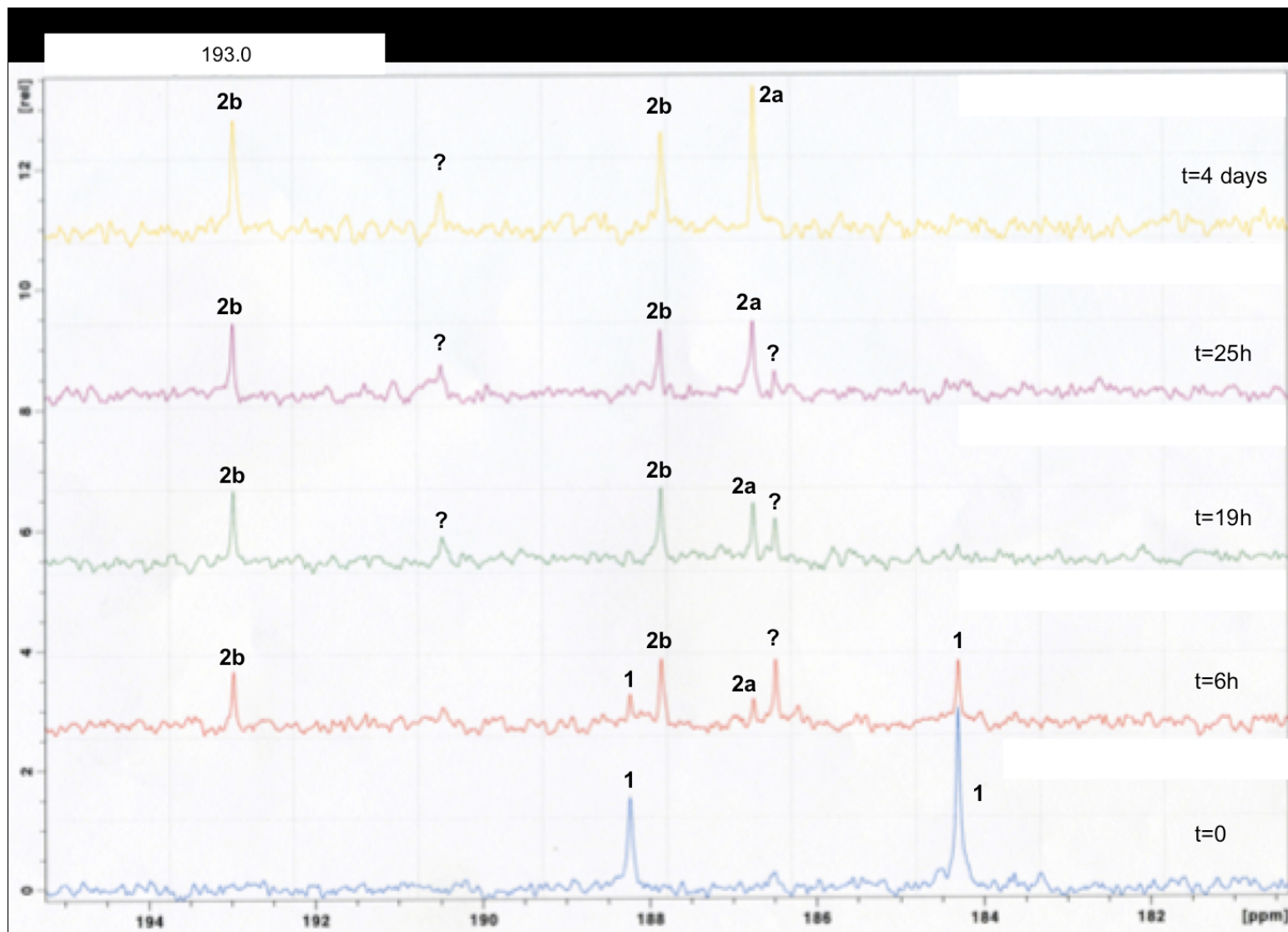
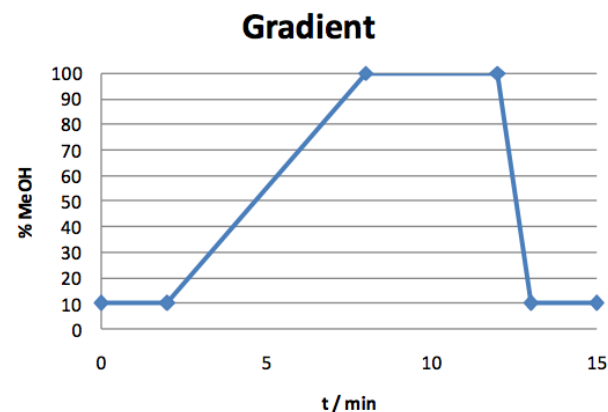
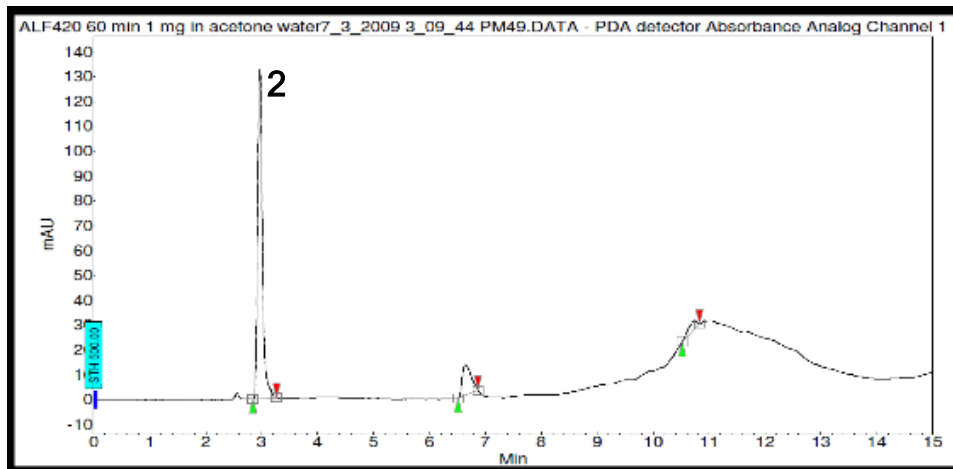
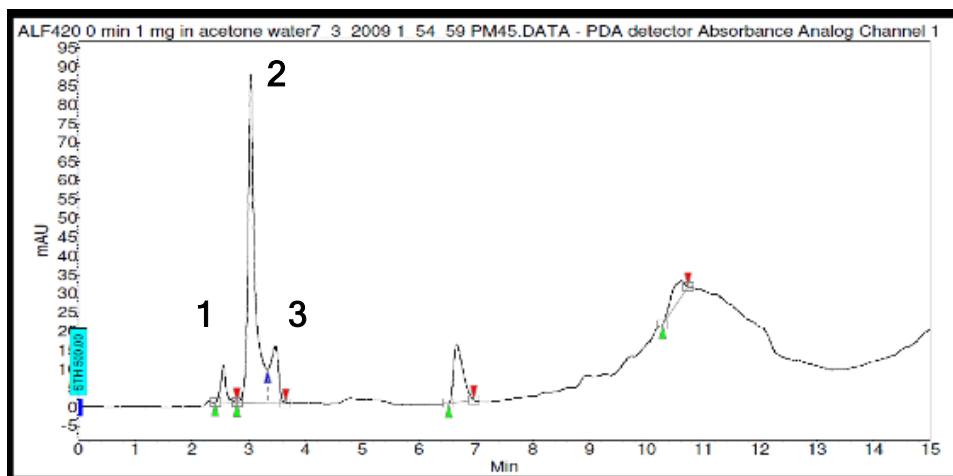
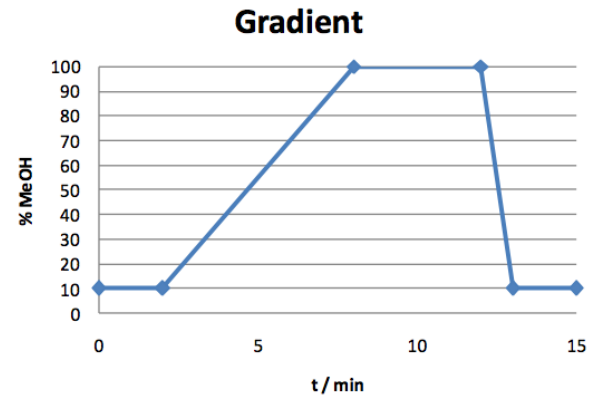
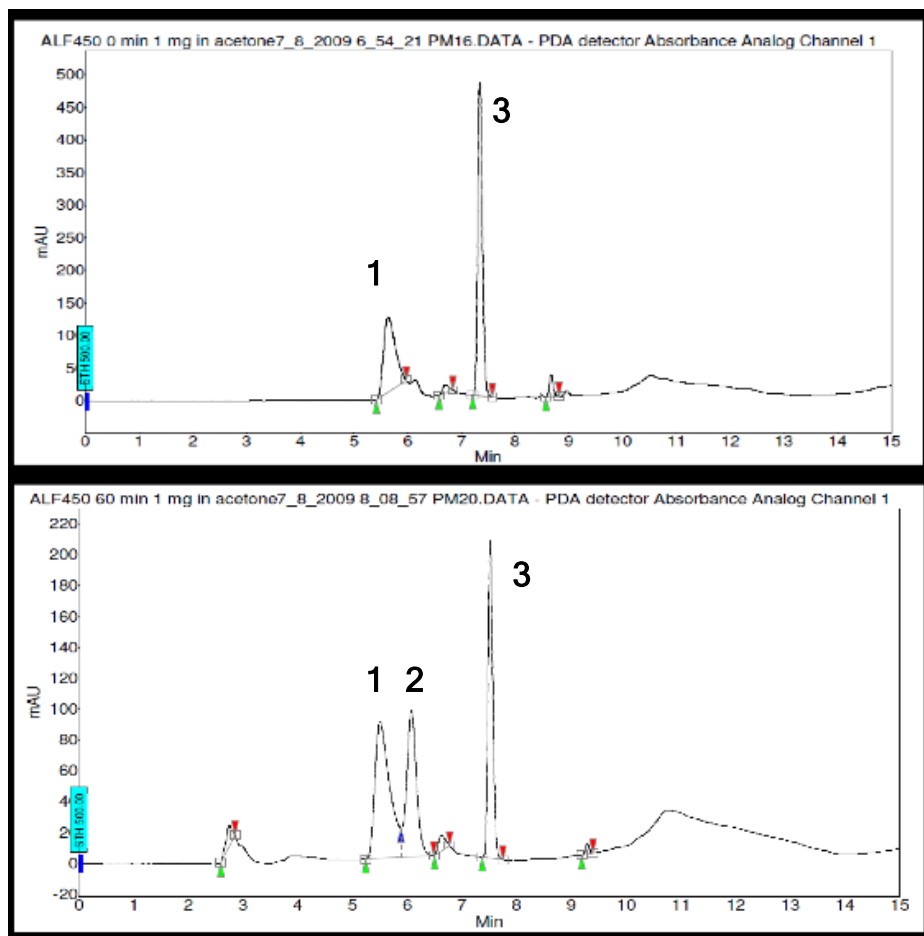


