Supporting Information

$[Au_2(phen^{2Me})_2(\mu\text{-}O)_2](PF_6)_2$, a novel dinuclear gold(III) complex showing excellent antiproliferative properties.

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Experimental Section

General experimental details

Solvents were purchased from Carlo Erba Reagenti and distilled prior to use, while MeCN was used as received. Elemental analyses were performed with a Perkin-Elmer Elemental Analyzer 240B by Mr. A. Canu (Dipartimento di Chimica, Università di Sassari). Conductivity measurements were performed with a Philips PW 9505 conductimeter. Infrared spectra were recorded with a Jasco FTIR-480 Plus spectrophotometer using Nujol mulls; ^{1}H NMR spectra were recorded at 293 K with a Varian VXR 300 spectrometer operating at 300.0 MHz, chemical shifts are given in ppm relative to internal tetramethylsilane.

Synthesis of $[Au(phen^{2Me})(\mu\text{-}O)]_2[PF_6]_2$, 1-$(PF_6)_2$. To a stirred solution of $[Au(phen^{2Me})Cl_3]$ (511.7 mg, 1.0 mmol) in CH_3CN (3 ml) were added an aqueous solution of AcONa (164.9 mg, 2.0 mmol, 100 ml) and KPF_6 (552.2 mg, 3.0 mmol). The resulting suspension was refluxed for about 3 hours until the colour

of the solid changed from orange to light pink. After cooling, the solid was collected by filtration and washed with H_2O, EtOH, Et_2O. The crude product was extracted with several portions of chloroform to remove some unreacted starting adduct. Recrystallization of the residue from CH_3CN/Et_2O afforded the analytical sample (368.3 mg, 65%). Mp 203°-204°C. Elemental analysis (%) calcd for $C_{28}H_{24}Au_2F_{12}N_4O_2P_2$: C 29.70, H 2.14, N 4.95; found C 29.84. H 1.89, N 4.98. Λ_{MAX} ($5x10^{-4}$ mol·L^{-1}, CH_3CN) 246.6 $\Omega^{-1}cm^2mol^{-1}$. Selected IR bands (n_{max}/cm^{-1}): 842 s, 557 s, 687 m, 669 m. ^1H NMR (CD_3CN) δ: 3.22 (s, 6H, Me), 7.97 (d, J = 8.2 Hz, 2H, CH-3 and CH-8), 8.18 (s, 2H, CH-5 and CH-6), 8.82 (d, J = 8.2 Hz, 2H, CH-4 and CH-7).

Synthesis of 1-$(BAr_4')_2$. This could be obtained by methathesis reaction of **1**-$(PF_6)_2$ and Na[BAr'$_4$]. To a stirred suspension of **1**-$(PF_6)_2$ (100.7 mg, 0.09 mmol) in 50 ml of CH_2Cl_2 a dichloromethane solution of $NaBAr_4'$ (157.8 mg, 0.18 mmol, 20 ml) was added. The resulting suspension was stirred at room temperature for about 30 minutes until most of the solid was solubilized. After this period, the suspension was filtered through Celite and the filtered solution concentred to a small volume. Addition of diethyl ether to the concentrated solution gave **1**-$(Bar_4')_2$ (171.1 mg, 74%). Mp 142°C. Elemental analysis (%) calcd for $C_{92}H_{48}Au_2B_2F_{48}N_4O_2$: C 43.01, H 1.88, N 2.18; found C 42.94. H 1.69, N 2.34. Λ_{MAX} ($5x10^{-4}$ mol·L^{-1}, acetone) 169.9 $\Omega^{-1}cm^2mol^{-1}$. Selected IR bands (n_{max}/cm^{-1}): 682 m, 670 m, 550 s. ^1H NMR (CD_3COCD_3) δ: 3.43 (s, 6H, Me), 7.67 (s, 8H, CH-4 $BAr_4'^-$), 7.79 (t, 16H, CH-2 and CH-5 $BAr_4'^-$), 8.25 (d, J = 8.4 Hz, 2H, CH-3 and CH-8), 8.41 (s, 2H, CH-5 and CH-6), 9.13 (d, J = 8.4 Hz, 2H, CH-4 and CH-7). X-ray quality crystals of **1**-$(BAr_4')_2$ were grown from slow diffusion of diethyl ether into a saturated dichloromethane solution of the complex.

