

Article

A molecular networking strategy: High-throughput screening and chemical analysis of Brazilian Cerrado plant extracts against cancer cells

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Dedicated to the memory of Professor José Elias de Paula

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Table S1. Brazilian Cerrado plant extracts submitted to high-throughput screening against a set of 8 cancer cell lines: colon (Colo205 and Km12), renal (A498 and U031), liver (HEP3B and SKHEP) and osteosarcoma (MG63 and MG63.3).

Family/Plant Species	Voucher number	Part of plant (solvent)	Vernacular Name	Traditional Use(s)	Vegetation types/ Collection season/ Soil types
Alismataceae					
<i>Echinodorus macrophyllus</i> (Kunth) Micheli	(UB) 3748	L ^a (d ¹ , hs ²)	Chapéu de couro	Anti-inflammatory, diuretic and antiarrhythmic [1]	Cerrado Ralo/ *Dry season/ Oxisol
Anacardiaceae					
<i>Astronium fraxinifolium</i> Schott	(UB) 3814	L (h ³ , a ⁴ , e ⁵), SW ^b (h, e, w ⁶), SB ^c (h, a, e), RW ^d (a, e, w), RB ^e (h, a, e, w)	Gonçalo-alves, Pau-Gonçalves	Antimicrobial, used to treat diarrhea and hemorrhoids, skin ulcers and rheumatism [2]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Schinus terebinthifolia</i> Raddi	(UB) 3753	L (h, d, hs), SW (h, hs, al ⁷), SB (h, d, hs), RW (hs, al), RB (h)	Pimenta-rosa, Aroeira-vermelha	Treatment of tumors and leprosy [3]	Mata Ciliar/ Dry season/ Oxisol
Annonaceae					
<i>Annona crassiflora</i> Mart.	(UB) 3700	L (h, e), SW (h, e), SB (h, e), RW (e), RB (e)	Araticum	Treatment of fever and Chagas disease [4]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Cardiopetalum calophyllum</i> Schltldl.	(UB) 3703	L (h, e), SW (h, e), SB (h, e), R ^f (h, e)	Imbira	Treatment of fever [4]	Mata Ciliar/ Dry season/ Inceptisol

<i>Duguetia furfuracea</i> (A. St. Hil.) Saff.	(UB) 3679	L (h, e), SW (e), RW (h, e), RB (h, e), S ^s (h, e)	Pinha-de-guará, Araticum-seco	Treatment of rheumatism and stomach pains [5]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Xylopia aromatica</i> (Lam.) Mart	(UB) 3699	L (h, e), SW (h, e), SB (h, e), RW (h, e), RB (h, e)	Pimenta de macaco	Carminative properties [4]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Xylopia emarginata</i> Mart.	(UB) 3690	L (h, e), SW (h), SB (h, e), RW (h, e), RB (h, e)	Pindaíba-do-brejo	Bactericidal properties [4]	Mata Ciliar/ Dry season/ Oxisol
Apocynaceae					
<i>Aspidosperma macrocarpon</i> Mart.	(UB) 3692	L (h, e), SW (h, e), SB (h, e), RW (h, e), RB (h, e)	Pau-pereira, Peroba-gigante-do-cerrado	Used in the treatment of malaria and as an anti-inflammatory [6]	Cerrado sensu stricto/ *Rainy season/ Oxisol
<i>Aspidosperma tomentosum</i> Mart.	(UB) 3744	L (h, d, hs, al), SW (h, d, hs), SB (h, d, hs), R (d, hs)	Peroba-do-Cerrado	Treatment of malaria, leishmaniasis, cancer, inflammations, fever and rheumatism [7]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Condylocarpon isthmicum</i> (Vell.) A. DC.	(UB) 3663	L (h, e), SW (h, e), SB (h, e)	Cipó de leite	Used as an aromatic plant [8]	Mata Ciliar/ Rainy season/ Inceptisol
<i>Hancornia pubescens</i> Nees & C. Mart.	(UB) 3677	L (h, e), RW (h, e), RB (h, e)	Mangaba	Treatment of digestive problems [6]	Campo sujo de Cerrado/ Rainy season/ Oxisol
<i>Himatanthus obovatus</i> (Müll. Arg.) Woodson	(UB) 3678	L (h, e), RW (h, e), RB (h, e)	Tiborna, Pau-de-leite	Used to treat cancer, herpes and helminthiases [4]	Campo fechado de Cerrado/ Rainy season/ Oxisol

<i>Peschiera affinis</i> (Müll. Arg.) Miers	(UB) 3717	SW (h, e), SB (h, e), R (h, e)	Leiteiro, Mata-pasto, Grão de galo	Used as anti-microbial and anti-tumor [9]	Cerrado sensu stricto/ Rainy season/ Inceptisol
Araliaceae					
<i>Didymopanax macrocarpus</i> (Cham. & Schltdl.) Seem.	(UB) 3821	L (d), SB (h, a, e)	Mandiocão, Verga D'anta	Analgesic [10]	Cerrado sensu stricto/ Dry season/ Oxisol
Asteraceae					
<i>Eremanthus glomerulatus</i> Less.	(UB) 3721	L (h, e), SW (h, e), SB (h, e), RW (h, e), RB (h, e)	Candeia	Astringent [11]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Eremanthus sphaerocephalus</i> (DC.) Baker	(UB) 3708	Ch (e)	João-bobo	Treatment of gastric diseases [12]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Piptocarpha macropoda</i> (DC.) Baker	(UB) 3680	L (h, e), SB (h, e)	Cambará preto	No use reported	Mata Ciliar/ Rainy season/ Inceptisol
<i>Piptocarpha rotundifolia</i> (Less.) Baker	(UB) 3676	L (h, e), SB (h, e), RW (h), RB (h, e)	Paratudo, infalível	Treatment of wounds and used as an anti-syphilitic [2]	Cerrado sensu stricto/ Dry season/ Oxisol
Bignoniaceae					
<i>Anemopaegma arvense</i> (Vell.) Stellfeld ex J.F. Souza	(UB) 3691	L (h, e), S (h, e), R (h, e), Fi (h, e)	Catuaba	Aphrodisiac and central nervous system stimulant [13]	Cerrado sensu stricto/ Dry season/ Inceptisol

<i>Anemopaegma chamberlaynii</i> (Sims) Bureau & K. Schum.	(UB) 3715	L (h), S (h, d, e)	Cipó preto	No use reported	Mata Ciliar/ Dry season/ Inceptisol
<i>Arrabidaea florida</i> DC.	(UB) 3714	L (e), FS ⁱ (h, d, hs)	Cipó-neve	No use reported	Mata Ciliar/ Dry season/ Oxisol
<i>Cybistax antisyphilitica</i> (Mart.) Mart.	(UB) 3696	L (h, e), SW (h, e), SB (h, e), S (h, e), F (h, e)	Caroba-brava, ipê-branco	Depurative, antisyphilitic and diuretic [14]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Jacaranda ulei</i> Bureau & K. Schum.	(UB) 3791	Rz ^k (ch ^s , a, e), AP ⁱ (a)	Carobinha-do-campo	Treatment of prostate and ovary inflammations; allergies; scabies; syphilis; constipation; liver dysfunction; together with blood purification and cholesterol reduction [15]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Tabebuia caraiba</i> (Mart.) Bureau	(UB) 3701	L (h, e), SW (h, e, hs), SB (h, e), RW (e), RB (e)	Ipê-amarelo-do cerrado, pau-d'arco	Used to treat common colds, chills and inflammations; purgative and anti-syphilitic [2]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Zeyheria montana</i> Mart.	(UB) 3799	S (h, a, e), RW (h), RB (a)	Bolsa-de-pastor, Chapéu-de-frade	Used to treat skin conditions; anti-syphilitic [10]	Cerrado sensu stricto/ Dry season/ Oxisol