Figure S2. Time evolution of ^{13}C NMR spectrum of *fac*- $\text{RuCl}_2(\text{DMSO})(\text{CO})_3$ (**1**) in d^6 -DMSO, showing the formation of $\text{RuCl}_2(\text{DMSO})_2(\text{CO})_2$ (**2**). Each spectrum was acquired over 29 min, at room temperature, in the carbonyl region at $t=0$; $t=6\text{h}$; $t=19\text{h}$; $t=25\text{h}$; $t=4$ days. At the time of dissolution **1** has 2 resonances at δ 188.3 and δ 184.3 ppm in a 1:2 ratio, corresponding to the tricarbonyl compound and later while 4 new resonances from the dicarbonyl species **2** appeared at δ 193.0 and 187.9 ppm (**2b**; *cis,cis,cis*- $\text{RuCl}_2(\text{DMSO})_2(\text{CO})_2$) and 186.8 ppm (**2a**; *cis,trans,cis*- $\text{RuCl}_2(\text{DMSO})_2(\text{CO})_2$). The resonance at δ 186.5 ppm cannot be clearly assigned to any species. After 19h the tricarbonyl compound **1** was already totally converted into dicarbonyl species **2**. After 4 days in solution only the **2a** and **2b** isomers are present in solution and a new peak at δ 190.5 ppm is observed, from a newly formed species.



ALF420	Peak - AUC (236 nm)		
	1	2	3
time (min)	RT= 2.56	RT= 2.99	RT= 3.47
0	62	741	155
15	23.2	660	-
30	-	750.7	-
45	-	776	-
60	-	776	-

Figure S4: HPLC traces of **CORM-2 (ALF420)**. Initial concentration 1 mg/ml in Me₂CO. Column: Nucleosil C18 5µm 150mmx4,6mm Supelco (Z226173). Elution gradient 10%MeOH/H₂O 1ml/min. Top: Initial chromatogram (t = 0). Bottom: Chromatogram at t = 60 min. Right table: AUC along time for the three earlier peaks.



5	% max		
	1	2	3
time (min)	RT= 5.55	RT= 6.1	RT= 7.5
0	90.1	0.0	100.0
15	115.2	69.3	84.6
30	100.0	91.2	67.6
45	95.1	100.0	56.9
60	86.3	95.1	44.4
75	81.4	89.4	35.4

Figure S5. HPLC traces of (**5**). Initial concentration 1 mg/ml in Me₂CO. Column: Nucleosil C18 5 μ m 150mmx4,6mm Supelco (Z226173). Elution gradient 10%MeOH/H₂O 1mL/min. Top: Initial chromatogram (t = 0). Bottom: Chromatogram at t = 60 min. Right table: relative values of AUC in % of maximum area along time.