X-ray Data Collection and Structure Determination: Crystal data are summarized in Ref. 16 in the published paper, and in the full Crystallographic Table **S1**. The diffraction experiment was carried out on a Bruker APEX II CCD area-detector diffractometer at 150 K, using Mo_{Ka} radiation (l = 0.71073), with a graphite crystal monochromator in the incident beam. No crystal decay was observed, so that no time-decay correction was needed. The collected frames were processed with the software SAINT,[1] and an empirical absorption correction was applied (SADABS)[2] to the collected reflections. The calculations were performed using the Personal Structure Determination Package[3] and the physical constants tabulated therein.[4] The structure was solved by direct methods (SHELXS)[5] and refined by full-matrix least

[1] SAINT Reference manual, Siemens Energy and Automation, Madison, W1, **1994-1996**

[2] G.M. Sheldrick, SADABS, Empirical Absorption Correction Program, University of Gottingen, **1997**
[3] B.A. Frenz, *Comput. Phys.* **1988**, 2, 42

[4] *Crystallographic Computing 5*, Oxford University Press: Oxford, U.K., **1991**; Chapter 11, 126
[5] G.M. Sheldrick, (1985) SHELXS 86. Program for the solution of crystal structures. University

squares using all reflections and minimizing the function $Sw(F_o^2 - kF_c^2)^2$ (refinement on F^2). In the anion three out of the eight CF_3 moieties are disordered (as often happens with this anion) in their nine F atoms, each of which appears to be split into two half F atoms, with occupancy factors of 0.50 each. This disorder has been fully rationalized. All the non-hydrogen atoms, including the F atoms with occupancy 0.50, were refined with anisotropic thermal parameters. The three hydrogen atoms bonded to the methylic atom C(13) of the cation, and the three hydrogen atoms bonded to the corresponding methylic atom C(14), were detected in the final Fourier maps and not refined. All the other hydrogen atoms were placed in their ideal positions (C-H = 0.97 Å), with the thermal parameter *U* being 1.10 times that of the carbon atom to which they are attached, and not refined. In the final Fourier map the maximum and minimum residuals were +1.48(11) $e \cdot Å^{-3}$ at 0.44 Å from Au, and –1.22(11) $e \cdot Å^{-3}$.

Table S1. Full crystallographic data.

Compound	**1**-$[B\{C_6H_3(CF_3)_2\}_4]_2$
Formula	$C_{92}H_{48}Au_2B_2F_{48}N_4O_4$
M	2568.91
Colour	yellow
Crystal system	triclinic
Space group	P-1
a/Å	13.0530(6)
b/Å	13.5091(6)
c/Å	15.1301(7)
a/°	63.879(1)
b/°	82.525(1)
g/°	76.795(1)
V/$Å^3$	2330.8(2)
Z	1
F(000)	1244
D_c/g cm^{-3}	1.830
T/K	150
l(Mo Ka)	0.71073
Crystal dimensions (mm)	0.17 x 0.22 x 0.34
m(Mo Ka) / cm^{-1}	32.80
Min. and max. transmiss. factors	0.805-1.000
Scan mode	w
Frame width / °	0.30
Time per frame / sec	15
No. of frames	3060
Detector-sample distance / cm	6.00
q-range	3.00-27.00
Reciprocal space explored	full sphere
No. of reflections (total; independent)	36769, 11918
R_{int}	0.022

of Gottingen, Germany.

Final R_2 and R_{2w} indices [a]		
(F^2, all reflections)	0.037, 0.057	
Conventional R_1 index		
[I>2s(I)]	0.021	
Reflections with I>2s(I)		11058
No. of variables		758
Goodness of fit [b]	0.943	

[a] R_2= [S(|F_o^2-kF_c^2|/SF_o^2], R_{2w}= [Sw(F_o^2-kF_c^2)^2/Sw(F_o^2)^2]$^{1/2}$
[b] [Sw(F_o^2-kF_c^2)^2/(N_o-N_v)]$^{1/2}$, where w=4F_o^2/s(F_o^2)^2, s(F_o^2)=[s^2(F_o^2)+(0.04F_o^2)^2]$^{1/2}$, N_o is the number of observations and N_v the number of variables.

