Supporting Information for

Mononuclear and dinuclear gold(I) complexes with a caffeine-based di(*N*-heterocyclic carbene) ligand: synthesis, reactivity and structural DFT analysis

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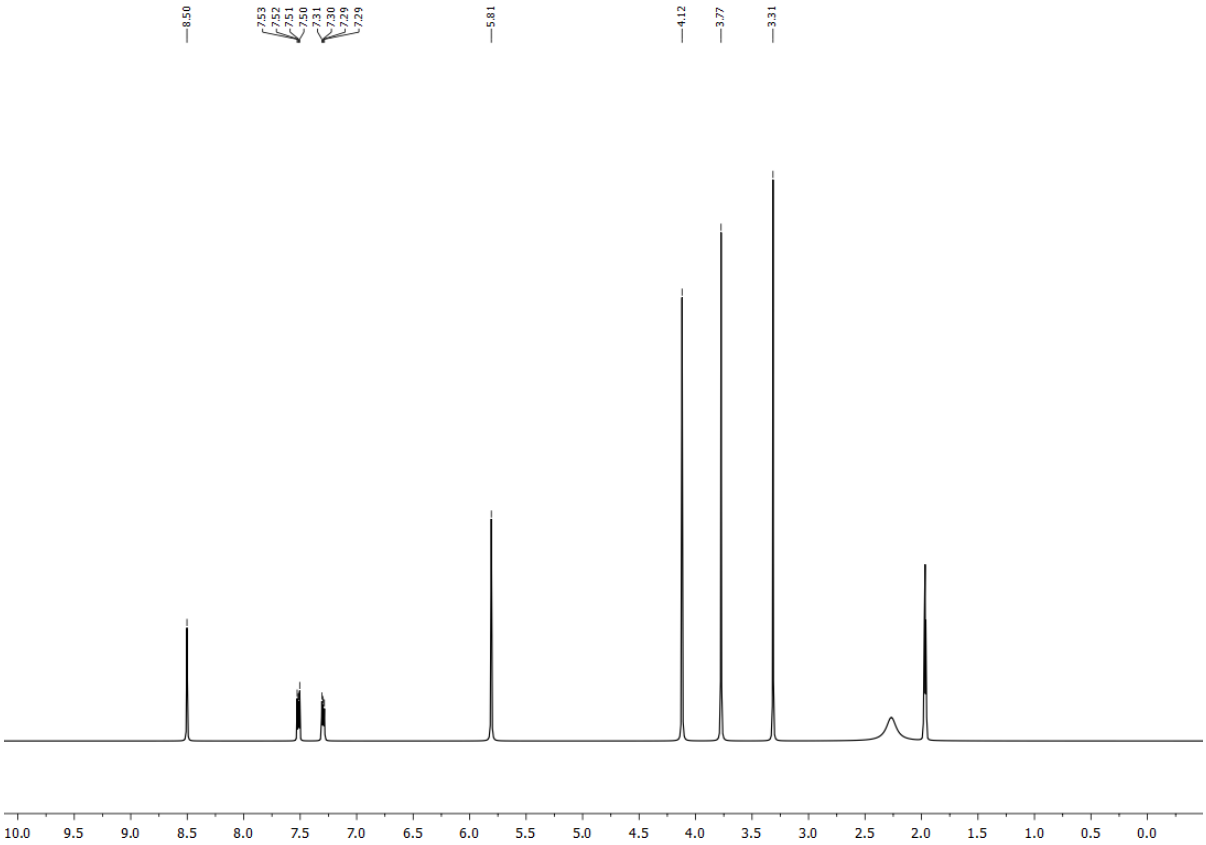

Figure S1. ^{1}H NMR spectrum of **1·2HBF$_4$** in CD_3CN.

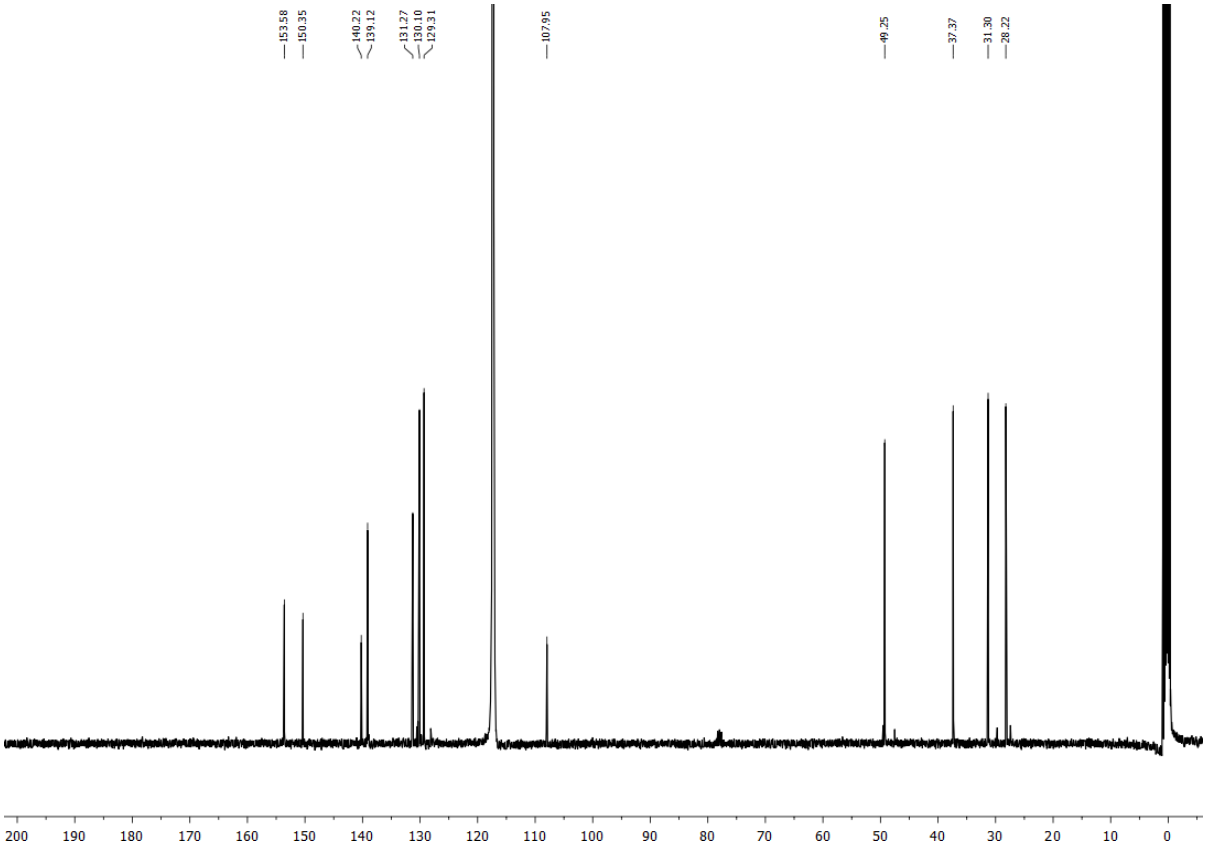

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **1·2HBF$_4$** in CD_3CN.

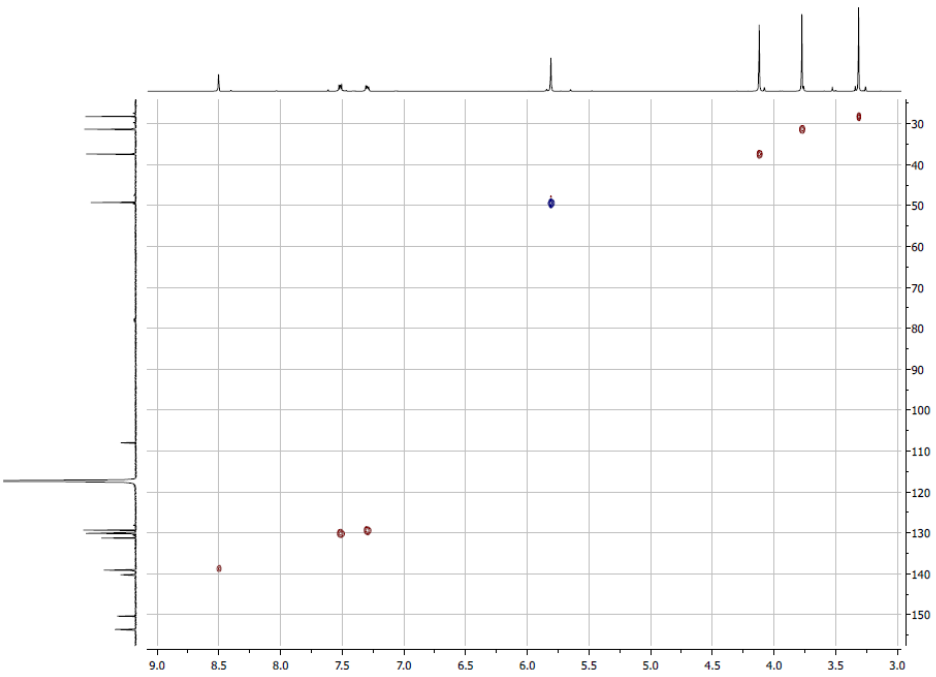

Figure S3. $^{13}C,^{1}H$-HSQC spectrum of **1·2HBF$_4$** in CD_3CN.

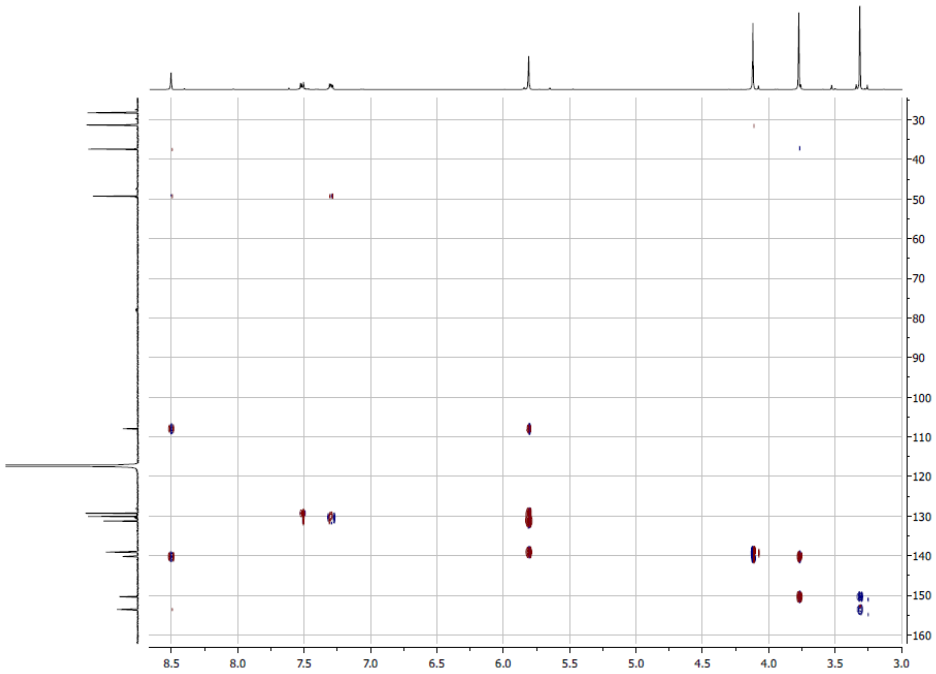

Figure S4. $^{13}C,^{1}H$-HMBC spectrum of **1·2HBF$_4$** in CD_3CN.