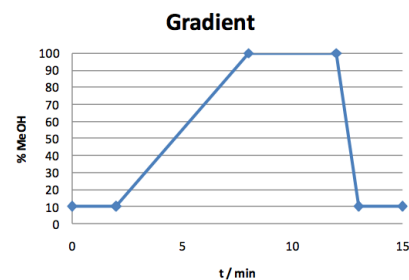
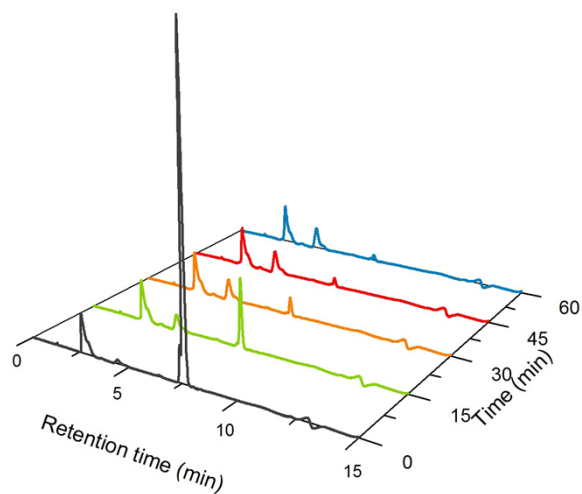
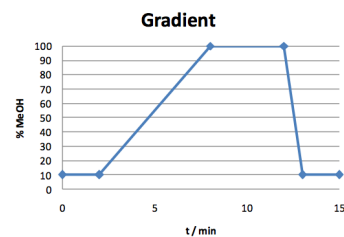
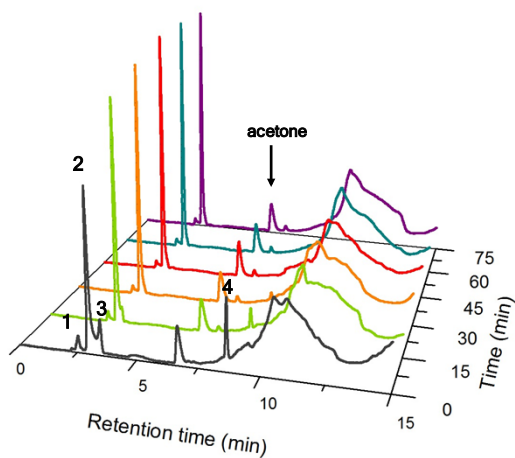


Figure S6. HPLC traces of **4**. Initial concentration: 1 mg/ml in 10%DMSO/H₂O. Column: Nucleosil C18 5 μ m 150mmx4,6mm Supelco (Z226173). Elution gradient 10%MeOH/H₂O 1mL/min.



3	Peak - AUC (236 nm)			
	1	2	3	4
time (min)	RT= 2.58	RT= 2.96	RT= 3.49	RT= 8.79
0	53.2	584.3	133.1	126.5
15	21.4	525.9	0.0	42.2
30	31.2	615.6	0.0	12.9
45	10.8	636.5	0.0	0.0
60	11.8	635.5	0.0	0.0

Figure S7. HPLC traces of **3**. Initial concentration: 1 mg/ml in 10%DMSO/H₂O. Column: Nucleosil C18 5 μ m 150mmx4,6mm Supelco (Z226173). Elution gradient 10%MeOH/H₂O 1mL/min

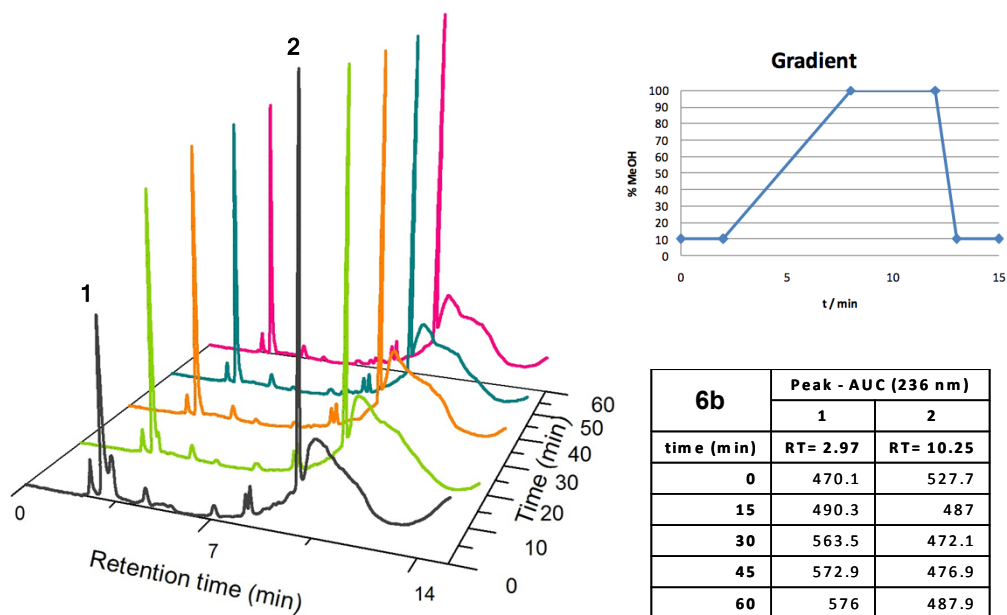


Figure S8. HPLC traces of (**6b**). Initial concentration: 1 mg/ml in 10%DMSO/H₂O. Column: Nucleosil C18 5 μ m 150mmx4,6mm Supelco (Z226173). Elution gradient 10%MeOH/H₂O 1mL/min