Burseraceae

<i>Protium heptaphyllum</i> (Aubl.) Marchand	(UB) 3689	L (h, e), SW (e), SB (e), RW (e), RB (h, e)	Breu-branco-verdadeiro, almecegueira-vermelha	Used as a wound healer and expectorant, antiulcerogenic and anti-inflammatory [16]	Mata Ciliar/ Dry season/ Oxisol
<i>Protium ovatum</i> Engl.	(UB) 3694	L (h, d, e), SB (h), S (h, e), R (h, e), F (h, e)	Breu-do-cerrado	Analgesic, expectorant and wound healer [17]	Cerrado sensu stricto/ Dry season/ Inceptisol
Calophyllaceae					
<i>Calophyllum brasiliense</i> Cambess.	(UB) 3754	L (h, d, hs), SW (h, d, a, hs), SB (h, d, hs), RW (h, d, hs), RB (h, d), R (hs, al)	Guanandi, guarandi	Used to treat rheumatism, varicose veins, hemorrhoids and chronic ulcers [16]	Mata Ciliar/ Dry season/ Inceptisol
<i>Kielmeyera coriacea</i> Mart. & Zucc.	(UB) 3745	L (h, d, hs), SW (h, d, a, hs), SB (h, d, hs), RW (h, d), RB (h, d), F (h, hs)	Pau-santo	Used to treat fungal and bacterial infections, malaria, schistosomiasis, leishmaniasis [18]	Cerrado sensu stricto/ Dry season/ Oxisol
Celastraceae					
<i>Cheiloclinium cognatum</i> (Miers) A.C. Sm.	(UB) 3805	L (h, a), SW (h, a, e), SB (h, w)	Saputá	Treatment of fever and edema [19]	Mata Ciliar de Interfluvio/ Rainy season/ Inceptisol
<i>Plenckia populnea</i> Reissek	(UB) 3747	L (a, e), SW (a), SB (a, e)	Marmeleiro-do-campo	Allergy treatments and wound healing [10]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Salacia crassifolia</i> (Mart. ex Schult.) G. Don	(UB) 3776	L (a, e, w), SW (h, a, e), SB (h, a, e), RW (h)	Bacupari-do-Cerrado, Bacupary de caapuêra,	Used as anti-microbial and anti-tumor [20]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Salacia elliptica</i> (Mart.) G. Don	(UB) 3819	L (a, e), SW (h, a), RW (a)	Laranjeira do Cerrado	Laxative [21]	Campo sujo de Cerrado/ Dry season/ Inceptisol

Clusiaceae

<i>Clusia pernambucensis</i> G. Mariz	(UB) 3771	L (h), SW (h, a), SB (h, a, e)	Cebolinha da mata	No use reported	Mata Ciliar em galeria/ Dry season/ Inceptisol
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Combretaceae

<i>Terminalia fagifolia</i> Mart. & Zucc.	(UB) 3812	L (h, a, e, w), SW (a, e, w), SB (h, a, e, w), RB (h), M ^m (a)	Capitão-do-Cerrado	Used to treat canker sores and tumors [22]	Campo aberto de Cerrado/ Dry season/ Oxisol
<i>Terminalia argentea</i> Mart. & Zucc.	(UB) 3808	L (h, d)	Cachaporra-do-gentio	Used to treat coughs, canker sores and common colds [2]	Cerrado sensu stricto/ Rainy season/ Oxisol

Connaraceae

<i>Connarus suberosus</i> Planch.	(UB) 3820	L (a), SW (h, a), RW (h, a, e), RB (h, a)	Cabelo-de-negro	Used to treat diarrhea [2]	Cerrado sensu stricto/ Dry season/ Oxisol
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Dilleniaceae

<i>Davilla elliptica</i> A. St.-Hil	(UB) 3773	L (h, a), SW (e), SB (h)	Cipó cabloco, sambaibinha	Used as an anti-inflammatory, anti-ulcerogenic, laxative and aphrodisiac [23]	Cerrado sensu stricto/ Dry season/ Inceptisol
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Ebenaceae

<i>Diospyros hispida</i> A. DC.	(UB) 3760	SW (h, d, hs), SB (h, d, hs), RW (w), R (h, a, e)	Caqui do Cerrado, fruta de boi	Treatment of infectious diseases [24]	Campo aberto de Cerrado/ Dry season/ Inceptisol
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Euphorbiaceae

<i>Croton goyazensis</i> Müll. Arg.	(UB) 3793	R (ch, e), AP (ch, a, e)	Pé-de-perdiz	Treatment of infections and general inflammation(s) [25]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Croton urucurana</i> Baill.	(UB) 3813	L (h, hs), SW (h, hs), SB (hs)	Sangue de dragão	Treatment of rheumatism, wounds, ulcers, diarrhea, and cancer [13]	Mata Ciliar/ Rainy season/ Oxisol
<i>Maprounea guianensis</i> Aubl.	(UB) 3772	L (d), SW (e), SB (h, a, e), RB (h, a, e)	Pinga-orvalho, milho-torrado	Used as an anti-diarrhea compound and to treat leg rashes [26]	Mata Ciliar em galeria/ Dry season/ Inceptisol
Fabaceae					
<i>Andira humilis</i> Mart. ex. Benth.	(UB) 3764	L (h, e), SW (a, e), SB (e), RW (h), RB (e)	Angelim rasteira, mata barata	Treatment of common colds, helminthiases and vaginal discharge [27]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Andira vermifuga</i> Mart. ex. Benth.	(UB) 3763	L (h)	Angelim	Purgative, emetic and narcotic effects [8]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Chamaecrista desvauxii</i> (Collad.) Killip	(UB) 3800	AP (a, e)	Rabo de pitu, vassourinha	Laxative and purgative [28]	Cerrado sensu stricto/ Rainy season/ Oxisol
<i>Enterolobium ellipticum</i> Benth.	(UB) 3739	L (h, d, hs), SW (h, hs), SB (h), S (h, hs), RW (h, d, hs, al), RB (h)	Tamboril, Favela branca	Used to treat lung infections [8]	Cerrado sensu stricto/ Rainy season/ Oxisol
<i>Enterolobium gummiferum</i> (Mart.) J.F. Macbr.	(UB) 3807	L (a), SW (h, a), SB (h), RW (h, a, e), RB (a)	Timburi, Orelha de macaco	Used to treat the lungs and dermatitis, antihelminthic [29]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Plathymenia reticulata</i> Benth.	(UB) 3794	SW (a), SB (h, e), RW (h), RB (h)	Vinhático-do-cerrado	Used to treat varicose veins, some inflammatory diseases, infections and cases of hemorrhaging resulting from an insect/tick bite [30]	Cerrado sensu stricto/ Dry season/ Oxisol

<i>Sclerolobium aureum</i> (Tul.) Baill.	(UB) 3818	L (a), SW (h, a, e), SB (a), RW (h, a, e), RB (a)	Gonçalo do campo	Used to treat fungal infections and as a hepatoprotector [31]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Stryphnodendron adstringens</i> (Mart.) Coville	(UB) 3740	L (h, d, hs, al), SW (h, d), SB (h, d, hs), RW (h, d), RB (h)	Barbatimão	Used as an anti-inflammatory, astringent and for healing wounds and vaginal infections [16]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Vatairea macrocarpa</i> (Benth.) Ducke	(UB) 3815	L (a), SW (h, a, e), SB (a), RW (h, a), RB (h, a)	Amargoso, angelim-do-Cerrado, maleiteira	Treatment of diabetes, superficial mycoses and cancer [31]	Cerrado sensu stricto/ Dry season/ Inceptisol
Hypericaceae					
<i>Vismia decipiens</i> var. <i>pyrifolia</i> Schlttdl. & Cham.	(UB) 3769	L (h, a, e), SW (h, a, e), SB (h, a, e, w), RW (h), RB (e), F (h, a)		No use reported	Mata Ciliar/ Dry season/ Oxisol
Magnoliaceae					
<i>Talauma ovata</i> A.St.-Hil.	(UB) 3738	L (h, e), SW (h, e), SB (h, e)	Baguaçu	Treatment of diabetes and fever [6]	Mata Ciliar/ Rainy season/ Oxisol
Malpighiaceae					
<i>Byrsonima coccolobifolia</i> Kunth	(UB) 3774	RW (h, a), SW (e), RB (h, e), SB (h, e)	Murici-pequeno	Treatment of gastrointestinal disorders [26]	Campo sujo de Cerrado/ Dry season/ Inceptisol
<i>Byrsonima crassa</i> Nied.	(UB) 3743	L (h, d, hs), SW (h, hs), SB (h, hs, al), RW (d, hs), RB (h)	Murici-cascudo, murici-vermelho	Antiemetic, diuretic, febrifuge, used to treat ulcers, gastritis and diarrhea [32]	Cerrado sensu stricto/ Dry season/ Oxisol

