Electronic Supplementary Information (ESI) for:

Structural analysis of monometallic ruthenium–arene complexes using ion mobility mass spectrometry, collision-induced dissociation, and density functional theory

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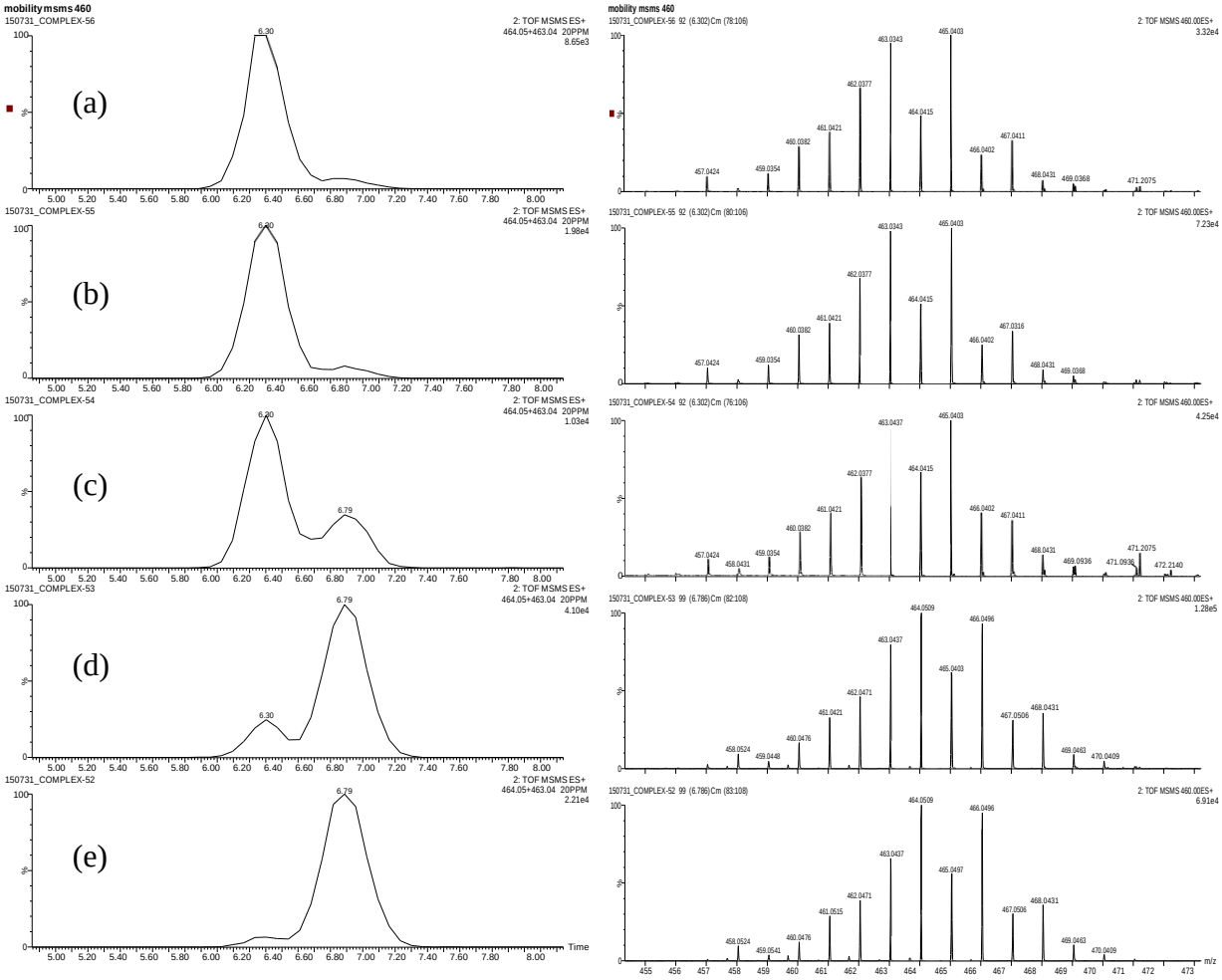

Fig. S1 Influence of flushing the ESI source on the IM-MS analysis of complex **3** in 1,2-dichloroethane: arrival drift time distributions (ATDs) of the ions (left) and MS spectra generated at once from both peaks for each ATD (right). Experimental conditions: extensive flushing with 1,2-dichloroethane between each infusion (a), flushing with 1,2-dichloroethane (b), no flushing (c), flushing with water (d), and extensive flushing with water (e).