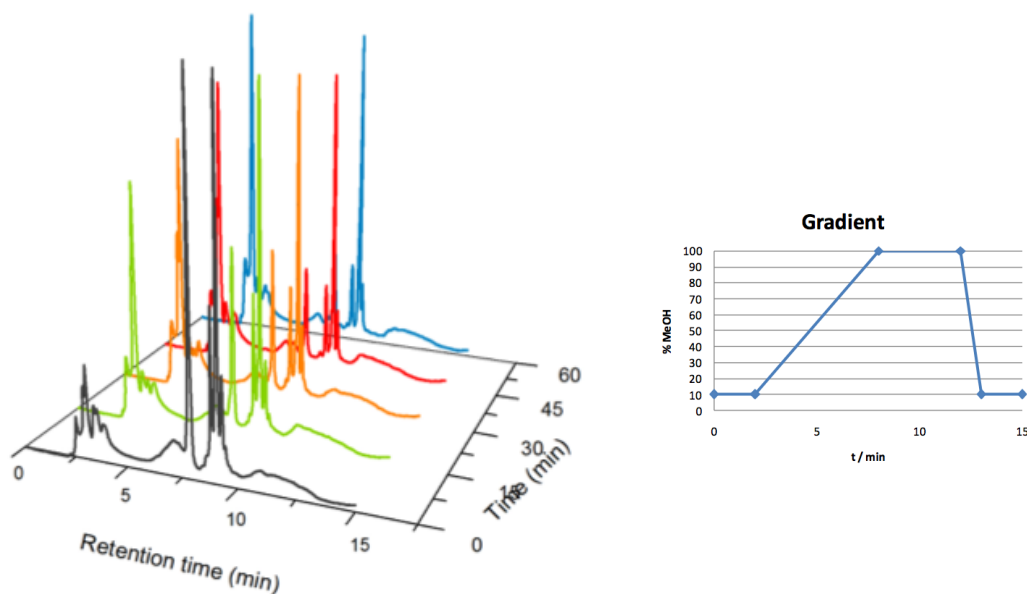
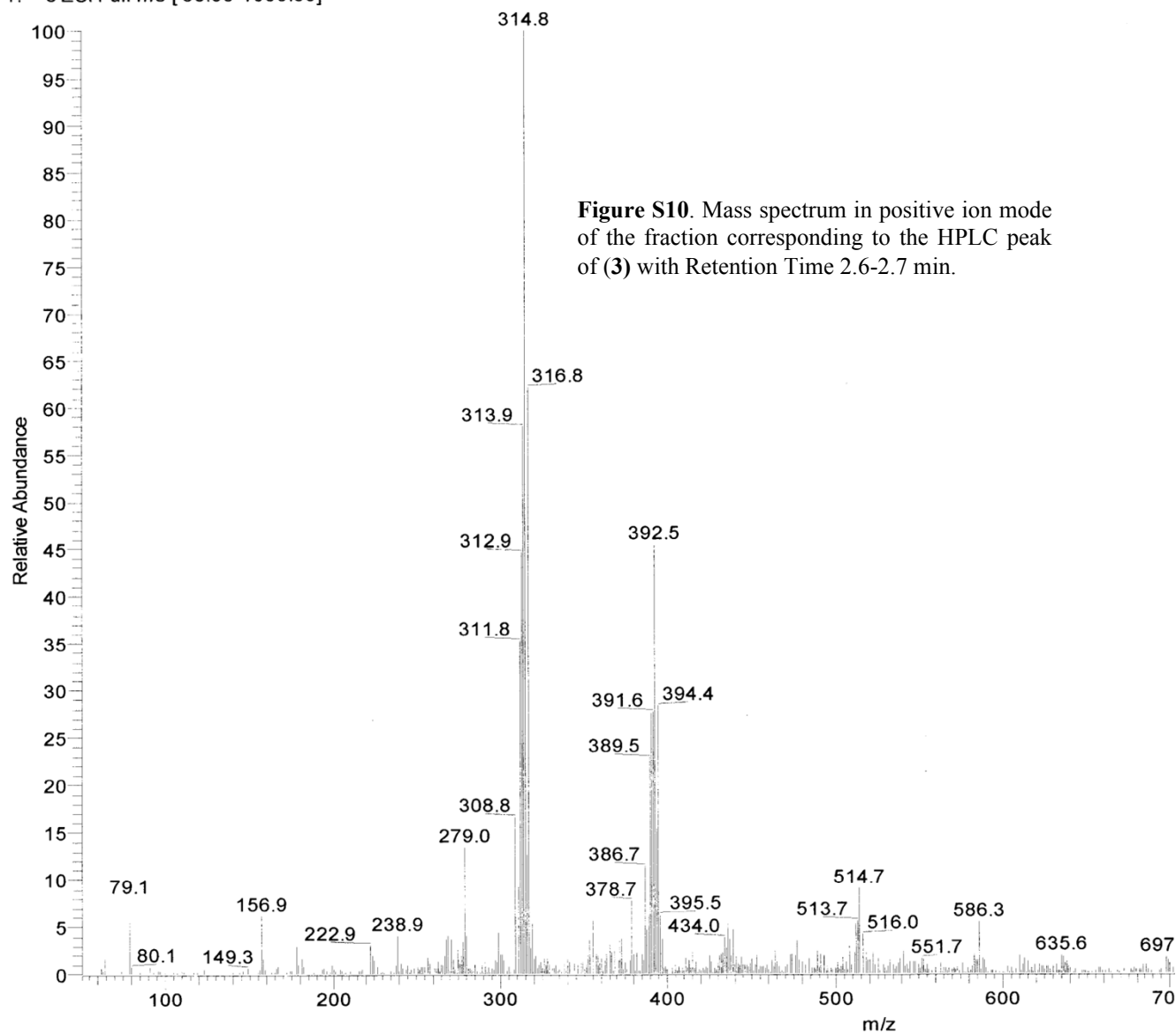


Figure S9. HPLC traces of **10**. Initial concentration: 1 mg/ml in 10%DMSO/H₂O. Column: Nucleosil C18 5 μ m 150mmx4,6mm Supelco (Z226173). Elution gradient 10%MeOH/H₂O 1mL/min

Average Mass Spectrum at RT 2.6 min

A456 #106-110 RT: 2.58-2.68 AV: 5 NL: 2.26E5
T: + c ESI Full ms [50.00-1000.00]



475_131009_POS #118-144 RT: 2.01-2.42 AV: 27 NL: 7.93E6
T: + c ESI Full ms [50.00-1000.00]

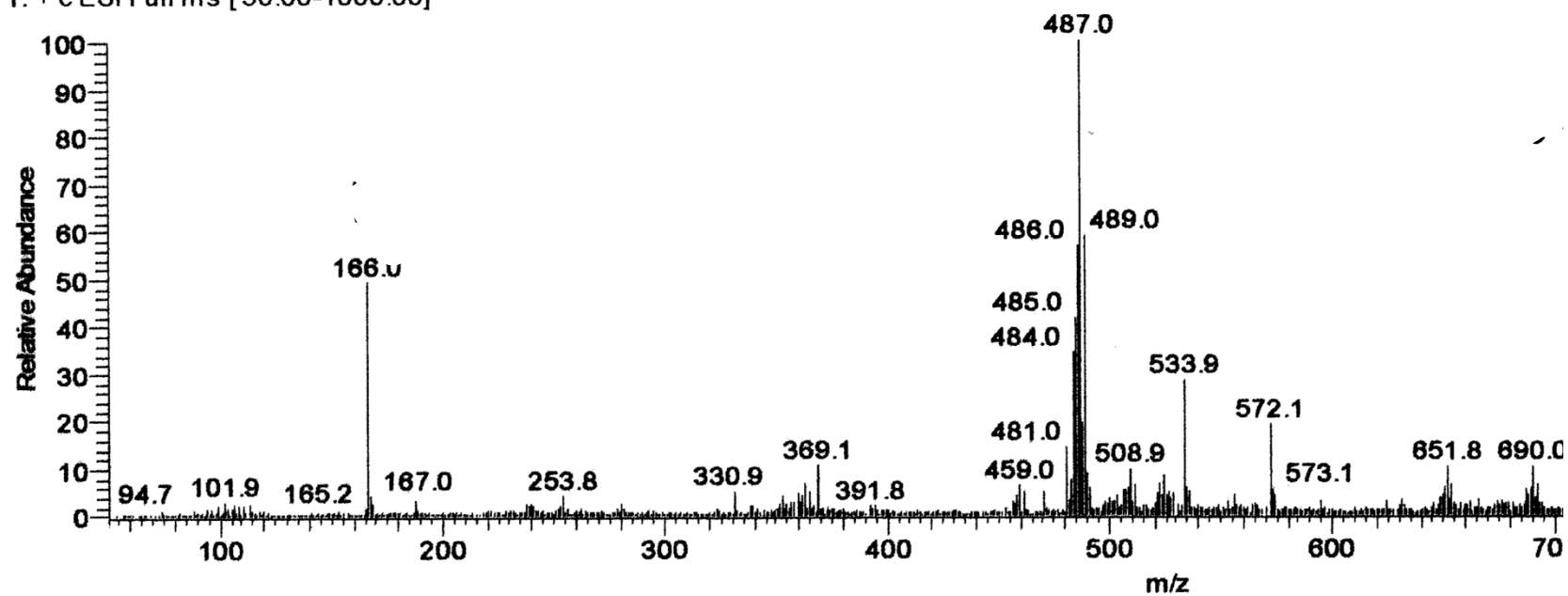


Figure S11. Mass spectrum in positive ion mode of the fraction corresponding to the HPLC peak of **6b** with Retention Time 2.0-2.4 min.