Meliaceae

<i>Guarea guidonia</i> (L.) Sleumer	(UB) 3712	L (h, e), S (h, e), R (h, e)	Cedro-macho, açafroa	Astringent, purgative, febrifuge, emetic and abortive [16]	Mata Ciliar/ Dry season/ Oxisol
<i>Guarea kunthiana</i> A. Juss.	(UB) 3710	L (h, e), S (h, d, e), R (h, d, e), F (e)	Jatuaúba	Antimalarial and used to treat stomach pains [6]	Mata Ciliar/ Dry season/ Oxisol
Myrtaceae					
<i>Blepharocalyx salicifolius</i> (Kunth) O. Berg	(UB) 3798	L (h, a, e, w), SW (h, a), SB (h, a), RB (w)	Anacahuita	Used as an external astringent, treatment of diarrhea, leucorrhoea, urethritis, rectal prolapse; antirheumatic, hypoglycemic, diuretic [16]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Eugenia dysenterica</i> DC.	(UB) 3803	L (hs)	Cagaita	The fruit is a laxative and the leaves are used to treat diarrhea [33]	Cerrado sensu stricto/ Rainy season/ Oxisol
<i>Myrcia linearifolia</i> Cambess.	(UB) 3817	R (h, a), AP (a)	Ratanhia, araçazinho	An edible fruit, with leaves used for their allelopathic activity [34]	Cerrado sensu stricto/ Dry season/ Inceptisol
<i>Psidium laruotteanum</i> Cambess.	(UB) 3810	L (h, a), SW (h, a), SB (h)	Araça cascudo	Used against stomachache and colic, colds, diarrhea, sore throat and worms [26]	Cerrado sensu stricto/ Rainy season/ Oxisol

Nyctaginaceae

<i>Guapira noxia</i> (Netto) Lundell	(UB) 1537	SW (a), RW (a), RB (a)	Pau-lepra, capa-rosa	No use reported	Cerrado sensu stricto/ Dry season/ Inceptisol
<i>Neea theifera</i> Oerst.	(UB) 3821	L (a), SW (h, a), RW (h, a, e), RB (a)	Capa-rosa-do-campo	Used to treat diarrhea, enterocolitis and enterorrhagia [8]	Cerrado sensu stricto/ Dry season/ Inceptisol
Ochnaceae					
<i>Ouratea floribunda</i> Engl.	(UB) 3713	L (d), F (h)	Caju bravo	Used as an astringent, tonic, vermifuge and to treat paralysis, erysipelas, wounds in the uterus, ulcers, gastric disorders and wound healing [35]	Cerrado sensu stricto/ Dry season/ Oxisol
Opiliaceae					
<i>Agonandra brasiliensis</i> Miers ex Benth. & Hook. f.	(UB) 3797	L (h, a, e), R (h)	Pau-marfim, quina de veado	Used to treat rheumatism, healing and treating bronchitis [29]	Cerrado sensu stricto/ Dry season/ Oxisol
Primulaceae					
<i>Myrsine guianensis</i> (Aubl.) Kuntze	(UB) 3795	L (h, a), SB (h, a, e, w), R (a)	Capororoca branca	No use reported	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Rapanea guianensis</i> Aubl.	(UB) 3804	L (h, a, e), SW (h, e), RW (h, a, e), RB (w)	Capororoca	Used to treat snake bites, cleanse tumors and wounds [9]	Cerrado sensu stricto/ Rainy season/ Oxisol
Rubiaceae					
<i>Chomelia pohliana</i> Mull. Arg.	(UB) 3741	L (d, hs), S (d), R (hs)	Limaorana, mentolzinho	No use reported	Mata Ciliar/ Dry season/ Inceptisol

<i>Palicourea rigida</i> Kunth	(UB) 3722	L (h, d), R (h, d, hs), AP (h, e)	Congonha-dourada, douradinha	Treatment of urinary tract inflammation [36]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Sabicea brasiliensis</i> Wernham	(UB) 3709	R (h, e), F (h, e)	Sangue de cristo	Treatment of infections in female genitalia [37]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Tocoyena formosa</i> (Cham. & Schltdl.) K. Schum.	(UB) 3792	L (h, a, e)	Genipa-brava, Trombeta, Genipaparaná	Use for the treatment of rheumatic pains [38]	Cerrado sensu stricto/ Dry season/ Oxisol
Rutaceae					
<i>Spiranthera odoratissima</i> A. St.-Hil.	(UB) 3768	L (h, a, e), R (h, a, e), F (h)	Manacá	Used for the treatment of rheumatism, gout, acne, boils, kidney infections and inflammation [39]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Zanthoxylum rhoifolium</i> Lam.	(UB) 3770	L (ch, a, e), SW (h, a, e, w), SB (a), RW (h, a, e, w), RB (ch, h, a, e)	Mamica-de-cadela, mamica-de-porca	Treatment and prevention of malaria [40]	Cerrado sensu stricto/ Dry season/ Inceptisol
Salicaceae					
<i>Casearia sylvestris</i> var. <i>lingua</i> (Cambess.) Eichler.	(UB) 3693	L (h, e), SW (h), SB (e), RW (h, e), RB (e), F (h, e)	Erva de Lagarto	Used as an anti-inflammatory, analgesic, antibiotic and in anti- cancer treatments [4]	Cerrado sensu stricto/ Dry season/ Inceptisol
Sapindaceae					
<i>Cupania vernalis</i> Cambess.	(UB) 3695	L (h, e), SW (h, e), SB (h, e), RW (h, e), RB (h, e), R (e)	Camboatã vermelho, olho de cotia	Treatment of fever and inflammation or as a tonic [4]	Mata Ciliar de Galeria/ Rainy season/ Oxisol

<i>Magonia pubescens</i> A.St. -Hil.	(UB) 3702	L (h, e), SB (h, e), RW (h, e), RB (h, e), R (h, e), F (h), FS (e)	Tingui	Insecticide and used to kill lice [29]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Matayba guianensis</i> Aubl.	(UB) 3697	SW (h, e), SB (h, e), RW (h, d, hs), RB (h, e), R (al)	Camboatá, assa-leitão	Edible fruit	Cerrado sensu stricto/ Rainy season/ Inceptisol
<i>Serjania lethalis</i> A. St. -Hil.	(UB) 3716	L (h, e), SW (h, e), SB (e), RB (h, e)	Timbó do cerrado	Used as an analgesic, anti-inflammatory and piscicide; Ichthyotoxic properties [4]	Cerrado sensu stricto/ Rainy season/ Inceptisol
Sapotaceae					
<i>Chrysophyllum soboliferum</i> Rizzini	(UB) 3733	L (h, e)	Fruta de tatu	Edible fruit	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Pouteria gardneri</i> (Mart. & Miq.) Baehni	(UB) 3672	L (h, e), SW (e), RW (h, e), RB (h, e), R (h, e)	Sapotinha	Edible fruit	Mata Ciliar/ Rainy season/ Inceptisol
<i>Pouteria ramiflora</i> (Mart.) Radlk.	(UB) 3671	L (h, e), SW (h, e), SB (h, e), RW (h, e), RB (h, e)	Abiu do cerrado, pitomba de leite	Used on bruises [41]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Pouteria torta</i> (Mart.) Radlk.	(UB) 3674	L (h, d, e), SW (e), RW (h, e), RB (h)	Curiola; Grao de galo	Edible fruit and the stem used in the treatment of dysentery	Cerrado sensu stricto/ Rainy season/ Inceptisol
Simaroubaceae					
<i>Simaba suffruticosa</i> Engl.	(UB) 3790	L (a)	Calunga	Abortive [42]	Cerrado sensu stricto/ Rainy season/ Oxisol