Description of the interionic hydrogen bonds in the packing of 1·[B{$C_6H_3(CF_3)_2$}$_4$]$_2$

In the packing of **1·[**B{$C_6H_3(CF_3)_2$}$_4$]$_2$ there are two interionic H···F hydrogen bonds, involving two different anionic fluorine atoms belonging to the same, ordered, CF_3 moiety (in the anion three out of eight CF_3 moieties are disordered), one cationic hydrogen atom, and one anionic hydrogen atom. Fig. S1 shows an isolated cation, including all its hydrogen atoms, with a label for each atom, including hydrogens. Fig. S2 shows an isolated anion, including all its hydrogen atoms, but only two fluorine atoms, those involved in the two hydrogen bonds. The other fluorine atoms have been omitted for clarity. Also in Fig. S2 each shown atom carries its label, including hydrogens. The stronger hydrogen bond is formed by cationic hydrogen atom H(3), bonded to C(8), and fluorine atom F(19), bonded to C(147) (see Figures). Bond and non-bond parameters for this interaction are:

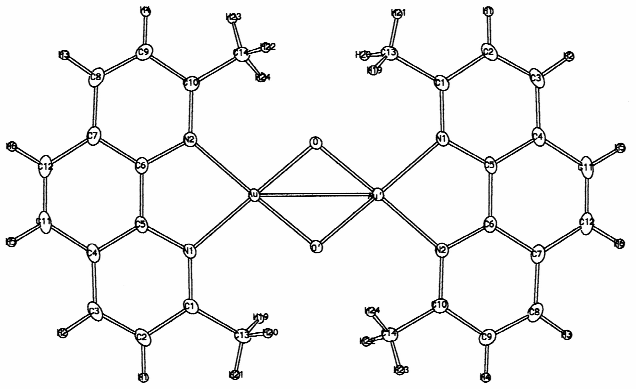


Figure S1

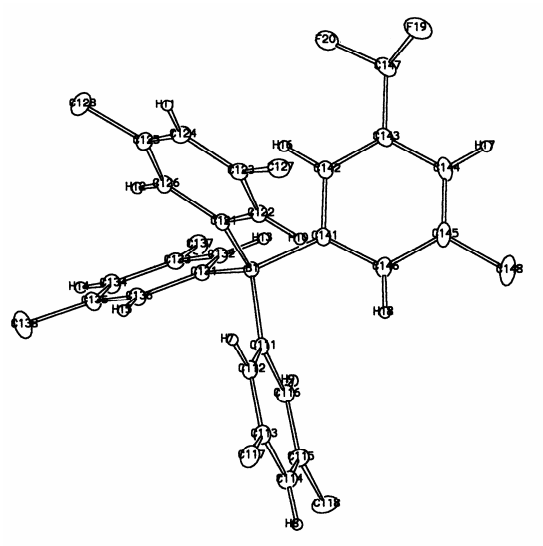


Figure S2

C(8)-H(3) = 0.970 Å (hydrogen atom placed in its ideal position)
H(3)···F(19) = 2.312 Å
C(8)···F(19) = 3.259(3) Å
angle C(8)-H(3)···F(19) = 165.2(2)°

The second hydrogen bond is formed by anionic hydrogen atom H(14), bonded to C(134), and fluorine atom F(20), bonded to C(147) (see Fig. S2). Bond and non-bond parameters for this interaction are:

C(134)-H(14) = 0.970 Å (hydrogen atom placed in its ideal position)
H(14)···F(20) = 2.498 Å
C(134)···F(20) = 3.457(2) Å
angle C(134)-H(14)···F(20) = 169.7(1)°

UV-visible spectrophotometry. UV-vis absorption spectra **1**-$(PF_6)_2$ were recorded on a Varian Cary 50 UV-Vis spectrophotometer. Solutions of **1**-$(PF_6)_2$ (10^{-5} M) in 50 mM phosphate buffer pH = 7.4 were monitored collecting the electronic spectra over 24 h at room temperature.

ESI Mass Spectrometry. Horse heart cytochrome c, red blood cell ubiquitin and bovine erythrocytes superoxide dismutase were purchased from Sigma (C7752, U6253 and S2515, respectively) and used as received. The sample was prepared by mixing equivalent amounts of the three proteins (100 μM) in 25 mM tetramethylammonium acetate buffer (TMeAmAc) (pH 7.4). Then **1**-$(PF_6)_2$ was added (3:1 metal/protein ratio) to the solution and incubated at 37 °C for 24h. After a 20-fold dilution with HCOOH 0.1%, ESI-MS spectrum was recorded by direct introduction at 5 μl/min flow rate in an LTQ-Orbitrap

high-resolution mass spectrometer (Thermo, San Jose, CA, USA), equipped with a conventional ESI source. The working conditions were the following: spray voltage 3.1 kV, capillary voltage 45 V and capillary temperature 220 °C. The sheath and the auxiliary gases were set, respectively, at 17 (arbitrary units) and 1 (arbitrary units). For acquisition, Xcalibur 2.0. software (Thermo) was used and monoisotopic and average deconvoluted masses were obtained by using the integrated Xtract tool. For spectrum acquisition a nominal resolution (at m/z 400) of 100,000 was used.