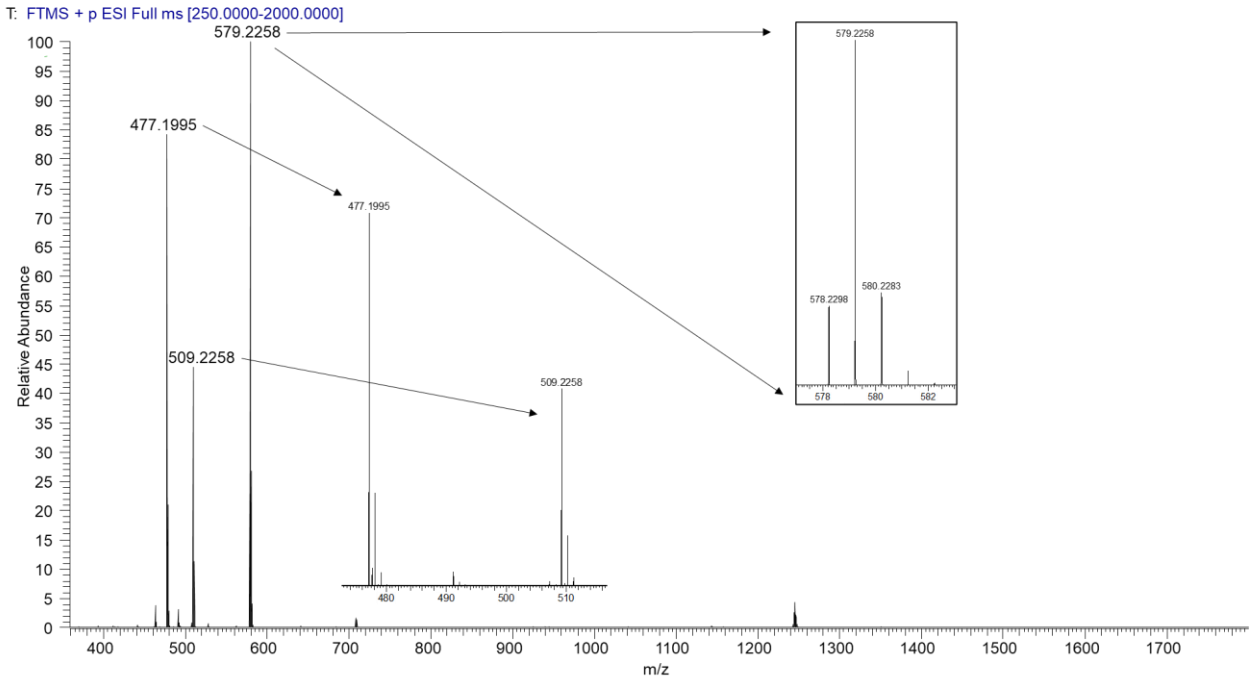

Figure S5. HRMS of **1·2HBF$_4$** (in CH_3CN).

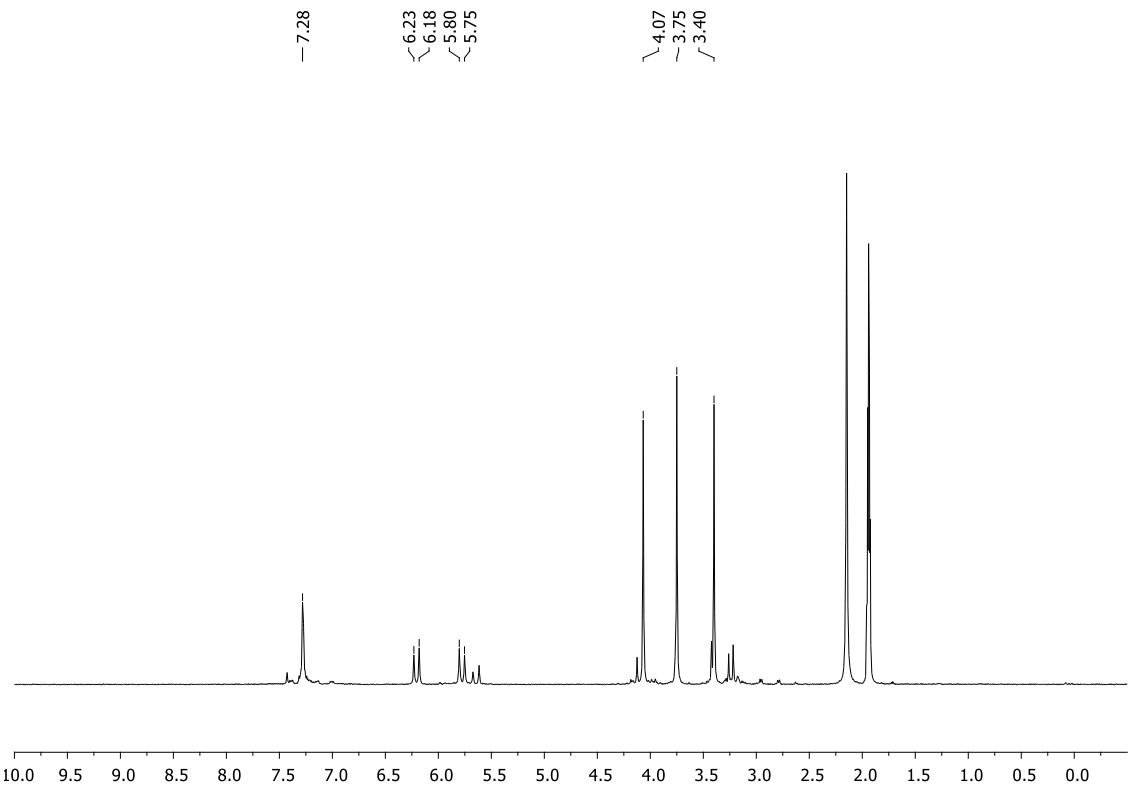

Figure S6. ^{1}H NMR spectrum of complex **2** in CD_3CN.

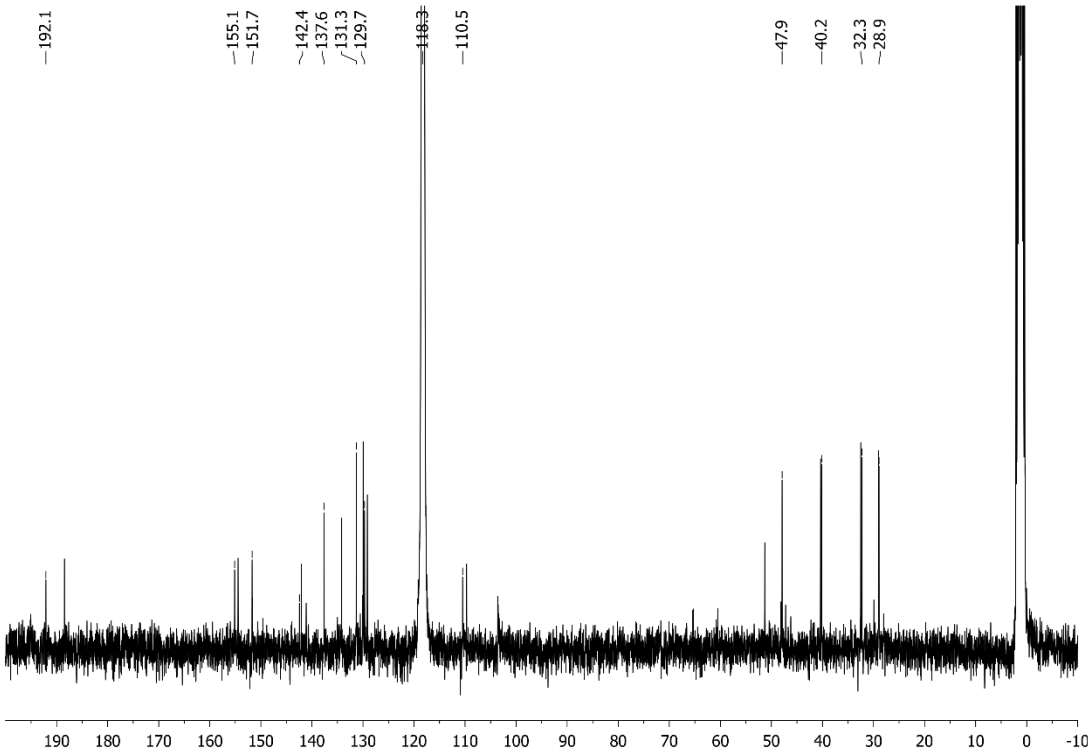

Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of complex **2** in CD_3CN. The spectrum was registered overnight so that also signals of complex **3** are present.

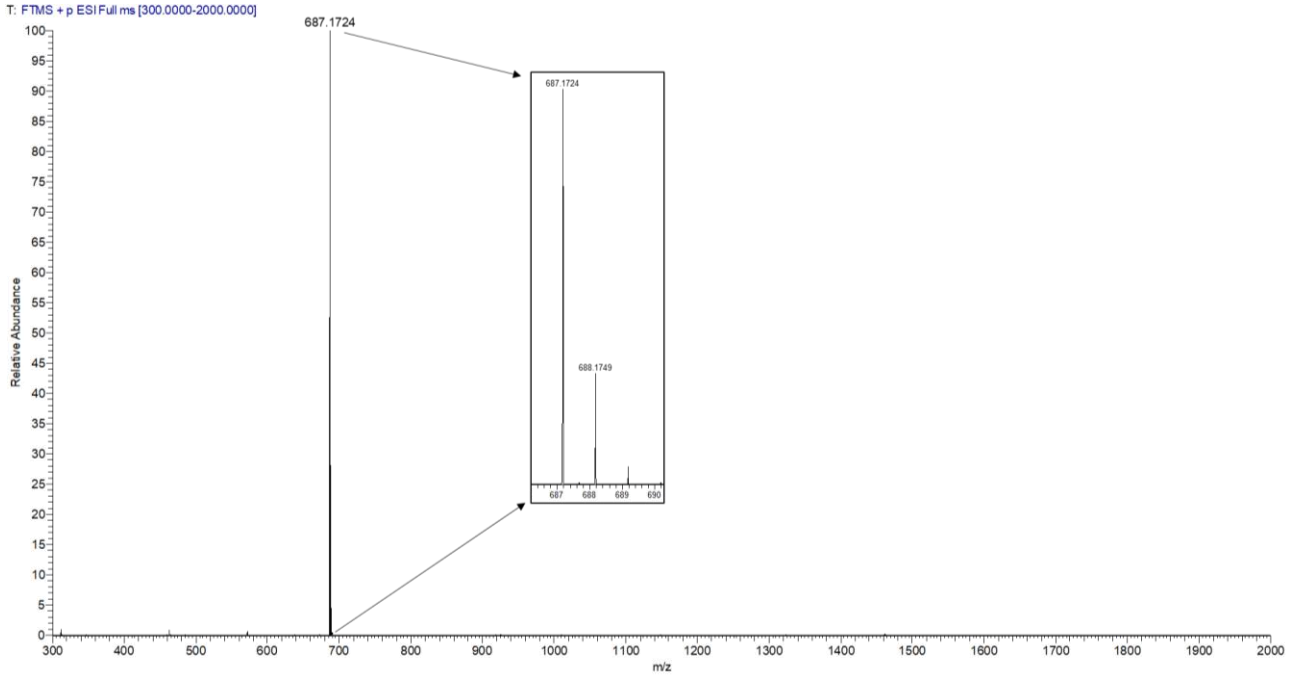

Figure S8. HRMS of complex **2** (in CH_3CN).