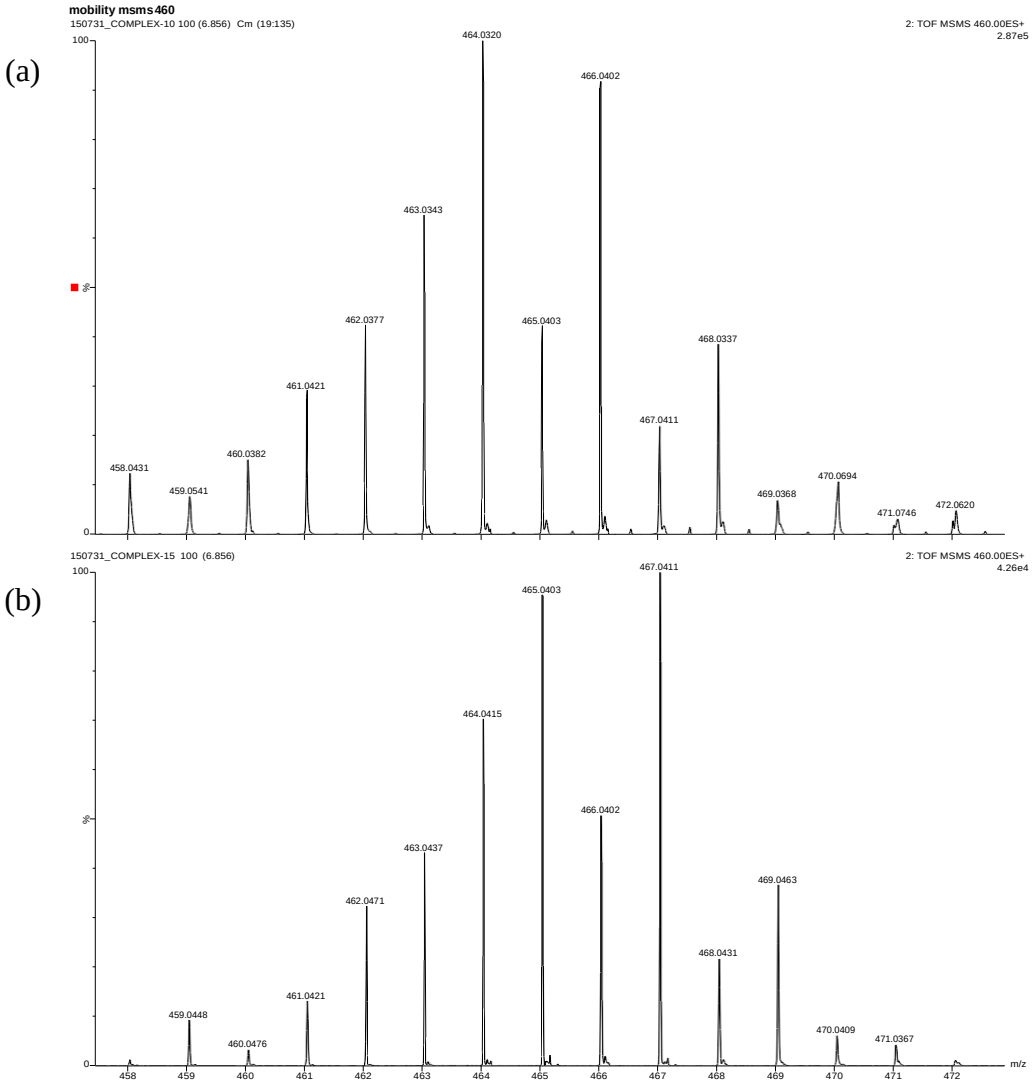

Fig. S2 ESI-MS spectra of complex **3** in H_2O (a) and D_2O (b).

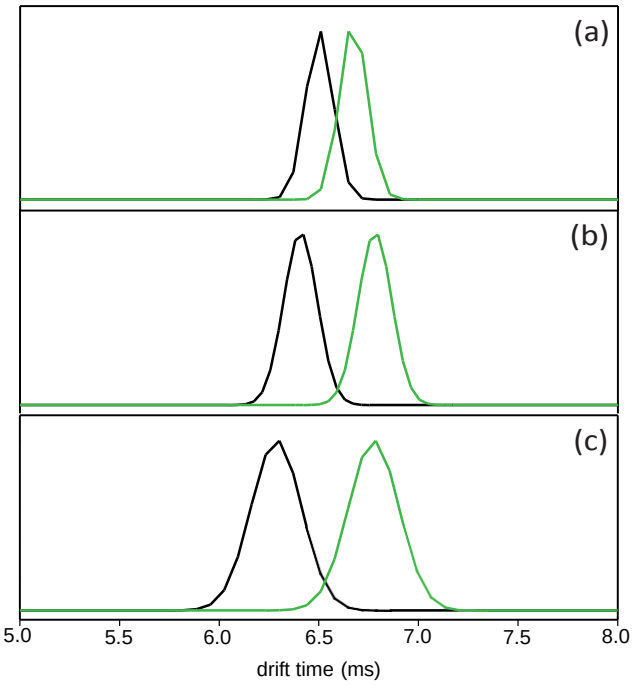

Fig. S3 Deconvoluted and normalized ATDs of the [$Ru^{III}Cl_2$(*p*-cymene)(PTA)]+ (black curves) and [$RuCl_2$(*p*-cymene)(PTA+H)]$^+$ ions (green curves) using helium (a), dinitrogen (b), or carbon dioxide (c) as buffer gas.

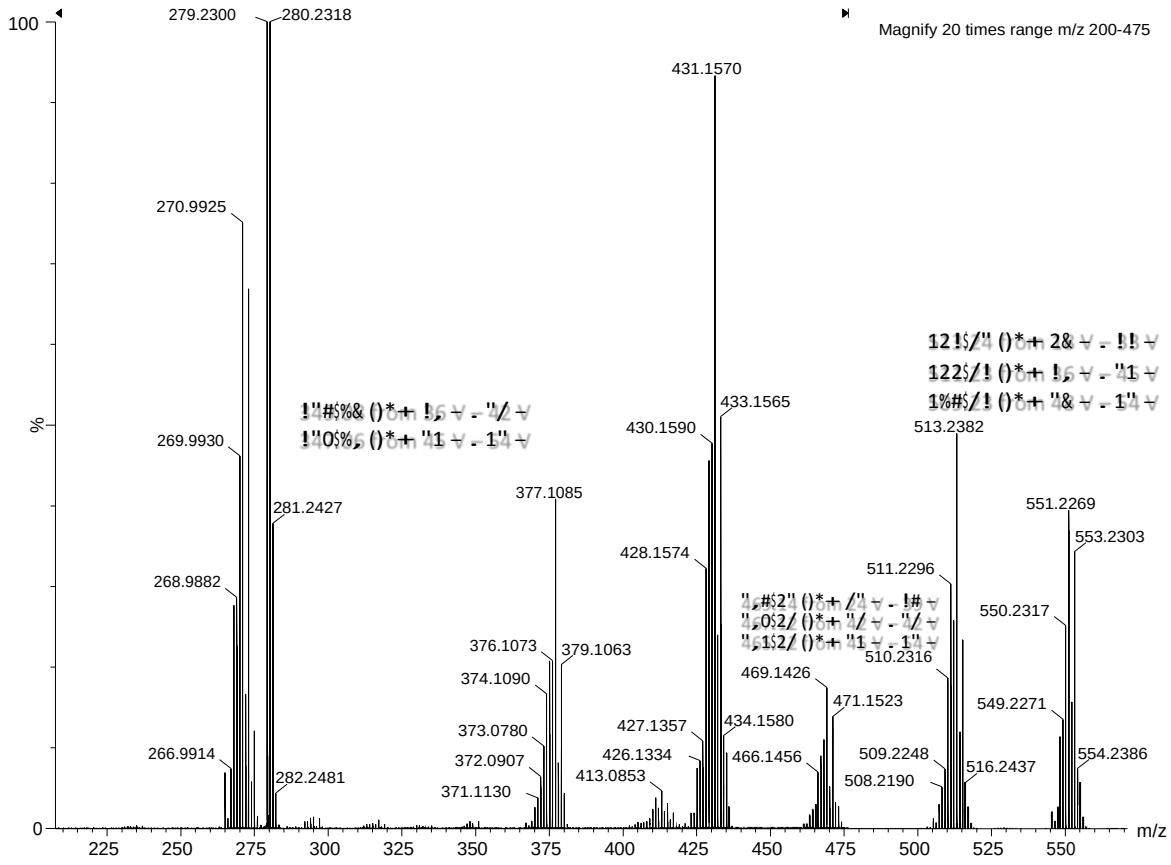

Fig. S4 MS/MS spectrum of complex **1** obtained upon CID in the transfer cell of the IM-MS spectrometer.