Tumor Cell Lines. Twenty-four out of the 36 cell lines were established from patient-derived tumor xenografts passaged subcutaneously in nude mice.[6] The origin of the donor xenografts has been already described.[7,8] The other 12 cell lines were commercially available and purchased from ATCC (Rockville, MD) or DSMZ (Braunschweig, Germany) or were kindly provided by the NCI (Bethesda. MD). The 36 cell line panel included 14 different tumor histotypes, each represented by 1-6 cell lines (see supplementary material). All cells were grown at 37°C in a humidified atmosphere (95% air, 5% CO_2) in RPMI 1640 medium (PAA, Cölbe, Germany) supplemented with 10% fetal calf serum (PAA) and 0.1 mg/ml gentamicin (PAA).

Cytotoxicity Assays (Monolayer Assay) and Compare Analysis. A modified propidium iodide assay [9] was used to assess the effects of compounds. Tumor derived cell lines were incubated in 96 multi-well plates. After one day, the compounds under test were added to the plates at 5 concentrations in the range from 0.01 µg/ml to 100 µg/ml and left for further four days. The inhibition of proliferation was determined by measuring the DNA content using an aqueous propidium iodide solution (7 µg/ml). Fluorescence was measured using the Cytofluor 4000. All compounds were tested in 2 to 4 independent experiments. In each experiment, all data points were determined in triplicate.

The Compare Algorithm uses *in vitro* activity data to obtain clues as to the mechanism of action of a test compound.[10] The individual IC_{50} and IC_{70}-values of the test compounds in 36 test cell lines obtained in the monolayer assay were correlated to the corresponding IC_{50}/IC_{70}-values for 110 standard agents determined in exactly these 36 cell lines. A list of these standard agents is available in the supplementary material (Table 1S). These standard agents represent the main mechanisms of action of

[6] Roth T, Burger, A. M., Dengler, W., Willmann, H., Fiebig, H.H. (1999) In: Fiebig HH, Burger, A. M. (ed) Contrib. Oncol., pp. 145-156

[7] Fiebig HH, Dengler, W.A., Roth, T. (1999) In: Fiebig HH, Burger, A. M. (ed) Contrib. Oncol., pp. 29-50

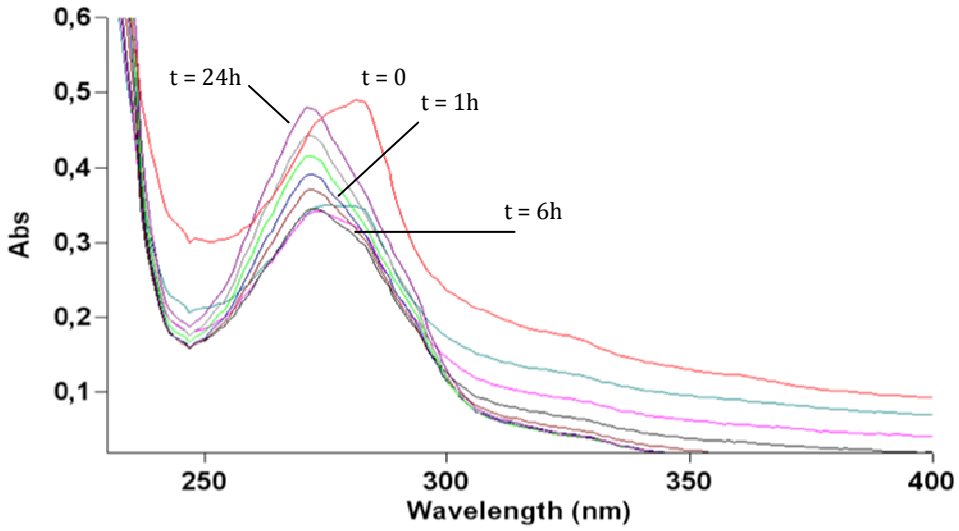
[8] Fiebig HH, Berger D. P., Dengler, W. A., Wallbrecher, E., Winterhalter, B. R. (1992) In: Fiebig HH, Berger, D. P. (ed) Relevance of Tumor Models for Anticancer Drug Development. Karger, Basel, pp. 321-351

[9] Dengler WA, Schulte J, Berger DP, Mertelsmann R, Fiebig HH (1995) Anti-Cancer Drug 6:522-532

[10] Paull KD, Shoemaker RH, Hodes L, Monks A, Scudiero DA, Rubinstein L, Plowman J, Boyd MR (1989) J Natl Cancer I 81:1088-1092; Huang RL, Wallqvist A, Covell DG (2005) Biochem, Pharmacol 69:1009.

current anti-cancer drugs. Similarities between the sensitivity pattern of a test compound and those of standard drugs are expressed quantitatively as Spearman correlation coefficients.[11] High correlations ($\rho>0.6$) between the sensitivity patterns of two compounds (referred to as Compare-positive) are indicative of similar mechanism of action. Low correlations between the sensitivity profile of a test compound and the profiles of all standard compounds (referred to as Compare-negative) indicate that the mechanism of action of the test compound is not represented by the selected standard compounds.

