Supplementary Materials: The *Trans* Influence in Unsymmetrical Pincer Palladacycles: An Experimental and Computational Study

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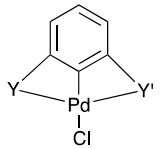
S1. QTAIM Analysis Data

Table S1. Topological analysis of AIM at BCP of Pd–Cl bond. The electron density $\rho(\mathbf{r})$, Laplacian of the electron density $\nabla^2\rho(\mathbf{r})$, total energy $H(\mathbf{r})$, bond pressure $|H(\mathbf{r})/\rho(\mathbf{r})|$, ellipticity ε, and delocalization index δ(Pd–Cl) and Pd–Cl bond lengths. All values of AIM are in a.u. (atomic units) and Pd–Cl bond lengths are in Å.

Compound	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	$H(\mathbf{r})$	$\lvert H(\mathbf{r})/\rho(\mathbf{r})\rvert$	ε	δ(Pd–Cl)	Bond Length
I	0.080	0.254	−0.017	0.213	0.102	1.361	2.334
II	0.077	0.247	−0.016	0.208	0.108	1.313	2.352
III	0.070	0.232	−0.013	0.186	0.124	1.239	2.395

Table S2. The electron density $\rho(\mathbf{r})$, Laplacian of the electron density $\nabla^2\rho(\mathbf{r})$, total energy $H(\mathbf{r})$, bond pressure $|H(\mathbf{r})/\rho(\mathbf{r})|$, ellipticity ε, delocalisation index δ(Pd–Y) in symmetrical and unsymmetrical pincer palladacycles (values are in atomic units). The donor atoms are shown in bold.



PdYCY′	Y	Y′	Pd–Y						Pd–Y′					
			$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	$H(\mathbf{r})$	$\lvert H(\mathbf{r})/\rho(\mathbf{r})\rvert$	ε	δ(Pd–Y)	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	$H(\mathbf{r})$	$\lvert H(\mathbf{r})/\rho(\mathbf{r})\rvert$	ε	δ(Pd–Y′)
PdNCN *	**N**Me$_2$CH$_2$	**N**Me$_2$CH$_2$	0.086	0.383	−0.014	0.163	0.033	0.908	0.086	0.383	−0.014	0.163	0.033	0.908
PdSCS *	**S**MeCH$_2$	**S**MeCH$_2$	0.091	0.257	−0.025	0.275	0.040	1.157	0.091	0.257	−0.025	0.275	0.040	1.157
PdPCP *	**P**Me$_2$CH$_2$	**P**Me$_2$CH$_2$	0.101	0.183	−0.036	0.356	0.022	1.124	0.101	0.183	−0.036	0.356	0.022	1.124
IV	**S**MeCH$_2$	**N**Me$_2$CH$_2$	0.097	0.271	−0.028	0.289	0.039	1.217	0.083	0.369	−0.013	0.157	0.046	0.883
V	**P**Me$_2$CH$_2$	**S**MeCH$_2$	0.110	0.170	−0.043	0.391	0.012	1.194	0.082	0.241	−0.021	0.256	0.064	1.073
VI	**P**Me$_2$CH$_2$	**N**Me$_2$CH$_2$	0.114	0.169	−0.046	0.404	0.006	1.243	0.075	0.333	−0.010	0.133	0.064	0.828
1a	**S**MeCH$_2$	2-**N**C$_5$H$_4$	0.096	0.273	−0.027	0.281	0.047	1.208	0.098	0.465	−0.018	0.184	0.012	0.979
1b	**S**EtCH$_2$	2-**N**C$_5$H$_4$	0.095	0.270	−0.027	0.284	0.044	1.203	0.098	0.463	−0.018	0.184	0.012	0.977
1c	**S**PrCH$_2$	2-**N**C$_5$H$_4$	0.095	0.269	−0.027	0.284	0.046	1.202	0.098	0.463	−0.018	0.184	0.011	0.977
1d	**S**PhCH$_2$	2-**N**C$_5$H$_4$	0.092	0.267	−0.025	0.272	0.041	1.188	0.098	0.456	−0.018	0.184	0.015	0.977
1e	**S**(*p*-MePh)CH$_2$	2-**N**C$_5$H$_4$	0.092	0.266	−0.025	0.272	0.039	1.189	0.098	0.458	−0.018	0.184	0.015	0.977
1f	**S**(*p*-MeOPh)CH$_2$	2-**N**C$_5$H$_4$	0.092	0.265	−0.025	0.272	0.037	1.187	0.098	0.458	−0.018	0.184	0.015	0.977
2a	**P**Ph$_2$O	2-**N**C$_5$H$_4$	0.114	0.191	−0.045	0.395	0.020	1.235	0.087	0.409	−0.013	0.149	0.006	0.919
2b	**P**Ph$_2$OCH$_2$	2-**N**C$_5$H$_4$	0.113	0.180	−0.044	0.389	0.023	1.206	0.089	0.426	−0.014	0.157	0.036	0.928
3a	**N**Me$_2$CH$_2$	2-**N**C$_5$H$_4$	0.086	0.380	−0.014	0.163	0.039	0.903	0.102	0.478	−0.020	0.196	0.023	1.004
3b	**N**Et$_2$CH$_2$	2-**N**C$_5$H$_4$	0.085	0.373	−0.014	0.165	0.041	0.900	0.102	0.476	−0.020	0.196	0.018	1.000
3c	**N**(C$_4$H$_8$O)CH$_2$	2-**N**C$_5$H$_4$	0.084	0.372	−0.013	0.155	0.038	0.896	0.102	0.477	−0.020	0.196	0.021	1.004

* Taken from reference [36].

S2. Cartesian Coordinates

Compound **I**

C	−2.05277800	−1.54143900	0.03010600
C	−3.44312100	−1.40137100	−0.12997700
C	−4.01170500	−0.14901600	−0.41113400
C	−3.18958500	0.98297400	−0.53091800
C	−1.79779600	0.85873700	−0.38395800
C	−1.23349400	−0.40473400	−0.08377000
H	−1.61561800	−2.51695700	0.25012000
H	−4.08159800	−2.28529300	−0.03124200
H	−5.09444300	−0.05156500	−0.53513400
H	−3.62877700	1.96432100	−0.74355800
C	−0.84574000	2.00946700	−0.54827000
H	−0.46602800	2.05047900	−1.58488800
H	−1.31158300	2.98873500	−0.31802500
N	0.34606100	1.78948400	0.33320400
C	1.44135600	2.71642000	−0.04795400
H	1.09654500	3.76152900	0.07308400
H	2.31276900	2.53725400	0.59654600
H	1.74138400	2.52945100	−1.08680500
C	−0.00674700	2.01398800	1.76456700
H	0.85686800	1.75365500	2.39356400
H	−0.26653500	3.07877000	1.92578800
H	−0.86115800	1.38213300	2.04200600
Pd	0.75965900	−0.34104100	0.16291200
Cl	1.05225400	−2.59427500	0.40993300
Cl	2.75887100	−0.02579400	−1.04287300
Optimization using PBE/6-31+G(d,p)[SDD]			
Energy = −1452.3633527 a.u.			
Zero-point energy correction = 0.190005 a.u.			
Single point energy using ωB97XD/6-311++G(2df,2p)[DGDZVP]			
Energy = −6265.1681887 a.u.			

Compound **II**

C	−1.75470500	−1.71701100	0.18204900
C	−3.15092500	−1.82196100	0.05737800
C	−3.91682000	−0.72315900	−0.35894300
C	−3.28445100	0.49510700	−0.65156000
C	−1.88662000	0.61599200	−0.54596300
C	−1.11556400	−0.49383300	−0.10252200
H	−1.16827500	−2.57723400	0.50824000
H	−3.63522300	−2.77567400	0.29082600
H	−5.00324300	−0.81060600	−0.45486400
H	−3.87799300	1.35963000	−0.96994700
C	−1.18752200	1.90301400	−0.88227700
H	−0.77335000	1.90147400	−1.90597900
H	−1.82538400	2.79563800	−0.77027000
S	0.30833800	2.07653600	0.18715900
C	−0.47697500	2.31280000	1.82458100

H	0.31847100	2.21720400	2.57725800
H	−0.90261100	3.32735700	1.86687100
H	−1.25088800	1.55170100	1.99782600
Pd	0.87783500	−0.20541400	0.13389000
Cl	1.43368200	−2.41937900	0.37313900
Cl	2.88668100	0.40816000	−0.92784000
Optimization using PBE/6-31+G(d,p)[SDD]			
Energy = −1755.8262745 a.u.			
Zero-point energy correction = 0.145848 a.u.			
Single point energy using ωB97XD/6-311++G(2df,2p)[DGDZVP]			
Energy = −6568.7076067 a.u.			

Compound **III**

C	−2.20330800	−1.41797200	0.11668300
C	−3.59168600	−1.24546300	−0.00502600
C	−4.12934100	0.00212200	−0.35561200
C	−3.27181100	1.08827700	−0.58283500
C	−1.87661400	0.93522400	−0.47251000
C	−1.33313900	−0.32634100	−0.09975200
H	−1.79811200	−2.39289600	0.39057800
H	−4.25144800	−2.09973200	0.17853300
H	−5.21165600	0.13104400	−0.45326800
H	−3.68497300	2.06634100	−0.85398400
C	−0.93900100	2.09200500	−0.73130400
H	−0.62689300	2.12887300	−1.79219000
H	−1.37663500	3.07246100	−0.47403300
P	0.56938100	1.70607400	0.25933300
C	1.92978300	2.77298900	−0.34840000
H	1.63230000	3.83287300	−0.28059700
H	2.83283200	2.59803600	0.25512800
H	2.16539100	2.50580200	−1.38870600
C	0.22003000	2.28836400	1.96975300
H	1.05277300	2.00529100	2.63160600
H	0.09436800	3.38383600	1.98777400
H	−0.69771100	1.80177400	2.33272100
Pd	0.69326500	−0.56365500	0.11533000
Cl	0.74103700	−2.87769000	0.37918100
Cl	2.82422100	−0.40653900	−0.88945800
Optimization using PBE/6-31+G(d,p)[SDD]			
Energy = −1738.8896856 a.u.			
Zero-point energy correction = 0.182235 a.u.			
Single point energy using ωB97XD/6-311++G(2df,2p)[DGDZVP]			
Energy = −6551.81864 a.u.			

Compound **IV**

Pd	0.70174700	0.01412000	−0.15268100
C	−1.25872000	−0.06521300	−0.09074700
C	−1.97075900	−1.27816300	0.04730000
C	−3.37823200	−1.24924300	0.10831400
C	−4.05918900	−0.02056700	0.07031000

C	−3.34926600	1.18937100	−0.04591500
C	−1.94839300	1.16689100	−0.14265000
C	−1.16691100	−2.54804900	0.17039600
C	−1.08004000	2.37722100	−0.38174000
C	1.29423700	2.98745900	−0.59991500
Cl	3.10559300	0.14529300	−0.00477300
H	−5.15145900	−0.00514000	0.13277700
H	−3.89419900	2.14020400	−0.07344800
H	−3.94669000	−2.18206400	0.19855800
H	−1.60860400	−3.40325300	−0.36837000
H	−1.02781100	−2.83832900	1.22704000
H	−0.99928900	2.56338600	−1.46766500
H	−1.47601000	3.30327100	0.08275600
H	1.06343800	4.05572500	−0.41432800
H	2.30669000	2.74498300	−0.24668500
H	1.24419100	2.77847900	−1.67831500
C	0.40946100	2.37934500	1.57648900
H	1.41030100	2.08959000	1.92816900
H	0.23644400	3.45522200	1.78376000
H	−0.34895000	1.77852100	2.09828200
N	0.32243200	2.12025700	0.11279900
S	0.54889100	−2.23699600	−0.51352800
C	1.60636800	−3.09241100	0.70916300
H	1.52359000	−4.18102300	0.56940800
H	2.63079300	−2.74888000	0.50064300
H	1.33153200	−2.79989500	1.73270000
Optimization using PBE/6-31+G(d,p)[SDD]			
Energy = −1468.9266824 a.u.			
Zero-point energy correction = 0.244944 a.u.			
Single point energy using ωB97XD/6-311++G(2df,2p)[DGDZVP]			
Energy = −6281.8376981 a.u.			

Compound **V**

Pd	−0.61788300	−0.34361900	−0.12767500
C	−2.43610900	2.56072100	−0.91175400
C	1.28604900	0.29950400	−0.06492700
C	1.62302900	1.67759500	−0.17625400
C	2.97011600	2.08396500	−0.12650500
C	3.99513200	1.13442300	0.00446000
C	3.67832800	−0.22897500	0.10237000
C	2.33453100	−0.64861000	0.08834000
C	0.50324200	2.68049000	−0.38168800
C	1.98925000	−2.10382200	0.29894300
Cl	−2.90254700	−1.08291300	−0.07428200
H	5.04073800	1.45639300	0.02741200
H	4.48108800	−0.96854900	0.20340100
H	3.22240100	3.14790600	−0.20398700
H	0.41008700	2.94810700	−1.45166200
H	0.65641400	3.62262200	0.17510900
H	2.75433800	−2.78601500	−0.10746000

H	1.86090600	−2.32810000	1.37323700
H	−3.36965800	2.03386700	−0.65902700
H	−2.54541100	3.64214300	−0.72478800
H	−2.22445400	2.38457800	−1.97727000
C	−1.45870600	2.38711500	1.81950100
H	−1.61156800	3.47882200	1.86104100
H	−2.36713400	1.87050700	2.16622600
H	−0.62223500	2.10461600	2.47644300
P	−1.08612100	1.83514500	0.10230700
S	0.35327900	−2.46556700	−0.50353400
C	−0.40833400	−3.65096100	0.65952400
H	−1.47641300	−3.67736300	0.39484200
H	0.04620200	−4.64549500	0.53692400
H	−0.30916600	−3.29482100	1.69533200
Optimization using PBE/6-31+G(d,p)[SDD]			
Energy = −1755.4562478 a.u.			
Zero-point energy correction = 0.237261 a.u.			
Single point energy using ωB97XD/6-311++G(2df,2p)[DGDZVP]			
Energy = −6568.491708 a.u.			

Compound **VI**

Pd	0.55265100	0.42163900	−0.03944700
P	1.36061000	−1.64786800	−0.02686500
C	2.01157200	−2.26360300	−1.63771200
C	−1.19716000	−0.50964000	−0.04261200
C	−1.35940100	−1.90159200	0.17071600
C	−2.65681600	−2.45108100	0.20115600
C	−3.78144500	−1.62492000	0.04118100
C	−3.62469600	−0.24210500	−0.16375200
C	−2.33595100	0.31423500	−0.21851100
C	−0.10942100	−2.73341600	0.38895700
C	−2.06621200	1.76476300	−0.54485800
N	−0.74405300	2.20157000	0.01904400
C	−0.88173700	2.54980400	1.45698000
C	−0.20963700	3.36699600	−0.72341800
C	2.69067900	−2.06113600	1.17455900
Cl	2.65869700	1.58009400	0.04971100
H	−4.78516600	−2.05950200	0.07843100
H	−4.50859400	0.39437600	−0.28964500
H	−2.79383000	−3.52703600	0.36069400
H	−0.09828000	−3.66433700	−0.20735300
H	−0.01066800	−3.03317700	1.44977200
H	−1.99335900	1.88341300	−1.64119500
H	−2.87208100	2.44330300	−0.19525900
H	0.11548800	2.76640500	1.86761100
H	−1.53512500	3.43892100	1.57787600
H	−1.31881200	1.69863500	1.99882000
H	−0.88991900	4.23786800	−0.62770900
H	0.78529400	3.61437300	−0.32480200
H	−0.09722400	3.10276700	−1.78526900

H	3.55385900	−1.41061000	0.96351900
H	2.33994700	−1.84120700	2.19426600
H	2.98455500	−3.12168300	1.10072200
H	2.85428500	−1.62387800	−1.94266400
H	2.34952600	−3.31047200	−1.55538300
H	1.22089400	−2.18796600	−2.39940800
Optimization using PBE/6-31+G(d,p)[SDD]			
Energy = −1451.9901878 a.u.			
Zero-point energy correction = 0.281139 a.u.			
Single point energy using ωB97XD/6-311++G(2df,2p)[DGDZVP]			
Energy = −6264.9477105 a.u.			

Compound **1a**

Pd	0.46035700	−0.69569800	−0.09378100
C	−2.37511500	−1.81277600	0.05789200
H	−1.81864600	−2.75644100	0.04172000
C	−3.77207000	−1.74454300	0.10521600
H	−4.35782400	−2.66653500	0.12955400
C	−4.38481700	−0.48205100	0.11839600
H	−5.47486600	−0.39348000	0.15372600
C	−3.58883300	0.66814800	0.08565900
H	−4.04571700	1.66090900	0.09498000
C	−2.18806400	0.54866500	0.03969600
C	−1.21794900	1.64945200	0.01185800
C	−1.52584300	3.02507200	0.02851900
H	−2.56565300	3.36867200	0.05248200
C	−0.48893700	3.96974600	0.01046000
H	−0.72742600	5.03729000	0.01170600
C	0.85711500	3.55812500	−0.00329700
H	1.65221300	4.31263600	−0.00814100
C	1.18065000	2.18716500	−0.00068500
C	0.13993400	1.23318800	−0.01805800
C	2.59998300	1.68097800	0.07626400
H	2.97961400	1.70868900	1.11309500
H	3.30151400	2.24475400	−0.56125500
C	3.66443900	−0.88143300	0.85645800
H	4.71818500	−0.59479000	0.71975900
H	3.53757100	−1.96635900	0.72250200
H	3.29825500	−0.59438300	1.85241100
Cl	0.81729700	−3.07067500	−0.06705000
N	−1.61039300	−0.70206000	0.02720300
S	2.64388100	−0.11508500	−0.45434000
Optimization using PBE/6-31+G(d,p)[SDD]			
Energy = −1542.6834107 a.u.			
Zero-point energy correction = 0.213060 a.u.			
Single point energy using ωB97XD/6-311++G(2df,2p)[DGDZVP]			
Energy = −6355.6377844 a.u.			