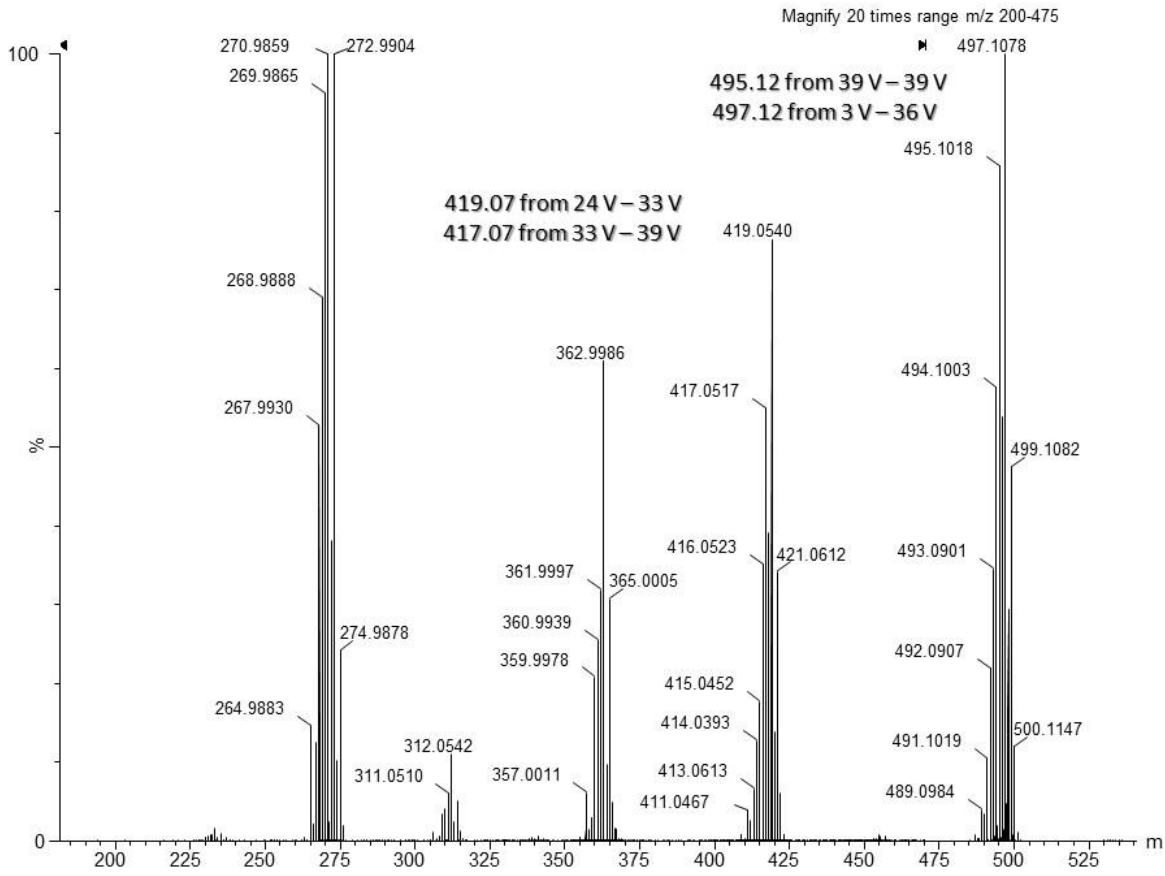

Fig. S5 MS/MS spectrum of complex **2** obtained upon CID in the transfer cell of the IM-MS spectrometer.

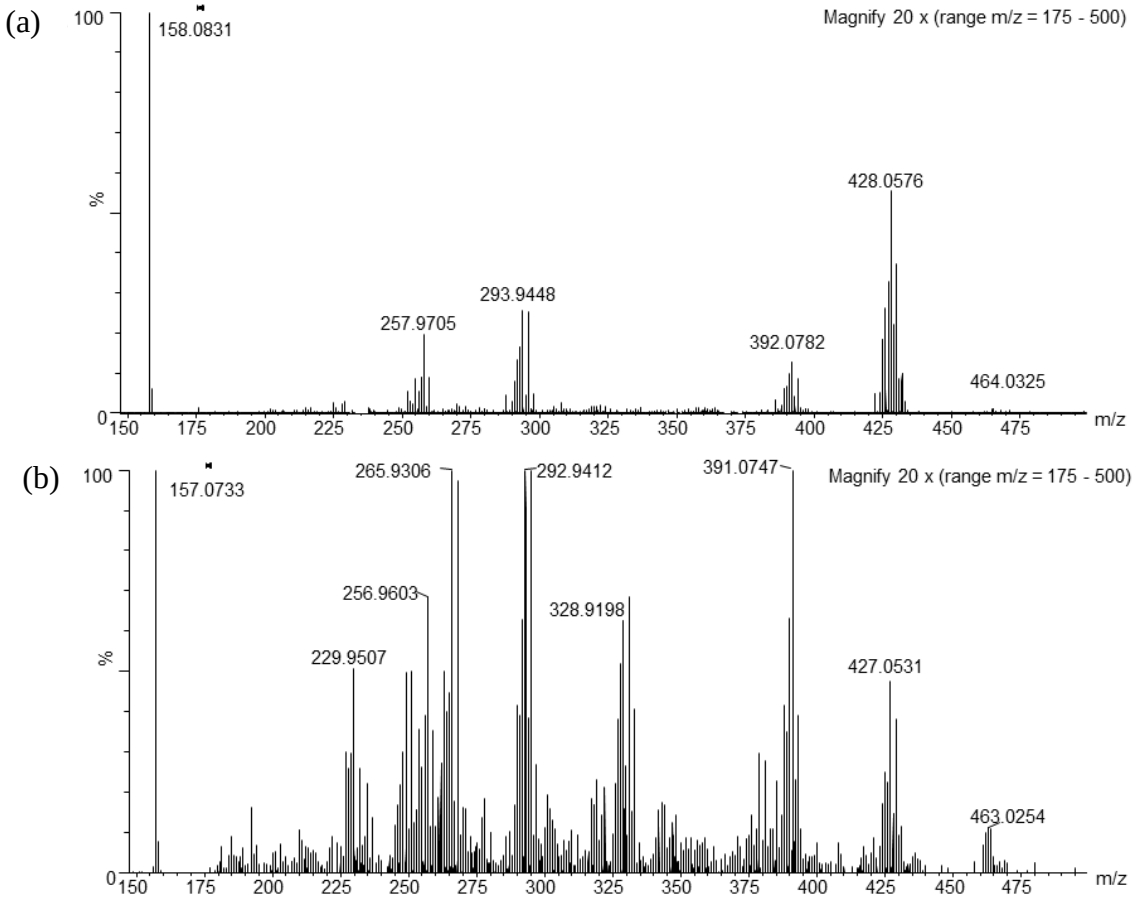

Fig. S6 IM-MS/MS spectra of complex **3** obtained upon CID in the transfer cell of the IM-MS spectrometer at 33 V of transfer performed at arrival drift times of 6.79 (a) and 6.30 ms (b).