<i>Simarouba versicolor</i> A. St. -Hil.	(UB) 3724	L (h, d, e), SB (h, e), S (e), RB (h, e), F (h, e)	Mata-cachorro	Used as a tonic to treat weakness; anti-helminthic, anti-hemorrhagic, anti-diarrhea, anti-dysenteric, anti-dyspepsia, anti-syphilitic, febrifuge and snake venom neutralizer [43]	Cerrado sensu stricto/ Dry season/ Oxisol
Siparunaceae					
<i>Siparuna cujabana</i> (Mart. ex Tul.) A. DC.	(UB) 3737	L (e), S (h, e), R (h, e), F (h, e)	Pau-limão	Anti-spasmodic [8]	Mata Ciliar/ Rainy season/ Oxisol
<i>Siparuna guianensis</i> Aubl.	(UB) 3106	L (h, e), SW (h, e), SB (h, e)	Negramina, capitiú	Used to relieve fever and body pain [44]	Mata Ciliar/ Rainy season/ Oxisol
Solanaceae					
<i>Solanum lycocarpum</i> A. St.-Hil.	(UB) 3720	L (h)	Lobeira	Used as tonic, emollient and antirheumatic; used to treat asthma, flu and colds [10]	Cerrado sensu stricto/ Rainy season/ Oxisol
Styracaceae					
<i>Styrax ferrugineus</i> Nees & Mart.	(UB) 2621	SW (h)	Laranjeira do campo	Used to treat fevers, burns and coughs; depurative [10]	Cerrado sensu stricto/ Dry season/ Oxisol
Symplocaceae					
<i>Symplocos rhamnifolia</i> A. DC.	(UB) 3331	SW (a), SB (a), RW (a), RB (a)	Congonha	Used when experiencing kidney problems; taken as a coffee or tea-like infusion [45]	Cerrado sensu stricto/ Dry season/ Inceptisol
Verbenaceae					

<i>Lippia rotundifolia</i> Cham.	(UB) 3796	L (h, a, e), SW (h, a), SB (a), R (h), FL ^a (h, a)	Rosmaninho, cha de pedestre	Used for relaxing baths and feet scaling [46]	Cerrado sensu stricto/ Dry season/ Inceptisol
Vochysiaceae					
<i>Qualea grandiflora</i> Mart.	(UB) 3746	L (h, d, hs), SW (h, d, e, hs), SB (h, d, hs), S (d), RB (d, hs), R (e, hs), FS (h, d, hs)	Pau-terra-do-cerrado	Antiseptic; indicated to treat diarrhea with blood, intestinal colic and amoebae [10, 29]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Qualea parviflora</i> Mart.	(UB) 3742	SW (h, d, hs), SB (d, hs), RW (h, d, hs, al), RB (hs), F (h)	Pau-terra-mirim	Used as an antiseptic and antiulcerogenic, and in the treatment of gastrointestinal disorders [47]	Cerrado sensu stricto/ Dry season/ Oxisol
<i>Salvertia convallariodora</i> A.St.-Hil.	(UB) 3777	L (h, a, e), SW (h, a, e)	Colher de vaqueiro	Gastro-protectant [48]	Cerrado sensu stricto/ Dry season/ Oxisol
Zingiberaceae					
<i>Renealmia alpinia</i> (Rottb.) Maas	(UB) 3719	L (h, e), Rz (h, d, hs), P ^o (h), LP ^p (h)	Paco-seroca	Used as febrifuge and to treat snake bites [49]	Mata Ciliar/ Rainy season/ Oxisol

All individuals were adults.

*The Cerrado climate is highly seasonal marked with dry (May-September) and rainy (October-April) seasons.

Solvent: d¹: dichloromethane, hs²: 90% hydroethanol, h³: hexane, a⁴: ethyl acetate, e⁵: ethanol, w⁶: water, al⁷: alkaloid extract, ch⁸: cyclohexane

Part of plant: ^aL: Leaf, ^bSW: Stem Wood, ^cSB: Stem Bark, ^dRW: Root Wood, ^eRB: Root Bark, ^fR: Root (Wood+ Bark), ^gS: Stem (Bark + Wood), ^hC:

Capitulum, ⁱF: Fruit, ^jFS: Fruit+Seed, ^kRz: Rhizome, ^lAP: Aerial Parts, ^mM: Mucilage, ⁿFL: Flower, ^oP: Pseudostem, ^pLP: Leaf + pseudostem

Table S2. Z-factors for plates used in initial screening and secondary dose response testing [50].

Cell line	Primary screening	Secondary D/R screening*
COLO205 (colon)	0.35, 0.50	0.41, 0.58, 0.58, 0.50
KM12 (colon)	0.54, 0.40	0.87, 0.68, 0.46
UO31 (renal)	0.51, 0.42	0.42, 0.43, 0.44, 0.74
A498 (renal)	0.39, 0.41	0.39, 0.57, 0.42, 0.41
MG63 (osteosarcoma)	0.73, 0.78	0.62, 0.59, 0.72
MG63.3 (osteosarcoma)	0.58, 0.66	0.51, 0.58, 0.80
HEP3B (hepatocellular)	0.56, 0.67	Not tested
SKHEP (hepatocellular)	0.64, 0.72	Not tested

*The number of plates varied according to the number of active samples with that cell line.

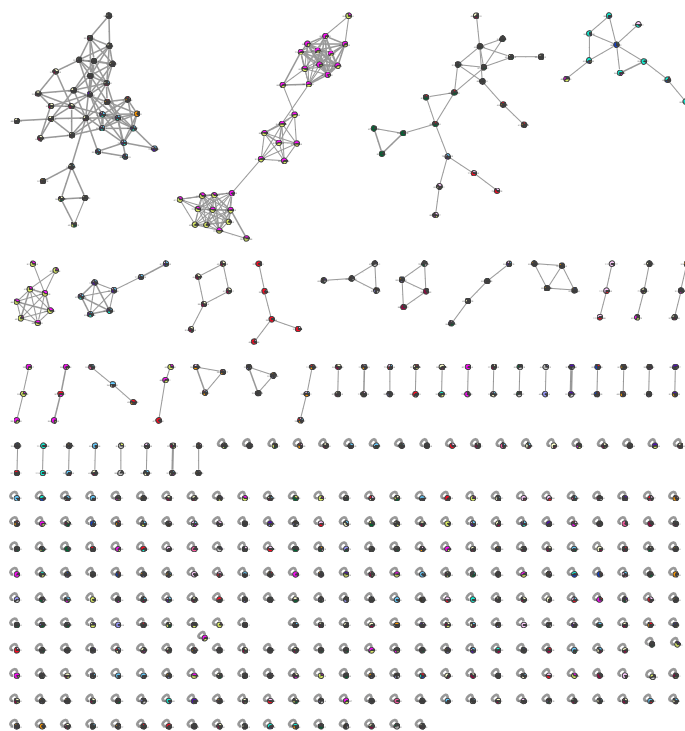
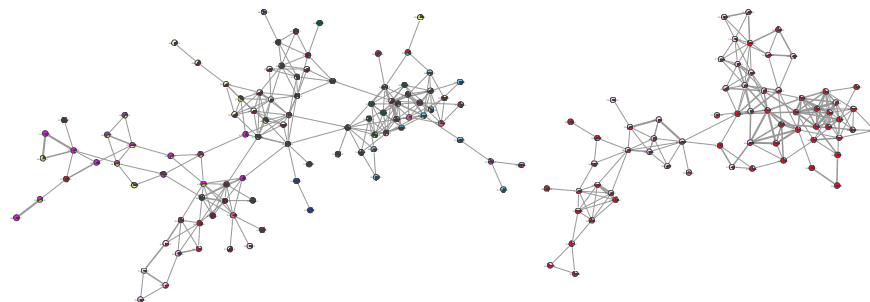


Figure S1. Complete molecular networking (MN) of 17 more active Cerrado plants.