Compound **1b**

Pd	0.36667100	−0.61998600	−0.23173000
C	−2.34270200	−1.99639700	0.07415700
H	−1.70737800	−2.88574800	−0.00313900
C	−3.73404200	−2.05720800	0.21145800
H	−4.23176800	−3.02927400	0.24597800
C	−4.45552000	−0.85674100	0.29987200
H	−5.54448200	−0.86908400	0.40621000
C	−3.76949600	0.36163400	0.25049600
H	−4.31188300	1.30807900	0.31748600
C	−2.36948500	0.37144100	0.11183300
C	−1.50697400	1.55726900	0.05124500
C	−1.93719600	2.89739800	0.13097500
H	−2.99956900	3.14126200	0.23872900
C	−0.99464900	3.93448900	0.06935200
H	−1.32833600	4.97498100	0.12047300
C	0.37848100	3.64980200	−0.05250400
H	1.09884400	4.47510300	−0.09200800
C	0.82554600	2.31541200	−0.11465100
C	−0.12221600	1.26942200	−0.08538800
C	2.28712200	1.94498500	−0.16537700
H	2.74781000	2.00220100	0.83630200
H	2.87441300	2.57938000	−0.85016200
C	3.69321500	−0.53028000	0.43351300
H	4.61478800	0.06209700	0.29624600
H	3.86484900	−1.53649000	0.01705000
Cl	0.93527400	−2.95550600	−0.27198000
N	−1.68382300	−0.82030900	0.02642000
S	2.45361600	0.17239900	−0.74142000
C	3.25340700	−0.61634100	1.89081100
H	2.36606800	−1.26251900	1.98101000
H	4.06914300	−1.05413000	2.49208800
H	3.01694700	0.37156900	2.31998100
Optimization using PBE/6-31+G(d,p)[SDD]			
Energy = −1581.944827 a.u.			
Zero-point energy correction = 0.240616 a.u.			
Single point energy using ωB97XD/6-311++G(2df,2p)[DGDZVP]			
Energy = −6394.9562865 a.u.			

Compound **1c**

Pd	0.20652300	−0.52775500	−0.40644400
C	−2.27898900	−2.21860000	0.12925800
H	−1.55890100	−3.02307100	−0.05771900
C	−3.62997200	−2.44550000	0.41529400
H	−4.00881700	−3.46939300	0.45930400
C	−4.46616800	−1.34048800	0.63710200
H	−5.52769700	−1.48287400	0.86116300
C	−3.93110900	−0.04947500	0.56912200
H	−4.56537100	0.82426500	0.73866100
C	−2.56600000	0.12784100	0.27909500

C	−1.85311500	1.40682400	0.18092400
C	−2.41780800	2.68433200	0.37108800
H	−3.48145500	2.79962100	0.60591500
C	−1.60984500	3.82535900	0.25650400
H	−2.04909900	4.81762800	0.39456900
C	−0.23689400	3.70612100	−0.02960100
H	0.37801200	4.61016100	−0.10845900
C	0.34590500	2.43561600	−0.20467500
C	−0.46938300	1.28617700	−0.12001900
C	1.82378200	2.24260100	−0.43929900
H	2.39645600	2.34610400	0.49884800
H	2.24206000	2.95082800	−1.17422000
C	3.53900800	−0.07121500	−0.03758700
H	4.36763500	0.64002700	−0.20827400
H	3.80763600	−1.03033100	−0.51251400
Cl	1.01577400	−2.78245000	−0.62114800
N	−1.76636000	−0.97281100	0.06332100
S	2.13324700	0.51140600	−1.08151700
C	3.23708900	−0.27509600	1.44751100
H	2.41635700	−1.00851700	1.53134000
H	2.87509900	0.66643200	1.89980500
C	4.47748200	−0.76989000	2.20659000
H	4.24408500	−0.92511700	3.27258200
H	4.83491300	−1.73146100	1.80069000
H	5.30955600	−0.04639500	2.14742400
Optimization using PBE/6-31+G(d,p)[SDD]			
Energy = −1621.2043503 a.u.			
Zero-point energy correction = 0.268431 a.u.			
Single point energy using ωB97XD/6-311++G(2df,2p)[DGDZVP]			
Energy = −6434.27147 a.u.			

Compound **1d**

Pd	−0.27180500	−0.51370000	−0.33108200
C	−2.75851800	−2.23208600	0.10782400
H	−2.02479700	−3.02629000	−0.07070700
C	−4.11492200	−2.47538100	0.35129300
H	−4.48334400	−3.50380300	0.37183300
C	−4.96938900	−1.38228500	0.56073800
H	−6.03551600	−1.53790700	0.75170600
C	−4.44551000	−0.08566600	0.52347700
H	−5.09271900	0.78009300	0.68451900
C	−3.07409300	0.10834100	0.27774900
C	−2.37216700	1.39437500	0.22137200
C	−2.95994100	2.66362500	0.39841300
H	−4.03411300	2.76326400	0.58773500
C	−2.16327900	3.81557600	0.32687400
H	−2.62085600	4.80117300	0.45243000
C	−0.77811500	3.71498300	0.09992500
H	−0.16966300	4.62550300	0.05595800
C	−0.17430100	2.45218500	−0.05758000

C	−0.97620700	1.29192900	−0.02069500
C	1.31227700	2.27188300	−0.20458800
H	1.81765100	2.25028600	0.77577900
H	1.79116800	3.04231100	−0.83100300
Cl	0.46827600	−2.78018300	−0.62314200
N	−2.25632600	−0.98058300	0.07285800
S	1.63971800	0.59144800	−0.98410600
C	3.14412500	0.10388800	−0.10754600
C	4.34823400	0.73515100	−0.47333400
C	3.12353800	−0.89584700	0.87829500
C	5.53707100	0.38459400	0.18393900
H	4.35868500	1.48608000	−1.26983400
C	4.32333900	−1.24796300	1.51670700
H	2.18634800	−1.41051400	1.10984200
C	5.52538000	−0.60623600	1.17944000
H	6.47398800	0.87679400	−0.09440000
H	4.31318500	−2.03336700	2.27846100
H	6.45599200	−0.88578000	1.68273500
Optimization using PBE/6-31+G(d,p)[SDD]			
Energy = −1734.1834206 a.u.			
Zero-point energy correction = 0.264283 a.u.			
Single point energy using ωB97XD/6-311++G(2df,2p)[DGDZVP]			
Energy = −6547.3573409 a.u.			

Compound **1e**

Pd	−0.52519100	−0.48257200	−0.38692800
C	−2.89245600	−2.33997700	0.13325300
H	−2.12921600	−3.08960200	−0.10474300
C	−4.22024000	−2.66059700	0.43735300
H	−4.53406600	−3.70715300	0.44695800
C	−5.11776300	−1.61968900	0.72047300
H	−6.16328400	−1.83604700	0.96014200
C	−4.66381400	−0.29667600	0.69332700
H	−5.34533100	0.52978700	0.90981200
C	−3.31861700	−0.02445300	0.38443600
C	−2.68808900	1.29808000	0.32544200
C	−3.32957400	2.52982900	0.56897200
H	−4.39482400	2.56783600	0.82082800
C	−2.59819600	3.72344300	0.48423600
H	−3.09768600	4.68041900	0.66111600
C	−1.22456000	3.70152400	0.17860900
H	−0.66743900	4.64390800	0.12544500
C	−0.56593800	2.47667900	−0.04541800
C	−1.30450300	1.27528200	0.00455100
C	0.91727500	2.37703300	−0.27882900
H	1.47760100	2.35788300	0.67129800
H	1.32215600	3.18530600	−0.90996200
Cl	0.32804500	−2.69424100	−0.76330200
N	−2.45749800	−1.06333500	0.10901200
S	1.28653200	0.73411100	-1.11903500

C	2.85050900	0.29132300	−0.33622600
C	4.02843600	0.87569000	−0.83493300
C	2.90861300	−0.62866100	0.72372500
C	5.26086400	0.55899000	−0.24586200
H	3.98546000	1.56890100	−1.68112600
C	4.15068300	−0.94213400	1.29143800
H	1.99220200	−1.11382200	1.07213200
C	5.34445500	−0.35559900	0.82324400
H	6.17474500	1.02204000	−0.63393800
H	4.19099700	−1.66587000	2.11282800
C	6.67851700	−0.72944200	1.42558000
H	7.05531900	−1.67271000	0.99057200
H	7.43873400	0.04602300	1.24032700
H	6.60101200	−0.88277900	2.51438500
Optimization using PBE/6-31+G(d,p)[SDD]			
Energy = −1773.4473545 a.u.			
Zero-point energy correction = 0.290848 a.u.			
Single point energy using ωB97XD/6-311++G(2df,2p)[DGDZVP]			
Energy = −6586.6757952 a.u.			

Compound **1f**

Pd	−0.75088400	−0.43324100	−0.44558100
C	−2.97501700	−2.46002900	0.07874100
H	−2.18183100	−3.14786900	−0.23560000
C	−4.26517500	−2.87795900	0.42412100
H	−4.51563200	−3.94092600	0.38906500
C	−5.20775500	−1.91118900	0.80626600
H	−6.22554400	−2.20419800	1.08125700
C	−4.83511800	−0.56308900	0.83184200
H	−5.55329300	0.20690600	1.12464500
C	−3.52547500	−0.19179000	0.47680500
C	−2.97999600	1.16917600	0.45850800
C	−3.68224100	2.34449200	0.79556100
H	−4.73422400	2.30332700	1.09787800
C	−3.03004300	3.58467600	0.73903400
H	−3.57766100	4.49822000	0.98836200
C	−1.67428500	3.66476700	0.36934600
H	−1.17877800	4.64194200	0.33921900
C	−0.95412400	2.49654800	0.05198300
C	−1.61558500	1.25005900	0.07183000
C	0.51944300	2.50049700	−0.25336900
H	1.12504600	2.46077000	0.66783900
H	0.84638600	3.36613200	−0.85288800
Cl	0.22426800	−2.56517300	−0.95926300
N	−2.61772900	−1.15945200	0.10678000
S	0.94237500	0.93162700	−1.20421700
C	2.56351700	0.52941200	−0.53753600
C	3.69666800	1.13070700	−1.12468100
C	2.72042400	−0.38780600	0.51204600
C	4.97230100	0.83928000	−0.63980600

H	3.57982200	1.81929700	−1.96733200
C	4.00120000	−0.69315900	0.99606500
H	1.84188100	−0.89238100	0.92457200
C	5.13161100	−0.07510200	0.42448300
H	5.86311100	1.29427200	−1.08119600
H	4.10056800	−1.42193700	1.80283300
O	6.42168600	−0.30062000	0.81775000
C	6.64536800	−1.24588500	1.86818100
H	7.73436500	−1.27798700	2.00884800
H	6.16229000	−0.92423400	2.80916700
H	6.27989500	−2.25087600	1.58902900
Optimization using PBE/6-31+G(d,p)[SDD]			
Energy = −1848.585334 a.u.			
Zero-point energy correction = 0.296003 a.u.			
Single point energy using ωB97XD/6-311++G(2df,2p)[DGDZVP]			
Energy = −6661.8862933 a.u.			

Compound **2a**

Pd	−0.78268800	−0.62530300	−0.05774600
Cl	−0.28046200	−2.95797500	−0.29195900
P	1.23595600	0.29211800	0.03860900
O	0.98890400	1.97107000	0.22325100
N	−2.90373900	−0.80291300	−0.08406800
C	−0.36279500	2.29912700	0.24996100
C	−0.76456400	3.63435100	0.38763400
H	−0.01893000	4.42953400	0.47577100
C	−2.14403500	3.92319300	0.40932900
H	−2.46735200	4.96272100	0.51590900
C	−3.10439500	2.90749700	0.29826700
H	−4.16748500	3.16698800	0.31989900
C	−2.68748900	1.56391500	0.16097700
C	−1.30528800	1.26303800	0.13659800
C	−3.56945200	0.39498800	0.03689300
C	−4.97670900	0.41458100	0.03498500
H	−5.50477600	1.36641600	0.13174100
C	−5.68801200	−0.78387700	−0.08945900
H	−6.78226300	−0.77366600	−0.09105400
C	−4.98672500	−1.99323200	−0.21130500
H	−5.50541100	−2.94978300	−0.31065200
C	−3.58729800	−1.95742400	−0.20419300
H	−2.96668300	−2.85626500	−0.29498900
C	2.30143000	0.23141000	−1.44730300
C	3.01687300	1.36193900	−1.89063200
H	2.91173100	2.31635900	−1.36682500
C	3.84509700	1.25921900	−3.01808400
H	4.39574400	2.13835400	−3.36738000
C	3.96364500	0.03596200	−3.69839100
H	4.61013600	−0.03904700	−4.57843600
C	3.24434100	−1.08683400	−3.25741900
H	3.32400300	−2.03716900	−3.79406900

C	2.40652200	−0.99465600	−2.13607600
H	1.82181900	−1.86098300	−1.80332200
C	2.32535200	−0.09326400	1.45613300
C	3.23795100	0.85859600	1.95629400
H	3.28116100	1.86127600	1.52081200
C	4.07580800	0.51879200	3.02737700
H	4.77845100	1.25933700	3.42221200
C	4.01347500	−0.76677000	3.59245000
H	4.67078500	−1.02768100	4.42788400
C	3.10577200	−1.71263300	3.09099500
H	3.05065300	−2.71193600	3.53350600
C	2.25389900	−1.38028800	2.02601200
H	1.53508900	−2.11068400	1.63569600
Optimization using PBE/6-31+G(d,p)[SDD]			
Energy = −1944.6510198 a.u.			
Zero-point energy correction = 0.330003 a.u.			
Single point energy using ωB97XD/6-311++G(2df,2p)[DGDZVP]			
Energy = −6758.111324 a.u.			

Compound **2b**

Pd	0.71182600	−0.42493200	0.26715500
Cl	−0.23300700	−2.54195900	0.92812100
P	−1.31668900	0.39072500	−0.18279500
O	−1.28148200	1.93091100	−0.82015000
N	2.71431800	−1.09235300	0.38912400
C	−0.38138700	2.85010700	−0.15494000
H	−0.59245500	2.84092500	0.93332100
H	−0.65624000	3.84437700	−0.54142500
C	1.08763700	2.56976700	−0.41020700
C	1.90377400	3.65541000	−0.78579000
H	1.44537300	4.63744400	−0.95440600
C	3.29004500	3.50251600	−0.93927200
H	3.91009200	4.35335900	−1.23618100
C	3.87173800	2.25438400	−0.69979000
H	4.95615900	2.14118100	−0.79831600
C	3.06778100	1.15426200	−0.33077400
C	1.64949400	1.29004300	−0.20745000
C	3.63608300	−0.16318300	−0.01150500
C	4.99964100	−0.51435900	−0.06919700
H	5.73962100	0.22119600	−0.39262100
C	5.40070700	−1.80607600	0.28574000
H	6.45866800	−2.08241400	0.24114800
C	4.43609200	−2.73884400	0.69646700
H	4.70704500	−3.75805500	0.98230500
C	3.09591600	−2.33954100	0.73043600
H	2.27915500	−3.00768700	1.02561400
C	−2.25883800	−0.43298900	−1.51860100
C	−2.30550700	0.12325700	−2.81280900
H	−1.79678600	1.06906900	−3.01578700
C	−3.01386500	−0.53580500	−3.82947600

H	−3.05262600	−0.09761300	−4.83176500
C	−3.66576400	−1.75027100	−3.56393700
H	−4.21461000	−2.26328500	−4.36004600
C	−3.60906200	−2.30871400	−2.27613000
H	−4.10879600	−3.25921700	−2.06570200
C	−2.90776900	−1.65665500	−1.25264000
H	−2.84397200	−2.10570300	−0.25714100
C	−2.48426200	0.52757600	1.22978200
C	−3.74014500	1.14415200	1.03982200
H	−4.02504000	1.51069500	0.04816600
C	-4.61958900	1.28597300	2.12136500
H	−5.59291600	1.76385900	1.97183100
C	−4.25382700	0.81026300	3.39323000
H	−4.94451900	0.91897500	4.23553900
C	−3.00775900	0.19324000	3.58225600
H	−2.72418100	−0.18398600	4.56959200
C	−2.11955200	0.05253200	2.50394000
H	−1.15436500	−0.44689200	2.63480100
Optimization using PBE/6-31+G(d,p)[SDD]			
Energy = −1983.9041486 a.u.			
Zero-point energy correction = 0.358281 a.u.			
Single point energy using ωB97XD/6-311++G(2df,2p)[DGDZVP]			
Energy = −6797.4232729 a.u.			

Compound **3a**

C	−2.38241400	−1.78986800	−0.05639400
H	−1.82840400	−2.73371800	−0.09804200
C	−3.77953500	−1.72057600	−0.00349900
H	−4.36596900	−2.64241200	−0.01182400
C	−4.39151700	−0.45938400	0.06164400
H	−5.48133400	−0.37179100	0.10458100
C	−3.59394800	0.69066700	0.07205100
H	−4.04694500	1.68423200	0.12335100
C	−2.19441700	0.57326200	0.01410200
C	−1.21993500	1.66943100	0.00667900
C	−1.46345600	3.05805600	0.07170000
H	−2.48317500	3.45173900	0.14721100
C	−0.37887800	3.95042400	0.04391000
H	−0.56701200	5.02633500	0.10466000
C	0.95095300	3.48669300	−0.06816500
H	1.77331100	4.21096200	−0.10232300
C	1.20328600	2.10649000	−0.14644700
C	0.11628400	1.21790000	−0.09036700
C	2.53329700	1.43536700	−0.39563300
H	2.73493000	1.42580100	−1.48171900
H	3.39110500	1.93892300	0.09326600
C	2.84414400	−0.12340600	1.48741300
H	2.71065400	−1.16647600	1.80890000
H	2.18146000	0.52574700	2.07737900
H	3.89846100	0.18620400	1.63869200

C	3.42580000	−0.83614800	−0.75997600
H	4.46257700	−0.46408500	−0.63624200
H	3.13637400	−0.78553100	−1.81959400
H	3.35140700	−1.88208700	−0.42906600
Cl	0.85433200	−3.05241600	0.04383200
N	−1.61361900	−0.68095900	−0.05085200
N	2.48266200	−0.01701700	0.04464200
Pd	0.44581800	−0.67783400	−0.07919600
Optimization using PBE/6-31+G(d,p)[SDD]			
Energy = −1239.2122694 a.u.			
Zero-point energy correction = 0.257010 a.u.			
Single point energy using ωB97XD/6-311++G(2df,2p)[DGDZVP]			
Energy = −6052.0888771 a.u.			