475_131009_NEG #103-117 RT: 2.74-3.09 AV: 15 NL: 2.07E5
T: -c ESI Full ms[50.00-1000.00]

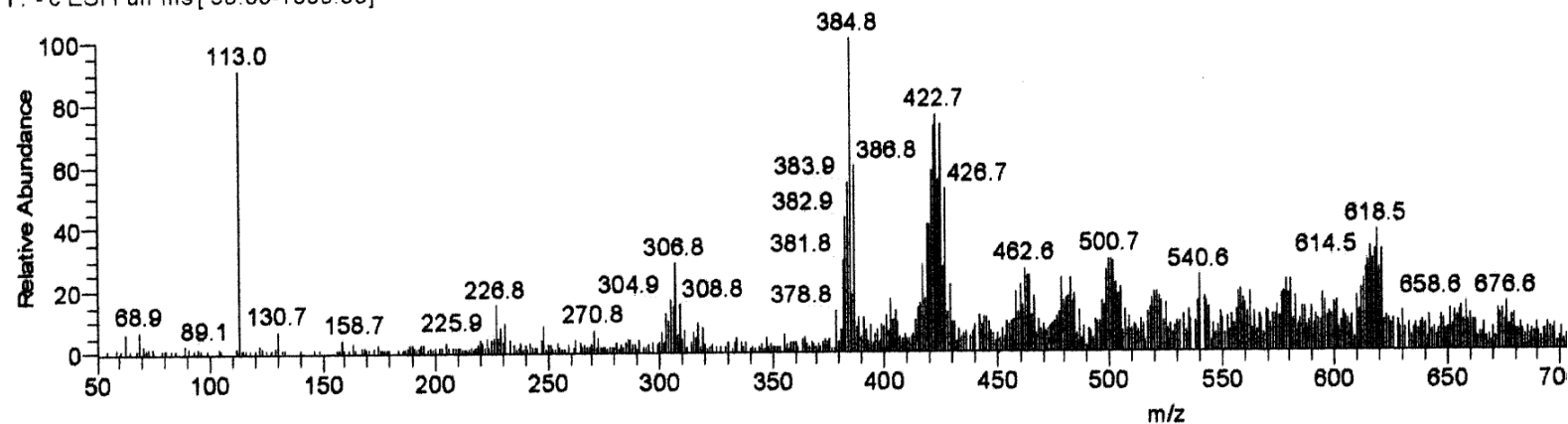


Figure S12. Mass spectrum in negative ion mode of the fraction corresponding to the HPLC peak of **6b** with Retention Time 2.74-3.09 min.

475_131009_NEG #390-432 RT: 9.86-10.89 AV: 43 NL: 4.78E5
T: -c ESI Full ms[50.00-1000.00]

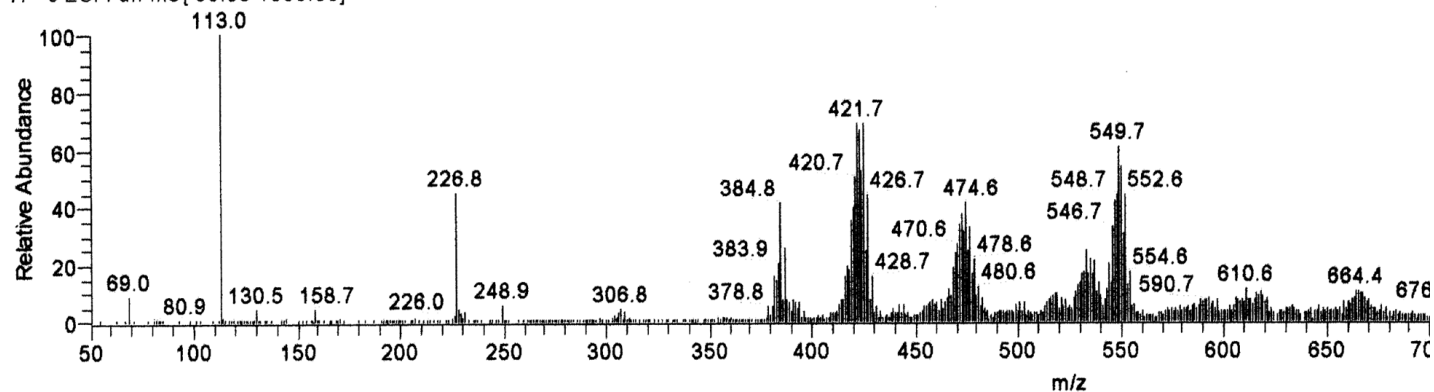


Figure S13. Mass spectrum in negative ion mode of the fraction corresponding to the HPLC peak of **6b** with Retention Time 9.86-10.89 min.

475_131009_NEG #390-432 RT: 9.86-10.89 AV: 43 NL: 4.78E5
T: -c ESI Full ms[50.00-1000.00]

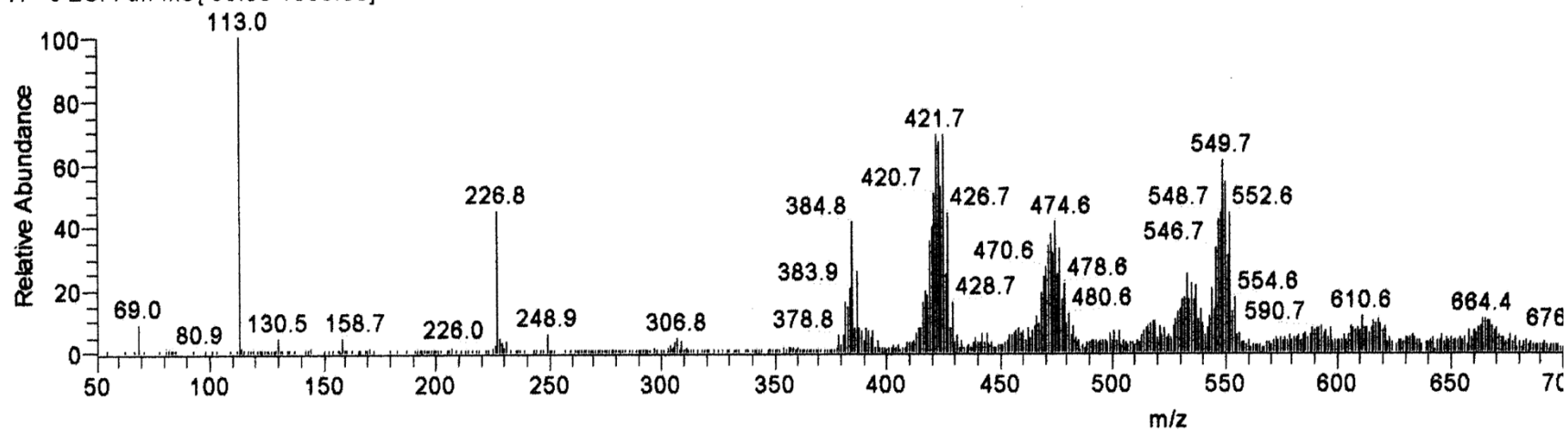


Figure S13. Mass spectrum in negative ion mode of the fraction corresponding to the HPLC peak of **6b** with Retention Time 9.86-10.89 min.