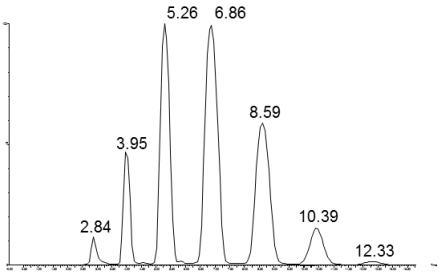

Fig. S7 ATDs of the seven tetraalkylammonium ions used for mobility calibration with drift times in milliseconds (tetraethylammonium, tetrapropylammonium, tetrabutylammonium, tetrapentylammonium, tetrahexylammonium, tetraheptylammonium, and tetraoctylammonium).

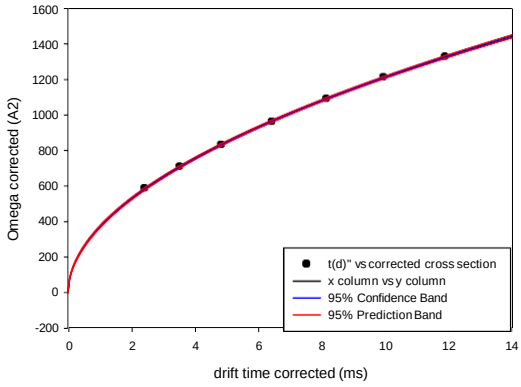

Fig. S8 Calibration curve of the drift time (corrected for mass-dependent flight time spent between the transfer region and the mass analyzer) *vs.* collision cross section (corrected for reduced mass and charge) for a wave velocity of 1000 m s^{-1} and a wave height of 40 V.

Table S1 Optimization of the peak separation for the IM-MS analysis of complex **3**

Run	Wave velocity/m s^{-1}	Wave height/V	Drift time of the first peak/ms	Drift time of the second peak/ms
1	800	40	4.99	5.40
2	1100	40	6.99	7.55
3	1000	35	8.03	8.43
4	1000	45	6.23	6.50
5	1000	40	6.30	6.79

Table S2 Comparison of experimental CCS values determined in dinitrogen for complexes **1**–**3** with theoretical values computed in helium using MOBCAL

Molecular ion	CCS/Å^2			
	Exp.[a]	PA[b]	EHSS[b]	TM[b]
[RuCl(*p*-cymene)(PCy_3)]$^+$	211 ± 1	145	161	152
[RuCl(*p*-cymene)(PPh_3)]$^+$	203 ± 1	140	156	146
[$Ru^{III}Cl_2$(*p*-cymene)(PTA)]$^+$	179 ± 1	115	124	118
[$RuCl_2$(*p*-cymene)(PTA+H)]$^+$	187 ± 1	115	124	116

[a]Experimental CCS values obtained by TWIG in dinitrogen *vs.* tetraalkylammonium bromide calibrants. [b]Theoretical CCS values in helium computed using the Projection Approximation (PA) Monte Carlo method, the Exact Hard Sphere Scattering (EHSS) method, and the Trajectory Method (TM) of the MOBCAL software.

Table S3 Molecular ion and fragments derived from complex **1** ($C_{28}H_{47}Cl_2PRu$) detected by MS/MS CID at 33 V in the transfer cell

Elemental composition	**Measured mass/Da**	**Theoretical mass/Da**	**Difference/ppm**	**Intensity/a.u.**
$C_{28}H_{47}ClPRu^+$	551.2269	551.214631	22	300000
$C_{28}H_{44}PRu^+$	513.2382	513.222629	30	380000
$C_{22}H_{37}ClPRu^+$	469.1521	469.136208	34	6520
$C_{22}H_{34}PRu^+$	431.1570	431.144734	28	37200
$C_{21}H_{28}PRu^+$	413.0764	413.097228	–50	1620
$C_{16}H_{24}PRu^+$	349.0805	349.065797	42	400
$C_{12}H_{18}PRu^+$	295.0305	295.018739	40	603
$C_{18}H_{32}P^+$	279.2300	279.223614	23	771000
$C_7H_{19}ClPRu^+$	270.9925	270.994941	–9	30700
$C_{10}H_{11}Ru^+$	232.9939	232.990142	16	806

Table S4 Molecular ion and fragments derived from complex **2** ($C_{28}H_{29}Cl_2PRu$) detected by MS/MS CID at 33 V in the transfer cell

Elemental composition	**Measured mass/Da**	**Theoretical mass/Da**	**Difference/ppm**	**Intensity/a.u.**
$C_{28}H_{29}ClPRu^+$	533.0818	533.073704	15	348
$C_{28}H_{28}PRu^+$	497.1078	497.097423	21	6270000
$C_{22}H_{23}ClPRu^+$	455.0399	455.026653	29	2170
$C_{22}H_{22}PRu^+$	419.0540	419.050302	9	240000
$C_{18}H_{14}PRu^+$	362.9986	362.987589	30	191000
$C_{16}H_{16}PRu^+$	341.0098	341.003187	19	1740
$C_{13}H_{23}PRu^+$	312.0542	312.057893	–12	34500
$C_7H_{19}ClPRu^+$	270.9859	270.994941	–33	551000
$C_{10}H_{11}Ru^+$	232.9941	232.990142	17	4820

Table S5 Molecular ion and fragments derived from the oxidized form of complex **3** ($C_{16}H_{26}Cl_2N_3P$) detected by MS/MS CID at 33 V in the transfer cell

Elemental composition	Measured mass/Da	Theoretical mass/Da	Difference/ppm	Intensity/a.u.
$C_{16}H_{26}Cl_2N_3PRu^+$	463.0254	463.027749	–5	62
$C_{16}H_{25}ClN_3PRu^+$	427.0531	427.051353	4	381
$C_{16}H_{24}N_3PRu^+$	391.0747	391.075007	–1	812
$C_6H_{12}Cl_2N_3PRu^+$	328.9198	328.917903	6	547
$C_6H_{11}ClN_3PRu^+$	292.9412	292.941516	–1	1050
$C_7H_7N_3PRu^+$	265.9306	265.941729	–42	998
$C_6H_{10}N_3PRu^+$	256.9603	256.965179	–19	548
$C_3H_{12}ClNPRu^+$	229.9507	229.943122	33	406
$C_6H_{12}N_3P^+$	157.0733	157.076335	–19	16000

Table S6 Molecular ion and fragments derived from the protonated form of complex **3** ($C_{16}H_{26}Cl_2N_3P$) detected by MS/MS CID at 33 V in the transfer cell

Elemental composition	Measured mass/Da	Theoretical mass/Da	Difference/ppm	Intensity/a.u.
$C_{16}H_{27}Cl_2N_3PRu^+$	464.0325	464.035574	–7	4
$C_{16}H_{26}ClN_3PRu^+$	428.0576	428.059178	–4	2060
$C_{16}H_{25}N_3PRu^+$	392.0782	392.082833	–12	476
$C_6H_{12}ClN_3PRu^+$	293.9448	293.949341	–15	959
$C_6H_{11}N_3PRu^+$	257.9705	257.973004	–10	736
$C_6H_{13}N_3P^+$	158.0831	158.08416	–7	74400

DFT-computed Cartesian coordinates for all of the optimized structures reported in this study. IMoS input is also included (Core, Valence, Rydberg, and Total are absolute computed energies in Hartree).