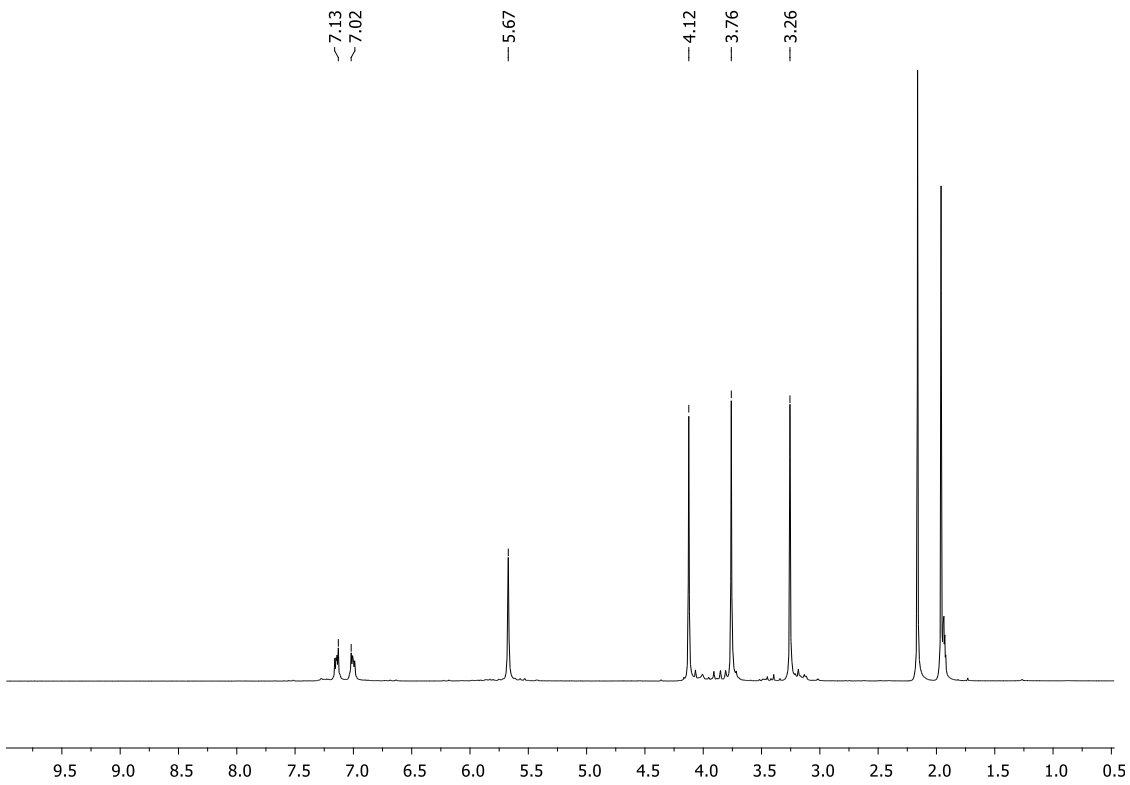

Figure S9. ^{1}H NMR spectrum of complex **3** in CD_3CN.

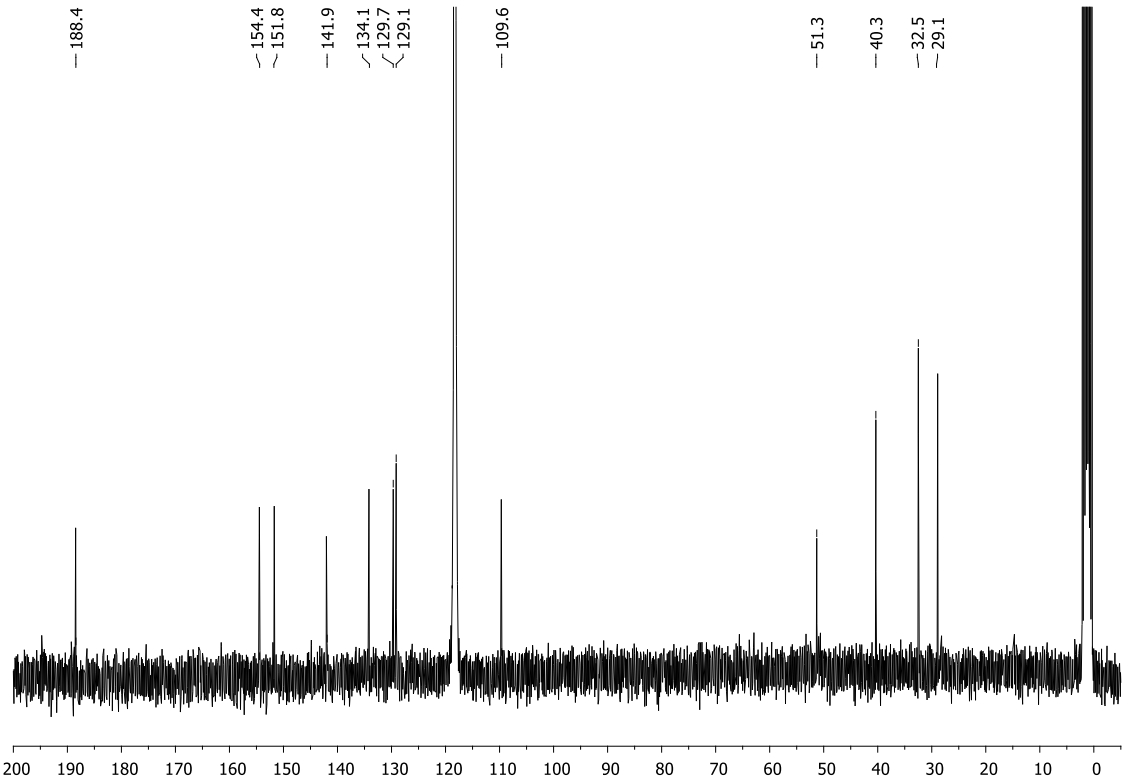

Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of complex **3** in CD_3CN.

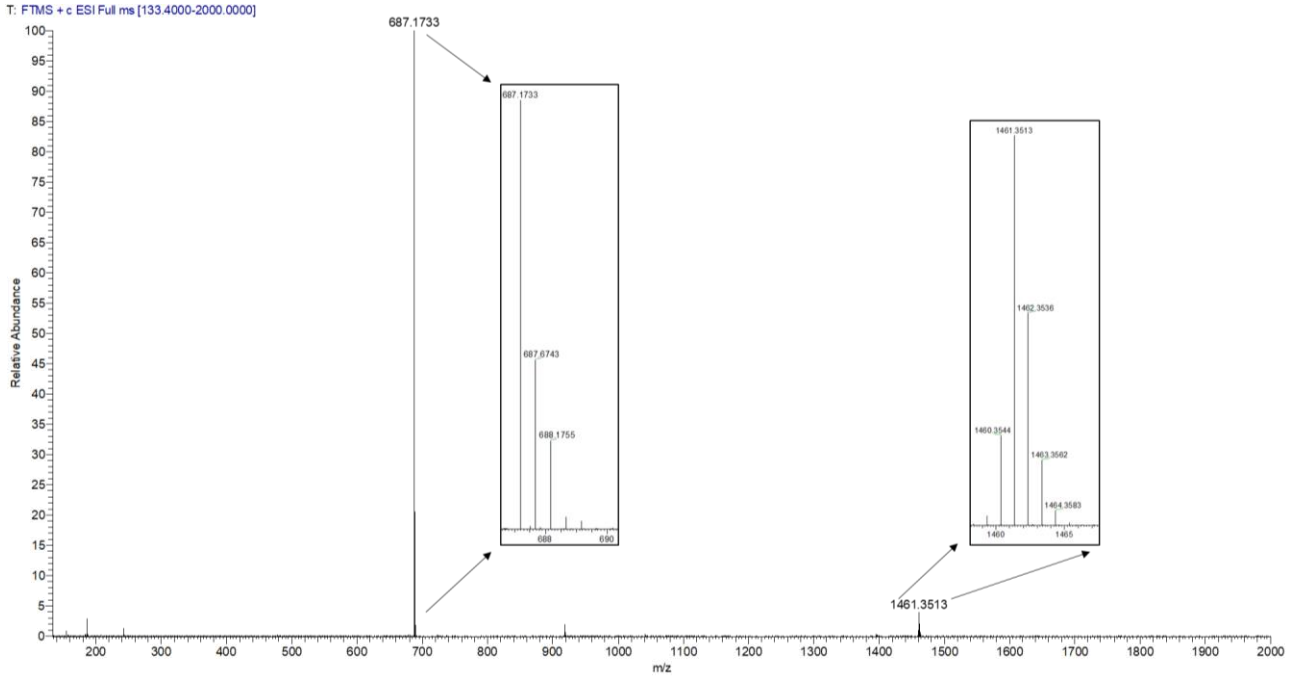

Figure S11. HRMS of complex **3** (in CH_3CN).