Compound **3b**

Pd	0.27026900	−0.63823000	−0.01593600
Cl	0.81527300	−2.98581600	0.17478900
N	−1.78937800	−0.75414500	−0.02363900
N	2.28480800	0.10755900	0.03652700
C	−2.50083600	−1.90014600	0.01620600
H	−1.90048600	−2.81592000	0.04186300
C	−3.90066600	−1.90193400	0.02869900
H	−4.43882900	−2.85231000	0.06083400
C	−4.57787800	−0.67306800	0.00140800
H	−5.67155200	−0.64037600	0.01115400
C	−3.84035900	0.51563400	−0.03802200
H	−4.34523900	1.48503500	−0.05941500
C	−2.43525800	0.46860100	−0.05108300
C	−1.51941500	1.61324800	−0.09346200
C	−1.84433600	2.98577500	−0.11457100
H	−2.88699600	3.32227000	−0.10013500
C	−0.81176700	3.93733400	−0.15030800
H	−1.06201000	5.00228700	−0.16154900
C	0.54431200	3.54561200	−0.17397800
H	1.32539200	4.31457500	−0.20741000
C	0.88072600	2.17990600	−0.15849400
C	−0.15629100	1.23345600	−0.11215500
C	2.27506100	1.60654400	−0.25176700
H	2.99127000	2.10553700	0.42862600
H	2.66453600	1.74942800	−1.27410000
C	2.84211500	−0.15976500	1.40988800
H	3.89303200	0.19987500	1.42353200
H	2.85084500	−1.25614700	1.52255000
C	2.04991400	0.47033800	2.55149300
H	2.00841900	1.56998300	2.48939200
H	2.53233600	0.20478300	3.50669000
H	1.01617000	0.08730100	2.56378900
C	3.15329000	−0.61403800	−0.95808100
H	3.23929600	−1.64767700	−0.58702300
H	4.16066900	−0.14781200	−0.93709600

C	2.59100600	−0.64524100	−2.37618200
H	2.45986800	0.35702500	−2.81690700
H	1.61813800	−1.16359900	−2.38778400
H	3.28740100	−1.20421900	−3.02314400
Optimization using PBE/6-31+G(d,p)[SDD]			
Energy = −1317.7330461 a.u.			
Zero-point energy correction = 0.311645 a.u.			
Single point energy using ωB97XD/6-311++G(2df,2p)[DGDZVP]			
Energy = −6130.7249275 a.u.			

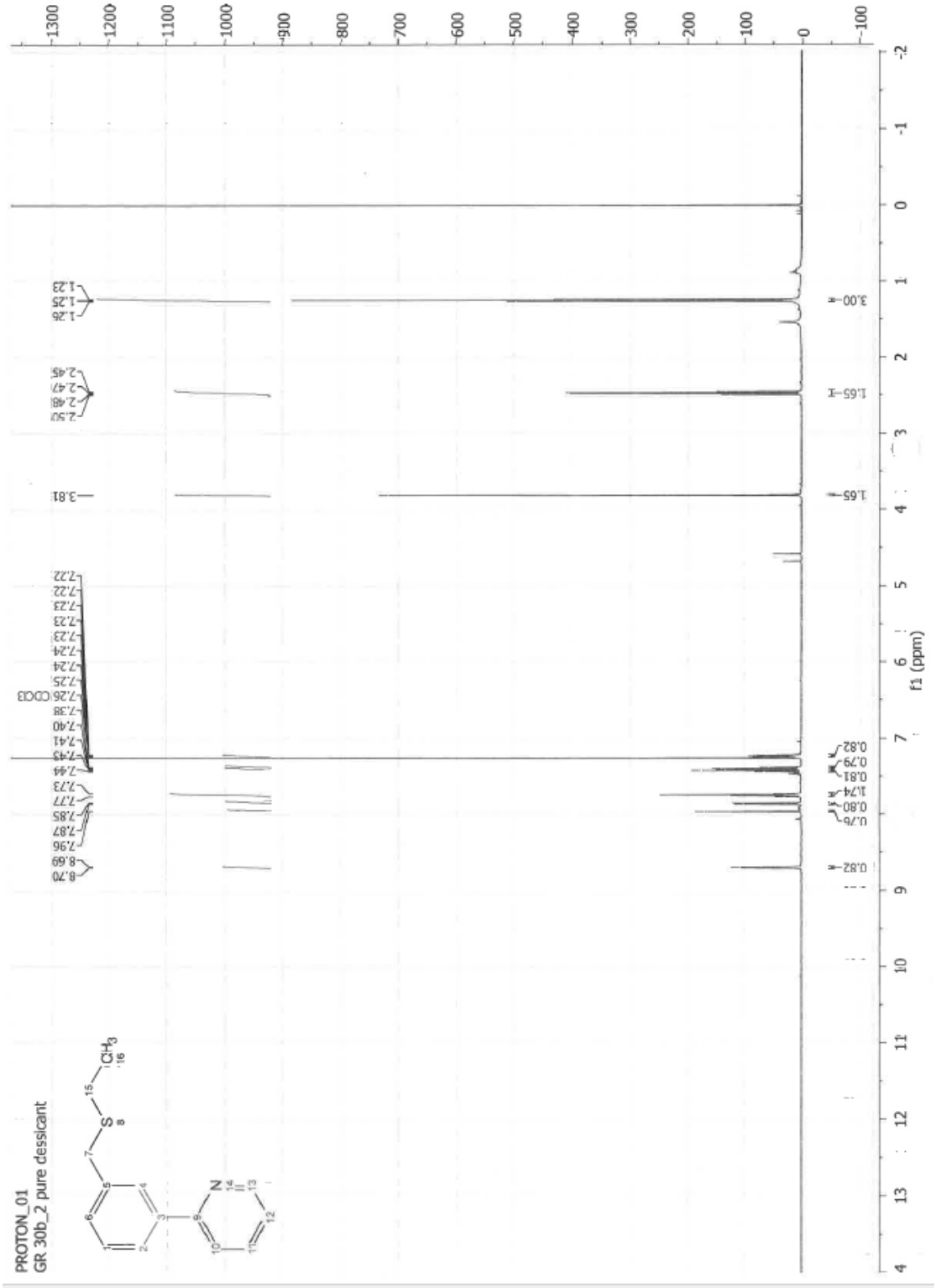
Compound **3c**

Pd	0.06872600	−0.63258100	−0.15098300
Cl	−0.49243900	−2.97834600	−0.05697400
O	−4.71370600	−0.44776900	0.57506400
N	2.11889600	−0.77521000	−0.00741900
N	−1.93298100	0.16325200	−0.14996700
C	2.81215400	−1.93265400	0.02875600
H	2.20236900	−2.83940800	−0.04440600
C	4.20586700	−1.95590400	0.15840100
H	4.72875100	−2.91499600	0.18219600
C	4.89639800	−0.73841700	0.25719500
H	5.98560100	−0.72346200	0.36044400
C	4.17762000	0.46193000	0.22282400
H	4.69223200	1.42347900	0.29830700
C	2.77865300	0.43732100	0.08770400
C	1.88227500	1.59601800	0.02310500
C	2.21508300	2.96531700	0.09483300
H	3.25321300	3.29033600	0.22598100
C	1.19656400	3.92845700	0.00163200
H	1.45315800	4.98983300	0.06780400
C	−0.15282600	3.55351200	−0.18183000
H	−0.92151900	4.33100600	−0.26507000
C	−0.49314200	2.19226800	−0.26795000
C	0.52600800	1.23393900	−0.14649800
C	−1.85477700	1.62177500	−0.58349800
H	−2.00732700	1.62715300	−1.67797800
H	−2.67957000	2.20965500	−0.14306600
C	−2.86716500	−0.62978400	−1.01795100
H	−2.69716700	−1.68998000	−0.76633200
H	−2.57206500	−0.47744500	−2.06923900
C	−4.33383900	−0.25615500	−0.79134700
H	−4.54215000	0.79334700	−1.09735300
H	−4.97996400	−0.91840300	−1.38964100
C	−3.90269900	0.35868600	1.43153000
H	−4.21533800	0.13244900	2.46379800
H	−4.11306000	1.43473600	1.24387000
C	−2.41148400	0.03665600	1.27464900
H	−1.79352200	0.69819900	1.90359100
H	−2.22346400	−1.00782700	1.57270800
Optimization using PBE/6-31+G(d,p)[SDD]			

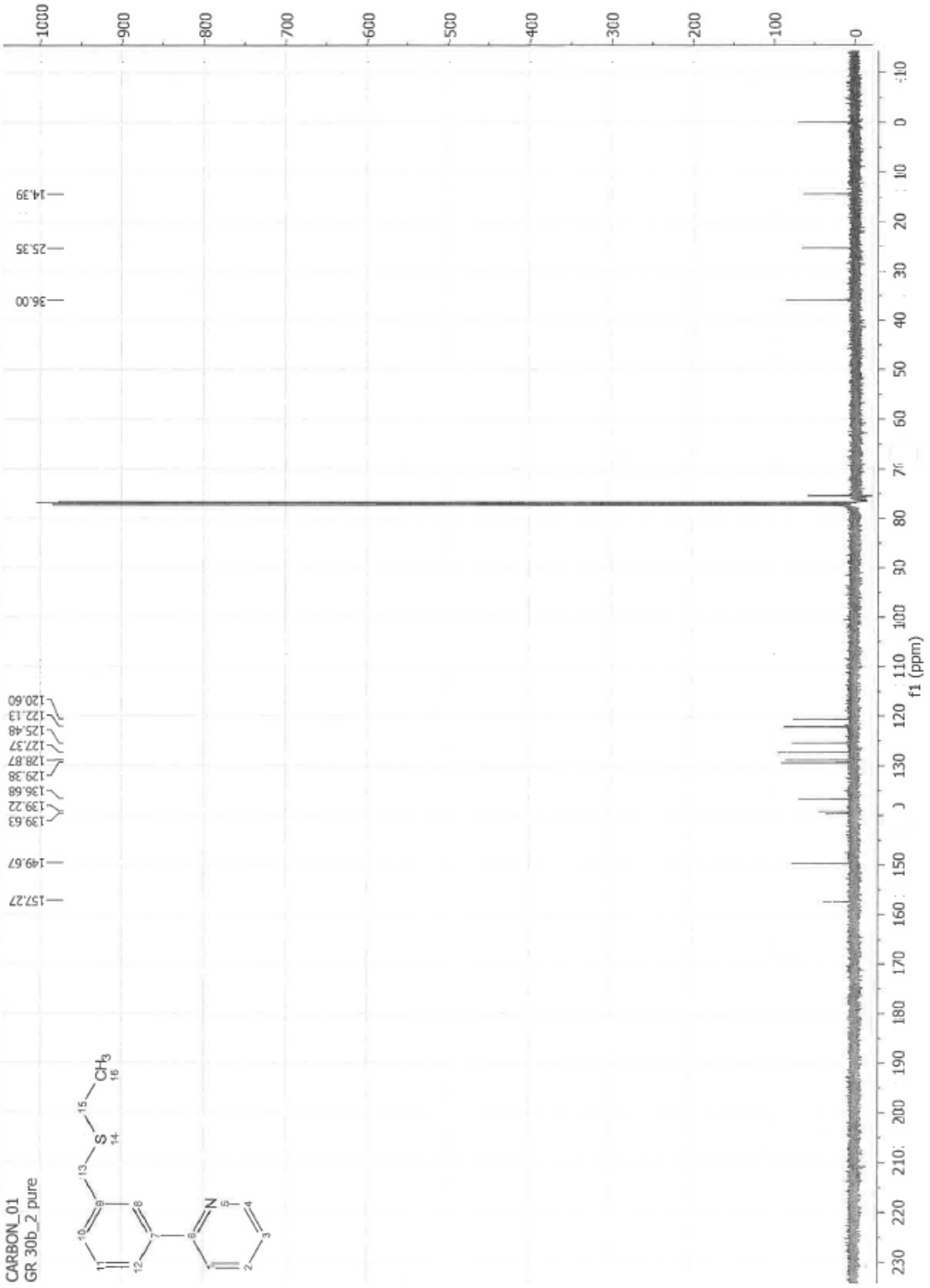
Energy = −1391.6718472 a.u.
Zero-point energy correction = 0.297406 a.u.
Single point energy using ωB97XD/6-311++G(2df,2p)[DGDZVP]
Energy = −6204.7210608 a.u.

S3. Experimental Spectral Data

2-3-[(Ethylsulfanyl)methyl]phenylpyridine, 6b, ^{1}H NMR.



2-3-[(Ethylsulfanyl)methyl]phenylpyridine, 6b, ^{13}C NMR.

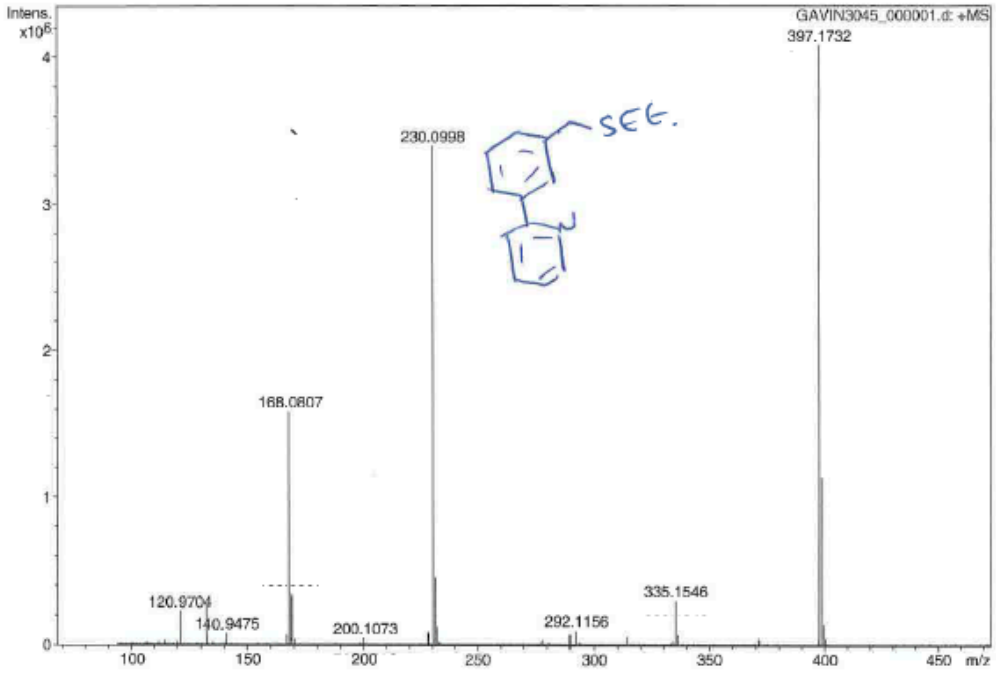


2-3-[(Ethylsulfanyl)methyl]phenylpyridine, 6b, ^{13}C HRMS.