Figure S3. UV-visible absorption spectra of **1**-$(PF_6)_2$ 10^{-5}M in 50 mM phosphate buffer (pH=7.4) recorded over 24 h at 25°C.



[11] Fang XL, Shao L, Zhang H, Wang SM (2004) J Chem Inf Comp Sci 44:249-257

Figure S4. Anticancer activity profile of compound **1**-$(PF_6)_2$ in a panel of 36 cell lines (IC_{70} mean graph).

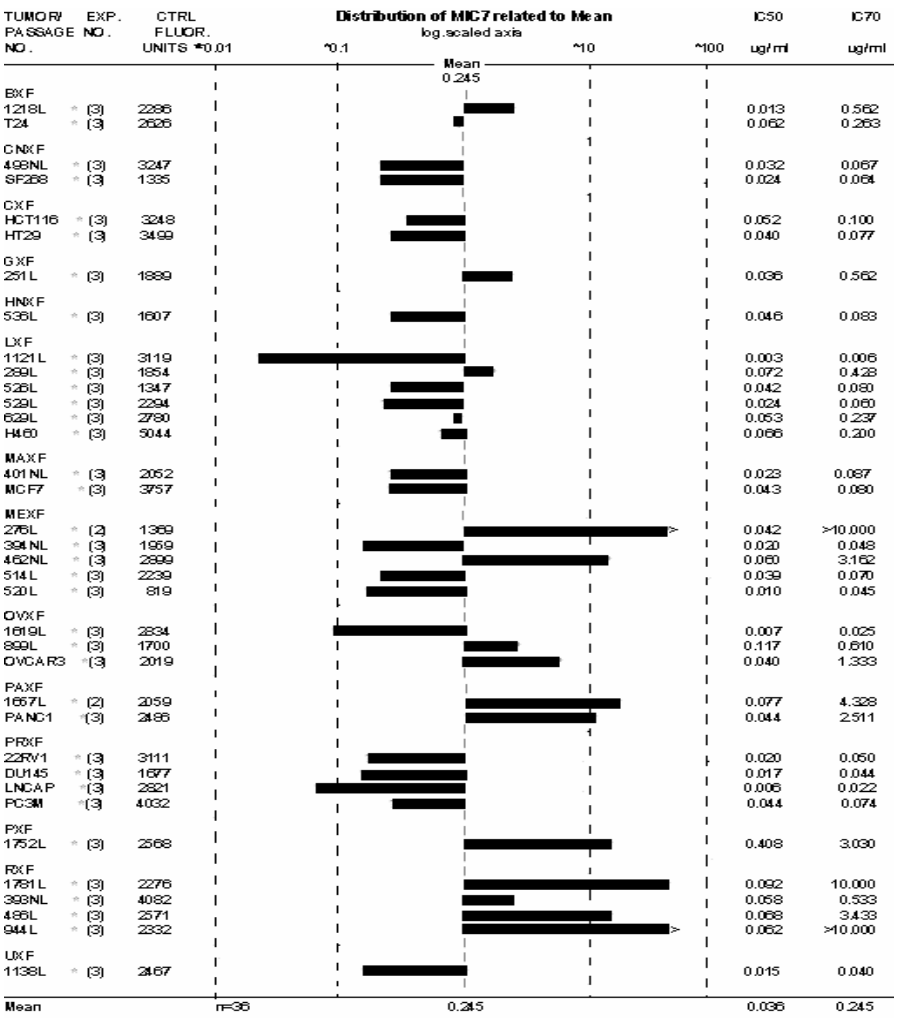


Table S2. Reference compounds used for Compare Analysis as available in the Oncotest Database.