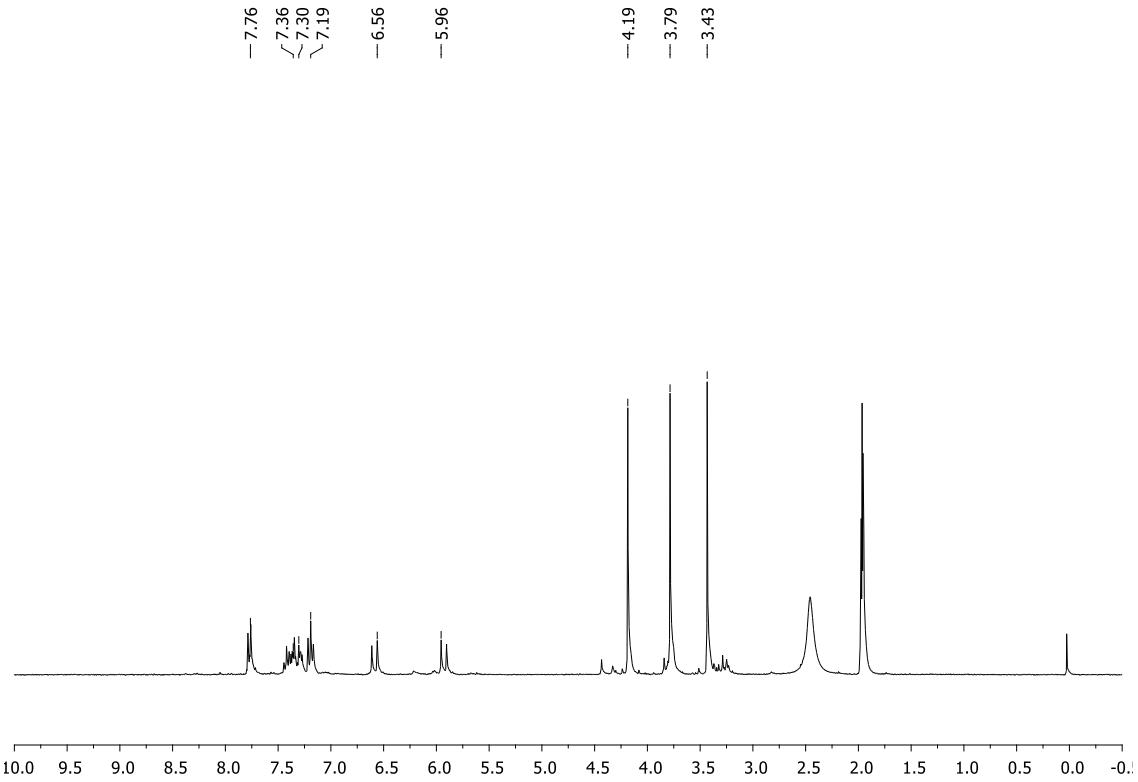

Figure S12. ^{1}H NMR spectrum of complex **4** in CD_3CN.

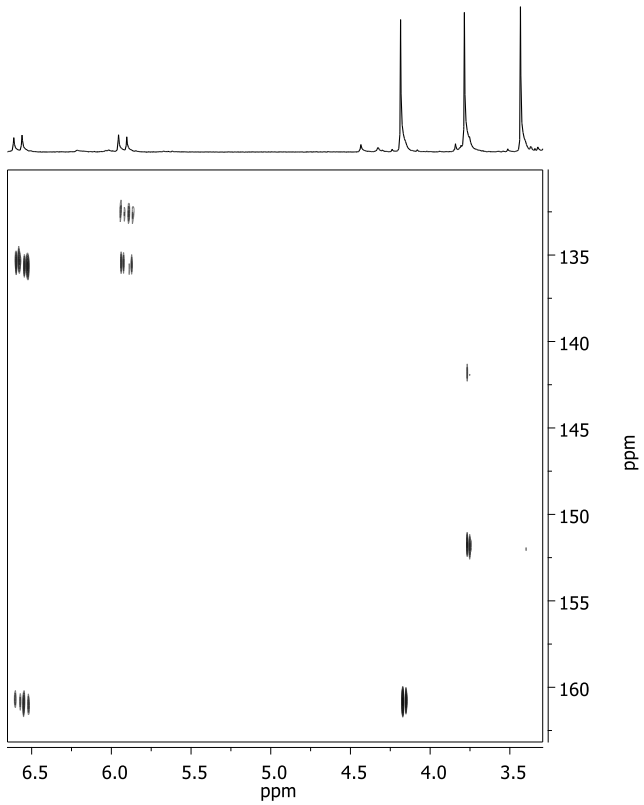

Figure S13. ^{13}C,^{1}H-HMBC spectrum of **4** in CD_3CN (detail on CH_3 and CH_2 signals).

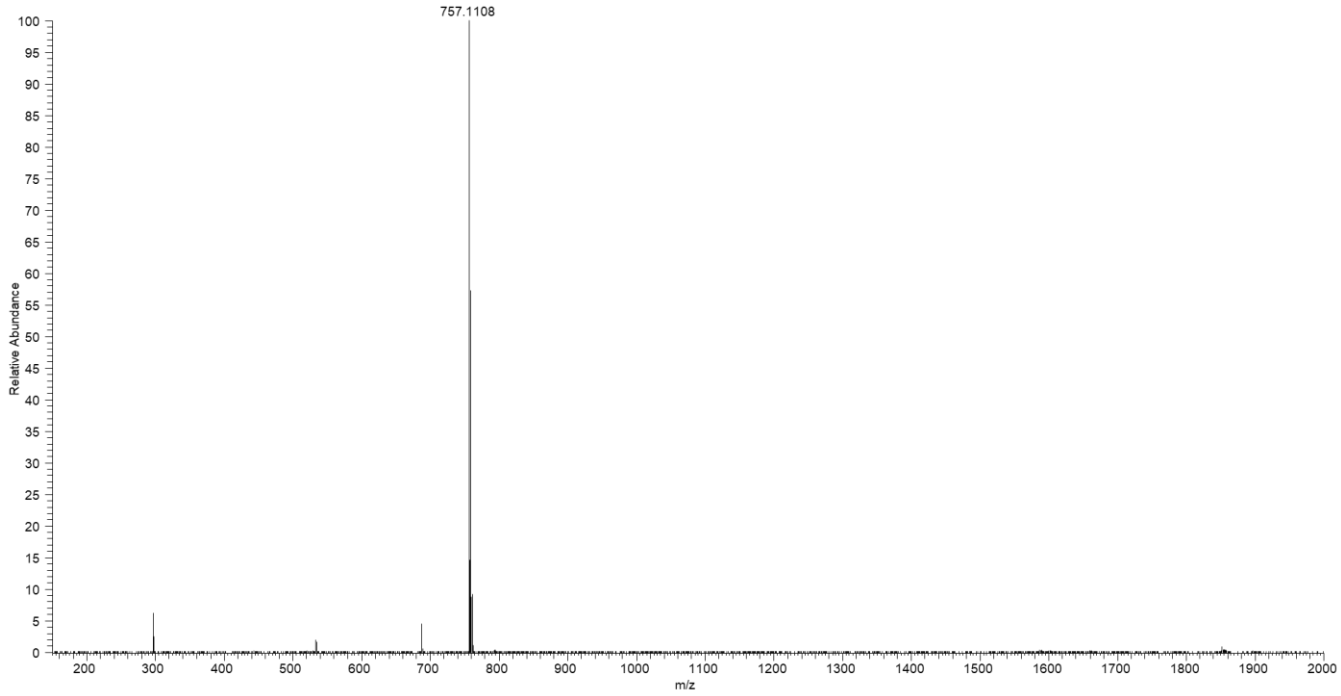

Figure S14. HRMS of complex **4** (in CH_3CN).

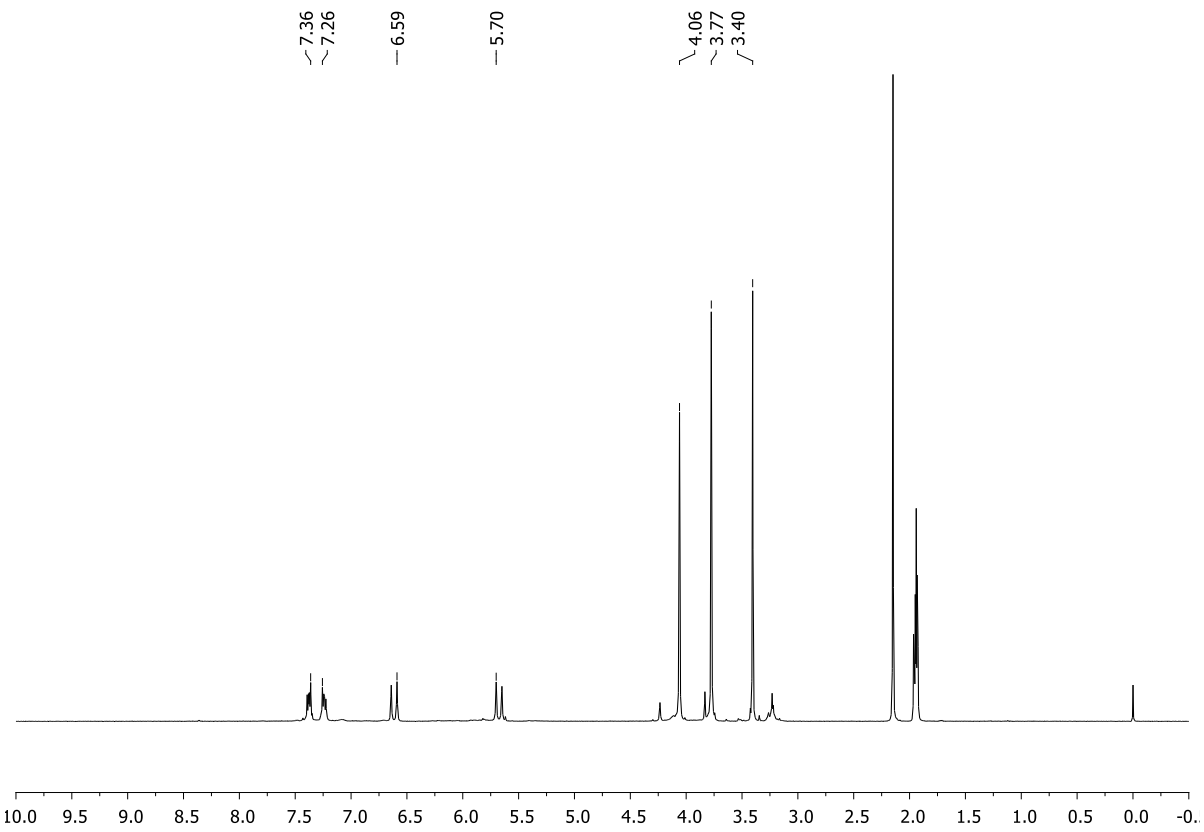

Figure S15. ^{1}H NMR spectrum of complex **5** in CD_3CN.