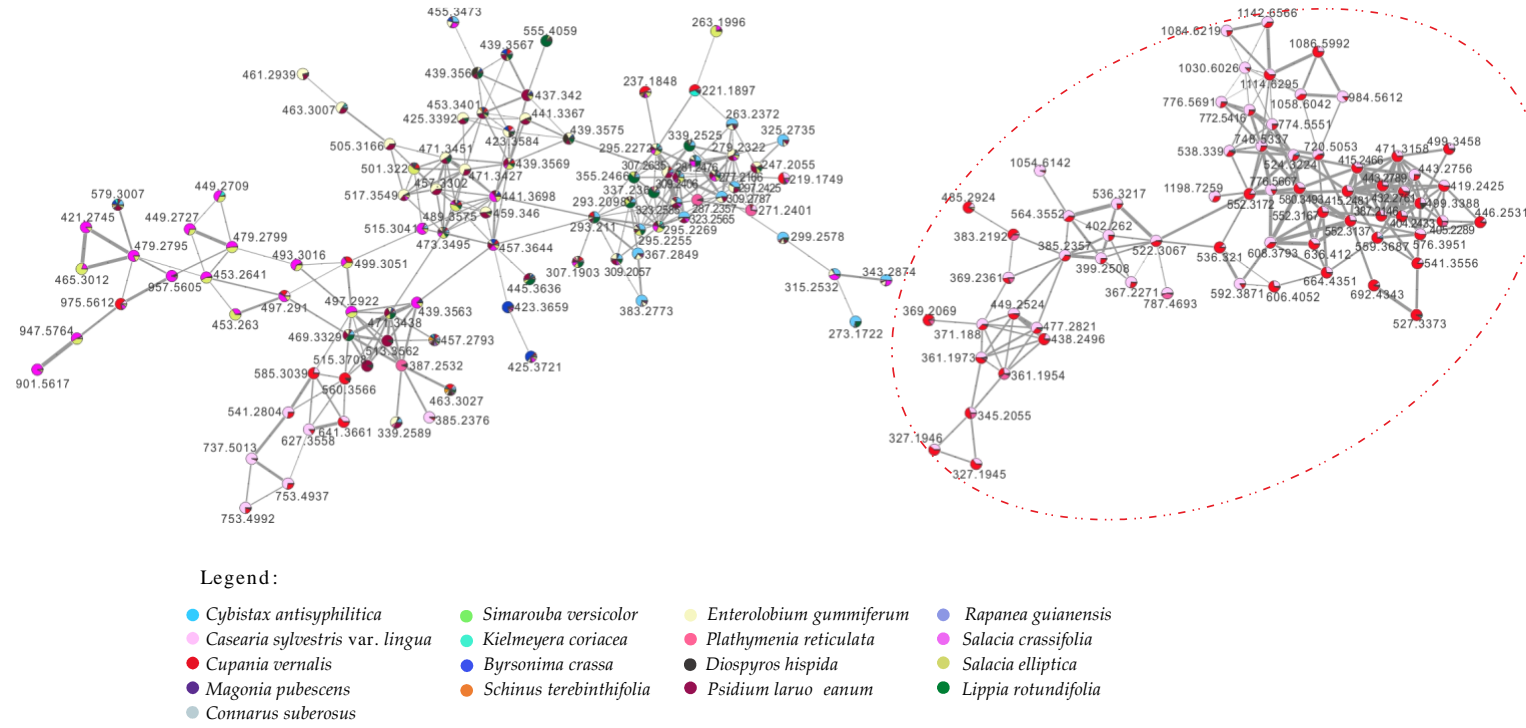


Figure S2. Expansion of the network, top portion.

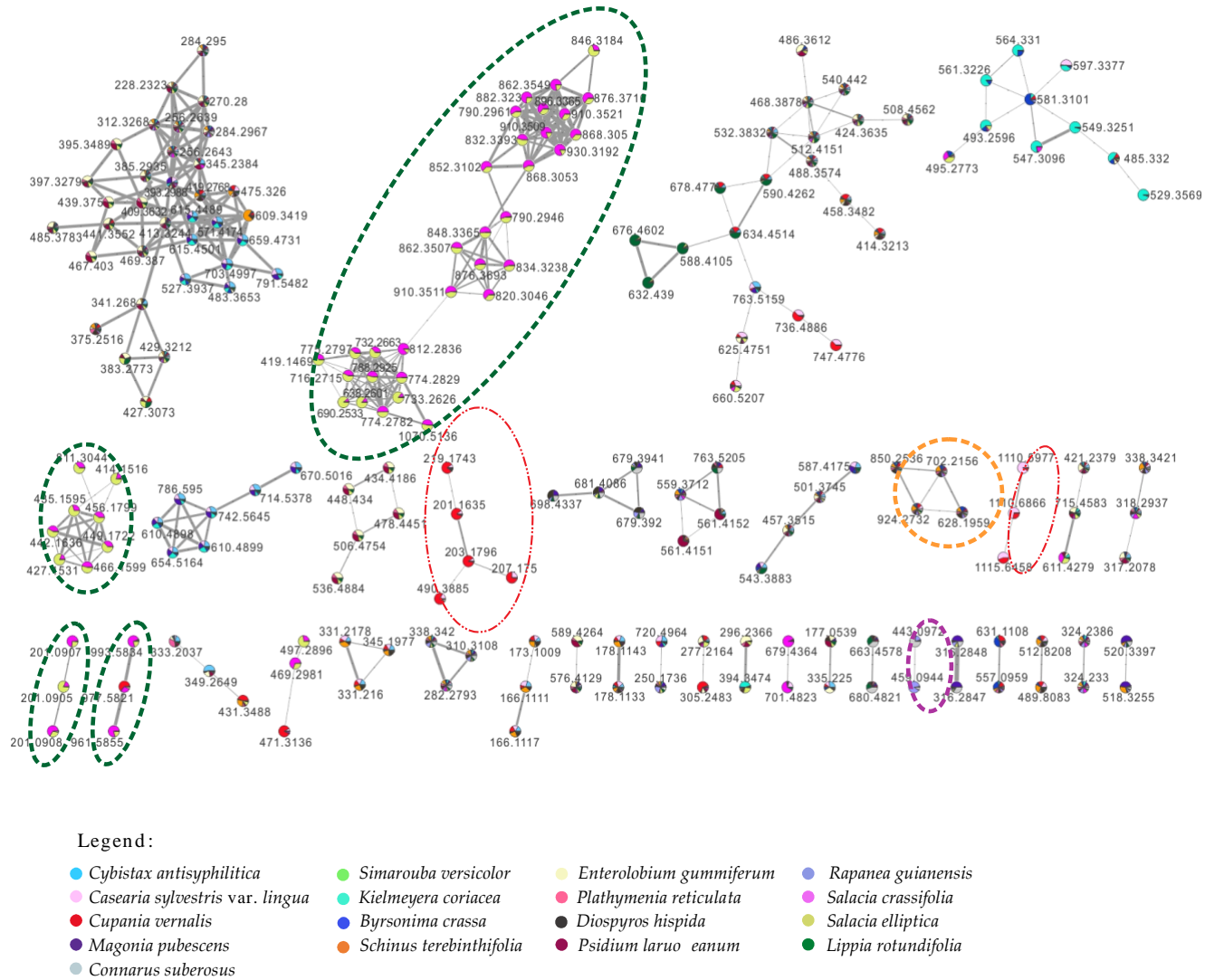


Figure S3. Expansion of the network, central portion.



Legend:

- | | | | |
|---|--|--|--|
| ● <i>Cyrtopogon antisyphilitica</i> | ● <i>Simarouba versicolor</i> | ● <i>Enterolobium gummiferum</i> | ● <i>Rapanea guianensis</i> |
| ● <i>Casearia sylvestris</i> var. <i>lingua</i> | ● <i>Kielmeyera coriacea</i> | ● <i>Plathymenia reticulata</i> | ● <i>Salacia crassifolia</i> |
| ● <i>Cupania vernalis</i> | ● <i>Byrsonima crassa</i> | ● <i>Diospyros hispida</i> | ● <i>Salacia elliptica</i> |
| ● <i>Magonia pubescens</i> | ● <i>Schinus terebinthifolia</i> | ● <i>Psidium laruotteanum</i> | ● <i>Lippia rotundifolia</i> |
| ● <i>Commersonia bartramia</i> | | | |

Figure S4. Expansion of the network, bottom portion.