[RuCl(*p*-cymene)(PCy_3)]$^+$

Atom	No	X	Y	Z	Charge	Core	Valence	Rydberg	Total
Ru	1	1.254.812	–0.720994	–0.570686	–0.10673	3.598.566	809.537	0.0257	4.410.673
Cl	2	1.159.799	0.543527	–2572931	–0.24038	999.975	723.725	0.00337	1.724.038
C	3	1.578.301	–2833807	0.387018	0.0105	199.866	397.323	0.01762	59.895
C	4	2.334.765	–2694144	–0.832504	–0.1759	199.869	416.125	0.01596	61.759
C	5	3.328.405	–1694021	–0.986618	–0.20584	199.868	419.142	0.01574	620.584
C	6	3.503.945	–0.690036	0.007584	0.05471	199.865	392.601	0.02062	594.529
C	7	2.656.812	–0.751712	1.174.476	–0.20075	199.866	418.633	0.01576	620.075
C	8	1.762.192	–1843357	1.387.941	–0.20781	199.869	419.281	0.01632	620.781
C	9	0.665875	–4012829	0.575581	–0.71082	19.992	47.044	0.00722	671.082
C	10	4.561.607	0.382532	–0.176463	–0.27047	199.903	426.031	0.01114	627.047
C	11	5.876.834	–0.109876	0.489928	–0.6914	199.926	468.579	0.00634	66.914
C	12	416.352	1.774.477	0.347873	–0.70203	199.928	469.627	0.00648	670.203
P	13	–0.940613	0.303441	0.076873	113.469	999.728	383.479	0.03324	1.386.531
C	14	–2138036	0.302611	–1443149	–0.54336	199.911	45.338	0.01045	654.336
C	15	–223408	–1079855	–2128146	–0.46058	199.916	445.217	0.00925	646.058
C	16	–3029071	–0.965831	–3448137	–0.4717	199.919	446.298	0.00953	64.717
C	17	–4426479	–0.358348	–3216591	–0.47705	199.919	446.889	0.00897	647.705
C	18	–4334687	0.998705	–2493252	–0.46942	199.919	446.085	0.00938	646.942
C	19	–3540333	0.888607	–1170056	–0.47431	199.915	446.519	0.00997	647.431
C	20	–1776521	–0.52896	1.613.723	–0.53957	199.914	453.026	0.01018	653.957
C	21	–2375298	–19172	1.304.355	–0.47356	199.917	446.558	0.00881	647.356
C	22	–2664208	–2683934	2.624.069	–0.46998	199.921	446.228	0.00848	646.998
C	23	–3121184	–1735764	3.766.064	–0.4816	19.992	447.347	0.00892	64.816
C	24	–3811292	–0.486045	3.193.858	–0.47529	19.992	446.703	0.00907	647.529
C	25	–2830191	0.363737	2.337.656	–0.47421	199.918	446.518	0.00985	647.421
C	26	–0.776213	2.158.053	0.613153	–0.52964	199.912	452.026	0.01027	652.964
C	27	0.220645	2.308.418	1.784.077	–0.46624	199.916	445.816	0.00893	646.624
C	28	0.268743	3.771.254	227.924	–0.47005	199.919	446.146	0.0094	647.005
C	29	0.607416	4.742.517	113.257	–0.47622	199.918	446.808	0.00895	647.622
C	30	–0.367099	4.572.587	–0.047902	–0.47145	199.919	446.288	0.00938	647.145
C	31	–0.416049	3.109.707	–0.546434	–0.47218	199.915	446.289	0.01014	647.218
H	32	214.859	–3387688	–1644227	0.30276	0	0.69604	0.00121	0.69724
H	33	3.877.373	–1624384	–1917122	0.30415	0	0.69451	0.00134	0.69585
H	34	2.726.014	0.024441	1.923.759	0.29809	0	0.70077	0.00114	0.70191
H	35	117.349	–1882548	2.295.687	0.29199	0	0.70684	0.00117	0.70801
H	36	1.268.421	–4903934	0.797001	0.28505	0	0.71405	0.00091	0.71495
H	37	0.087041	–4227955	–0.327954	0.27063	0	0.72827	0.0011	0.72937
H	38	–0.02564	–3866596	1.407.403	0.26089	0	0.73804	0.00107	0.73911
H	39	4.742.684	0.470377	–1255332	0.27633	0	0.72134	0.00233	0.72367
H	40	5.755.327	–0.212511	1.574.589	0.24319	0	0.75554	0.00128	0.75681