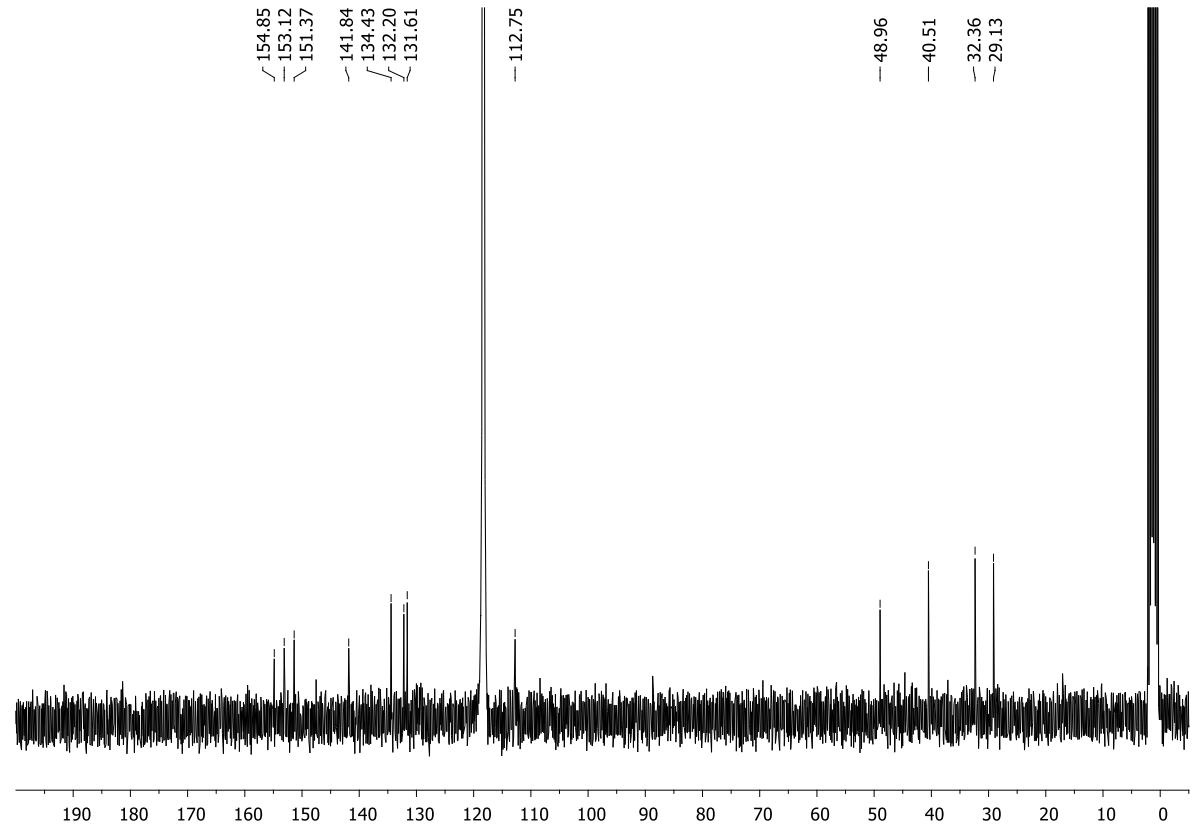

Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum of complex **5** in CD_3CN.

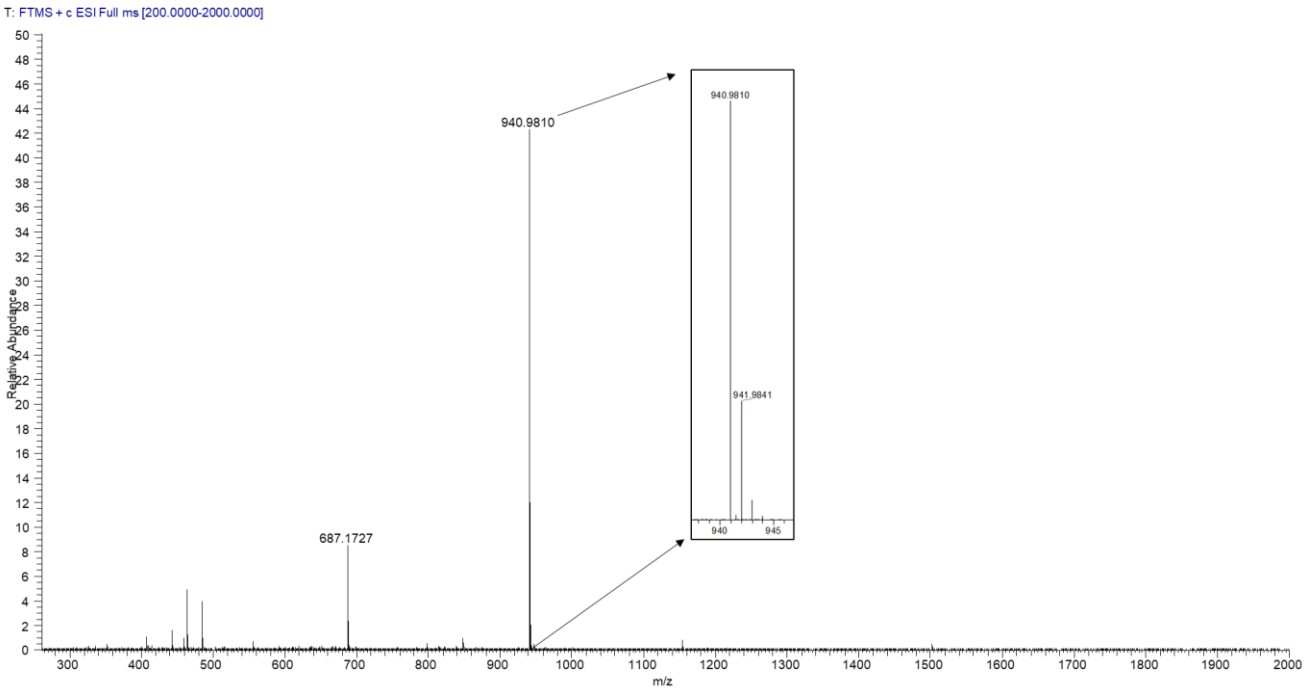

Figure S17. HRMS of complex **5** (in CH_3CN).

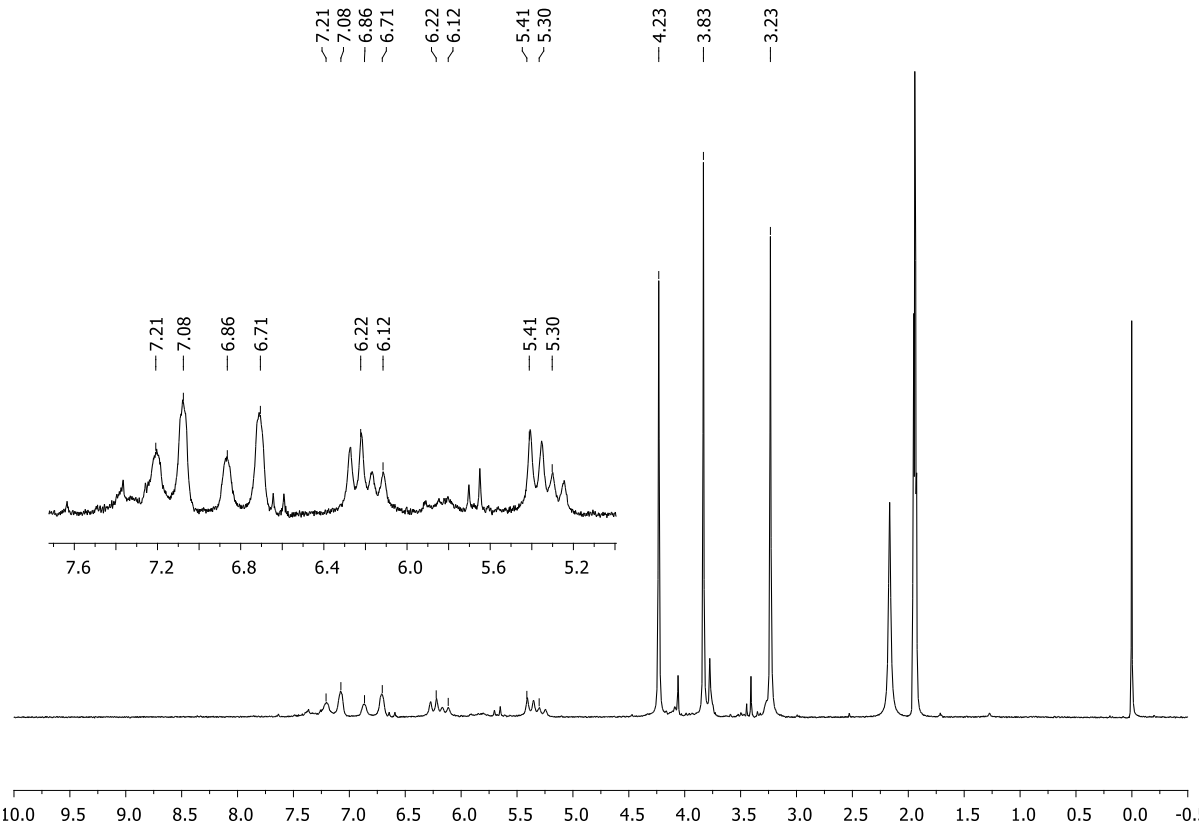

Figure S18. ^{1}H NMR spectrum of complex **7** in CD_3CN.