Generic Display Report

Analysis Info

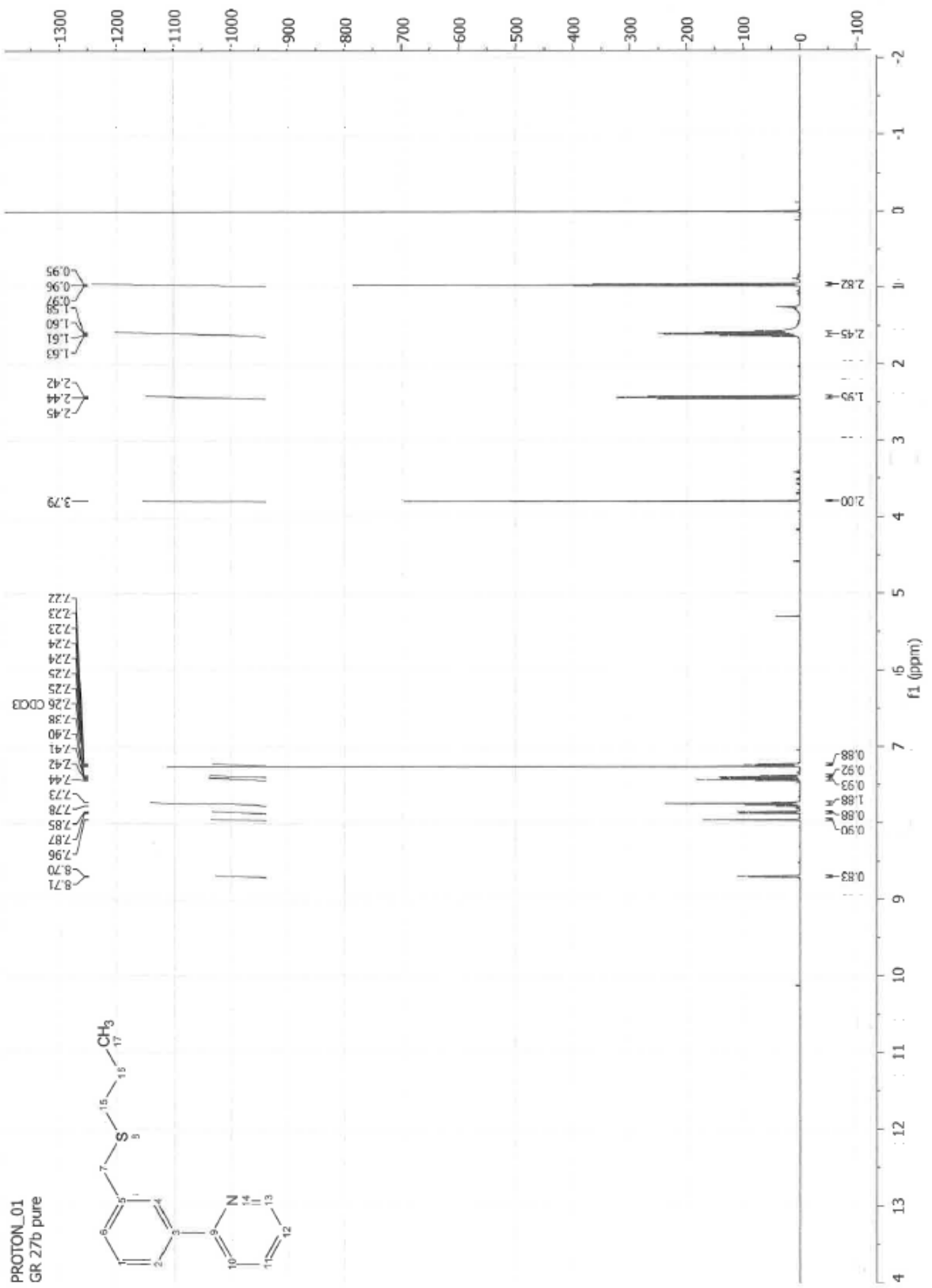
Analysis Name	D:\Data\Alinanopos\GAVIN3045_000001.d	Acquisition Date	12/06/2013 15:43:28
Method	pos20090608esi	Operator	Administrator
Sample Name	POS ESI GR 30B-2	Instrument	apex-III
Comment			



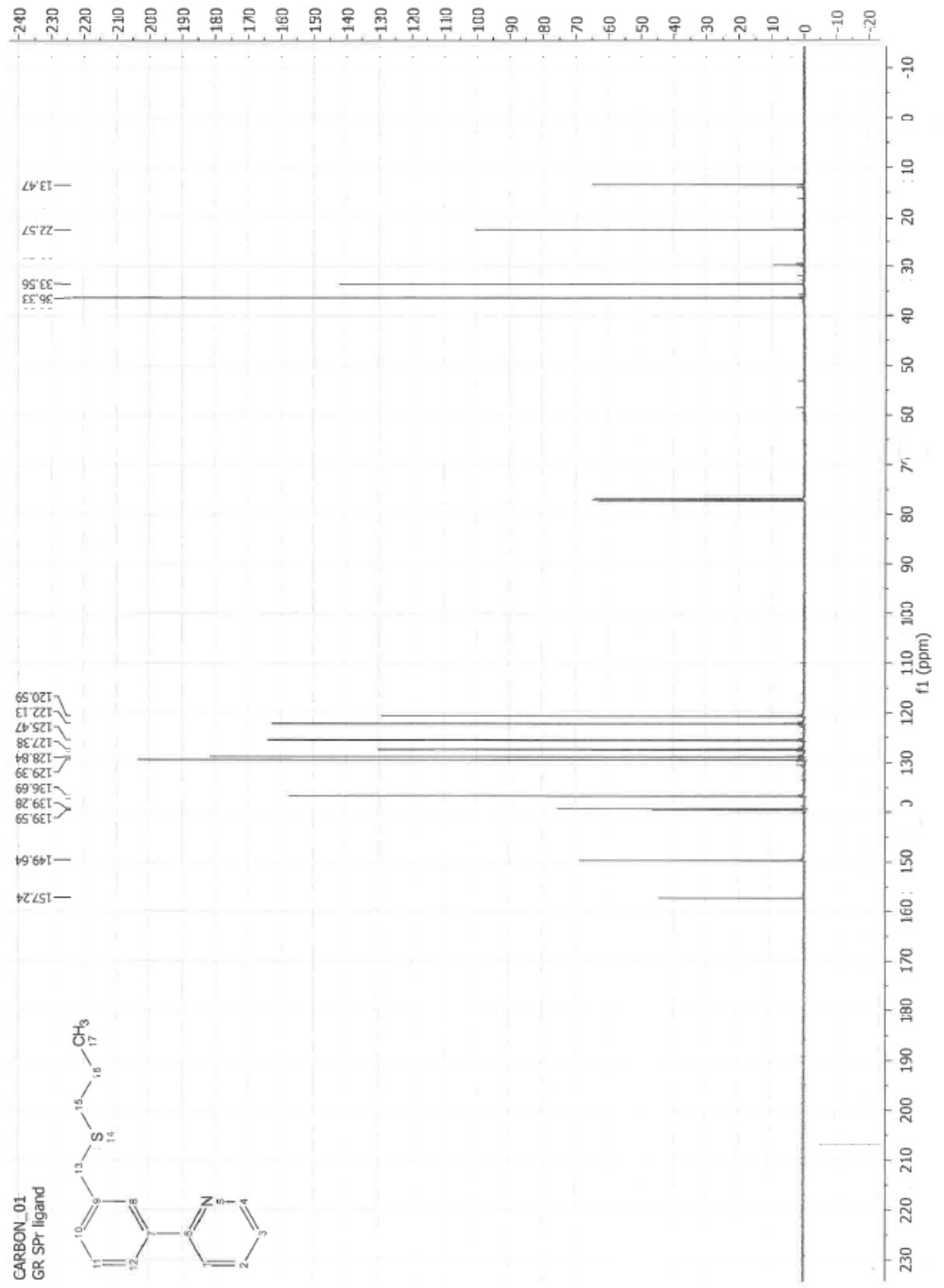
Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 14 H 16 N 1 S 1	0.033	230.0998	0.09	-0.85	-0.20	7.50	ok	even

Bruker Daltonics DataAnalysis 3.4 printed: 12/06/2013 15:44:41 Page 1 of 1

2-3-[(Propylsulfanyl)methyl]phenylpyridine, 6c. ^{1}H NMR



2-3-[(Propylsulfanyl)methyl]phenylpyridine, 6c. ^{13}C NMR



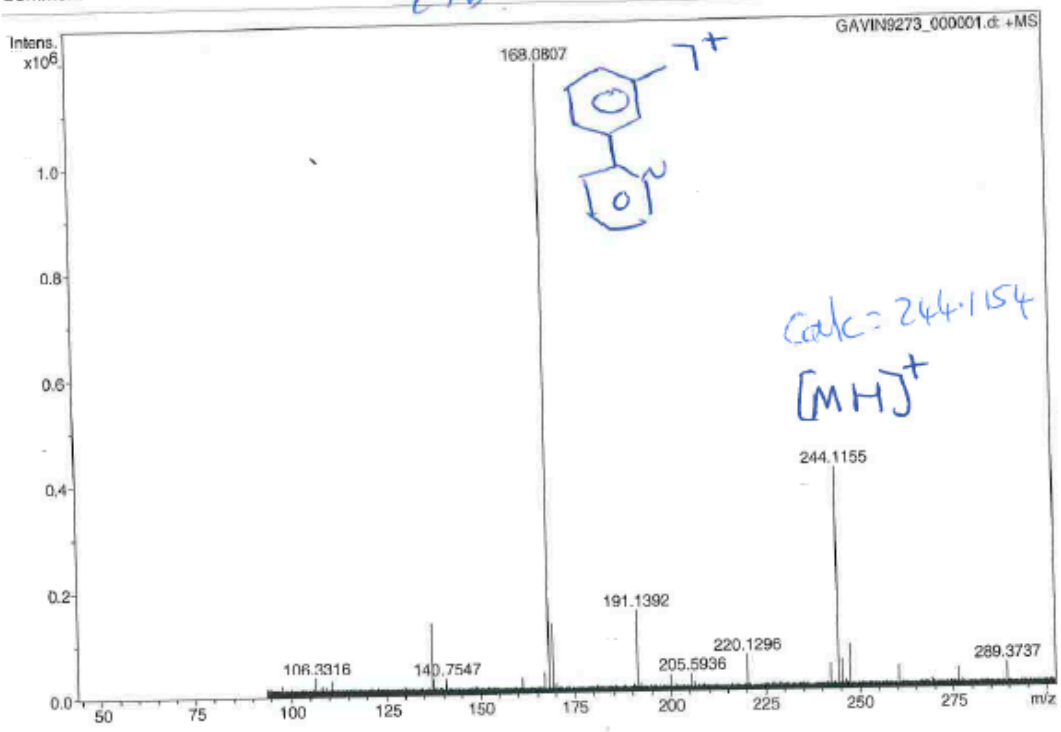
2-3-[(Propylsulfanyl)methyl]phenylpyridine, 6c. HRMS

Generic Display Report

Analysis Info

Analysis Name D:\Data\Alinanopos\GAVIN9273_000001.d
Method pos20090608esi
Sample Name POS ESI ~~GB3275~~ GR 27b
Comment

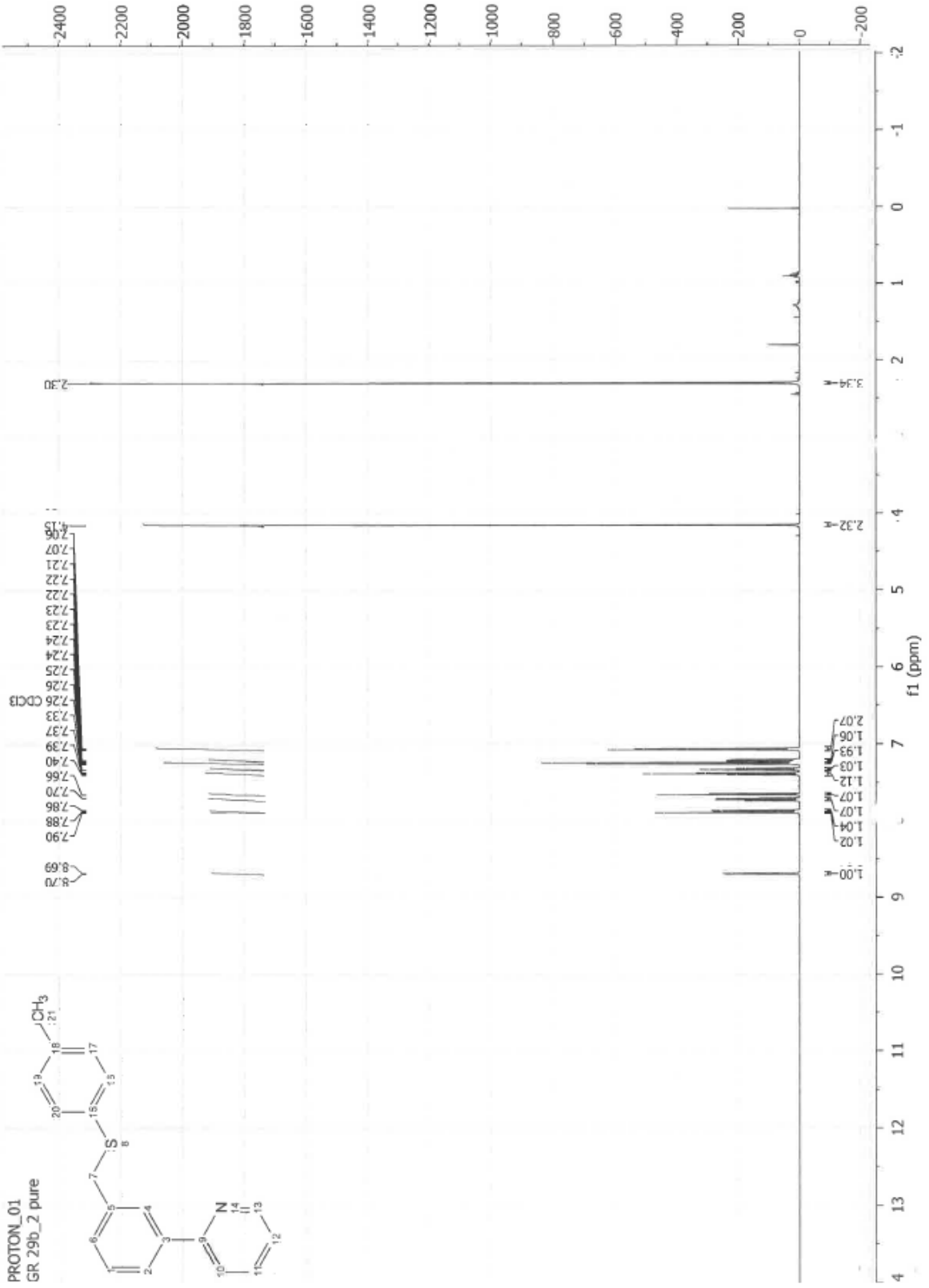
Acquisition Date 07/05/2013 12:23:10
Operator Administrator
Instrument apex-III



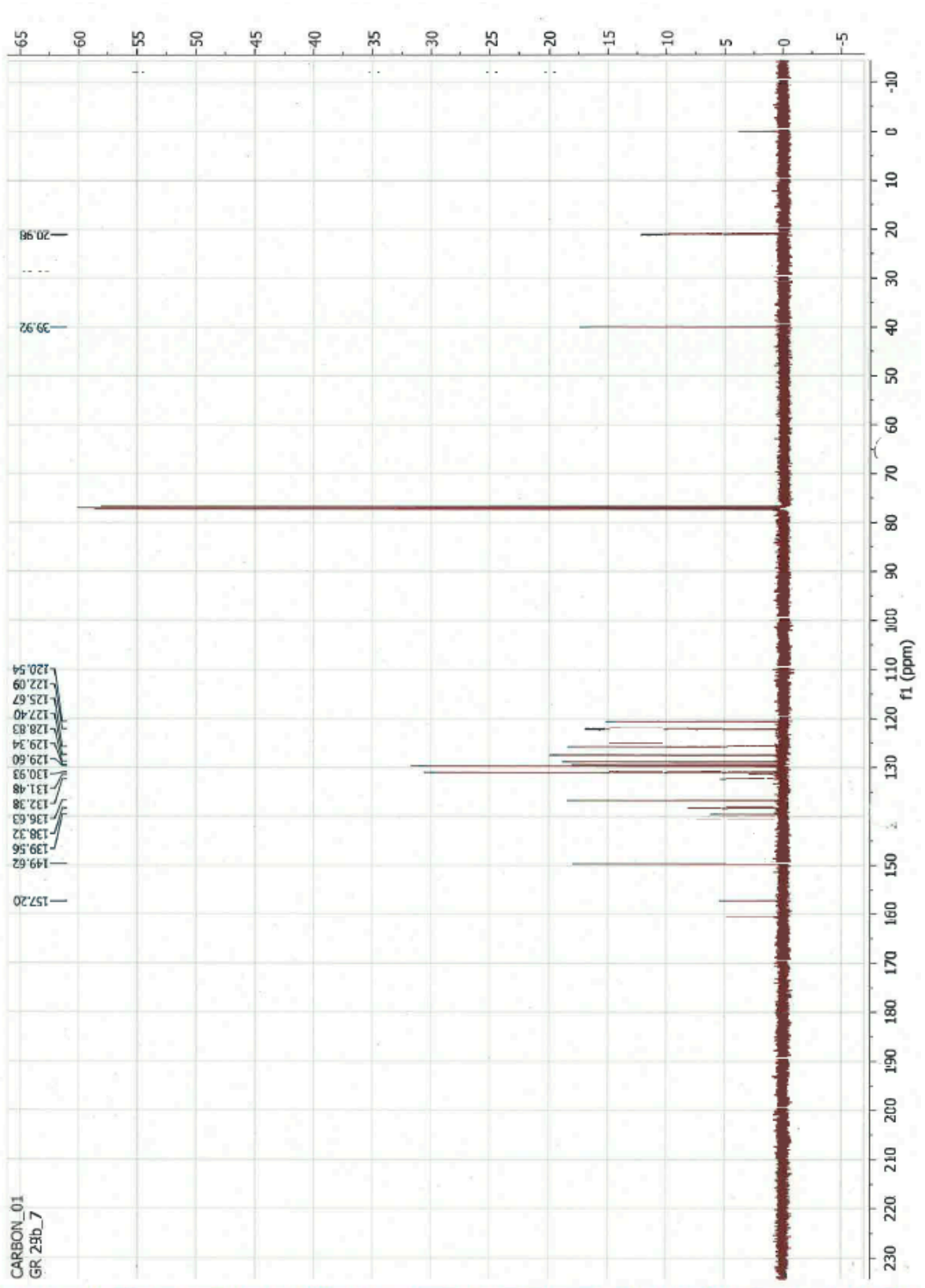
Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 15 H 18 N 1 S 1	0.085	244.1154	-0.35	-41.53	-10.16	7.50	ok	even