Results graphs of NCI-60 screening S5 to S55

A. *Cybistax antispyhilitica*

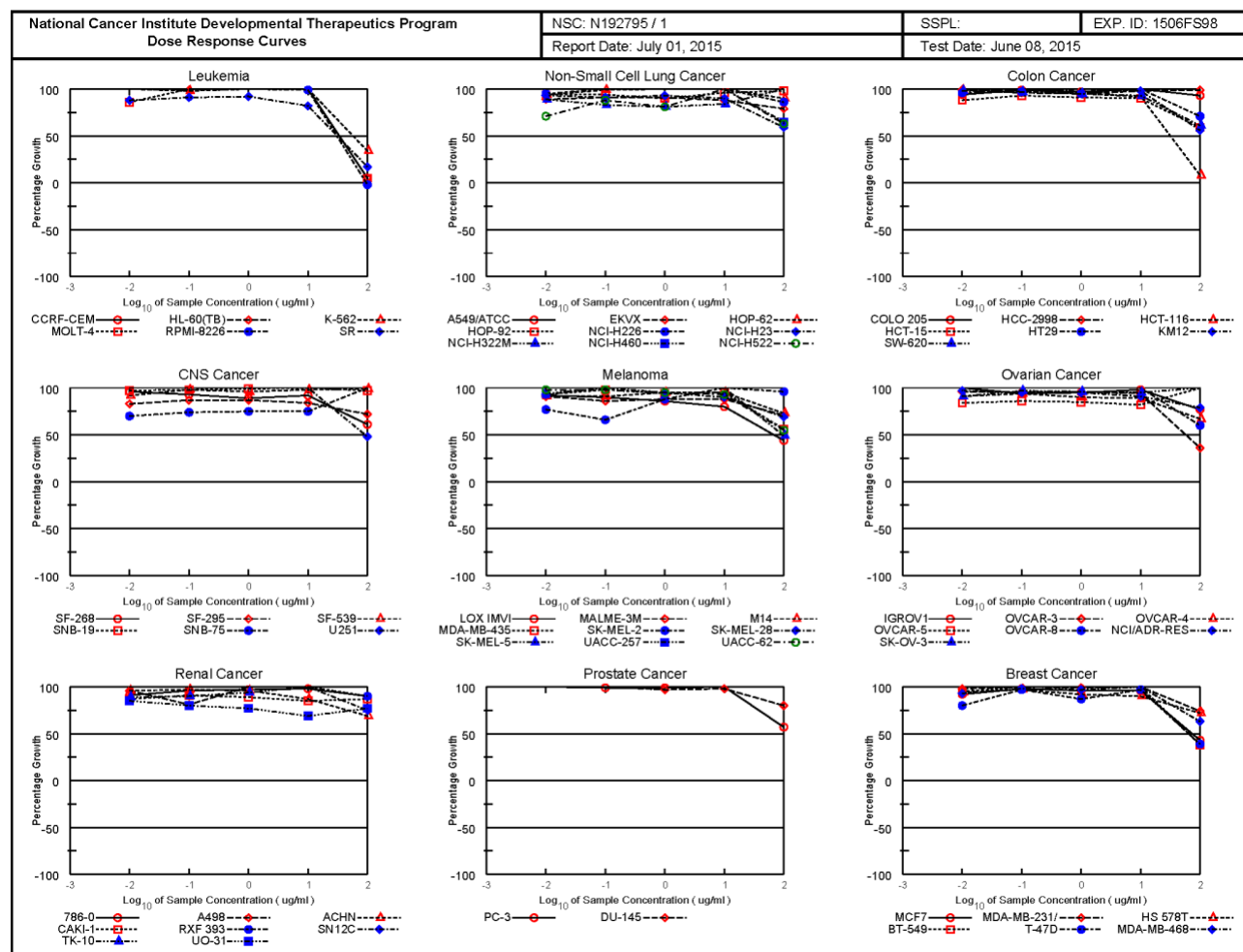


Figure S5. Dose response curves of the *Cybistax antispyhilitica* stem bark hexane extract (BR 125/N192795) against 9 cell panels with different susceptibility.

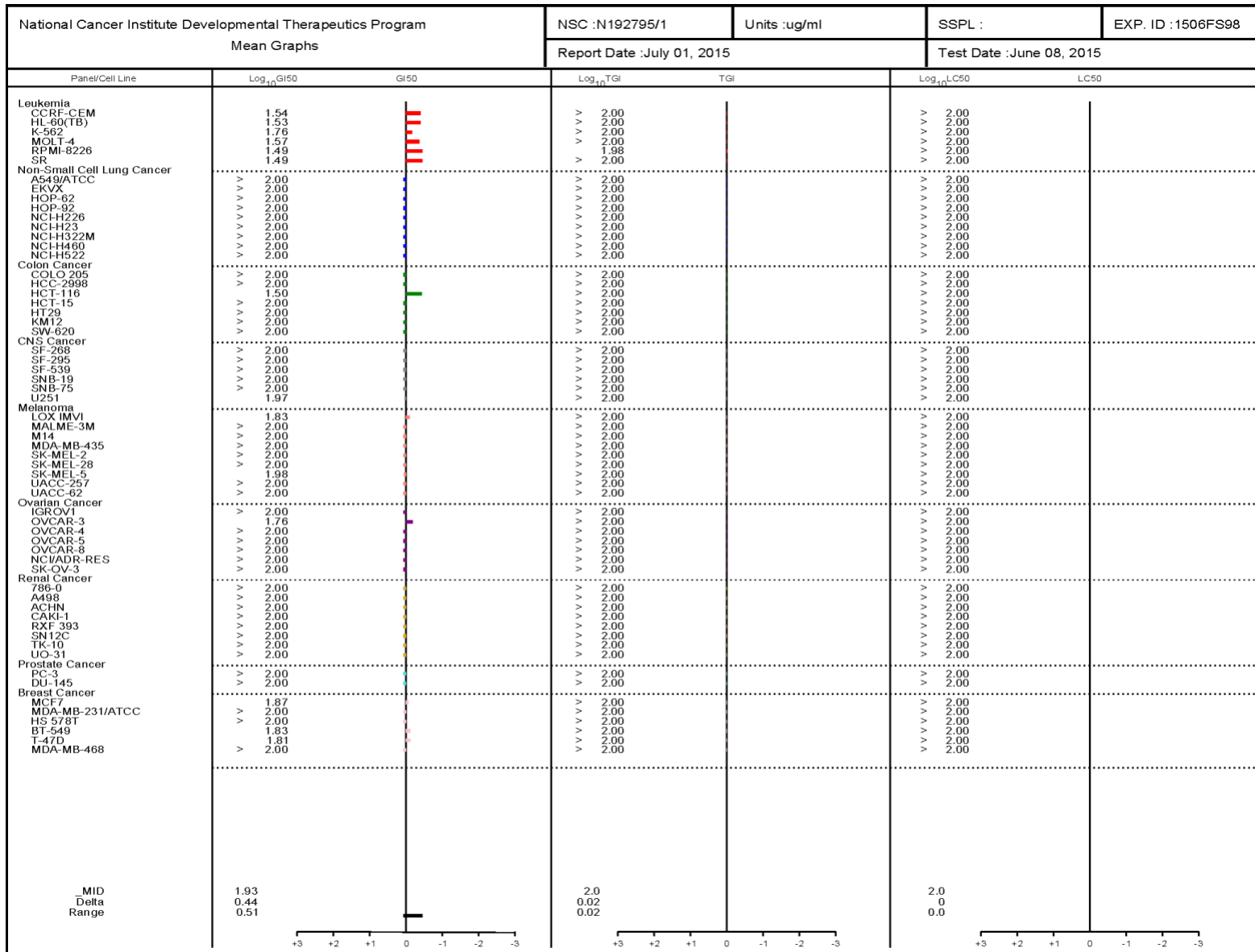


Figure S6. Mean bar graph of the *Cybistax antispyhilitica* stem bark hexane extract (BR 125/N192795) in the NCI-60 cell five-dose screen.