#	designation 1 Intern	designation 2	MoA 1	MoA 2
1	BCNU	Carmustin	Alkylating Agent	Nitrosourea
2	HECNU	Chloroethyl-nitroso-hydroxyethyl-urea	Alkylating Agent	Nitrosourea
3	CCNU	Lomustin	Alkylating Agent	Nitrosourea
4	MCCNU	Semustine, Methyl-CCNU	Alkylating Agent	Nitrosourea
5	CARBOPLA	Carboplatin	Alkylating Agent	Platin
6	PLAT	Cisplatin	Alkylating Agent	Platin
7	OXPLAT	Oxaliplatin	Alkylating Agent	Platin
8	TETPLAT	Tetraplatin	Alkylating Agent	Platin
9	CHLORAMB	Chlorambuzil	Alkylating Agent	
10	CYACT	Cyclophosphamid (act. metabolite)	Alkylating Agent	
11	AZQ	Diaziquone	Alkylating Agent	
12	NCI17	Hepsulfam	Alkylating Agent	
13	MITO	Mitomycin C	Alkylating Agent	
14	TEX	Teroxirone, Triglycidylisocyanurate	Alkylating Agent	
15	THT	Thio-tepa	Alkylating Agent	
16	TREO	Treosulfan	Alkylating Agent	
17	MTX	Methotrexat	Antimetabolite	Folic acid activation
18	TOMUDEX	Raltitrexed	Antimetabolite	Folic acid activation
19	DON	6-Diazo-5-oxo-L-norleucine	Antimetabolite	GMP Synth. Inh.
20	ACV	Acivicin, Antibiotic AT-125	Antimetabolite	GMP Synth. Inh.
21	MP	6-Mercaptopurin	Antimetabolite	Purin-Analoga
22	THG	6-Thioguanin, 6-TG	Antimetabolite	Purin-Analoga
23	CDA	Cladribin	Antimetabolite	Purin-Analoga
24	FUDR	5-Fluoro-2'-deoxyuridine, Floxurine	Antimetabolite	Pyrimidin-Analoga
25	5FU	5-Fuorouracil (s.a. N88)	Antimetabolite	Pyrimidin-Analoga
26	FTF	Ftorafur, Fluorofur	Antimetabolite	Pyrimidin-Analoga
27	GEMZAR	Gemcitabine	Antimetabolite	Pyrimidin-Analoga
28	CCD	Cyclocytidine, Ancitabine HCl	Antimetabolite	
29	NCI14	Cyclopentenylcytosine	Antimetabolite	
30	ARAC	Cytarabin, ara-C	Antimetabolite	
31	DUP785	DUP785, Brequinar sodium	Antimetabolite	
32	N224131	PALA, L-Aspartic acid	Antimetabolite	
33	ALIMTA	Pemetrexed, LY231514	Antimetabolite	
34	DASATNB	Dasatinib	Bcl/Abl Kinhase Inh.	
35	GLEEVEC	Imatinib Mesylat, STI571	Bcl/Abl Kinhase Inh.	
36	FLT3I2	Bisinolatderivative	Broad-spectrum Kinase inh.	FLT3-inhibitor
37	VATALNB	Vatalinib	Broad-spectrum Kinase inh.	KDR/PDGFR
38	SORAFNB	Sorafinib, Nexavar	Broad-spectrum Kinase inh.	Multikinase-inh.
39	SUNITNB	Sunitinib, Eurasia	Broad-spectrum Kinase inh.	Multikinase-inh.
40	STAUROSP	Staurosporine	Broad-spectrum Kinase inh.	PKC
41	UCN01	UCN-01 (N638850)	Broad-spectrum Kinase inh.	PKC
42	TRD	Tetrandrine	Ca2+-channel blocker	
43	APL	Alsterpaullone	CDK Inh	
44	CYC202	CYC202	CDK Inh	
45	FCL	Fascaplysin	CDK Inh	
46	N101	Flavopiridol	CDK Inh	
47	PURA	Purvalanol A	CDK Inh	
48	SU9516	SU9516	CDK Inh	
49	NIME	Nimesulide	COX II Inh.	
50	APHIDICO	Aphidicolin	DNA-Synth. Inh.	
51	W020	Aphidicolin glycinate	DNA-Synth. Inh.	