Bruker Daltonics DataAnalysis 3.4 printed: 07/05/2013 12:25:44 Page 1 of 1

2-(3-[(4-Methylphenyl)sulfanyl]methylphenyl)pyridine, 6e. ^{1}H NMR



2-(3-[(4-Methylphenyl)sulfanyl]methylphenyl)pyridine, 6e. ^{13}C NMR

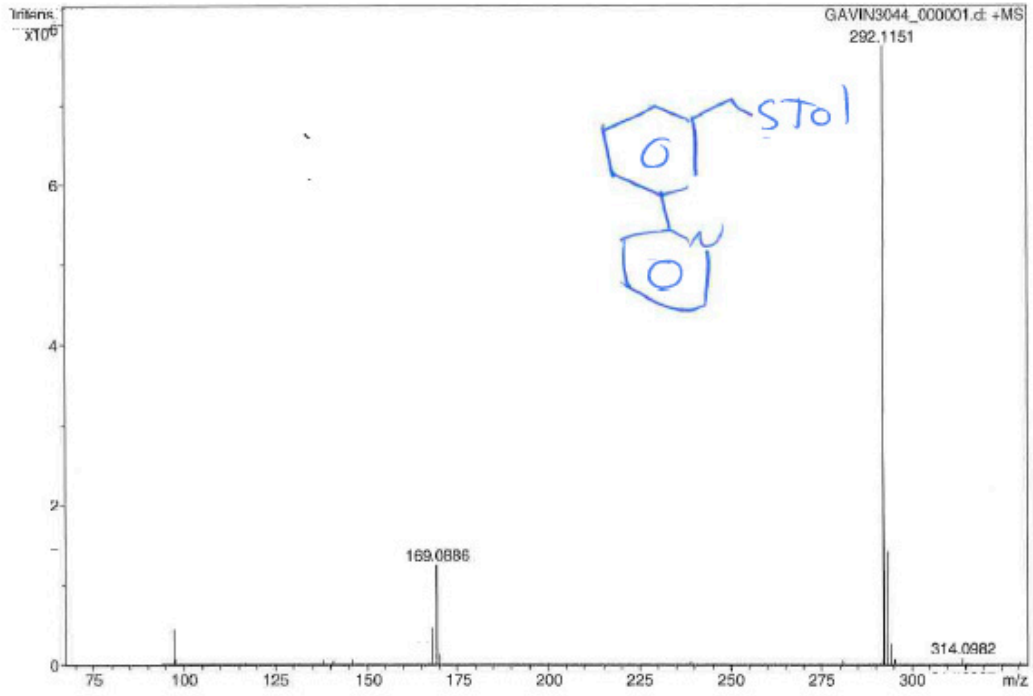


2-(3-[(4-Methylphenyl)sulfanyl]methylphenyl)pyridine, 6e. HRMS

Generic Display Report

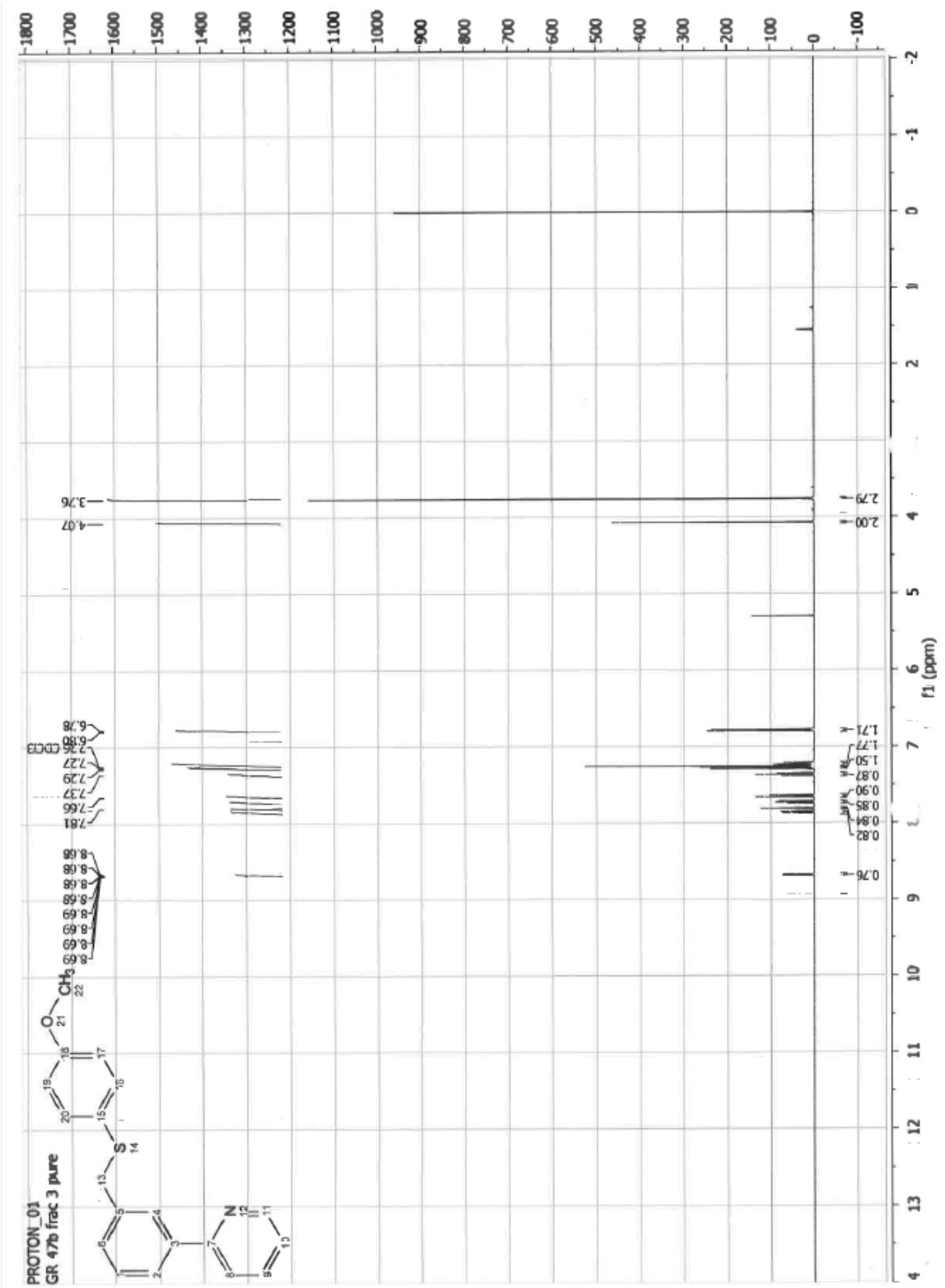
Analysis Info

Analysis Name	D:\Data\Alinanopos\GAVIN3044_000001.d	Acquisition Date	12/06/2013 15:38:22
Method	pos20090608esi	Operator	Administrator
Sample Name	POS ESI GR 29B	Instrument	apex-III
Comment			

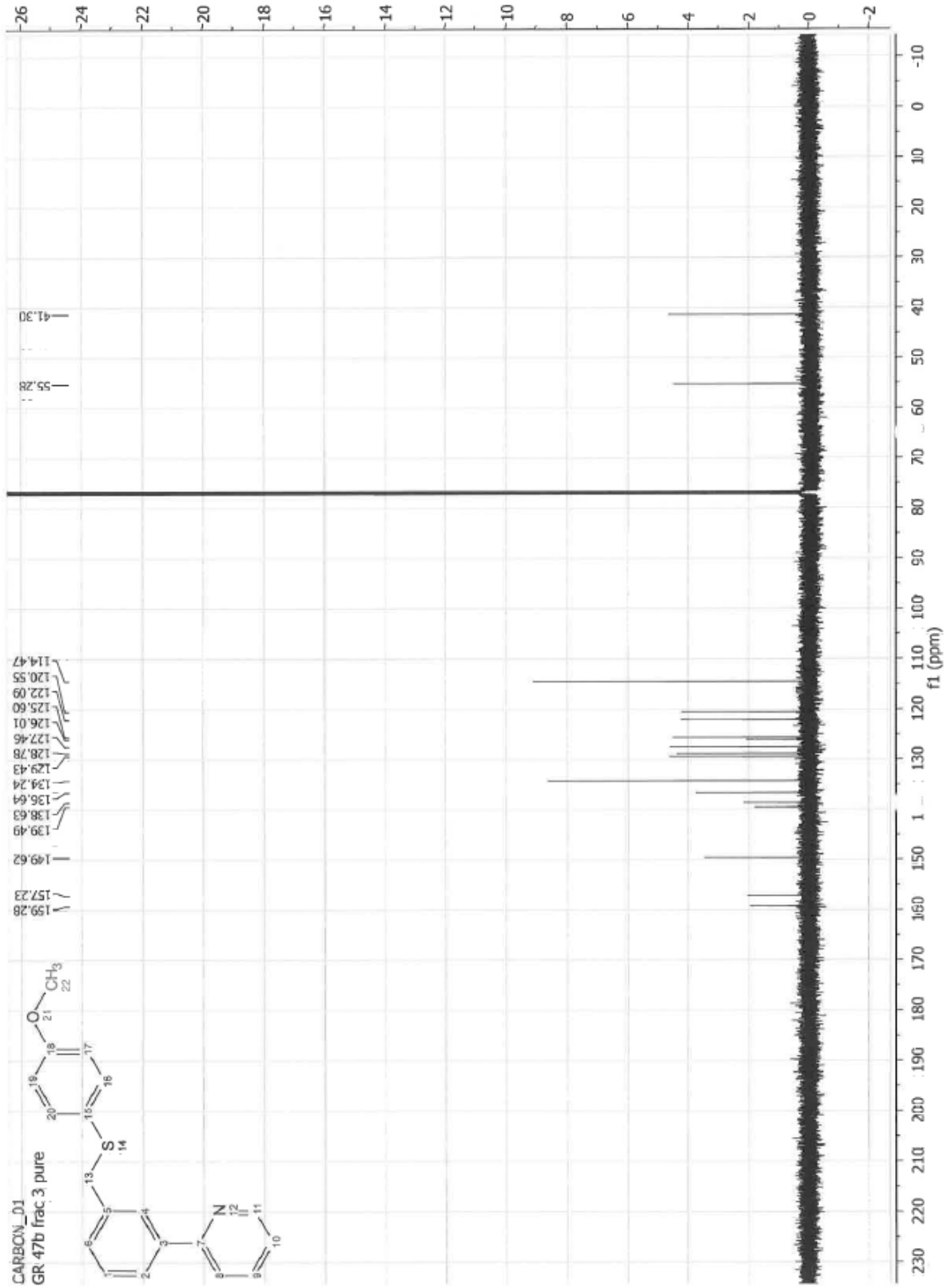


Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 19 H 18 N 1 S 1	0.027	292.1154	1.11	0.75	0.22	11.50	ok	even

2-(3-[(4-Methoxyphenyl)sulfanyl]methylphenyl)pyridine, 6f. ^{1}H NMR



2-(3-[(4-Methoxyphenyl)sulfanyl]methylphenyl)pyridine, 6f. ^{13}C NMR

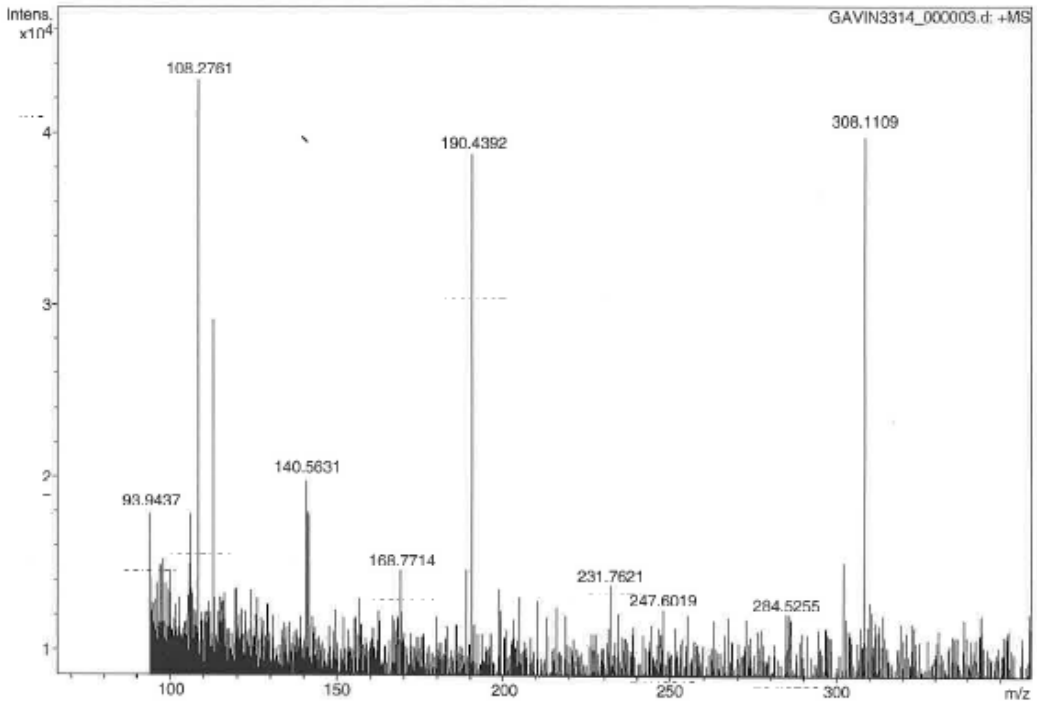


2-(3-[(4-Methoxyphenyl)sulfanyl]methylphenyl)pyridine, 6f. HRMS

Generic Display Report

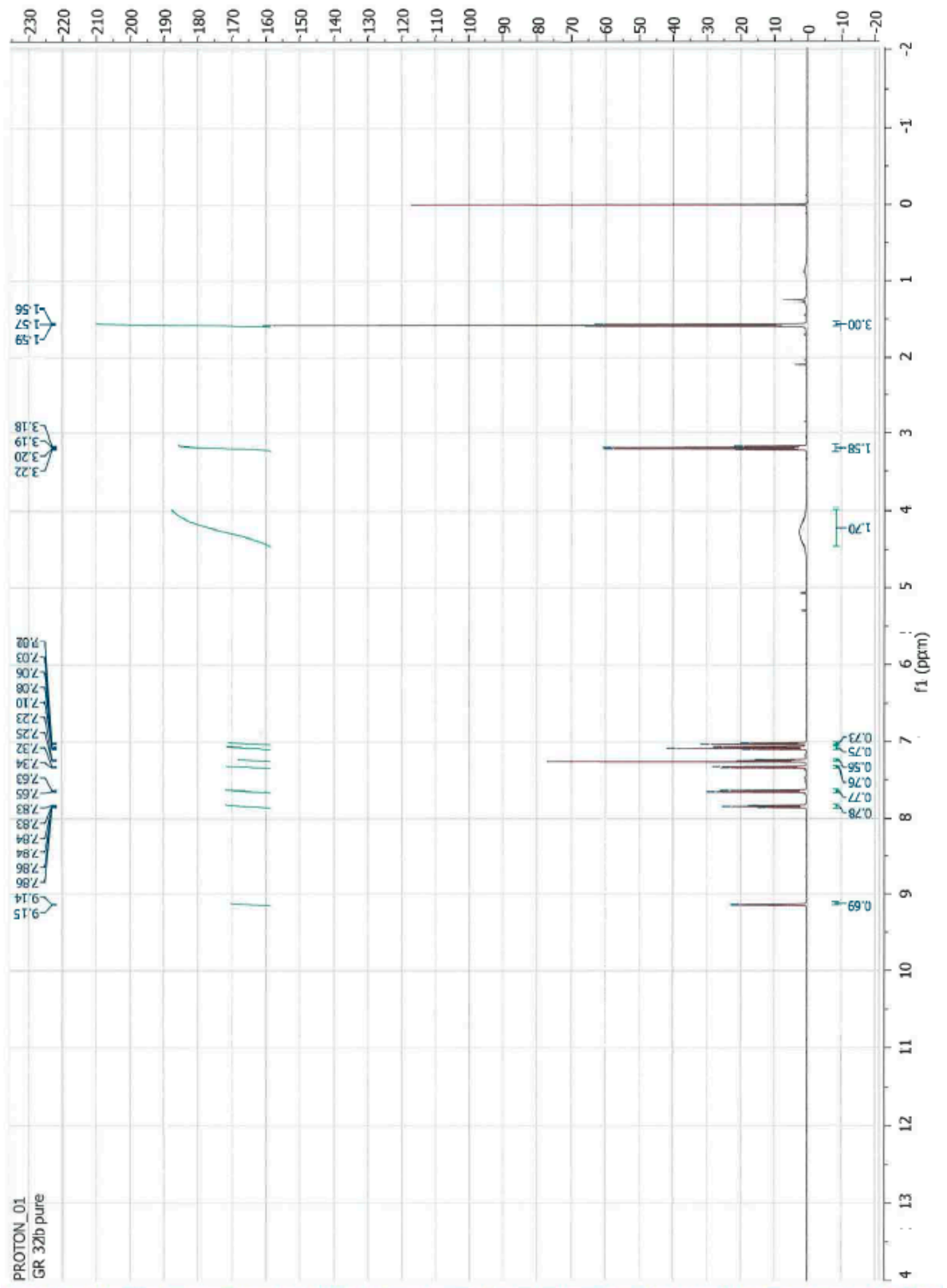
Analysis Info

Analysis Name	D:\Data\Alinanopos\GAVIN3314_000003.d	Acquisition Date	28/10/2013 15:53:24
Method	pos20090608esi	Operator	Administrator
Sample Name	POS ESI GR47B	Instrument	apex-III
Comment			