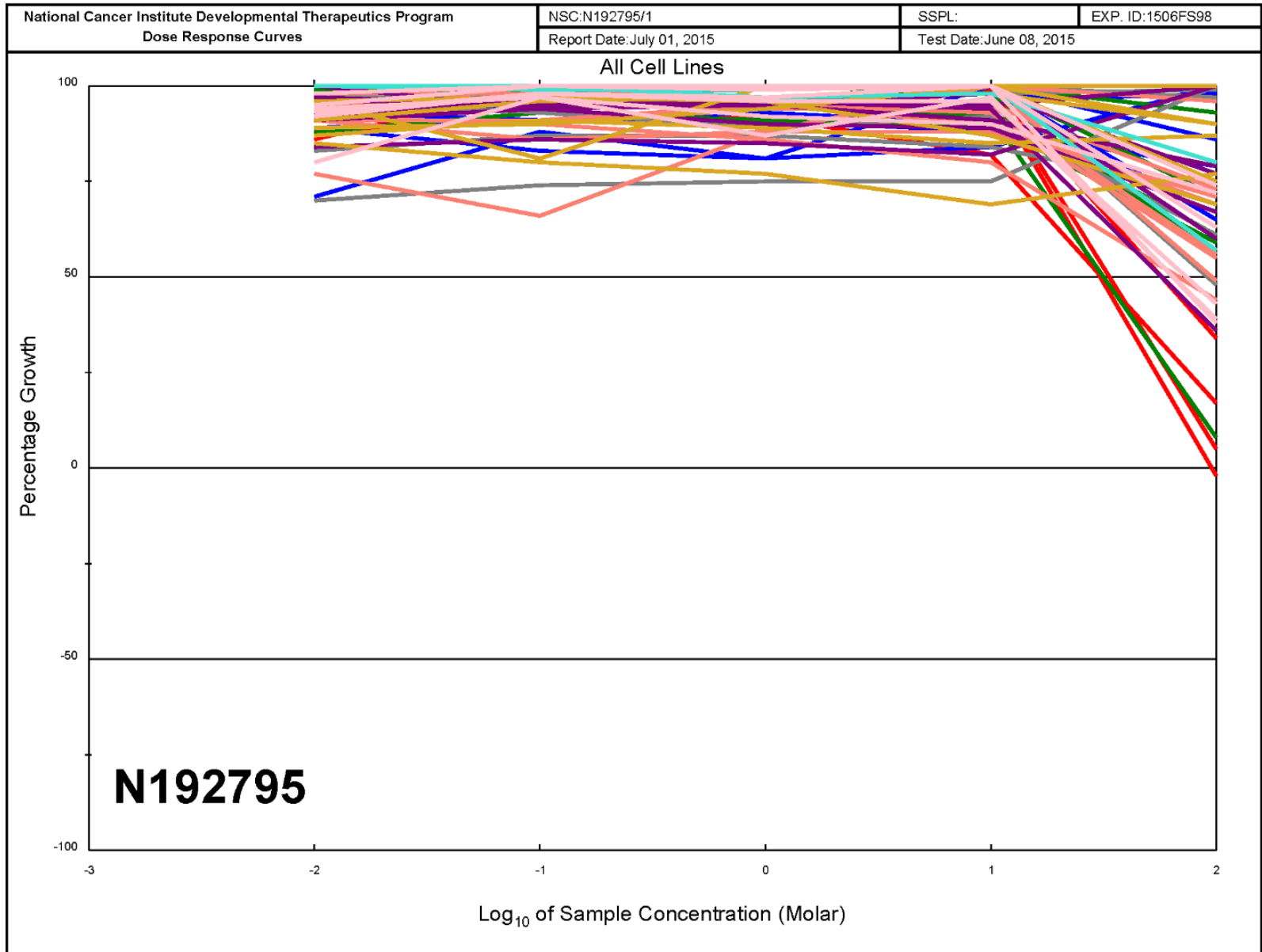


Figure S7. Composite of the NCI-60 dose response curves for the *Cybastax antisiphilitica* stem bark hexane extract (BR 125/N192795).

B. *Magonia pubescens*

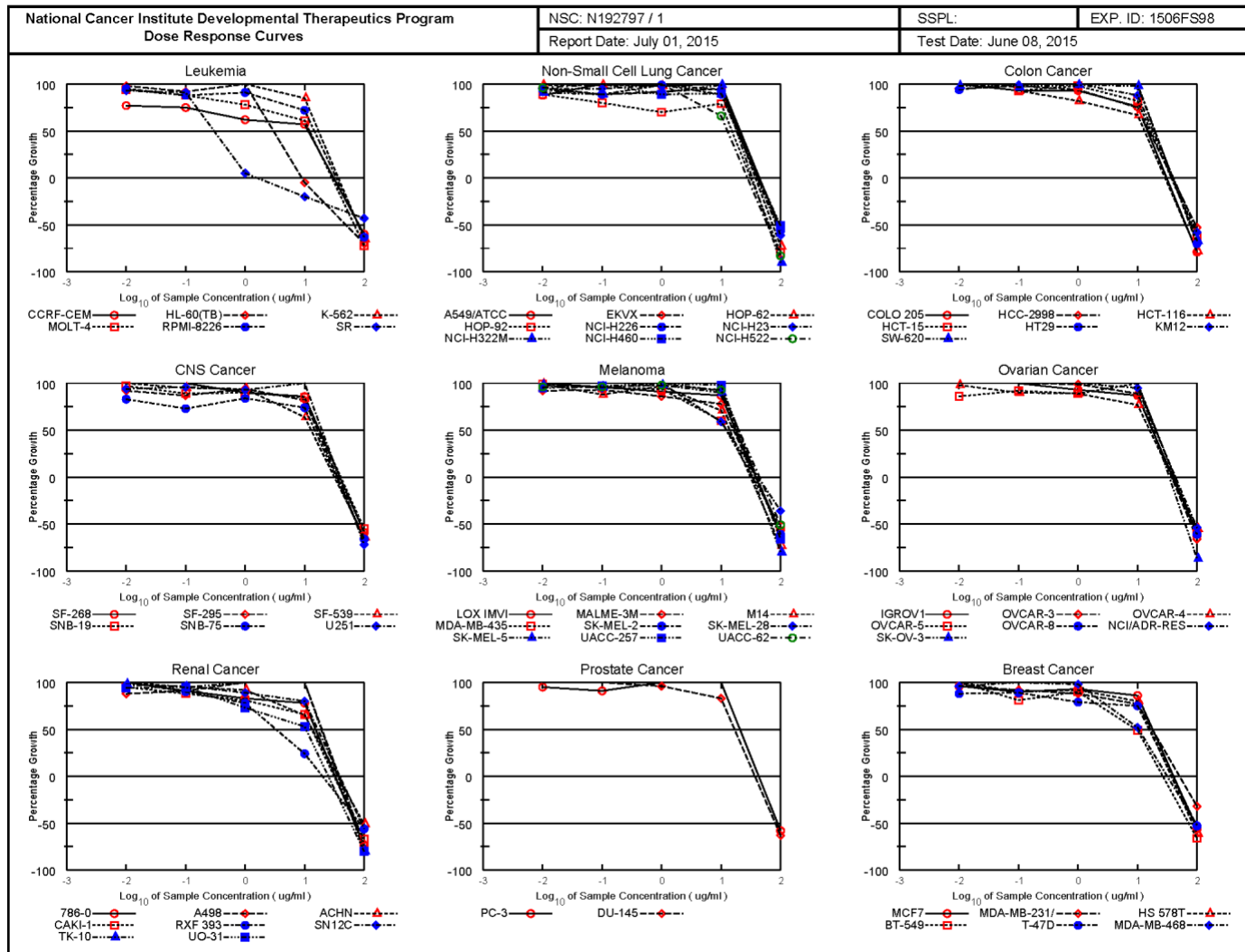


Figure S8. Dose response curves of the *Magonia pubescens* root wood ethanol extract (BR 204/N192797) against 9 cell panels with the highest activity against the leukemia SR cell line.