H	41	6.672.345	0.619209	0.306084	0.26475	0	0.73442	0.00083	0.73525
H	42	6.200.654	–1074956	0.086548	0.25085	0	0.74817	0.00099	0.74915
H	43	3.237.256	2.127.363	–0.115667	0.25245	0	0.74642	0.00112	0.74755
H	44	4.954.278	2.490.959	0.104994	0.26699	0	0.73213	0.00088	0.73301
H	45	4.043.364	1.785.757	1.437.662	0.2333	0	0.76548	0.00122	0.7667
H	46	–1607481	0.969496	–2134148	0.28679	0	0.71077	0.00245	0.71321
H	47	–2736654	–1797353	–1467532	0.23475	0	0.76306	0.00219	0.76525
H	48	–1228956	–1469186	–2333498	0.24708	0	0.7514	0.00152	0.75292
H	49	–3116093	–1957013	–3910036	0.25628	0	0.74238	0.00135	0.74372
H	50	–2465909	–0.336858	–4152386	0.24438	0	0.75359	0.00203	0.75562
H	51	–5030614	–105235	–2613045	0.23516	0	0.76273	0.00211	0.76484
H	52	–4948743	–0.239335	–4173273	0.25986	0	0.73883	0.00131	0.74014
H	53	–5337906	1.389.285	–2283469	0.25908	0	0.73956	0.00136	0.74092
H	54	–3841387	1.730.966	–3148855	0.24067	0	0.75728	0.00205	0.75933
H	55	–3469161	1.877.702	–0.701155	0.24605	0	0.75232	0.00164	0.75395
H	56	–4091375	0.238751	–0.476781	0.23608	0	0.76173	0.00219	0.76392
H	57	–0.924065	–0.674853	2.290.698	0.25534	0	0.74228	0.00238	0.74466
H	58	–1713269	–250778	0.662763	0.24284	0	0.75537	0.00178	0.75716
H	59	–330809	–1785243	0.744167	0.24723	0	0.75103	0.00174	0.75277
H	60	–1767482	–3234173	2.942.708	0.23111	0	0.7673	0.00158	0.76889
H	61	–3435507	–3438969	2.429.349	0.257	0	0.74146	0.00154	0.743
H	62	–2257157	–1424455	437.006	0.2339	0	0.76424	0.00186	0.7661
H	63	–3793777	–2266905	4.448.166	0.26387	0	0.73489	0.00125	0.73613
H	64	–4218592	0.135898	3.998.776	0.26372	0	0.73498	0.0013	0.73628
H	65	–4667862	–0.796958	2.581.092	0.24211	0	0.75609	0.00181	0.75789
H	66	–3409735	0.951339	1.618.457	0.24717	0	0.75114	0.00168	0.75283
H	67	–2310037	1.080.416	2.984.215	0.24711	0	0.75115	0.00174	0.75289
H	68	–1779975	2.419.719	0.974471	0.26792	0	0.72916	0.00292	0.73208
H	69	1.221.418	2.012.191	1.439.372	0.23169	0	0.76611	0.00219	0.76831
H	70	–0.045596	164.405	2.616.526	0.23955	0	0.75887	0.00157	0.76045
H	71	1.003.989	3.861.094	3.088.725	0.25532	0	0.7433	0.00138	0.74468
H	72	–0.706852	4.039.205	2.710.656	0.24053	0	0.75741	0.00206	0.75947
H	73	1.635.036	4.554.165	0.786483	0.23336	0	0.76455	0.00209	0.76664
H	74	0.584491	5.776.643	1.496.276	0.25989	0	0.73879	0.00132	0.74011
H	75	–0.078517	5.227.366	–0.878797	0.26133	0	0.73736	0.00131	0.73867
H	76	–1374869	4.885.219	0.263379	0.23779	0	0.76012	0.00208	0.76221
H	77	–1145799	3.026.863	–1359578	0.25112	0	0.74734	0.00154	0.74888
H	78	0.556295	283.075	–0.969748	0.25113	0	0.74698	0.00189	0.74887

[RuCl(*p*-cymene)(PPh$_3$)]$^+$

Atom	No	X	Y	Z	Charge	Core	Valence	Rydberg	Total
Ru	1	1.170.328	–0.826111	–0.554642	–0.1379	3.598.539	812.648	0.02603	441.379
Cl	2	0.398601	–1203266	–2753014	–0.21536	999.974	721.253	0.00309	1.721.536
P	3	–1026562	0.158703	0.031022	115.768	999.706	380.862	0.03664	1.384.232
C	4	–2401724	–1113426	0.212761	–0.363	199.883	434.859	0.01558	6.363
C	5	–2419091	–2233094	–0.6358	–0.20767	19.989	419.645	0.01231	620.767
C	6	–3460484	–3163364	–0.538729	–0.22697	199.898	421.597	0.01202	622.697
C	7	–4483413	–2982341	0.399355	–0.2089	199.899	419.828	0.01163	62.089

C	8	–4469672	–1863308	1.240.069	–0.22698	199.897	421.595	0.01206	622.698
C	9	–3432873	–0.926907	1.150.061	–0.23349	19.989	422.207	0.01252	623.349
C	10	–0.949719	105.293	168.709	–0.35168	199.883	433.566	0.01719	635.168
C	11	–0.90907	0.31307	2.883.111	–0.24887	199.891	423.766	0.0123	624.887
C	12	–0.793438	0.970859	411.275	–0.23077	199.897	421.972	0.01208	623.077
C	13	–0.712769	2.369.111	4.157.491	–0.21836	199.898	420.758	0.0118	621.836
C	14	–0.757042	3.106.884	2.969.712	–0.22592	199.898	42.149	0.01204	622.592
C	15	–0.876399	2.453.579	1.735.705	–0.22449	19.989	421.357	0.01202	622.449
C	16	–164264	1.442.205	–1193869	–0.34533	199.881	432.961	0.01692	634.533
C	17	–0.715762	2.173.168	–195309	–0.22407	19.989	421.367	0.0115	622.407
C	18	–1161361	3.159.849	–2839244	–0.22681	199.897	421.573	0.01211	622.681
C	19	–253158	3.411.697	–2975445	–0.21082	199.899	420.022	0.01161	621.082
C	20	–3456433	2.676.406	–2224857	–0.22197	199.898	421.113	0.01187	622.197
C	21	–3016584	1.691.378	–133326	–0.20968	199.888	419.832	0.01248	620.968
H	22	–1641041	–236947	–1377792	0.25988	0	0.73878	0.00133	0.74012
H	23	–3472251	–4023637	–1199333	0.26086	0	0.73818	0.00095	0.73914
H	24	–528831	–3705787	0.472189	0.26098	0	0.73809	0.00093	0.73902
H	25	–5264268	–1714552	1.963.442	0.26127	0	0.73777	0.00096	0.73873
H	26	–3432933	–0.064405	1.806.543	0.26058	0	0.73795	0.00147	0.73942
H	27	–1002047	–0.768288	2.861.293	0.25589	0	0.74286	0.00125	0.74411
H	28	–0.778443	0.395185	5.032.328	0.26041	0	0.73864	0.00095	0.73959
H	29	–0.626848	2.877.807	5.111.517	0.26171	0	0.73736	0.00093	0.73829
H	30	–0.709972	4.190.242	2.999.359	0.26113	0	0.73791	0.00095	0.73887
H	31	–0.927488	303.618	0.822759	0.25859	0	0.7399	0.00151	0.74141
H	32	0.344993	1.958.898	–1874834	0.2416	0	0.75709	0.00131	0.7584
H	33	–0.44289	3.718.374	–3429456	0.25727	0	0.74175	0.00097	0.74273
H	34	–2877039	4.170.717	–3668929	0.26	0	0.73907	0.00094	0.74
H	35	–4519176	2.862.671	–23357	0.26039	0	0.73864	0.00096	0.73961
H	36	–3741047	1.119.459	–0.76445	0.2573	0	0.74119	0.00151	0.7427
C	37	2.134.678	–2478604	0.652796	0.01052	199.864	397.338	0.01745	598.948
C	38	298.309	–2271412	–0.496537	–0.17025	199.867	41.552	0.01638	617.025
C	39	3.471.234	–0.990953	–0.800735	–0.20668	199.869	419.203	0.01597	620.668
C	40	31.565	0.149119	0.031756	0.05554	199.867	392.509	0.0207	594.446
C	41	2.408.692	–0.079871	1.229.816	–0.20445	199.866	418.954	0.01625	620.445
C	42	1.906.918	–1370936	1.534.718	–0.19606	199.869	41.812	0.01618	619.606
C	43	1.565.013	–3836745	0.948191	–0.70922	19.992	470.285	0.00717	670.922
C	44	3.719.428	1.509.513	–0.343931	–0.27045	199.903	426.037	0.01105	627.045
C	45	5.214.159	1.561.118	0.080882	–0.6927	199.927	468.701	0.00642	66.927
C	46	2.945.427	2.704.754	0.239294	–0.70095	199.928	469.527	0.0064	670.095
H	47	3.152.753	–3091512	–1183188	0.30285	0	0.69596	0.00118	0.69715
H	48	4.019.851	–0.832328	–1721428	0.3031	0	0.69561	0.00129	0.6969
H	49	2.148.574	0.750648	187.096	0.29824	0	0.70042	0.00134	0.70176
H	50	128.496	–1507366	2.409.166	0.30307	0	0.6956	0.00132	0.69693
H	51	2.290.504	–4419578	1.532.436	0.2829	0	0.71623	0.00087	0.7171
H	52	1.354.798	–439273	0.030708	0.26945	0	0.72933	0.00122	0.73055
H	53	0.643585	–3770116	1.532.286	0.26255	0	0.73605	0.00139	0.73745
H	54	3.684.052	1.579.242	–1440312	0.27314	0	0.72456	0.00229	0.72686
H	55	5.312.757	149.041	1.169.983	0.24112	0	0.75765	0.00123	0.75888
H	56	565.174	2.511.835	–0.239552	0.2646	0	0.73457	0.00084	0.7354
H	57	5.796.751	0.751462	–0.370885	0.25213	0	0.74687	0.00101	0.74787