Coordinates of fully optimized molecular structures; level of theory: (COSMO)-ZORA-BLYP-D3(BJ)/TZ2P

2 (gas-phase)

Au	1.979851	21.503547	12.745023
H	1.526232	25.306405	10.652850
C	1.763846	19.487578	12.989882
C	2.124161	17.535017	14.061733
C	3.570960	25.081691	14.217179
C	1.126050	17.316105	13.131085
C	1.105723	24.775761	11.508856
C	-0.042125	18.840794	11.395253
H	0.104375	19.891626	11.143334
H	-1.068704	18.690614	11.735088
N	2.098305	24.671168	12.593646
C	2.524751	23.444597	13.069965
H	0.203966	25.280724	11.860778
C	2.738581	25.690666	13.297194
H	0.856292	23.756019	11.213790
C	1.501327	20.775114	17.723026
C	1.763406	22.149146	17.752843
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C	2.620952	22.705382	16.807917
C	2.952969	20.532647	15.774171
C	3.217599	21.921473	15.804154
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O	5.124639	25.322165	16.003987

3-*anti closed* (gas-phase)

Au	1.48682679	1.84287671	3.20385388
Au	1.77892133	4.95953383	3.42941953
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H	6.35191146	4.99686297	10.21086075
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H	2.34512969	5.50161471	-2.48038800
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N	1.76397178	5.52085298	6.40829116
N	2.11102722	5.72553996	8.88368700
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C	3.08209479	5.56679506	9.93435260

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H	3.10397281	0.87179768	1.46505496	C	5.41117271	2.62521294	1.91792079
H	2.96802631	-0.23779254	0.08011634	C	5.79908723	3.64327761	1.04705540
H	3.58534748	1.42752599	-0.15008878	C	5.78759669	4.96815320	1.48795980
C	2.77581162	4.66774712	0.16242163	C	5.42697910	5.24239463	2.80612106
H	3.22062655	5.57282308	-0.25601839	H	5.46886588	6.26691232	3.16857047

H	6.09130423	5.77544319	0.82690045
H	6.12513542	3.40144964	0.03830833
H	5.44623802	1.59320027	1.57807602

3-*anti open* (gas-phase)

Au	1.61002700	2.07039500	3.33325300
Au	1.62172500	5.32771100	3.29644500
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H	6.65767700	3.80189800	9.48593000
C	5.07067800	4.43362000	7.67737500
O	6.01434000	3.73607700	7.33331700
C	4.00984100	4.94273200	6.81951700
C	2.91840400	5.61877700	7.34941300
N	1.41056400	2.16798700	0.23008100
C	0.78920100	1.93155200	1.44949600
N	-0.45038800	1.47921700	1.15669700
C	-1.71664400	0.80865900	-0.97767200
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N	-1.52114500	0.96113500	-2.37905800
H	-3.35560600	0.01375700	-2.66080000
C	-0.41378900	1.54062900	-3.00982300
O	-0.35565400	1.69141400	-4.21816900
N	0.68294800	1.94132600	-2.16844600
H	1.68176500	2.41504500	-3.91676800
C	0.53513200	1.84516800	-0.80939500
C	-0.62702900	1.39043500	-0.22457600
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H	-1.01568200	1.32820900	3.13230500
H	-1.83957000	0.19157600	2.04719400
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C	-3.97515300	1.53773600	1.89268000
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C	-5.14566600	2.29449100	1.82757600
H	-6.10434600	1.79676600	1.70893900
C	-5.07796600	3.68589600	1.91315800
H	-5.98278400	4.28599500	1.86754800
C	-3.83668800	4.30186600	2.05953100
H	-3.78016500	5.38660700	2.12818200
C	-1.37581300	4.30952700	2.34482400
H	-1.61339400	5.23840900	2.86913200
H	-0.68274100	3.74064000	2.96960700
N	-0.51246800	4.75099800	1.16909300
C	0.69084400	5.29950200	1.46099700
N	1.21332100	5.78130700	0.27653100
N	0.45087300	5.80962200	-2.09515600
H	1.29106500	6.74059300	-3.74012600
C	-0.58761900	5.39687400	-2.99406500
O	-0.52423700	5.64554300	-4.18355800
N	-1.65233200	4.68597600	-2.42843200
H	-3.43894300	3.69106700	-2.84377500
C	-1.84130400	4.35139600	-1.05530100
O	-2.78736400	3.66647800	-0.69295600
C	-0.77552600	4.87444700	-0.21197000
C	0.31818900	5.53215900	-0.75991500
C	7.07399600	4.29577600	4.56978900
H	7.02612600	5.37914800	4.47692900
C	4.61384600	4.31617900	4.27796100
H	4.86027400	5.23163700	3.73446200
H	3.91852600	3.73916500	3.66322900
N	3.74984800	4.78957000	5.44083900
C	2.55053200	5.33815400	5.13319900
N	2.02774700	5.84997400	6.30491600
N	2.78360100	5.92686200	8.67763500
H	1.93959700	6.89198600	10.30064300
C	3.81743200	5.52913500	9.58859800

O	3.75219100	5.80507800	10.77197700	H	2.92341500	6.45469200	1.23504700
N	1.80438700	2.24342900	6.43246400	H	3.20368900	5.94724100	-0.44818300
C	2.42765700	1.97374600	5.22094200	C	0.40489500	2.68968900	6.50770400
N	3.66376800	1.52158600	5.52817400	H	0.31981900	3.57914900	7.13107300
C	4.92000200	0.89552100	7.68214800	H	0.09313800	2.93219900	5.49107600
O	5.87900000	0.29084200	7.22151800	H	-0.23417200	1.89654600	6.90374800
N	4.72161900	1.08395600	9.07888000	C	0.72795900	6.54812000	6.33923300
H	6.55654300	0.14619700	9.38822400	H	0.85697500	7.58933000	6.63775300
C	3.61516300	1.68345600	9.69213600	H	0.32564700	6.51379000	5.32586800
O	3.55362600	1.86239900	10.89645400	H	0.03655500	6.04802100	7.01960300
N	2.52341700	2.07005500	8.83782700	C	5.91425900	4.38556200	10.02434000
H	1.52029900	2.58656800	10.57142500	H	6.36780400	5.27513100	10.46747200
C	2.67498600	1.94094200	7.48197000	H	5.44130600	3.79810700	10.81390800
C	3.83627400	1.46563300	6.91172200	C	1.70939800	6.77514000	9.24206100
C	4.73071000	1.23820900	4.53098700	H	1.70361300	7.75691400	8.76320900
H	4.23246200	1.31932200	3.55825300	H	0.73453500	6.29270200	9.14134600
H	5.04499900	0.20250400	4.67199700	C	5.76853400	0.57969900	10.00108400
C	5.88333600	3.55576300	4.53264100	H	6.15403900	1.40448600	10.60268900
C	5.94209300	2.14859100	4.63332900	H	5.33764000	-0.17257100	10.66595200
C	7.19068000	1.53515200	4.79807000	C	1.33573900	2.64406500	9.49893700
H	7.23821800	0.45605200	4.90597300	H	1.21084700	3.69389900	9.21865900
C	8.36695100	2.28398600	4.84867300	H	0.44001000	2.07015900	9.25175400
H	9.32149200	1.78158900	4.98022600	C	-2.69199400	4.25499100	-3.39814900
C	8.31014600	3.67367500	4.73251900	H	-3.13918800	5.13669600	-3.86283500
H	9.21947500	4.26767100	4.76692100	H	-2.22555700	3.64375200	-4.17344800
C	2.81239100	2.60406400	0.14018900	C	1.52542000	6.64340800	-2.68048500
H	3.12934300	2.86660300	1.15022300	H	1.53619500	7.63411900	-2.22049200
H	3.44526400	1.79866500	-0.24080800	H	2.49922800	6.15993900	-2.57470000
H	2.90044300	3.47929800	-0.50266600	C	-2.57361000	0.44069600	-3.28583700
C	2.51829000	6.46852300	0.22232600	H	-2.96695600	1.25558400	-3.89601900
H	2.39645600	7.50343400	-0.10007600	H	-2.14507300	-0.31928600	-3.94326200

C	1.86998400	2.49673600	-2.84648500
H	1.99850200	3.55240300	-2.59083200
H	2.76497400	1.92619900	-2.58908400

3-*syn* (gas-phase)

Au	9.86058800	0.45872200	19.23866800
Au	9.33013400	3.14390300	21.07516500
O	12.94710000	-3.67116600	22.39738200
C	12.98826800	-1.56217300	21.30076200
C	13.75363400	-0.57523300	20.71694000
C	13.20292100	1.37420000	19.11774400
H	12.25411700	1.81643500	18.81018500
H	13.75489400	1.04541500	18.23370300
C	9.01614400	1.50472800	16.09771900
H	8.85294700	0.82770800	15.25835000
H	9.91156100	1.19383500	16.63762700
N	7.89667000	1.42947000	17.05524400
C	8.08199300	1.01596100	18.36020800
N	6.86528200	1.03274000	18.95593800
C	4.45776900	1.72225500	18.17633200
O	3.78923100	1.60564900	19.19308900
N	3.87771900	2.19524200	16.96132100
H	2.04955900	2.31222200	17.96169700
C	4.52225100	2.42017500	15.74046400
O	3.93441800	2.81959800	14.75213300
N	5.93424300	2.16872000	15.70909100
H	6.96497300	1.31819700	14.05394300
C	6.54841100	1.70094100	16.84188400
C	5.88327700	1.45751200	18.03658300
C	6.78155200	0.49614600	20.37879400
H	7.60072400	1.00650400	20.89042800
H	7.04754300	-0.55961600	20.28774400
C	5.18990800	1.71268300	21.97788400
C	5.50749300	0.60340700	21.16402200
C	4.65742200	-0.51140800	21.15977100
H	4.91526600	-1.37060800	20.54359000
C	3.49130400	-0.53595900	21.92203600
H	2.84268900	-1.40750900	21.89878000
C	3.17039800	0.56484300	22.71768500
H	2.26523700	0.56350200	23.31904800
C	4.01598800	1.67461800	22.74133900
H	3.75313200	2.53414500	23.34961300
C	6.07269900	2.94016100	22.11916800
H	5.60181500	3.64637200	22.80541200
H	7.06676400	2.69143000	22.50742800
N	6.33539600	3.66778600	20.84543200
C	7.54903400	3.77621200	20.25890000
N	7.33524300	4.41728800	19.04612700
N	5.28890400	5.29692300	17.87538400
H	6.31454800	4.92049900	16.05438300
C	3.86097300	5.43964200	17.98502500
O	3.21707500	5.89221400	17.05415000
N	3.28100300	5.04135000	19.19793100
H	1.65200900	6.08728500	20.05854500
C	3.95311000	4.48985800	20.32111300
H	8.23561000	4.39626300	17.13265100
C	5.35231500	4.25129100	20.04559300
C	5.97607200	4.70704800	18.90423200
C	8.44223100	4.75697100	18.14003800
H	8.60997400	5.83659500	18.11878500
H	9.33201200	4.25828800	18.52728300
H	15.90985200	0.60763700	19.26680700
C	15.75500800	-1.47294600	21.72678800
O	16.94659800	-1.39369200	21.96998400
N	14.95809900	-2.51505200	22.21691900
H	16.20540900	-3.10862600	23.81694600