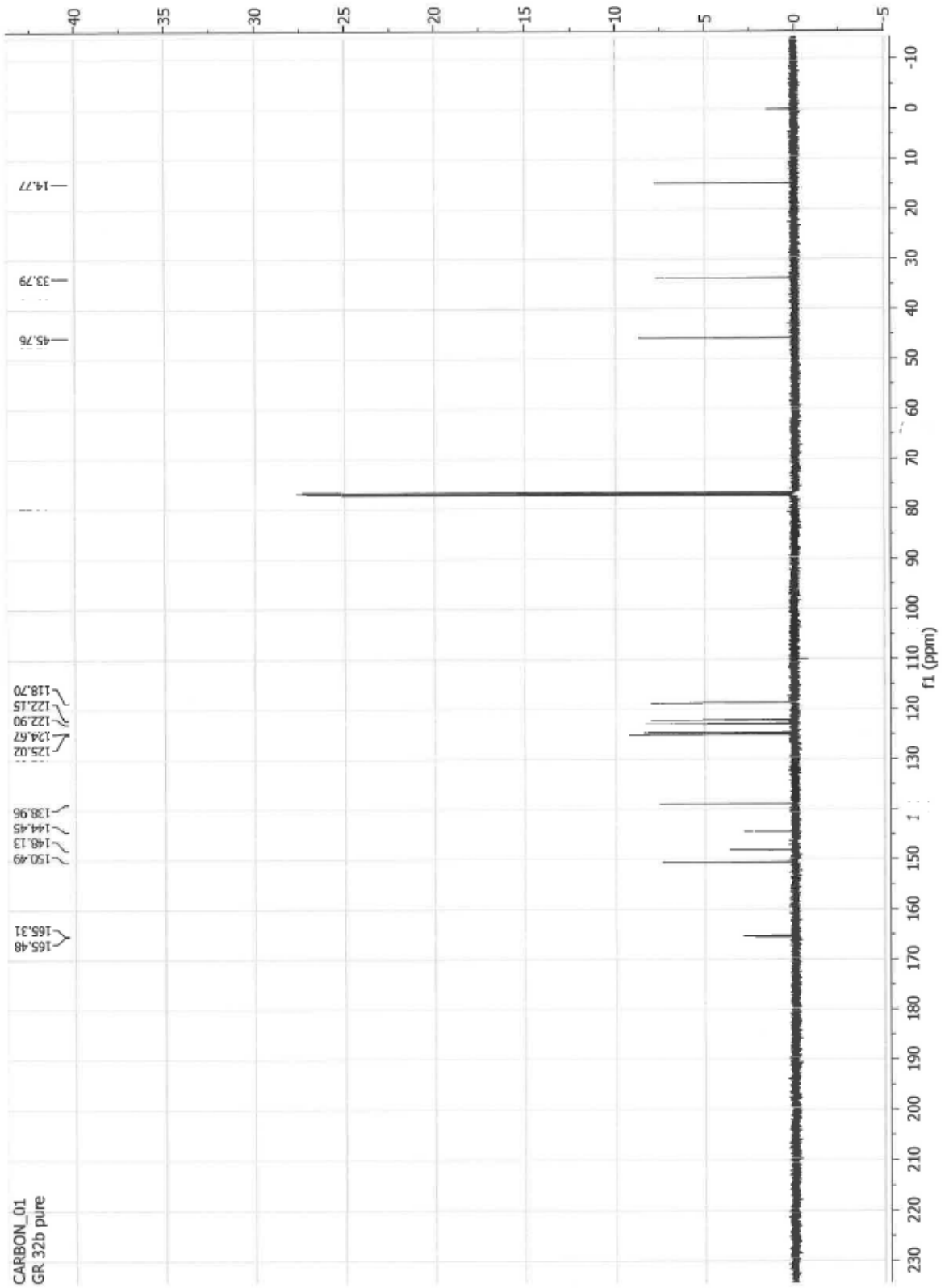


Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 19 H 18 N 1 O 1 S 1	0.147	308.1104	-1.76	-20.59	-6.36	11.50	ok	even

2-3-[(Ethylsulfanyl)methyl]phenylpyridine chloro-palladacycle, 1b. ^{1}H NMR



2-3-[(Ethylsulfanyl)methyl]phenylpyridine chloro-palladacycle, 1b. ^{13}C NMR



2-3-[(Ethylsulfanyl)methyl]phenylpyridine chloro-palladacycle, 1b. HRMS

Generic Display Report

Analysis Info

Analysis Name	D:\Data\Alinanopos\GAVIN3160_000001.d	Acquisition Date	12/08/2013 13:22:19
Method	pos20090608esi		
Sample Name	POS ESI GR32B	Operator	Administrator
Comment		Instrument	apex-III

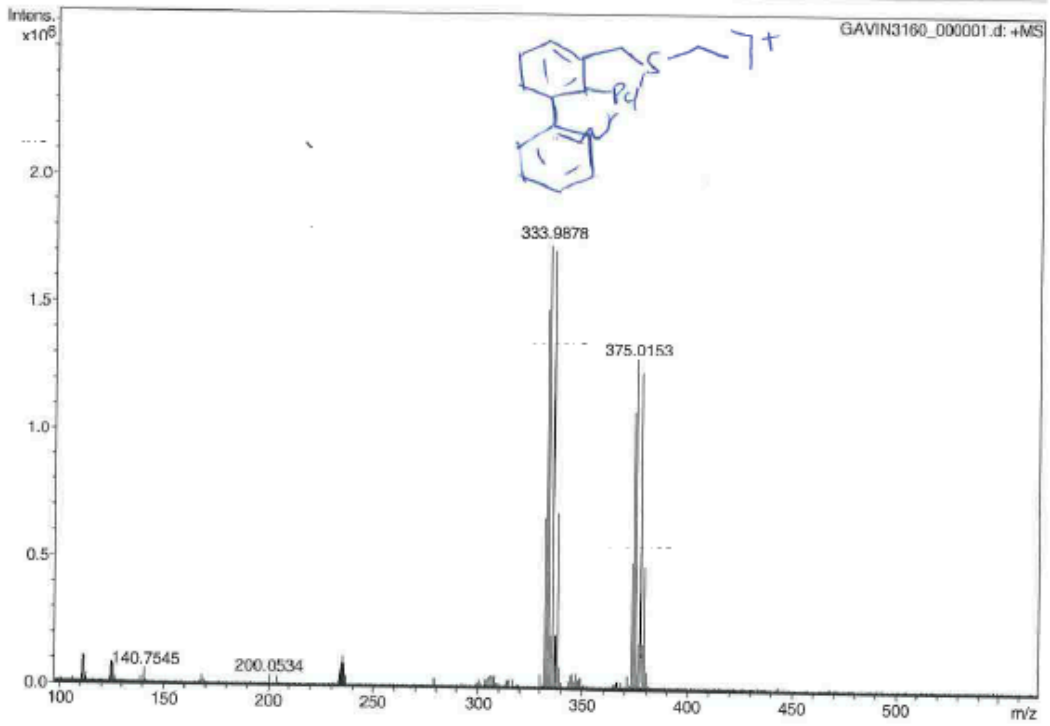


Table 'GenFormulaResults' could not be found in this analysis

2-3-[(Ethylsulfanyl)methyl]phenylpyridine chloro-palladacycle, 1b. Elemental Analysis

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metropolitan
university

tal Analysis Service

Please send completed form ... es to:

Stephen Boyer
School of Human Sciences
Science Centre
London Metropolitan University
29 Hornsey Road
London N7 7DD

Telephone: 020 7133 3605
Fax: 020 7133 2577
Email: s.boyer@londonmet.ac.uk

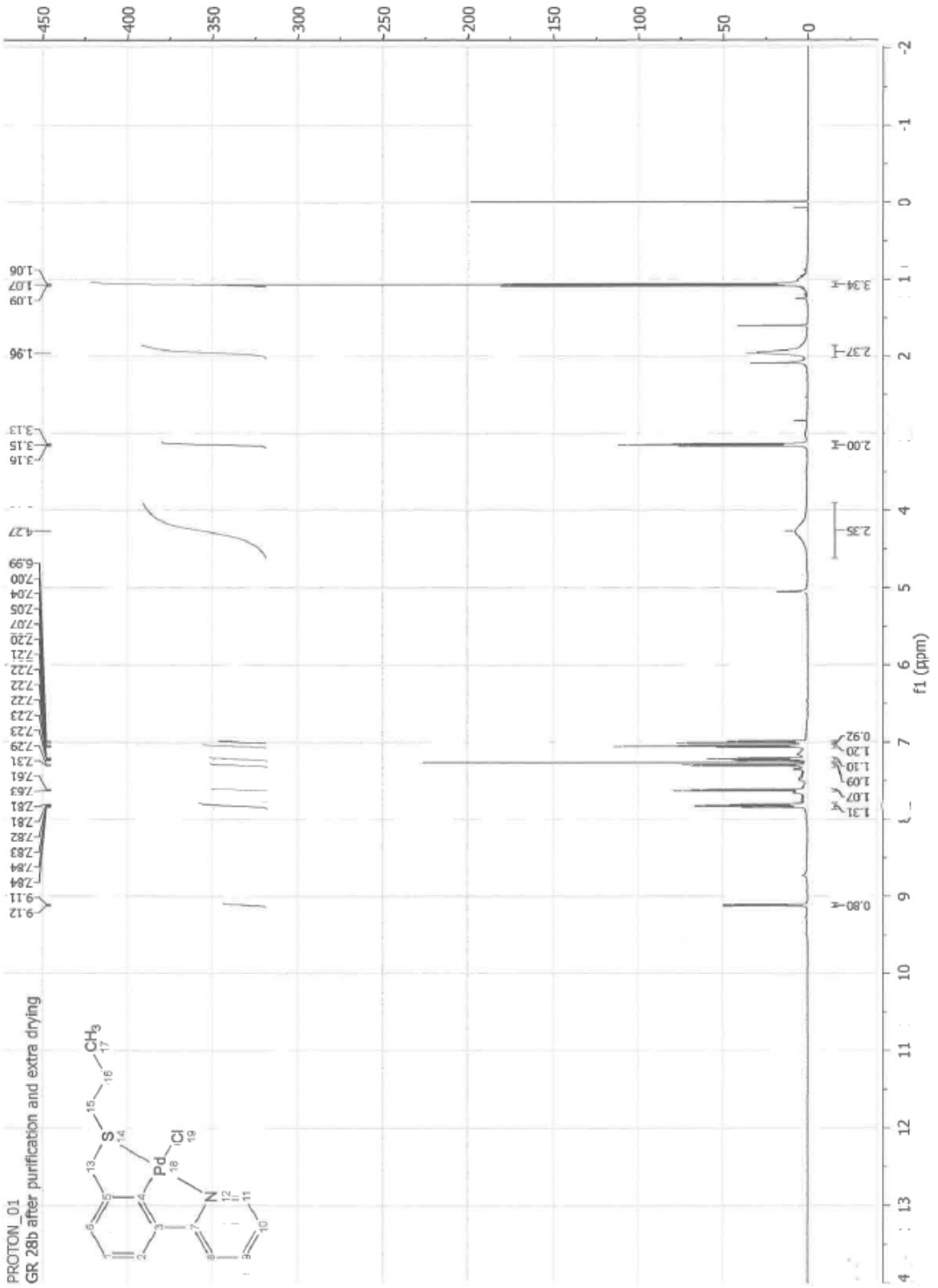
Sample submitted by: Gavin Roffe
Address: Department of Chemistry, Arundel building, Sussex University, Falmer, Brighton, BN1 9RH
Telephone: 07584 291754 Email: gwr20@sussex.ac.uk
Date Submitted: 12/7/13

Please submit ca. 5 mg of sample.

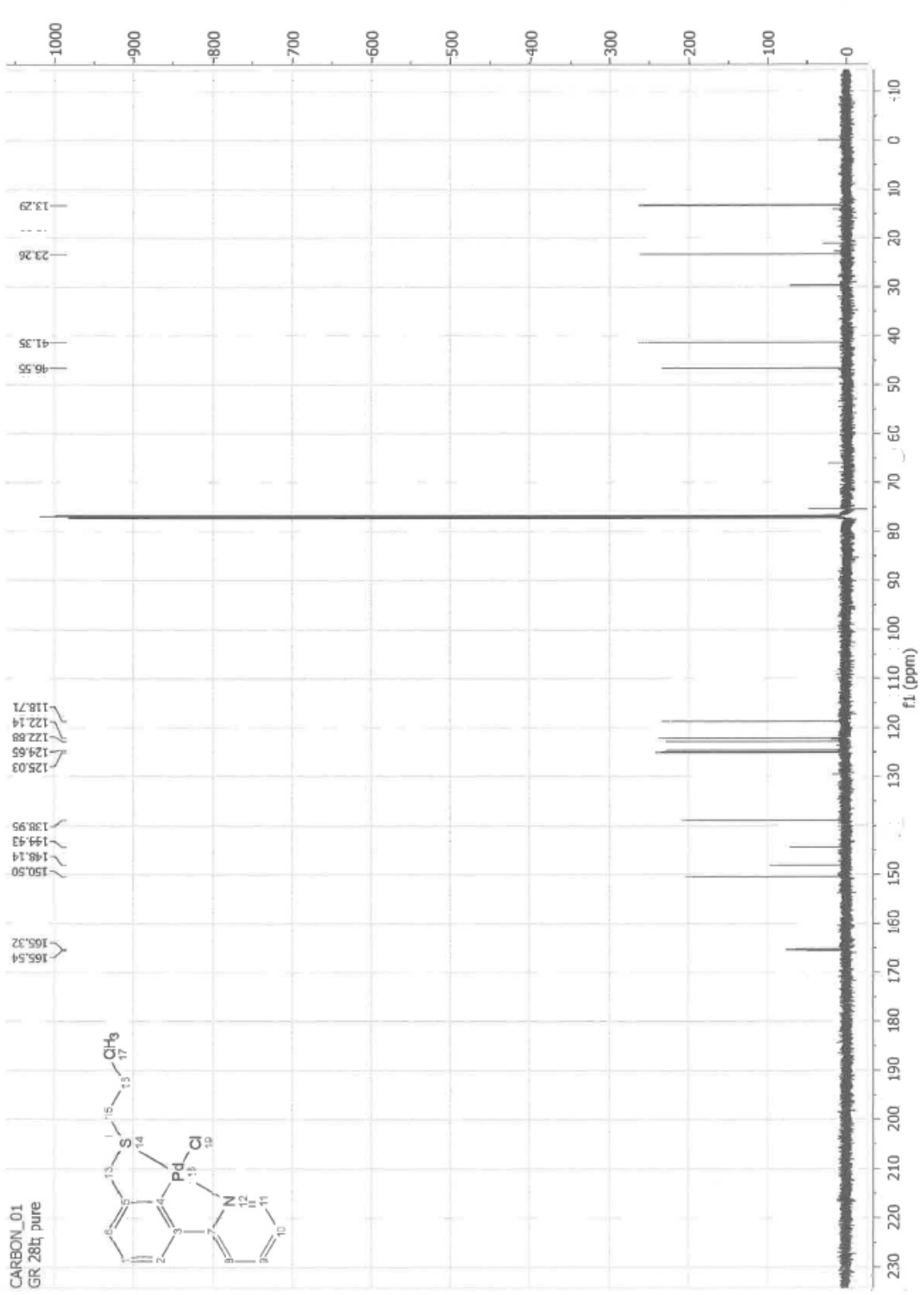
Sample Reference No.: GR 32b
Name of Compound: NCS Pincer Palladacycle - pyrSEt
Molecular Formula:$C_{14}H_{14}ClNPdS$
Stability: Stable to air and moisture
Hazards: Unknown. Standard PPE.
Other Remarks:

Element	Expected %	Found (1)	Found (2)	
Carbon	45.42	45.50	45.54	
Hydrogen	3.81	3.70	3.75	
Nitrogen	3.78	3.83	3.86	

2-3-[(Propylsulfanyl)methyl]phenylpyridine chloro-palladacycle, 1c. ^{1}H NMR



2-3-[(Propylsulfanyl)methyl]phenylpyridine chloro-palladacycle, 1c. ^{13}C NMR



2-3-[(Propylsulfanyl)methyl]phenylpyridine chloro-palladacycle, 1c. HRMS

Generic Display Report

Analysis Info

Analysis Name	D:\Data\Alinanopos\GAVIN3170_000002.d	Acquisition Date	19/08/2013 15:07:41
Method	pos20090608esi		
Sample Name	POS ESI GRSPR PDCYCLE	Operator	Administrator
Comment		Instrument	apex-III

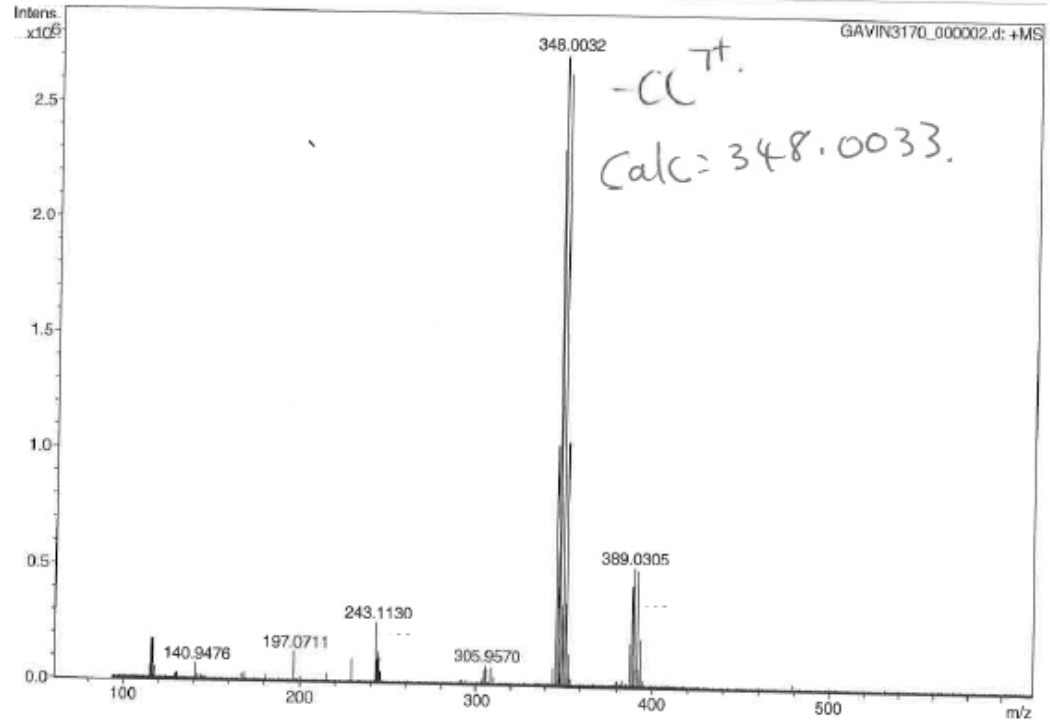


Table 'GenFormulaResults' could not be found in this analysis

2-3-[(Propylsulfanyl)methyl]phenylpyridine chloro-palladacycle, 1c. Elemental Analysis

LONDON metropolitan university

Elemental Analysis Service

Please send completed form and samples to:

Stephen Boyer
School of Human Sciences
Science Centre
London Metropolitan University
29 Hornsey Road
London N7 7DD