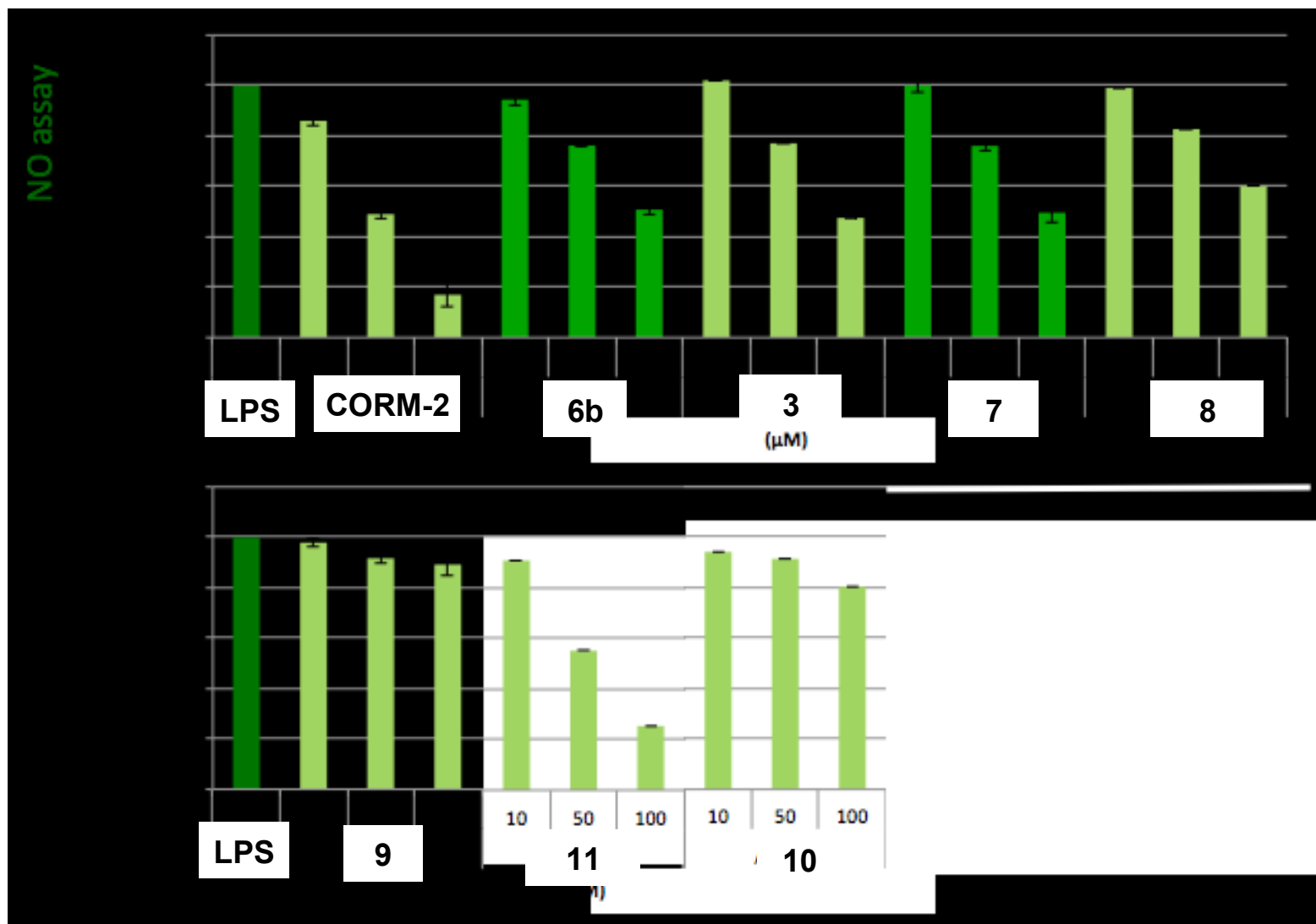


Figure S14. Inhibition of NO induced by LPS in RAW264.7 macrophages upon treatment with different doses of $[\text{Ru}^{\text{II}}\text{CO}_3]$ based CORMs.

Atomic coordinates for all the optimized molecules

fac-[RuCl₂(CO)₃(Me₂SO)]

Ru	0.648492	0.518063	0.318908
Cl	0.893251	1.026616	-2.032926
S	-1.294525	-1.213836	-1.411211
O	0.215181	-0.322975	3.213979
C	0.382109	0.009484	2.134487
H	-2.825198	-1.108387	-3.243250
Cl	1.536466	-1.711158	0.034791
O	-0.622621	3.280631	0.504317
C	-0.139333	2.247425	0.451184
H	-3.454820	-0.241248	-1.791751
O	3.483696	1.494695	0.741689
C	2.406219	1.145143	0.608938
H	-2.143352	0.479986	-2.785924
O	-1.265388	-0.288617	-0.152094
C	-2.577195	-0.447820	-2.408314
H	-2.454401	-3.291052	-1.630235
C	-2.199829	-2.636279	-0.792772
H	-1.519654	-3.153153	-0.113291
H	-3.095301	-2.305618	-0.261927

fac-[RuCl₂(CO)₃(Me₂SO)]

Ru	0.525036	0.654176	0.473499
C	-0.063368	1.675942	1.965974
S	-1.748162	0.180923	-0.216468
Cl	1.320843	-0.686706	-1.374329
O	-0.404614	2.277069	2.876408
H	-1.353733	-2.150391	-0.167816
C	0.597715	2.118989	-0.755850
Cl	0.375044	-1.293810	1.904318
O	0.649963	2.976328	-1.504004
H	-2.871464	-1.712425	-1.071110
C	2.391837	0.769790	0.950407
O	3.494433	0.785305	1.224889
H	-1.243976	-1.468120	-1.812273
C	-1.821035	-1.474464	-0.887677
O	-2.385382	1.155784	-1.144419
H	-2.274952	-0.714006	1.921733
C	-2.777971	-0.024631	1.239156
H	-2.891805	0.960064	1.695896
H	-3.753109	-0.399516	0.920464

A

Ru	-0.464665	-0.099366	-0.456622
C	1.124621	0.680205	-1.103914
O	2.098302	1.218762	-1.370314
H	0.686113	-1.448356	-3.670095
H	0.915613	0.393602	-3.813495
N	0.208435	0.240765	1.524272
O	1.413268	-0.872316	-3.409137
O	0.536332	1.353050	-4.092171
C	0.267384	-1.822553	-0.417393
H	-0.271408	1.138877	-4.570046
N	0.649841	-0.075581	3.633992
O	0.702827	-2.881152	-0.380158
H	1.126225	2.185558	1.368844
C	0.893186	1.339937	1.998212
C	0.079869	-0.599969	2.538536
C	1.177251	1.156940	3.323870
C	1.888747	2.007585	4.308336
H	-0.410412	-1.560779	2.511677
C	-1.222510	-0.370251	-2.178598
H	0.681456	-0.521662	4.541677
H	2.779611	1.502807	4.696564
Cl	-2.513137	-1.052577	0.459265
H	1.247051	2.255350	5.160101
H	2.202444	2.938364	3.831776
Cl	-1.452289	2.122706	-0.449169

O	-1.785953	-0.552449	-3.155609
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TS_{AB}