C	13.55827400	-2.68020500	22.02079400	H	10.62562900	-3.12372900	21.16080200
C	12.46421200	4.47158100	21.35732400	H	9.63261000	-1.67813100	20.89362300
H	13.23061100	4.39252900	20.58387500	N	11.66202300	-1.31909300	20.93865900
H	12.73608300	5.24666400	22.07474200	C	11.58250300	-0.24238800	20.12452400
N	12.26855500	3.17640100	22.03555800	N	12.87970000	0.23259200	19.98602400
C	11.05168500	2.52286900	22.01970700	N	15.10854600	-0.48871200	20.90066000
N	11.20288200	1.38973900	22.74698200	H	11.51024200	4.73111100	20.89640400
C	13.22241400	0.27352500	23.99283900	H	13.78776300	2.11528900	19.66240600
O	12.75772500	-0.78432900	24.39131200	H	9.14835500	2.52562100	15.73427000
N	14.59385600	0.60577100	24.20865300	O	3.38049800	4.28084000	21.38213900
H	16.31741600	-0.59296000	24.43768800	C	1.82250300	5.25934200	19.36485500
C	15.26960500	1.75486200	23.78539100	H	1.40101700	5.49292300	18.39014500
O	16.44585000	1.95161200	24.03046900	H	1.38297100	4.35234400	19.78326600
N	14.50553300	2.69975700	23.02393400	C	5.90502400	5.76369700	16.61745500
H	15.22404600	4.13538700	21.61978400	H	5.10769100	6.22036200	16.03210500
C	13.18105300	2.43887900	22.78375800	H	6.67992800	6.50591000	16.82065300
C	12.52243400	1.30341100	23.23743500	C	2.41518500	2.46057000	16.94834900
C	9.95835300	0.54331100	22.98024000	H	2.23968100	3.48173300	16.60627900
H	9.52657400	0.44766800	21.98130700	H	1.92846200	1.76643200	16.25890900
H	9.29994000	1.18415000	23.57126400	C	6.58612100	2.28802600	14.38511600
C	10.28047400	-1.99928800	22.95195100	H	5.81311400	2.62603400	13.69568700
C	10.05700800	-0.79407300	23.65282800	H	7.39076500	3.02606700	14.40900500
C	9.80433700	-0.83765500	25.03101500	C	15.67874100	-3.56550400	22.97750500
H	9.61609000	0.09225100	25.56395300	H	14.93538100	-4.27997600	23.32568200
C	9.79556900	-2.04424200	25.72802700	H	16.40753700	-4.05514800	22.32696200
H	9.60429100	-2.05474500	26.79766600	C	15.96433300	0.58431800	20.35736800
C	10.02887300	-3.23492100	25.03830000	H	15.68067400	1.55191000	20.78024400
H	10.02576600	-4.18527800	25.56528200	H	16.98343900	0.35245100	20.66567700
C	10.26651600	-3.20580600	23.66372100	C	15.18510600	3.97468300	22.69931100
H	10.46151600	-4.13308100	23.13478500	H	14.68708000	4.81197200	23.19390900
C	10.48675000	-2.08048700	21.44980700	H	16.20110600	3.88349000	23.08216100

C	15.41828000	-0.34197700	25.00268200
H	15.71126100	0.13198900	25.94284100
H	14.80752200	-1.22151200	25.19369400

3-*anti open* (acetonitrile)

Au	1.604900	2.024498	3.336078
Au	1.615120	5.243956	3.301773
N	4.938472	4.790607	8.995506
H	6.686933	3.749039	9.440180
C	5.154198	4.468632	7.619144
O	6.154707	3.848851	7.269906
C	4.062230	4.909636	6.780521
C	2.962069	5.563147	7.320137
N	1.456777	2.195518	0.246448
C	0.817018	1.912539	1.441844
N	-0.423734	1.485393	1.120148
C	-1.648032	0.930350	-1.070253
O	-2.636658	0.317272	-0.665268
N	-1.434132	1.167061	-2.455470
H	-3.460788	0.876745	-2.896303
C	-0.275228	1.694687	-3.039429
O	-0.163185	1.834620	-4.256606
N	0.775999	2.068649	-2.164696
H	1.913749	2.492979	-3.850089
C	0.596186	1.925470	-0.812141
C	-0.584254	1.462191	-0.266199
C	-1.479022	1.171028	2.111798
H	-0.982411	1.239514	3.085510
H	-1.779413	0.133522	1.959080
C	-2.664898	3.473209	2.156988
C	-2.703330	2.067166	2.044755
C	-3.947858	1.432558	1.929002
H	-3.977025	0.351883	1.825462
C	-5.139680	2.158058	1.940727
H	-6.090849	1.638761	1.852412
C	-5.101514	3.548901	2.070617
H	-6.021734	4.127529	2.088632
C	-3.869843	4.191332	2.181541
H	-3.832748	5.273247	2.286645
C	-1.401658	4.259782	2.382347
H	-1.655621	5.182001	2.908145
H	-0.701754	3.702155	3.009745
N	-0.556465	4.702294	1.205507
C	0.663180	5.224578	1.482498
N	1.184455	5.695178	0.297498
N	0.399542	5.761367	-2.060787
H	1.217357	6.813313	-3.652912
C	-0.631668	5.368556	-2.941113
O	-0.577524	5.615707	-4.145567
N	-1.703697	4.670591	-2.383587
H	-3.455047	3.624578	-2.805890
C	-1.924191	4.385039	-0.999804
O	-2.929012	3.780106	-0.637177
C	-0.831311	4.840885	-0.170296
C	0.273133	5.475213	-0.723912
C	7.094824	4.185470	4.443005
H	7.064719	5.265214	4.315581
C	4.627084	4.266102	4.241660
H	4.887117	5.174815	3.695678
H	3.923194	3.699665	3.626774
N	3.785103	4.740013	5.408659
C	2.568160	5.262688	5.120559
N	2.051075	5.764623	6.294516
N	2.839080	5.881730	8.649937
H	2.017023	6.957649	10.223492
C	3.870856	5.507154	9.537642

O	3.820819	5.784963	10.735596
N	1.755405	2.269696	6.420766
C	2.392630	1.953585	5.232293
N	3.631302	1.527721	5.563646
C	4.854866	1.022287	7.766508
O	5.839506	0.393084	7.376989
N	4.644402	1.297099	9.145166
H	6.671379	1.020524	9.595519
C	3.489258	1.846431	9.716553
O	3.379768	2.020326	10.929531
N	2.437858	2.200323	8.833683
H	1.300082	2.662297	10.509154
C	2.615495	2.021668	7.485082
C	3.792992	1.538624	6.949976
C	4.684045	1.183349	4.579225
H	4.187317	1.232760	3.604421
H	4.977464	0.147565	4.755492
C	5.885134	3.476086	4.483568
C	5.914371	2.072498	4.625277
C	7.154859	1.432160	4.752575
H	7.177039	0.353658	4.878400
C	8.351471	2.149282	4.724289
H	9.299293	1.625570	4.822030
C	8.322358	3.537421	4.565974
H	9.246333	4.109450	4.535202
C	2.867062	2.626446	0.204884
H	3.153717	2.864604	1.228721
H	3.500552	1.823809	-0.173907
H	2.978292	3.515397	-0.411519
C	2.509365	6.349507	0.234574
H	2.399466	7.408233	0.002368
H	2.959890	6.242751	1.221170
H	3.142726	5.861148	-0.504920
C	0.347509	2.709044	6.452662
H	0.241096	3.612559	7.048384
H	0.061799	2.925037	5.423652
H	-0.290168	1.918815	6.850031
C	0.731476	6.430851	6.342425
H	0.849577	7.491608	6.560565
H	0.284621	6.314361	5.355255
H	0.090405	5.958232	7.085587
C	5.990560	4.401309	9.960867
H	6.508913	5.292753	10.323489
H	5.528464	3.886194	10.803486
C	1.755505	6.737469	9.191750
H	1.696139	7.664839	8.622777
H	0.799904	6.210962	9.171141
C	5.706659	0.841761	10.069506
H	5.620657	1.400533	10.997745
H	5.595031	-0.228097	10.270386
C	1.189274	2.724254	9.429703
H	1.044754	3.768720	9.146435
H	0.338633	2.121680	9.112921
C	-2.755558	4.261630	-3.341062
H	-3.270325	5.145726	-3.726110
H	-2.294028	3.724678	-4.170287
C	1.483620	6.605491	-2.619786
H	1.548961	7.539647	-2.062864
H	2.437552	6.075866	-2.597608
C	-2.496875	0.693570	-3.370074
H	-2.415175	1.237784	-4.307403
H	-2.382175	-0.378920	-3.554667

C	2.025772	2.576327	-2.772194
H	2.173128	3.625913	-2.510134
H	2.875100	1.977945	-2.444090

3-*anti closed* (acetonitrile)

Au	1.494799	1.847794	3.204176
Au	1.770386	4.959550	3.429082
N	4.436115	5.206546	9.500218
H	6.393085	4.910278	10.150746
C	4.888594	4.987511	8.171287
O	6.072457	4.739031	7.918449
C	3.816115	5.072171	7.218429
C	2.530337	5.419358	7.575383
N	1.477500	1.330836	0.225602
C	0.675500	1.668837	1.316108
N	-0.553823	1.912310	0.807793
C	-1.624026	1.813352	-1.537649
O	-2.807908	2.061882	-1.284950
N	-1.171692	1.592714	-2.866361
H	-3.128781	1.887824	-3.517050
C	0.133422	1.273095	-3.260168
O	0.420402	1.091266	-4.441673
N	1.115316	1.185949	-2.244237
H	2.542971	0.984951	-3.741646
C	0.734463	1.383011	-0.941562
C	-0.551334	1.730440	-0.584876
C	-1.841130	2.199337	1.512855
C	-1.826424	2.601246	2.968510
H	-2.433344	1.286976	1.413114
H	2.749578	-0.167055	-2.402544
C	2.499458	0.862815	-2.662176
H	-2.195298	0.712219	-4.491147
H	-1.871704	2.460183	-4.655995
H	2.411602	5.543984	-2.276513
C	1.730274	4.806326	-2.696671
C	-2.162334	1.667543	-3.963787
H	2.170971	3.807966	-2.654646
H	3.199267	1.553476	-2.192296
H	-3.855280	4.287777	-2.500744
C	-1.581961	5.155856	2.497529
H	-1.306134	6.019389	3.105996
C	-1.783940	3.946613	3.399239
N	-0.563812	5.027276	1.431967
C	0.770139	4.918042	1.632064
N	1.336868	4.813107	0.372105
N	0.443703	4.841086	-1.964286
H	1.517175	5.052974	-3.733593
C	-0.742301	4.897589	-2.737273
O	-0.696838	4.807706	-3.962343
N	-1.948999	5.046366	-2.036933
H	-3.698753	6.058616	-2.641645
C	-2.102567	5.142421	-0.634047
O	-3.221047	5.281509	-0.121896
C	-0.852689	5.033740	0.062899
C	0.351238	4.900805	-0.598428
H	-2.515403	5.394301	1.982454
H	-2.348361	2.956503	0.917216
C	5.106280	4.605827	5.120462
H	5.698322	5.518246	5.220680
H	5.613484	3.848483	5.715929
N	3.818847	4.892368	5.825515
C	2.589674	5.136924	5.317300
N	1.787608	5.473692	6.408117
N	2.149327	5.614769	8.878264
H	0.721252	5.813478	10.375650
C	3.131045	5.526116	9.894223