H	58	187.928	2.664.121	–0.006574	0.25828	0	0.74051	0.00121	0.74172
H	59	3.349.353	3.634.894	–0.171922	0.26591	0	0.73321	0.00088	0.73409
H	60	3.047.069	2.763.405	1.329.162	0.23086	0	0.76793	0.00121	0.76914

$[Ru^{III}Cl_2(p\text{-cymene})(PTA)]^+$

Atom	No	X	Y	Z	Charge	Core	Valence	Rydberg	Total
Ru	1	–0.915812	–0.532785	0.40649	–0.24301	3.598.683	822.731	0.02887	4.424.301
Cl	2	–0.625238	0.982859	2.230.118	–0.16123	999.972	715.743	0.00408	1.716.123
Cl	3	0.040921	–2533318	1.295.057	–0.16082	999.972	715.695	0.00415	1.716.082
C	4	–2242145	–1895311	–1180732	0.04355	199.875	393.966	0.01804	595.645
C	5	–3065968	–1606161	–0.040227	–0.18737	199.878	417.083	0.01775	618.737
C	6	–3352239	–0.280813	0.333865	–0.18722	199.879	41.709	0.01753	618.722
C	7	–2826266	0.835952	–0.40018	0.05393	199.877	392.643	0.02087	594.607
C	8	–1940051	0.551559	–1471696	–0.21911	199.875	420.362	0.01675	621.911
C	9	–1657044	–0.7967	–1859526	–0.21734	199.874	420.113	0.01747	621.734
C	10	–1995399	–3315039	–160154	–0.7199	199.919	471.336	0.00735	67.199
C	11	–3242806	2.242.429	–0.009649	–0.27833	199.903	426.861	0.0107	627.833
C	12	–4679353	2.501.142	–0.549328	–0.69179	199.926	468.616	0.00637	669.179
C	13	–2274013	3.344.402	–0.469648	–0.70731	199.928	470.111	0.00691	670.731
P	14	1.385.047	0.018358	–0.026374	113.358	999.654	383.878	0.03109	1.386.642
N	15	3.983.513	0.233574	0.969337	–0.48836	199.937	547.819	0.0108	748.836
N	16	377.593	–0.477735	–1374955	–0.48946	199.938	547.906	0.01102	748.946
N	17	334.498	1.866.548	–0.753057	–0.48951	199.938	54.791	0.01103	748.951
C	18	2.656.463	–0.138787	1.449.518	–0.56023	199.922	45.458	0.01521	656.023
C	19	2.405.961	–0.989637	–1348719	–0.56933	199.924	455.546	0.01464	656.933
C	20	1.890.768	1.812.436	–0.606257	–0.56943	199.923	45.557	0.0145	656.943
C	21	4.503.752	–0.668161	–0.089368	–0.14168	199.922	412.049	0.02197	614.168
C	22	4.077.295	1.646.768	0.525213	–0.14151	199.922	412.031	0.02198	614.151
C	23	3.867.804	0.945068	–1796608	–0.14171	199.922	41.206	0.02189	614.171
H	24	–3461879	–2427738	0.545473	0.30817	0	0.69076	0.00107	0.69183
H	25	–3970065	–0.092751	1.204.415	0.30719	0	0.6917	0.00112	0.69281
H	26	–1496686	1.363.769	–2031773	0.29865	0	0.7003	0.00104	0.70135
H	27	–10092	–0.980985	–2708293	0.29738	0	0.70159	0.00103	0.70262
H	28	–290713	–3732688	–2048149	0.28771	0	0.7115	0.00078	0.71229
H	29	–1727955	–3940091	–0.744035	0.28827	0	0.71056	0.00117	0.71173
H	30	–1195238	–3384928	–2341685	0.26711	0	0.73199	0.0009	0.73289
H	31	–3286111	2.266.868	1.087.446	0.28716	0	0.71053	0.00232	0.71284
H	32	–4695257	2.491.525	–1644949	0.24689	0	0.75181	0.0013	0.75311
H	33	–5020096	348.502	–0.212814	0.26843	0	0.73075	0.00082	0.73157
H	34	–539472	1.754.964	–0.187643	0.24828	0	0.75077	0.00095	0.75172
H	35	–1258913	3.166.403	–0.099505	0.24679	0	0.75201	0.0012	0.75321
H	36	–2606166	43.074	–0.071263	0.27265	0	0.72654	0.00082	0.72735
H	37	–2248661	3.440.996	–1561922	0.23693	0	0.76179	0.00128	0.76307
H	38	2.320.143	0.520906	2.250.508	0.29071	0	0.7072	0.00209	0.70929
H	39	2.632.886	–1171064	1.801.167	0.29101	0	0.70692	0.00207	0.70899
H	40	2.388.055	–2042846	–105919	0.28589	0	0.71177	0.00235	0.71411
H	41	1.937.945	–0.87866	–2330475	0.26226	0	0.73537	0.00237	0.73774
H	42	1.401.996	2.038.353	–1557649	0.26334	0	0.7343	0.00236	0.73666