52	ECH	Echinomycin A	DNA-Synth. Inh.	
53	MTM	Mitramycin	DNA-Synth. Inh.	
54	DTB	Decitabine	DNMT inh.	
55	TARCEVA	Erlotinib, OSI-774	EGF/HER2 Inh.	
56	IRESSA	Gefitinib	EGF/HER2 Inh.	
57	LAPAT	Lapatinib	EGF/HER2 Inh.	
58	PD168393	PD 168393	EGF/HER2 Inh.	
59	MANUA	Manumycin A	Farnesyl Transf. Inh.	
60	ACDINAL	Acetyldinaline, CI-994	HDAC inh.	Benzamide
61	MS275	MS-275	HDAC inh.	Benzamide
62	APICID	Apicidin	HDAC inh.	Cyclic Peptide
63	N630176	Depsipeptide	HDAC inh.	Cyclic Peptide
64	M344	M344	HDAC inh.	Hydroxamate
65	SBHA	Suberic Bishydroxamat	HDAC inh.	Hydroxamate
66	SAHA	Suberoylanilide hydroxamic acid	HDAC inh.	Hydroxamate
67	TRISTAT	Trichostatin A	HDAC inh.	Hydroxamate
68	NM07	17AAG	HSP90 inh	
69	NM10	17DMAG	HSP90 inh	
70	NCI1	Rapamycin	mTOR-Inh	
71	LY294002	LY-294,002	PI3K/AKT Inh.	
72	MGAG	Mitoguazone, Guanylhydrazone	Polyaminsyn. Inh.	SAMD Inh.
73	VELCADE	Bortezomib, PS-341	Proteasome	
74	EPM	Epoxomicin	Proteasome	
75	MG132	MG-132	Proteasome	
76	TPA	Tyropeptin A	Proteasome	
77	DAS	Anguidine	Protein-Syn. Inh.	
78	HHT	Homoharringtonine	Protein-Syn. Inh.	
79	ML1	Mistellektin 1	Protein-Syn. Inh.	
80	PSPA	Pentyl-Sparsomycin	Protein-Syn. Inh.	
81	NCI2	Phyllanthoside	Protein-Syn. Inh.	
82	SPA	Sparsomycin	Protein-Syn. Inh.	
83	HYPHRE	Fenretinide, H-(4-Hydroxyphenyl)retinamide	Retinoic acid analog	
84	RIFA	Rifamycin SV	RNA Synth.	RNA-Polym. Inh.
85	HU	Hydroxyharnstoff	RNA Synth.	RNR Inh.
86	CMA3	Chromomycin A3	RNA Synth.	
87	APIGENIN	Apigenin	Serin/Threonin Kinase Inh.	
88	SB202190	SB-202190	Serin/Threonin Kinase Inh.	
89	MST312	MST-312	Telomerase Inh	
90	CAMPTO	Camptothecin	Topoisomerase I Inh.	
91	SN38	Irinotecan	Topoisomerase I Inh.	
92	TOPOT	Topotecan Hydrochlorid	Topoisomerase I Inh.	
93	DACT	Actinomycin-D	Topoisomerase II Inh.	
94	AMSA	Amsacrin	Topoisomerase II Inh.	
95	BLEO	Bleomycin Sulfat	Topoisomerase II Inh.	
96	DAUNORUB	Daunorubicin	Topoisomerase II Inh.	
97	ADR	Doxorubicin	Topoisomerase II Inh.	
98	VP16	Etoposide	Topoisomerase II Inh.	
99	IDA	Idarubicin	Topoisomerase II Inh.	
100	MITOXANT	Mitoxantron Hydrochlorid	Topoisomerase II Inh.	
101	NCI15	Pyrazolo-acridine-propanamine	Topoisomerase II Inh.	
102	VM26	Teniposid	Topoisomerase II Inh.	
103	TXT	Docetaxel	Tubulin interactin	Taxoid
104	TAXOL	Paclitaxel, Taxol	Tubulin interactin	Taxoid
105	VELBE	Vinblastin Sulfat	Tubulin interactin	Vincaalcaloid
106	VCR	Vincristin Sulfat	Tubulin interactin	Vincaalcaloid
107	VIND	Vindesin Sulfat	Tubulin interactin	Vincaalcaloid
108	NAVELBIN	Vinorelbin	Tubulin interactin	Vincaalcaloid
109	STC	S-trityl-L-cysteine	Eg5 inhibitor	
110	NCI6	Pancratistatin		

checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: compound_1.B{C6H3CF324}2

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: **a=13.0530(6) b=13.5091(6) c=15.1301(7)**
alpha=63.879(1) beta=82.550(1) gamma=76.795(1)
Temperature: 150 K

	Calculated	Reported
Volume	2330.84(19)	2330.8(2)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C32 H12 B F24, 0.5(C28 H24 Au2 N4 O2)	?
Sum formula	C46 H24 Au B F24 N2 O	C92 H48 AU2 B2 F48 N4 O2
Mr	1284.45	2568.91
Dx,g cm-3	1.830	1.830
Z	2	1
Mu (mm-1)	3.291	3.280
F000	1244.0	1244.0
F000'	1241.06	
h,k,lmax	16,17,19	
Nref	10179	
Tmin,Tmax	0.425,0.573	0.805,1.000
Tmin'	0.325	

Correction method= EMPIRICAL

Data completeness= 0.000 Theta(max)=

R(reflections)= 0.0370(******) wR2(reflections)= *****(11918)**

S = 0.943 Npar= 758

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

PLAT022_ALERT_3_A Ratio Unique / Expected Reflections too Low 0.00
PLAT026_ALERT_3_A Ratio Observed / Unique Reflections too Low .... 0 Perc.
PLAT215_ALERT_3_A Disordered F10A has ADP max/min Ratio 5.10
PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C128
PLAT224_ALERT_1_A Ueq(Rep) and Ueq(Calc) differ by -0.007 Ang**2 . F11A

Alert level B

```
PLAT215_ALERT_3_B Disordered F12B      has ADP max/min Ratio .....       4.50
PLAT215_ALERT_3_B Disordered F22A      has ADP max/min Ratio .....       4.40
PLAT215_ALERT_3_B Disordered F22B      has ADP max/min Ratio .....       4.10
PLAT215_ALERT_3_B Disordered F24A      has ADP max/min Ratio .....       4.30
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for       C138
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for       C148
PLAT731_ALERT_1_B Bond    Calc   3.0187(2), Rep  3.0190(10) ......       5.00 su-Ra
             AU   -AU      1.555   2.566
```

Alert level C

```
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......       0.96
PLAT215_ALERT_3_C Disordered F10B      has ADP max/min Ratio .....       3.50
PLAT215_ALERT_3_C Disordered F11A      has ADP max/min Ratio .....       3.80
PLAT215_ALERT_3_C Disordered F12A      has ADP max/min Ratio .....       3.40
PLAT215_ALERT_3_C Disordered F16A      has ADP max/min Ratio .....       3.80
PLAT215_ALERT_3_C Disordered F16B      has ADP max/min Ratio .....       4.00
PLAT215_ALERT_3_C Disordered F18A      has ADP max/min Ratio .....       3.30
PLAT215_ALERT_3_C Disordered F23A      has ADP max/min Ratio .....       3.40
PLAT215_ALERT_3_C Disordered F23B      has ADP max/min Ratio .....       3.50
PLAT215_ALERT_3_C Disordered F24B      has ADP max/min Ratio .....       3.20
PLAT220_ALERT_2_C Large Non-Solvent    F     Ueq(max)/Ueq(min) ...       3.46 Ratio
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C117
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C147
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT045_ALERT_1_C Calculated and Reported Z Differ by .............       2.00 Ratio
PLAT701_ALERT_1_C Bond    Calc   3.0187(2), Rep  3.0190(10), Dev..       1.50 Sigma
             AU   -AU      1.555   2.566
PLAT751_ALERT_4_C Bond    Calc     0.97000, Rep    0.970(2) ......  Senseless su
             C3   -H2      1.555   1.555
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1
             C32 H12 B F24
```

Alert level G

```
GOODF01_ALERT_1_G  _refine_ls_goodness_of_fit_obs is an old dataname which has
           been superceded by _refine_ls_goodness_of_fit_ref
RFACG01_ALERT_3_G  _refine_ls_R_factor_obs is an old dataname which has been
           superceded by _refine_ls_R_factor_gt
RFACR01_ALERT_3_G  _refine_ls_wR_factor_obs is an old dataname which has been
           superceded by _refine_ls_wR_factor_ref
SHFSU01_ALERT_2_G  _refine_ls_shift/esd_max is an old dataname which has been
           superceded by _refine_ls_shift/su_max
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................       9.00 Perc.
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal  (x 10000)        100 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF ......      15.40 Deg.
             F10A -C128 -F10B    1.555   1.555   1.555
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF ......      27.50 Deg.
             F11A -C128 -F11B    1.555   1.555   1.555
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF ......      28.90 Deg.
             F12A -C128 -F12B    1.555   1.555   1.555
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF ......      30.10 Deg.
             F16A -C138 -F16B    1.555   1.555   1.555
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF ......      39.80 Deg.
             F17A -C138 -F17B    1.555   1.555   1.555
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF ......      41.70 Deg.
             F18A -C138 -F18B    1.555   1.555   1.555
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF ......      33.80 Deg.
             F22A -C148 -F22B    1.555   1.555   1.555
PLAT808_ALERT_5_G No Parsable SHELXL style Weighting Scheme Found           !
```

5 **ALERT level A** = In general: serious problem
7 **ALERT level B** = Potentially serious problem
18 **ALERT level C** = Check and explain
14 **ALERT level G** = General alerts; check

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
20 ALERT type 3 Indicator that the structure quality may be low
9 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/08/2009; check.def file version of 12/08/2009

Datablock compound_1.B{C6H3CF324}2 - ellipsoid plot