O	2.843969	5.706718	11.075896
N	1.929337	1.992865	6.261270
C	2.495482	1.888847	5.000994
N	3.829408	1.778218	5.200427
C	5.368882	1.659203	7.265713
O	6.487109	1.520308	6.752957
N	5.215875	1.753398	8.668796
H	6.965245	0.739455	9.271747
C	4.009511	1.901821	9.369758
O	3.964473	1.989952	10.594976
N	2.823258	1.959982	8.597311
H	1.749838	1.742593	10.366089
C	2.915186	1.902403	7.231330
C	4.118794	1.769443	6.569391
C	4.846860	1.649672	4.134277
H	5.780431	1.410235	4.648659
H	4.570135	0.786746	3.525353
H	-2.191473	0.566824	3.559948
H	-2.763655	1.110521	5.907308
H	-2.770698	3.500716	6.647187
H	-2.128772	5.274992	5.052001
C	-2.116590	4.237342	4.731303
C	-2.487735	3.237838	5.631237
C	-2.489532	1.903745	5.217428
C	-2.152824	1.598907	3.899343
C	2.856962	0.831596	0.381423
H	3.028898	0.711738	1.449879
H	2.959097	-0.134758	-0.109575
H	3.576544	1.544205	-0.019806
C	2.784827	4.630412	0.203519
H	3.258848	5.555248	-0.125959
H	3.177062	4.349393	1.176744
H	2.986377	3.831532	-0.507829
C	0.481616	2.176851	6.430584
H	0.281158	2.972618	7.145706
H	0.089816	2.462956	5.458667
H	0.006293	1.251140	6.755763
C	0.408510	5.974056	6.252691
H	0.306915	6.939824	6.744981
H	0.236857	6.095449	5.184367
H	-0.311592	5.261375	6.652807
C	5.426649	5.130274	10.597651
H	5.459759	6.085008	11.126069
H	5.135798	4.336919	11.288946
C	0.765152	5.937571	9.296415
H	0.515449	6.967990	9.038594
H	0.065298	5.247997	8.825031
C	6.470180	1.695811	9.453345
H	7.122742	2.510370	9.132836
H	6.216541	1.798557	10.504546
C	1.537052	1.994550	9.330378
H	1.098858	2.994215	9.293120
H	0.853768	1.260541	8.907092
C	-3.203081	5.102338	-2.821976
H	-2.949023	4.998518	-3.872966
C	5.049273	2.859353	3.233236
C	5.092087	4.204484	3.664618
C	5.382281	2.569123	1.901138
C	5.754192	3.568881	1.001807
C	5.756433	4.902769	1.416259
C	5.419317	5.207107	2.734355
H	5.458242	6.239017	3.074237

H	6.031173	5.696214	0.726881
H	6.037359	3.306357	-0.014178
H	5.394240	1.531612	1.579976

4-*trans* (gas-phase)

Au	0.095817	6.214027	11.368940
Cl	0.110854	4.057910	12.316801
Cl	0.078015	8.448743	10.639823
C	-2.926875	7.536847	12.812107
H	-3.314139	8.525839	12.563602
H	-1.867888	7.624087	13.051952
H	-3.460429	7.117528	13.666419
N	-2.358588	5.326907	10.016765
C	-1.937597	6.058585	11.064815
N	-3.035926	6.639059	11.645659
C	-4.175050	6.256058	10.930042
N	-5.492730	6.574454	11.120835
H	-5.605495	8.424979	12.160901
C	4.371097	6.331863	10.985182
C	3.971423	5.504058	9.953634
O	4.574479	4.237412	8.031029
H	6.804625	4.234042	7.575408
H	3.582365	7.163416	13.719790
H	5.766026	8.538344	12.207931
H	3.478120	8.577545	12.620076
C	4.887260	4.950759	8.982495
C	6.156772	7.522267	12.305040
C	3.077231	7.590125	12.851700
C	-6.466038	6.052892	10.206345
O	-7.650405	6.309893	10.335230
N	-5.989685	5.240552	9.161549
H	-7.750600	4.129637	8.792110
C	-4.640888	4.870521	8.918156
O	-4.303333	4.164066	7.970015
H	7.243212	7.547999	12.229614
O	7.852296	6.446386	10.434909
C	6.674673	6.166554	10.292296
H	5.869615	7.088302	13.265554
N	5.680695	6.671729	11.193547
H	8.013756	4.265311	8.902950
N	6.226574	5.342205	9.244455
C	7.287502	4.849133	8.332613
H	2.011963	7.683220	13.059517
H	7.798234	5.699902	7.875522
C	-3.747817	5.436572	9.902950
C	-1.453967	4.565149	9.087643
H	-2.124454	3.996114	8.440804
H	-0.887328	3.869934	9.705897
C	0.828384	5.518743	8.274003
C	-0.585340	5.504774	8.263936
C	-1.266586	6.414607	7.434687
H	-2.353289	6.387451	7.406853
C	-0.584725	7.337006	6.648963
H	-1.136878	8.030759	6.020563
C	0.814460	7.351300	6.659422
H	1.361639	8.056302	6.039213
C	1.503191	6.442461	7.454877
H	2.590516	6.437392	7.443022
C	1.703493	4.594661	9.108401
H	1.141687	3.889055	9.719287
H	2.392025	4.037928	8.469823
N	3.216157	6.697218	11.684608
C	2.135555	6.097385	11.090297
N	2.582796	5.371761	10.048870
C	-7.029775	4.732063	8.234276
H	-7.552360	5.575426	7.776931

H	-6.525701	4.131894	7.478910
C	-5.998677	7.407955	12.232129
H	-7.082748	7.434398	12.128171
H	-5.737675	6.959402	13.193678

4-*cis open* (gas-phase)

Au	4.921690	13.036793	16.261404
Cl	4.220754	11.329111	17.719734
Cl	4.272947	14.748644	17.738975
C	7.525428	10.853143	16.292660
H	8.538299	10.872059	15.890725
H	7.417588	10.066082	17.041576
H	7.301699	11.805869	16.769553
N	6.541814	10.655651	15.210729
C	5.444545	11.473061	15.034419
N	4.661104	10.917147	14.098988
C	5.233383	9.712261	13.665231
C	4.689266	8.681998	12.807233
O	3.592495	8.714543	12.253287
N	6.610467	15.382694	15.241330
H	7.358669	14.168021	16.756300
C	4.814411	17.441140	12.865476
C	3.858119	14.471206	11.129404
H	2.981793	14.087678	14.409961
H	9.118772	18.616063	14.557675
H	4.166748	11.842425	8.993726
C	4.038606	12.390624	9.923651
H	6.101316	19.799026	11.113377
C	4.061756	13.786816	9.932614
H	4.208289	14.342336	9.009812
C	6.513125	16.502372	14.412072
C	5.490930	14.598935	15.052967
N	5.574780	7.580511	12.680515
H	5.911455	6.307016	11.027954
C	6.819895	7.422447	13.310995
O	7.522647	6.445622	13.121473
N	7.230051	8.465900	14.206302
H	8.977072	7.385123	14.450775
C	5.328134	16.386127	13.711872
N	5.729855	18.519420	12.754072
O	7.706249	19.595696	13.214274
H	8.602522	15.127658	15.918786
H	7.483239	15.895852	17.097087
H	3.820363	15.555406	11.129473
C	3.442817	14.632245	13.586156
O	3.718800	17.445015	12.308304
C	7.588849	15.137745	16.318346
H	2.820133	15.496271	13.350103
N	4.723174	15.190620	14.126610
N	7.356818	17.570202	14.272499
C	6.977132	18.635667	13.389410
C	6.414794	9.553218	14.362818
C	3.396938	11.519110	13.567173
H	2.953041	12.066741	14.398331
H	2.749008	10.676530	13.321610
C	3.660865	13.786296	12.341882
C	3.638624	12.373530	12.333025
C	3.813196	11.698037	11.111794
H	3.740927	10.615645	11.098325
C	5.162370	6.451811	11.809709
H	5.091585	5.539134	12.406180
H	4.194847	6.707492	11.382041
C	8.560655	8.315975	14.834331
H	9.209859	9.147803	14.547861
H	8.472710	8.249115	15.920754
C	5.350491	19.669426	11.896187
H	4.374326	19.448298	11.468879

H	5.310058	20.577548	12.502316
C	8.685474	17.681560	14.912445
H	8.590734	17.718804	15.999622
H	9.324335	16.848482	14.606549

4-*cis closed* (gas-phase)

Au	4.932919	4.723344	3.462104
Cl	4.147517	3.171225	1.877443
C	5.594849	0.789917	7.402054
N	7.454833	0.118482	5.262783
N	5.115288	2.737239	5.786244
N	6.546038	2.208155	4.204188
C	5.580900	3.119224	4.584025
C	5.764404	1.565329	6.192736
C	6.655695	1.228490	5.193990
C	7.274279	2.281697	2.920508
H	7.027264	3.232304	2.452819
H	6.945148	1.483728	2.253622
H	8.347808	2.222812	3.100266
C	4.056135	3.433907	6.591249
H	4.550101	4.231921	7.150154
H	3.713862	2.691609	7.314235
C	2.935930	3.936975	5.713541
C	2.129984	3.000258	5.053164
H	2.302855	1.938853	5.216824
C	1.131752	3.410995	4.170946
H	0.525271	2.671379	3.655942
N	6.466081	-0.329912	7.429566
C	7.382495	-0.709352	6.433334
N	4.889677	6.620062	5.868840
N	6.803718	6.738185	4.789603
C	5.571026	6.115800	4.827598
C	5.680143	7.581924	6.518685
C	6.875608	7.659556	5.837007
C	7.771144	6.530701	3.694233
H	7.381193	5.734874	3.061359
H	7.852619	7.437086	3.091349
H	8.744350	6.243306	4.092870
C	3.457166	6.382362	6.268811
H	3.476840	6.185088	7.342818
H	2.955858	7.344164	6.141235
C	2.716069	5.315114	5.501970
C	1.704011	5.715044	4.615339
H	1.539420	6.774906	4.441036
C	0.922865	4.773909	3.945964
H	0.155651	5.103513	3.251262
Cl	4.293389	6.578819	2.160438
C	5.380687	8.371519	7.692177
N	6.454712	9.243698	8.020308
N	7.883497	8.507619	6.207263
C	7.685536	9.352229	7.352989
O	4.808687	1.044264	8.312147
C	6.420274	-1.219851	8.616075
H	7.406085	-1.248474	9.086068
H	5.676295	-0.813104	9.298494
H	6.148504	-2.230275	8.301964
O	8.086598	-1.696900	6.546824
C	8.379781	-0.325108	4.196415
H	9.219084	0.368489	4.097310
H	8.760051	-1.298144	4.505042
H	7.846584	-0.424535	3.249221
C	9.192130	8.608591	5.526739
H	9.751614	9.382074	6.051780
H	9.734996	7.662079	5.597591
H	9.061809	8.902536	4.483157
O	8.556763	10.120190	7.721076
C	6.293726	10.132746	9.197197

H	6.410129	11.172514	8.883223
H	5.298631	9.957693	9.602207
H	7.061021	9.898542	9.939050
O	4.342952	8.315821	8.345710