H	43	1.548.775	252.168	0.151235	0.28372	0	0.71398	0.0023	0.71628
H	44	441.448	–1707124	0.23387	0.26295	0	0.73537	0.00168	0.73705
H	45	5.558.374	–0.438656	–0.255687	0.27126	0	0.72719	0.00155	0.72874
H	46	3.674.228	2.304.387	1.297.926	0.26254	0	0.73578	0.00168	0.73746
H	47	5.128.898	1.892.973	0.363692	0.27132	0	0.72713	0.00155	0.72868
H	48	3.315.315	1.091.099	–272793	0.25374	0	0.74444	0.00181	0.74626
H	49	4.918.898	1.184.594	–1970701	0.27324	0	0.7252	0.00156	0.72676

$[RuCl_2(p\text{-cymene})(PTA+H)]^+$

Atom	No	X	Y	Z	Charge	Core	Valence	Rydberg	Total
Ru	1	–0.948252	–0.506938	0.229544	–0.47748	3.598.592	845.824	0.03332	4.447.748
Cl	2	–0.083488	–2439484	1.453.709	–0.31468	999.972	73.075	0.00746	1.731.468
C	3	–2178459	–1899478	–1133999	0.0146	199.858	396.356	0.02326	59.854
C	4	–2960369	–1592368	0.035129	–0.16311	199.862	414.319	0.02129	616.311
C	5	–3229148	–0.270856	0.405012	–0.19127	199.864	417.156	0.02107	619.127
C	6	–2750563	0.843166	–0.377494	0.03926	199.862	393.589	0.02623	596.074
C	7	–1991317	0.547584	–1529201	–0.21128	199.863	419.314	0.01951	621.128
C	8	–1698784	–0.808475	–1893103	–0.19048	199.862	417.162	0.02024	619.048
C	9	–1896421	–3327197	–1504832	–0.69746	199.918	468.883	0.00945	669.746
C	10	–3118418	2.249.421	0.057922	–0.26912	1.999	425.608	0.01404	626.912
C	11	–4605031	2.510.632	–0.274805	–0.67832	199.926	467.028	0.00878	667.832
C	12	–2223518	3.348.021	–0.525511	–0.68658	199.927	467.829	0.00901	668.658
P	13	1.306.095	–0.104396	–0.092736	125.882	999.623	367.287	0.07208	1.374.118
N	14	3.715.236	–0.271957	–1481535	–0.49799	199.931	548.211	0.01657	749.799
N	15	326.486	1.896.976	–0.410498	–0.507	199.942	549.708	0.01051	7.507
N	16	3.883.183	–0.059039	0.941441	–0.4957	199.929	547.996	0.01645	74.957
C	17	2.320.385	–0.759687	–1533952	–0.59815	199.919	457.652	0.02244	659.815
C	18	1.768.594	170.881	–0.294233	–0.6079	199.919	458.698	0.02174	66.079
C	19	2.521.662	–0.517314	1.275.528	–0.59267	199.916	457.026	0.02325	659.267
C	20	3.833.622	1.135.513	–1648295	–0.08162	199.921	405.776	0.02465	608.162
C	21	4.420.982	–0.706773	–0.261402	–0.10556	199.921	407.878	0.02757	610.556
C	22	4.007.488	1.350.392	0.860379	–0.07889	199.921	405.474	0.02494	607.889
Cl	23	–0.488053	0.95794	2.156.568	–0.34286	999.973	733.593	0.0072	1.734.286
H	24	–3266199	–2402061	0.688701	0.30178	0	0.69648	0.00174	0.69822
H	25	–3747586	–0.074047	1.336.841	0.2989	0	0.6994	0.0017	0.7011
H	26	–1602083	1.352.694	–2140042	0.27763	0	0.72078	0.00159	0.72237
H	27	–1095403	–1004477	–277373	0.27778	0	0.72066	0.00157	0.72222
H	28	–2817162	–3815528	–1843579	0.26841	0	0.73018	0.00141	0.73159
H	29	–1514529	–3875887	–0.639475	0.28173	0	0.71622	0.00205	0.71827
H	30	–116238	–3392636	–2311392	0.24776	0	0.75074	0.0015	0.75224
H	31	–3000588	2.269.085	1.147.776	0.28443	0	0.71269	0.00287	0.71557
H	32	–4774167	2.505.951	–1357019	0.23706	0	0.76113	0.00181	0.76294
H	33	–4905699	3.489.205	0.11041	0.25432	0	0.74433	0.00135	0.74568
H	34	–5262326	1.759.597	0.173402	0.24295	0	0.75564	0.0014	0.75705
H	35	–1171824	3.173.508	–0.279556	0.23105	0	0.7671	0.00185	0.76895
H	36	–2506634	4.314.708	–0.100459	0.25915	0	0.73947	0.00138	0.74085
H	37	–2328598	3.432.702	–1613314	0.22664	0	0.77154	0.00182	0.77336
H	38	3.475.015	2.896.083	–0.50796	0.46946	0	0.52657	0.00397	0.53054

H	39	2.322.159	–1852528	–1493723	0.28645	0	0.71158	0.00197	0.71355
H	40	1.867.887	–0.467378	–2487123	0.26358	0	0.73435	0.00206	0.73642
H	41	1.303.593	2.131.165	–118919	0.26937	0	0.72866	0.00197	0.73063
H	42	1.403.202	2.243.789	0.58627	0.30142	0	0.69538	0.0032	0.69858
H	43	2.165.972	–0.055274	2.199.034	0.30055	0	0.69698	0.00247	0.69945
H	44	251.549	–1596898	1.427.301	0.30052	0	0.69733	0.00215	0.69948
H	45	3.279.687	1.494.227	–2519148	0.2629	0	0.73507	0.00203	0.7371
H	46	4.882.388	1.435.296	–1723294	0.26552	0	0.73249	0.00199	0.73448
H	47	4.329.466	–1789116	–0.159451	0.27106	0	0.72719	0.00174	0.72894
H	48	5.481.175	–0.454595	–0.362411	0.25802	0	0.74011	0.00187	0.74198
H	49	3.559.864	1.852.489	1.720.349	0.275	0	0.72302	0.00198	0.725
H	50	5.049.948	1.657.219	0.738421	0.26198	0	0.73601	0.00201	0.73802