Telephone: 020 7133 3605
Fax: 020 7133 2577
Email: s.boyer@londonmet.ac.uk

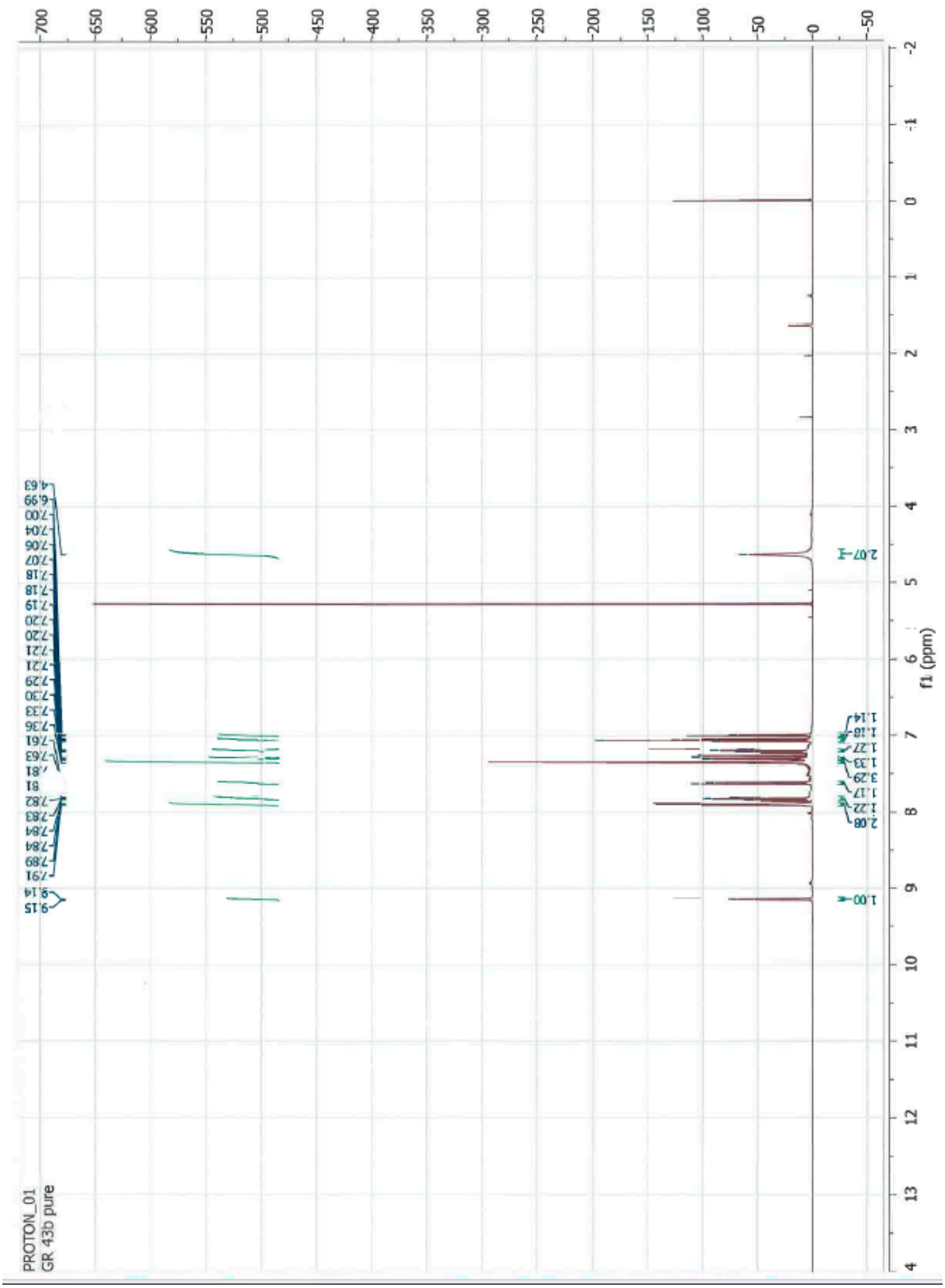
Sample submitted by:	Gavin Rolfe.
Address:	Department of Chem, Arundel Building, Uni of Sussex, BN1 9RH.
Telephone: Email:	gwr20@sussex.ac.uk
Date Submitted:	30/6/14

Please submit ca. 5 mg of sample.

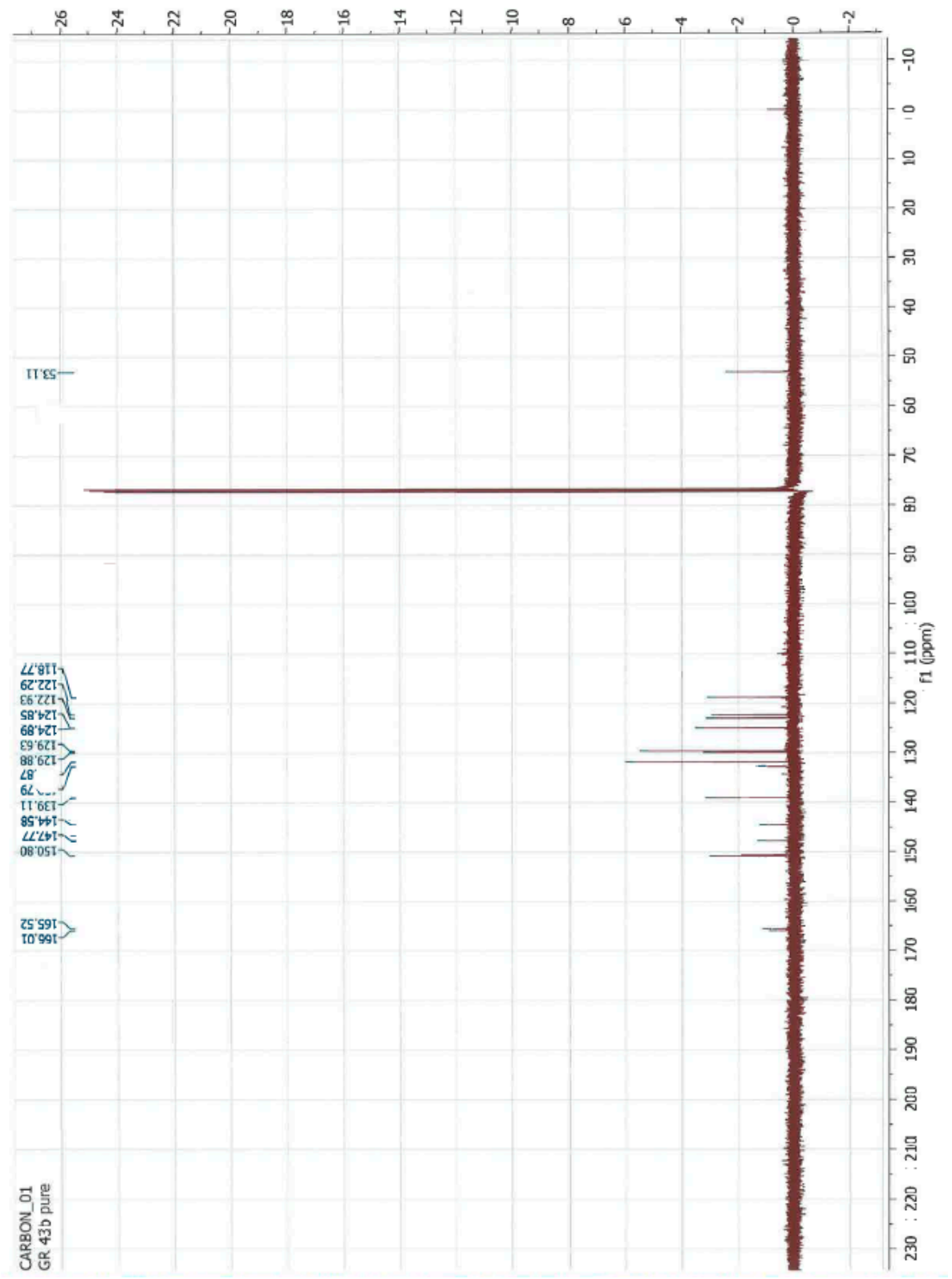
Sample Reference No.:	GR286-4
Name of Compound:	SPr Polycle
Molecular Formula:	
Stability:	✓
Hazards:	✓
Other Remarks:	

Element	Expected %	Found (1)	Found (2)	
Carbon	46.89	47.02	47.04	
Hydrogen	4.20	4.08	4.15	
Nitrogen	3.65	3.56	3.60	

2-3-[(Phenylsulfanyl)methyl]phenylpyridine chloro-palladacycle, 1d. ^{1}H NMR



2-3-[(Phenylsulfanyl)methyl]phenylpyridine chloro-palladacycle, 1d. ^{13}C NMR



2-3-[(Phenylsulfanyl)methyl]phenylpyridine chloro-palladacycle, 1d. HRMS

Generic Display Report

Analysis Info

Analysis Name	D:\Data\Alinanopos\GAVIN4406A_000001.d	Acquisition Date	16/05/2014 12:51:25
Method	pos20090608esi	Operator	Administrator
Sample Name	POS ESI GR 43B	Instrument	apex-III
Comment			

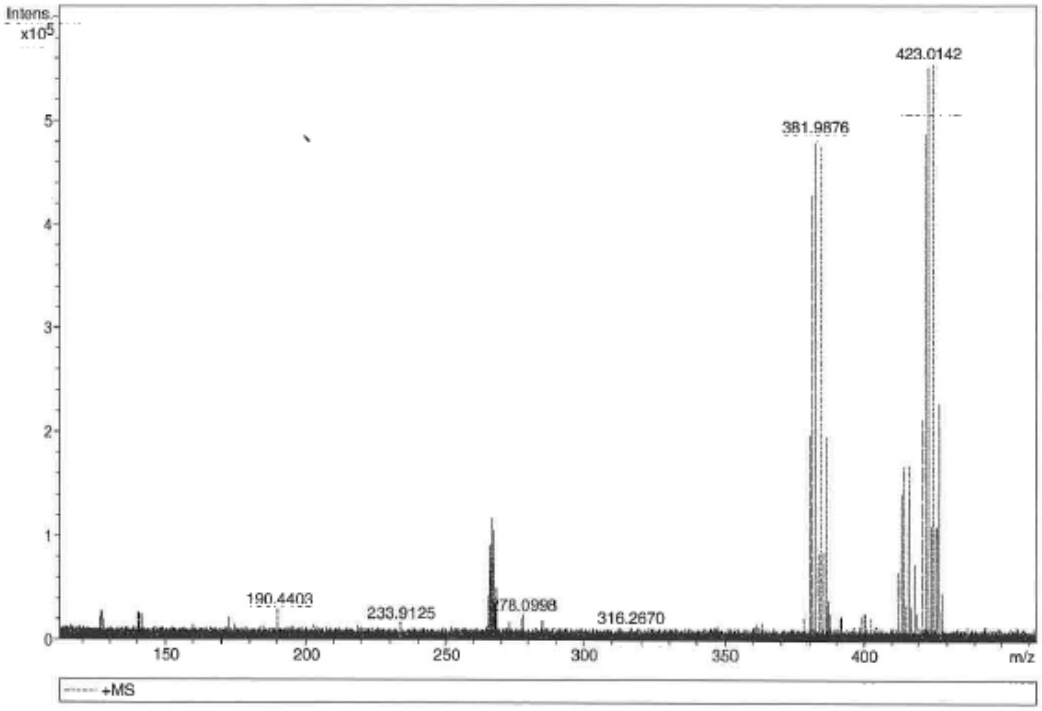


Table 'GenFormulaResults' could not be found in this analysis

2-3-[(Phenylsulfanyl)methyl]phenylpyridine chloro-palladacycle, 1d. Elemental Analysis

LONDON metropolitan university

Elemental Analysis Service

Please send completed form and samples to:

Stephen Boyer
School of Human Sciences
Science Centre
London Metropolitan University
29 Hornsey Road
London N7 7DD

Telephone: 020 7133 3605
Fax: 020 7133 2577
Email: s.boyer@londonmet.ac.uk

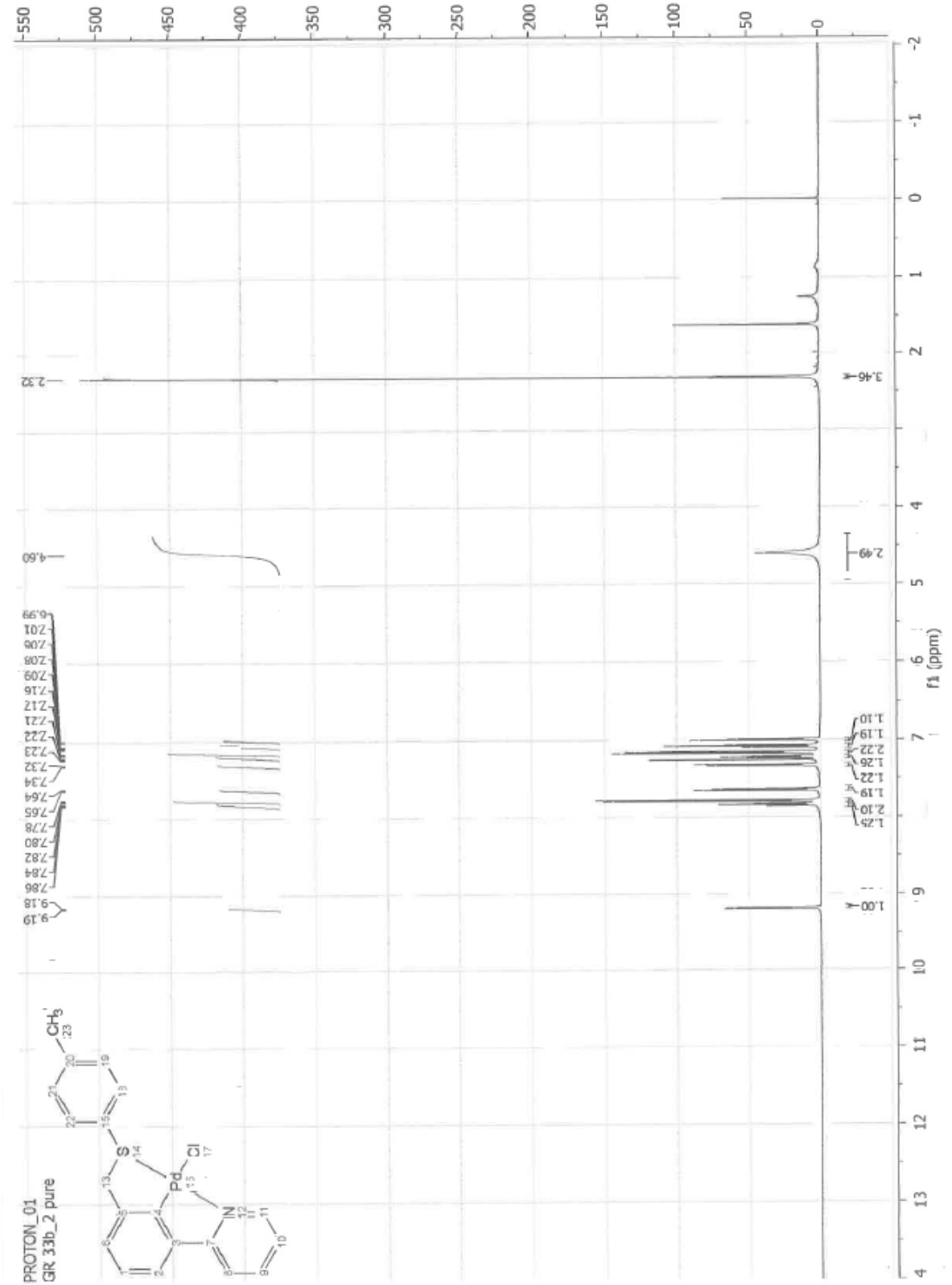
Sample submitted by: Gavin Rothe.
Address: Department of Chemistry, Arundel building, Sussex University, Falmer, Brighton, BN1 9RH
Telephone: 07584 291754 Email: gwr20@sussex.ac.uk
Date Submitted: 15/5/14.

Please submit ca. 5 mg of sample.