Ru	-0.481702	-0.071022	-0.469631
C	1.096211	0.734875	-1.121288
O	2.053894	1.311605	-1.367021
H	0.731773	-1.490004	-3.386593
H	0.940442	0.344333	-3.780964
N	0.211418	0.244549	1.508823
O	1.474171	-0.885503	-3.278452
O	0.553162	1.274605	-4.121289
C	0.271392	-1.784870	-0.479136
H	-0.238361	1.021701	-4.607260
N	0.664715	-0.093349	3.612944
O	0.716241	-2.840300	-0.460598
H	1.120968	2.194957	1.371565
C	0.894341	1.341013	1.991825
C	0.090910	-0.607475	2.514517
C	1.186276	1.144401	3.313793
C	1.900029	1.987148	4.303497
H	-0.396643	-1.569350	2.480013
C	-1.263263	-0.321224	-2.180924
H	0.703234	-0.550236	4.514999
H	2.791477	1.479051	4.686002
Cl	-2.512567	-1.057626	0.453477
H	1.260135	2.228777	5.158404
H	2.213215	2.921416	3.833442
Cl	-1.487908	2.143338	-0.413974
O	-1.830359	-0.496813	-3.157270

B

Ru	-0.510104	-0.204911	-0.543795
C	1.274658	0.266764	-1.375639
O	2.046155	1.123076	-0.979006
H	1.074979	-1.105045	-2.723597
H	0.995191	0.841404	-3.929288
N	0.318590	0.145933	1.402967
O	1.717907	-0.420930	-2.492765
O	0.420773	1.462977	-4.398724
C	-0.068383	-1.983608	-0.438806
H	-0.351350	0.925031	-4.607568
N	0.802713	-0.155571	3.511925
O	0.184558	-3.109543	-0.365714
H	1.042232	2.164101	1.269314
C	0.894397	1.297582	1.893465
C	0.276639	-0.712666	2.408828
C	1.205342	1.126782	3.215223
C	1.827532	2.031920	4.212318
H	-0.122279	-1.715033	2.380231
C	-1.381969	-0.429392	-2.163588
H	0.889167	-0.611902	4.410312
H	2.751091	1.606407	4.619121
Cl	-2.690371	-0.748547	0.637721
H	1.152601	2.225165	5.052978
H	2.070474	2.987090	3.742290
Cl	-1.171014	2.156369	-0.681818
O	-1.986327	-0.559451	-3.137486

C

Ru	-2.816482	-0.482983	-1.789564
H	-5.091682	-0.540802	1.235448
N	-2.234002	-0.070159	0.195190
O	-5.256261	0.243741	1.771241
O	-6.838445	1.264748	0.134881
C	-1.818306	-2.072357	-1.760281
H	-6.181049	0.848105	0.861676
H	-6.225907	1.453567	-0.585929
N	-1.753268	-0.316214	2.304166
O	-1.219621	-3.046264	-1.745517

H	-1.799225	2.038306	0.085099
C	-1.829922	1.149115	0.696391
C	-2.183457	-0.935368	1.195850
C	-1.529413	1.011514	2.023783
C	-1.373780	0.542814	-2.422545
C	-1.060747	1.987017	3.037276
H	-2.438041	-1.983240	1.152238
O	-0.502549	1.171580	-2.813057
C	-3.466102	-0.824590	-3.544241
H	-1.641290	-0.757144	3.207858
H	-0.108817	1.673512	3.478202
Cl	-4.691985	-1.806934	-0.986832
H	-1.785609	2.096373	3.850776
H	-0.918576	2.963997	2.571239
Cl	-4.112251	1.580417	-1.827979
O	-3.882511	-1.026850	-4.586764

TS_{CD}

Ru	-3.029676	-0.489815	-1.464483
H	-5.073983	-0.304220	0.952710
N	-2.203073	-0.105246	0.428789
O	-5.365667	0.598295	1.124244
O	-6.851548	0.764595	-0.908587
C	-1.881996	-1.889840	-1.709692
H	-6.277465	0.699672	-0.032721
H	-6.243131	1.254401	-1.479936
N	-1.572017	-0.371977	2.492879
O	-1.152491	-2.758632	-1.862973
H	-1.697491	1.989107	0.283328
C	-1.714260	1.098869	0.894751
C	-2.103022	-0.976030	1.422664
C	-1.314270	0.946328	2.193300
C	-1.830370	0.742892	-2.249586
C	-0.723017	1.897364	3.164227
H	-2.400309	-2.012912	1.396388
O	-1.021166	1.389178	-2.733856
C	-3.930587	-0.789244	-3.128485
H	-1.390782	-0.824002	3.380000
H	0.254936	1.549533	3.512781
Cl	-4.473684	-2.256897	-0.512299
H	-1.366320	2.019914	4.041545
H	-0.593272	2.873140	2.692425
Cl	-4.202300	2.112657	-2.246389
O	-4.484339	-0.987227	-4.104419

D

Ru	0.155316	-0.559467	-1.404198
H	-1.920437	-0.527162	0.926037
N	1.036567	-0.202665	0.465551
O	-2.259911	0.363678	1.067806
O	-3.603722	0.461329	-1.064809
C	1.369391	-1.858594	-1.792877
H	-3.076438	0.420600	-0.157620
H	-3.008672	1.018255	-1.587430
N	1.750411	0.855158	2.226761
O	2.134144	-2.674978	-2.039884
H	1.529021	-2.188766	1.144816
C	1.536442	-1.129915	1.355712
C	1.180966	0.991215	1.022396
C	1.992923	-0.478345	2.468055
C	1.246852	0.787689	-2.175979
C	2.635813	-0.974607	3.708088
H	0.886688	1.936250	0.590556
O	2.040717	1.468536	-2.640295
C	-0.789311	-0.856701	-3.043675
H	1.972851	1.620439	2.850859
H	2.069858	-0.676861	4.596587
Cl	-1.141091	-2.403607	-0.437294
H	3.652295	-0.580580	3.811900
H	2.691309	-2.064569	3.683363

Cl	-1.050376	2.141339	-2.139373
O	-1.362808	-1.055870	-4.007949

TS_{DE}

Ru	0.143747	-0.560492	-1.387631
H	-1.913513	-0.534669	0.909941
N	1.040457	-0.208424	0.476558
O	-2.245776	0.361430	1.034499
O	-3.588754	0.444917	-1.102624
C	1.373555	-1.836396	-1.796120
H	-3.063864	0.408812	-0.195663
H	-2.996686	1.008339	-1.622305
N	1.780670	0.848968	2.227495
O	2.148022	-2.641674	-2.049662
H	1.500378	-2.197947	1.167061
C	1.527136	-1.138171	1.371557
C	1.209747	0.986712	1.024288
C	1.999102	-0.486946	2.477788
C	1.212141	0.806670	-2.161823
C	2.636752	-0.984325	3.720088
H	0.930052	1.934345	0.588257
O	2.006821	1.486439	-2.627015
C	-0.804614	-0.862034	-3.024812
H	2.019449	1.614658	2.845056
H	2.077605	-0.670399	4.607364
Cl	-1.129603	-2.414180	-0.417689
H	3.659473	-0.605431	3.818682
H	2.674660	-2.075162	3.703997
Cl	-1.066657	2.174720	-2.153751
O	-1.375503	-1.066961	-3.989434