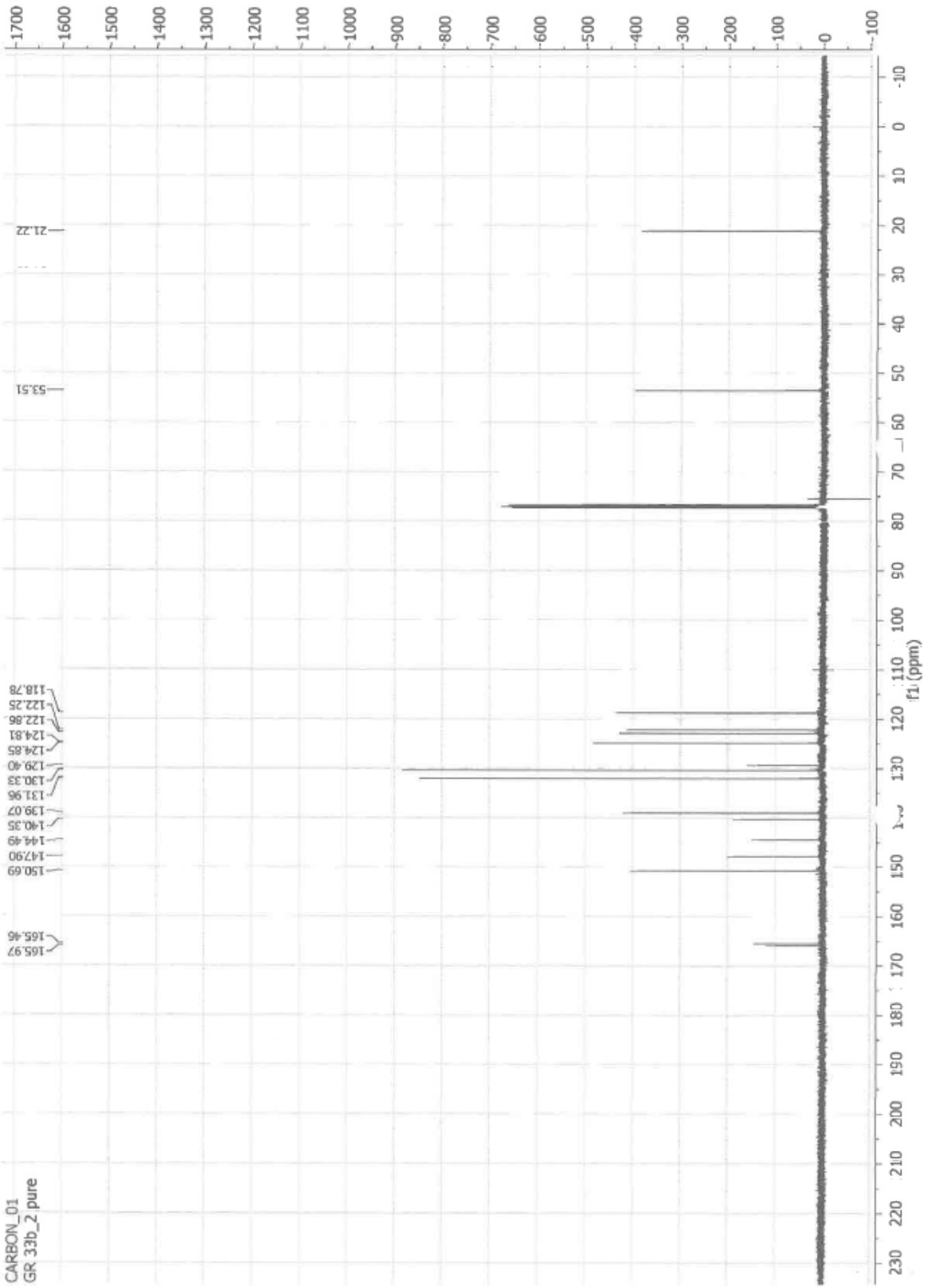
Sample Reference No.: GR43b.
Name of Compound: SPh palladacycle.
Molecular Formula: $C_{18}H_{14}ClNPdS$.
Stability: Stable to air and moisture
Hazards: Unknown. Standard PPE.
Other Remarks:

Element	Expected %	Found (1)	Found (2)	
Carbon	51.69	51.50	51.45	
Hydrogen	3.37	3.26	3.24	
Nitrogen	~~3.35~~ 3.35	3.41	3.47	

2-(3-[(4-Methylphenyl)sulfanyl]methylphenyl)pyridine, 1e. ^{1}H NMR



2-(3-[(4-Methylphenyl)sulfanyl]methylphenyl)pyridine, 1e. ^{13}C NMR



2-(3-[(4-Methylphenyl)sulfanyl]methylphenyl)pyridine, 1e. HRMS

Generic Display Report

Analysis Info

Analysis Name	D:\Data\Alinanopos\GAVIN3159_000001.d	Acquisition Date	12/08/2013 13:40:31
Method	pos20090608esi	Operator	Administrator
Sample Name	POS ESI GR STOL-PDCYCLE	Instrument	apex-III
Comment			

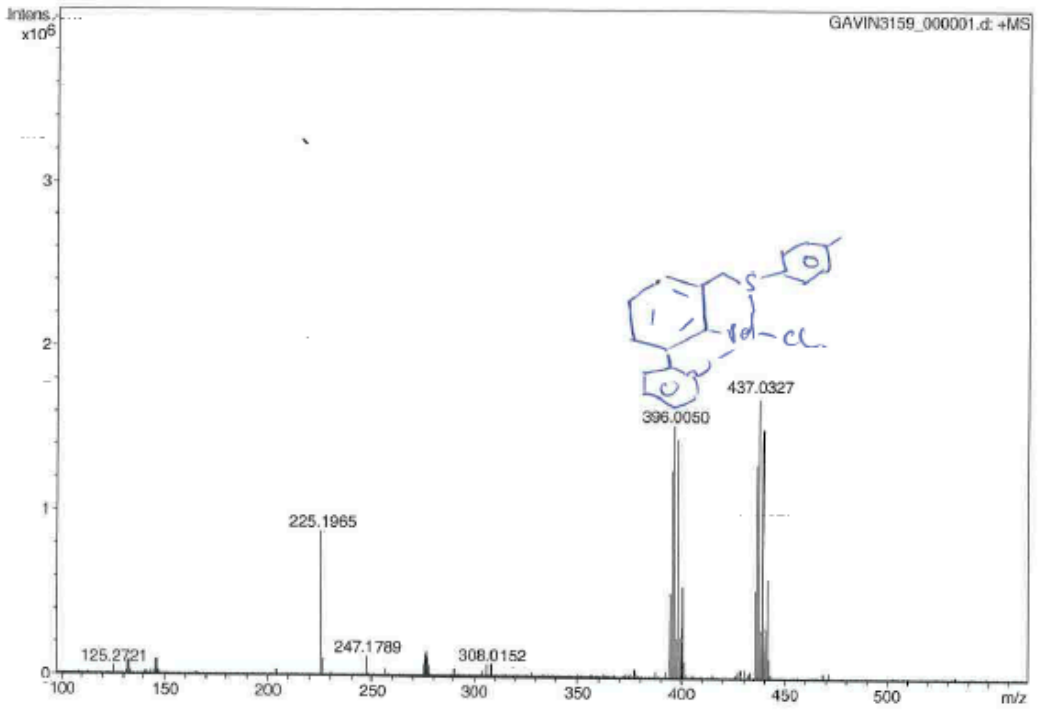


Table 'GenFormulaResults' could not be found in this analysis

Bruker Daltonics DataAnalysis 3.4 printed: 12/08/2013 13:41:20 Page 1 of 1

2-(3-[(4-Methylphenyl)sulfanyl]methylphenyl)pyridine, 1e. Elemental Analysis

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Stephen Boyer
School of Human Sciences
Science Centre
London Metropolitan University
29 Hornsey Road
London N7 7DD

Telephone: 020 7133 3605
Fax: 020 7133 2577
Email: s.boyer@londonmet.ac.uk

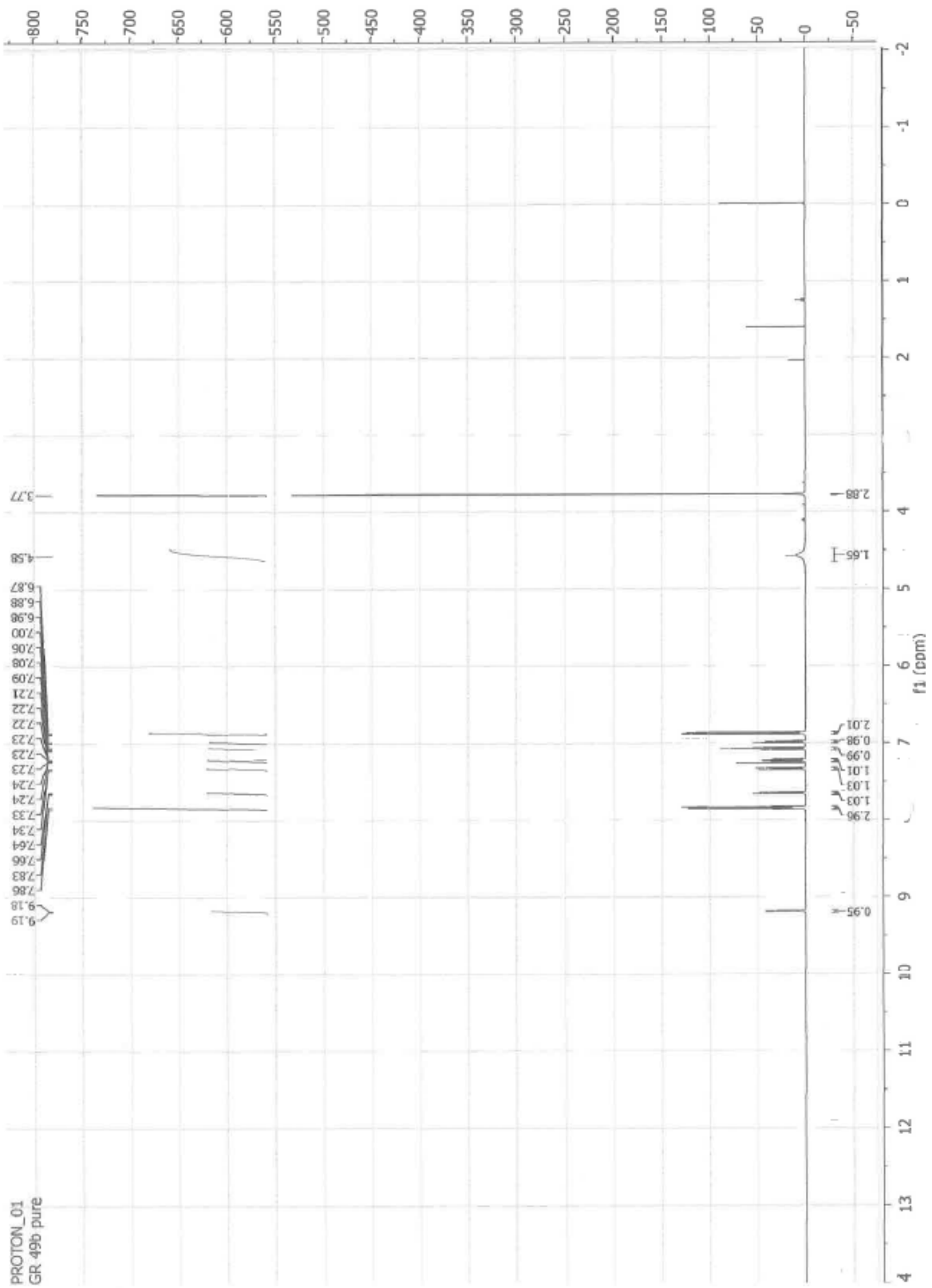
Sample submitted by: Gavin Roffe
Address: Department of Chemistry, Arundel building, Sussex University, Falmer, Brighton, BN1 9RH
Telephone: 07584 291754 Email: gwr20@sussex.ac.uk
Date Submitted: 12/7/13

Please submit ca. 5 mg of sample.

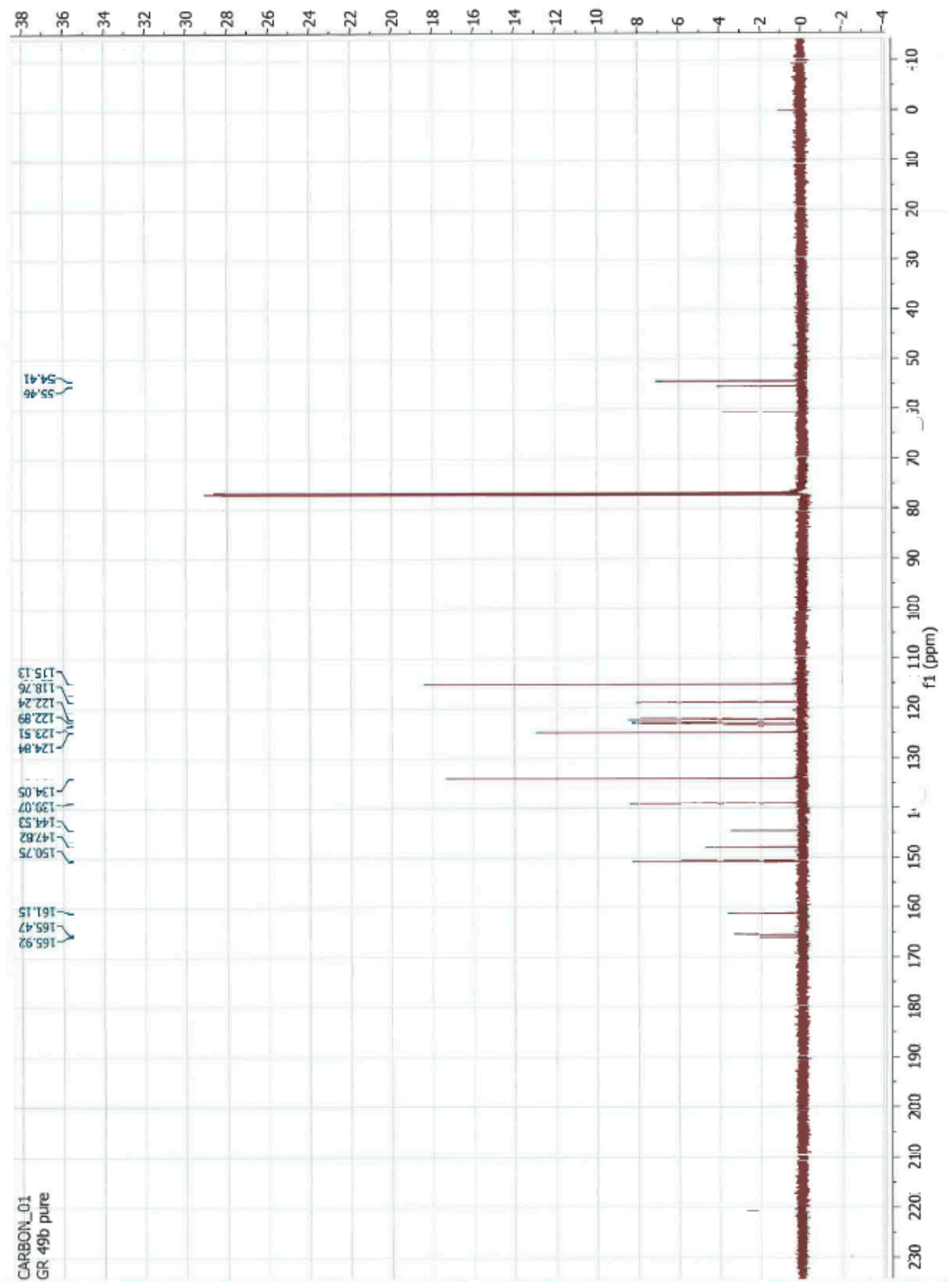
Sample Reference No.: GR 33b_2
Name of Compound: NCS Pincer Palladacycle - pyrSTol
Molecular Formula:$C_{19}H_{16}ClNPdS$
Stability: Stable to air and moisture
Hazards: Unknown. Standard PPE.
Other Remarks:

Element	Expected %	Found (1)	Found (2)	
Carbon	52.79	52.03	52.62	
Hydrogen	3.73	3.84	3.87	
Nitrogen	3.24	3.29	3.23	

2-(3-[(4-Methoxyphenyl)sulfanyl]methylphenyl)pyridine, 1f. ^{1}H NMR



2-(3-[(4-Methoxyphenyl)sulfanyl]methylphenyl)pyridine, 1f. ^{13}C NMR



2-(3-[(4-Methoxyphenyl)sulfanyl]methylphenyl)pyridine, 1f. HRMS

Generic Display Report

Analysis Info

Analysis Name	D:\Data\Alinanopos\GAVIN4411_000001.d	Acquisition Date	19/05/2014 16:39:58
Method	pos20090608esi	Operator	Administrator
Sample Name	POS ESI GR 49B	Instrument	apex-III
Comment			

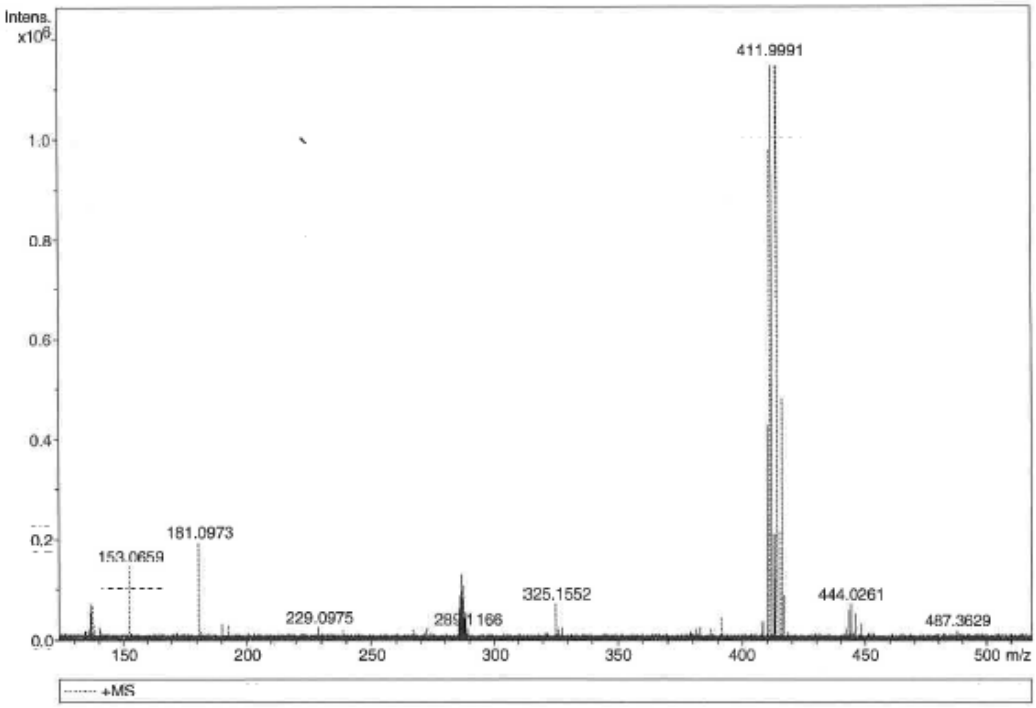


Table 'GenFormulaResults' could not be found in this analysis

2-(3-[(4-Methoxyphenyl)sulfanyl]methylphenyl)pyridine, 1f. Elemental Analysis

LONDON metropolitan university

Elemental Analysis Service

Please send completed form and samples to:

Stephen Boyer
School of Human Sciences
Science Centre
London Metropolitan University
29 Hornsey Road
London N7 7DD

Telephone: 020 7133 3605
Fax: 020 7133 2577
Email: s.boyer@londonmet.ac.uk

Sample submitted by: Gavin Roffe
Address: Department of Chemistry, Arundel building, Sussex University, Falmer, Brighton, BN1 9RH
Telephone: 07584 291754 Email: gwr20@sussex.ac.uk
Date Submitted: 18/11/13

Please submit ca. 5 mg of sample.

Sample Reference No.: GR 49b
Name of Compound: SCN Pincer Palladacycle - pyrNSOMe
Molecular Formula: $C_{19}H_{18}ClNOPdS$
Stability: Stable to air and moisture
Hazards: Unknown. Standard PPE.
Other Remarks:

Element	Expected %	Found (1)	Found (2)	
Carbon	50.91	50.73	50.80	
Hydrogen	3.60	3.51	3.47	
Nitrogen	3.12	3.14	3.19	