E

Ru	-0.157536	-0.623517	-0.914498
H	-2.051132	-0.151848	0.572513
N	0.961164	-0.314074	0.857309
O	-1.607988	0.497328	0.009384
O	-3.427096	0.926999	-1.905803
C	1.221364	-1.711051	-1.619188
H	-2.780071	0.807489	-1.167847
H	-2.874645	1.285807	-2.632681
N	1.828539	0.670841	2.595592
O	2.048727	-2.393119	-2.021696
H	1.811675	-2.260269	1.222869
C	1.720668	-1.234627	1.547618
C	1.048663	0.830342	1.515864
C	2.271043	-0.631538	2.645586
C	0.598170	0.940917	-1.630910
C	3.149736	-1.150395	3.721352
H	0.577542	1.762446	1.244259
O	1.121426	1.888952	-2.000158
C	-1.224367	-1.016735	-2.442155
H	2.052464	1.399227	3.261299
H	2.674729	-1.055181	4.703423
Cl	-1.156291	-2.571624	0.133017
H	4.098883	-0.605528	3.756717
H	3.365044	-2.205951	3.544835
Cl	-1.618374	2.063207	-4.188887
O	-1.811537	-1.394301	-3.346712

F

Ru	-0.267858	-0.609937	-1.714232
N	0.522374	-0.197190	0.130984
C	0.756626	-2.158637	-1.853596
N	1.401725	-0.389158	2.112508
O	1.371883	-3.114412	-1.930962
H	0.475387	1.968754	0.110826
C	0.716919	1.068969	0.654309
H	-1.398709	2.013613	-1.765347
C	0.959271	-1.063499	1.043700

C	1.268773	0.963747	1.903510
H	-2.355125	1.030514	-1.015687
C	1.117422	0.334325	-2.539638
C	1.680986	1.988584	2.894751
H	0.988232	-2.139600	0.953289
O	1.957637	0.921614	-3.033886
O	-1.422367	-1.021780	-3.482702
H	1.793462	-0.816497	2.942992
H	2.749144	1.911315	3.120885
O	-1.987949	-1.522351	-0.773449
H	1.125015	1.882407	3.831570
H	1.492919	2.988850	2.502328
O	-1.633678	1.082535	-1.658895
H	-1.940522	-0.274162	-3.815636
H	-1.051986	-1.479822	-4.250361
H	-2.517849	-2.135373	-1.303849
H	-1.966232	-1.857808	0.132991

G

Ru	-0.286937	-0.648547	-1.459124
N	0.469593	-0.214714	0.448925
C	0.907106	-2.061126	-1.692677
N	1.114053	-0.386157	2.522555
O	1.647714	-2.918088	-1.809964
H	0.931006	1.897773	0.244825
C	0.916921	1.025624	0.883577
H	-2.131636	1.476460	-1.675862
C	0.606236	-1.048629	1.474812
C	1.325397	0.931737	2.188705
H	-1.499474	1.494095	-0.249890
O	1.074340	0.800873	-2.167634
C	1.882952	1.933819	3.131003
H	0.349242	-2.097517	1.484763
H	1.215362	0.912327	-3.118947
C	-1.040828	-0.959984	-3.199558
H	1.315509	-0.799597	3.424989
H	2.886887	1.649379	3.461940
O	-1.712368	-1.857308	-0.486748
H	1.250664	2.039920	4.018140
H	1.952371	2.909374	2.647788
O	-1.715610	0.922407	-1.000916
O	-1.493941	-1.140313	-4.226387
H	1.948076	0.797343	-1.749030
H	-2.002912	-2.691230	-0.883505
H	-2.508824	-1.359824	-0.244079

H

Ru	-0.478624	-0.717496	-1.702599
N	0.317609	-0.300525	0.136914
O	0.753117	-2.429214	-1.896864
N	1.076836	-0.503746	2.166191
H	0.635325	-2.946230	-2.707123
H	0.654094	1.833595	-0.025642
C	0.717801	0.946168	0.586970
H	-1.958683	1.243903	-0.573150
C	0.548951	-1.161718	1.124168
C	1.199320	0.832317	1.865412
H	-2.458959	1.155359	-2.050009
C	0.889467	0.445062	-2.524306
C	1.759420	1.834445	2.806143
H	0.350235	-2.223459	1.110860
O	1.674637	1.113970	-2.994714
O	-1.248658	-1.247874	-3.683737
H	1.341795	-0.931715	3.044785
H	2.790803	1.588882	3.078218
C	-1.829010	-1.852831	-0.838356
H	1.168456	1.889482	3.725857
H	1.759963	2.823388	2.345811
O	-1.697034	1.007460	-1.474030
H	-1.017785	-0.760045	-4.484960

H	-2.118901	-1.640501	-3.830600
O	-2.606188	-2.499375	-0.323525
H	1.703813	-2.339701	-1.745115

I

Ru	0.080213	-0.451599	-1.768551
N	0.876074	-0.056755	0.071868
C	1.185269	-1.888774	-2.010021
N	1.672877	-0.215900	2.094191
O	1.882539	-2.787800	-2.153394
H	1.025231	2.103232	-0.058173
C	1.167501	1.215335	0.540998
H	-1.719694	1.591706	-2.268659
C	1.201251	-0.903111	1.043125
C	1.668583	1.129543	1.814312
H	-1.243844	1.852421	-0.807891
O	1.474463	0.950988	-2.500714
C	2.134146	2.165494	2.770156
H	1.128825	-1.979987	1.008179
H	2.315500	0.991166	-2.022591
O	-0.986190	-0.627362	-3.639154
H	1.996069	-0.632086	2.958758
H	1.683890	0.992853	-3.443838
H	3.180259	2.005657	3.049681
O	-1.558807	-1.595431	-1.083823
H	1.533515	2.159924	3.685269
H	2.053912	3.156515	2.321248
O	-1.361940	1.165978	-1.477120
H	-1.737032	-1.237078	-3.583527
H	-0.547463	-0.813570	-4.480164
H	-2.185214	-1.095895	-0.539548
H	-1.453932	-2.470564	-0.687416

J

Ru	-0.429605	-0.628425	-1.476326
N	0.366626	-0.252554	0.447442
O	1.195477	-1.951899	-1.772875
N	0.882154	-0.439018	2.560139
H	1.165914	-2.664602	-2.425487
H	1.259133	1.695929	0.163876
C	1.040057	0.890281	0.848305
H	-2.438782	1.238978	-1.606245
C	0.287267	-1.038518	1.518662
C	1.371041	0.788493	2.174243
H	-1.666195	1.378732	-0.254680
O	0.926403	0.833981	-2.178876
C	2.091089	1.705822	3.092916
H	-0.194389	-2.004001	1.565293
H	0.709352	1.328210	-2.981454
C	-1.148593	-0.948053	-3.185308
H	0.955212	-0.830231	3.490851
H	1.818104	0.476297	-2.308412
H	3.002949	1.242577	3.482956
O	-1.698932	-2.036587	-0.528286
H	1.464971	1.991321	3.944151
H	2.377098	2.616853	2.565417
O	-1.937839	0.749611	-0.939339
O	-1.587395	-1.143160	-4.223738
H	1.599784	-2.303634	-0.967255
H	-1.973895	-2.822793	-1.020284
H	-2.511006	-1.621812	-0.198386