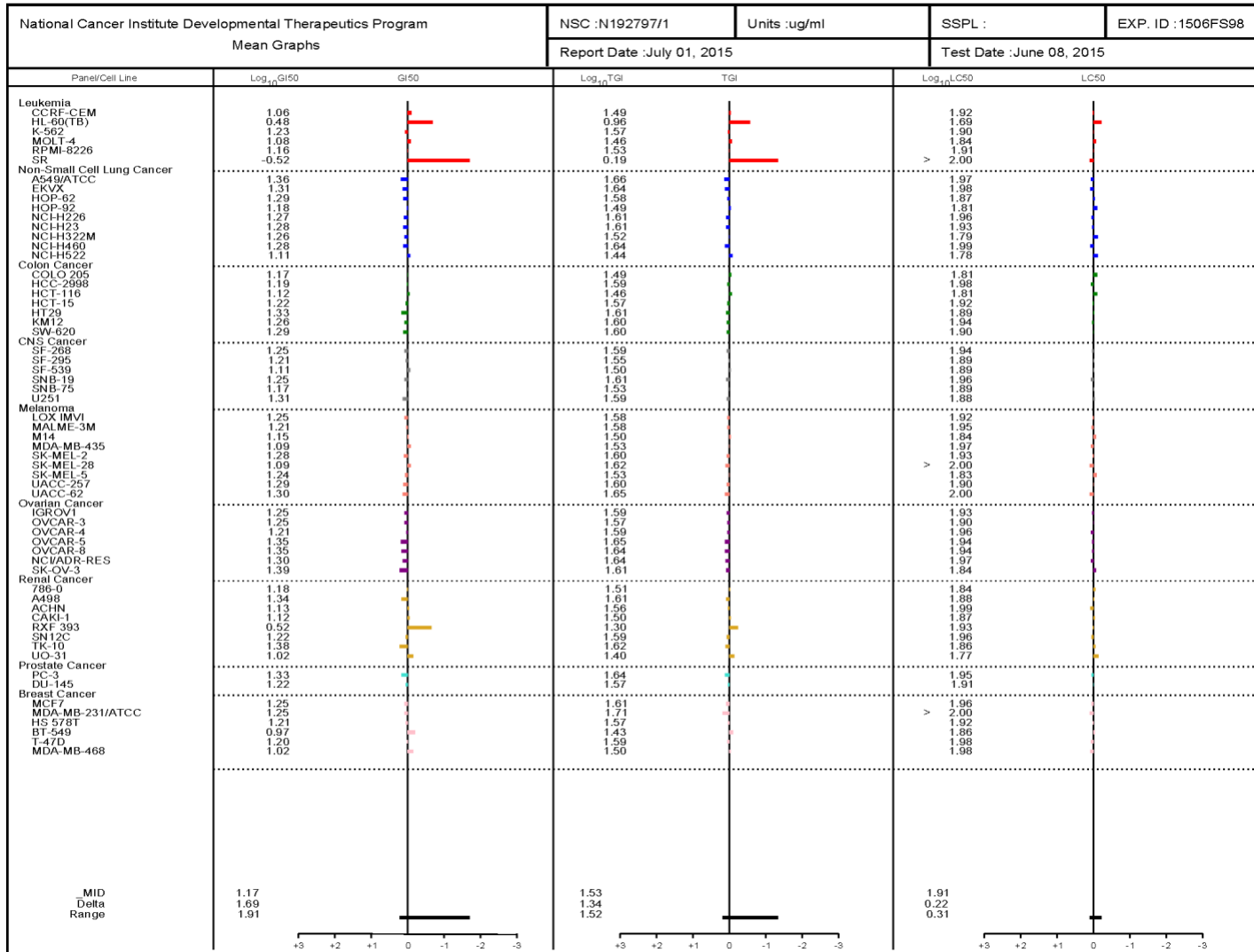


Figure S9. Mean bar graph of the *Magonia pubescens* root wood ethanol extract (BR 204/N192797) in the NCI-60 cell five-dose screen.

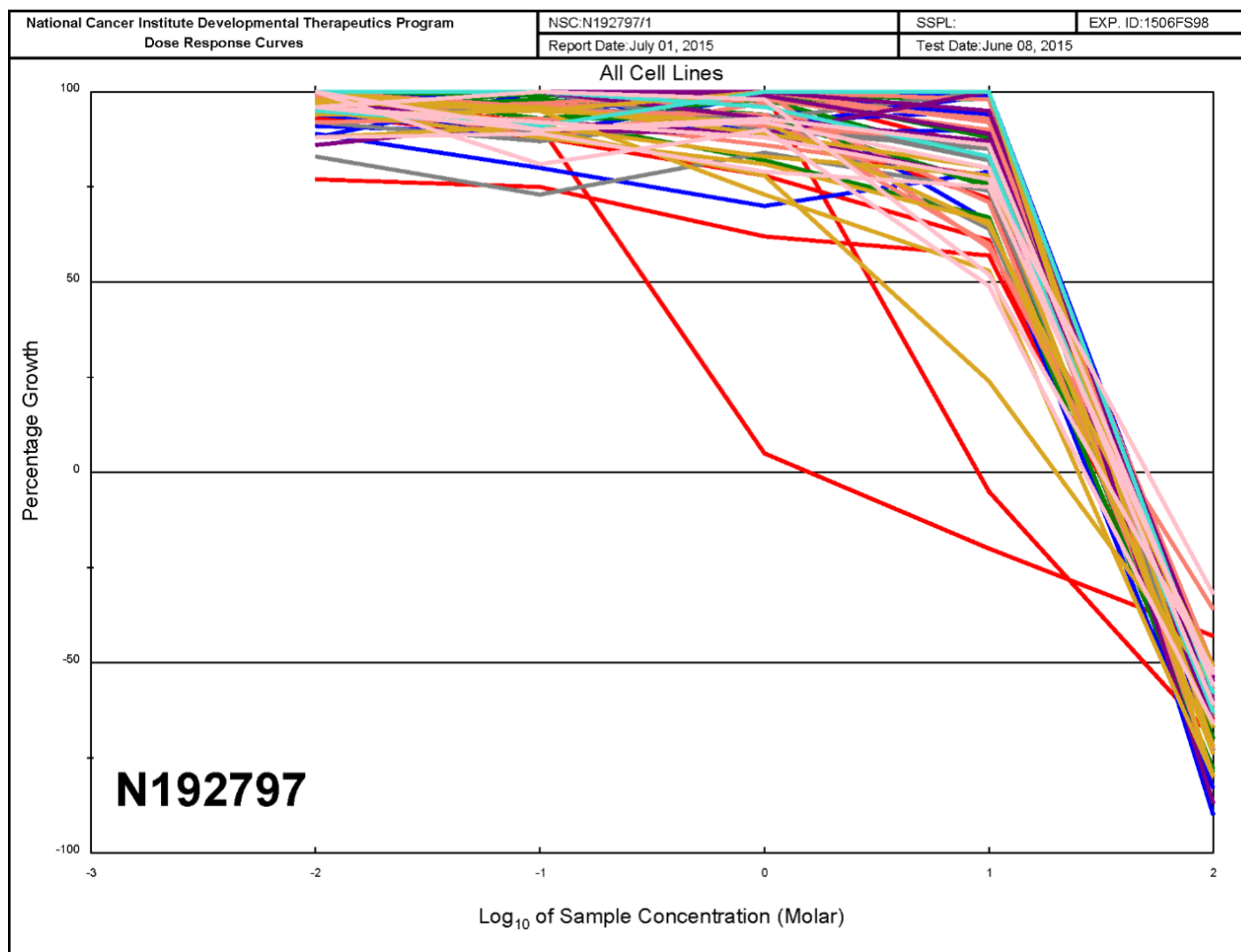


Figure S10. Composite of the NCI-60 dose response curve of the *Magonia pubescens* root wood ethanol extract (BR 204/N192797) with higher activity against the leukemia SR cell line.

C. Diospyros hispida

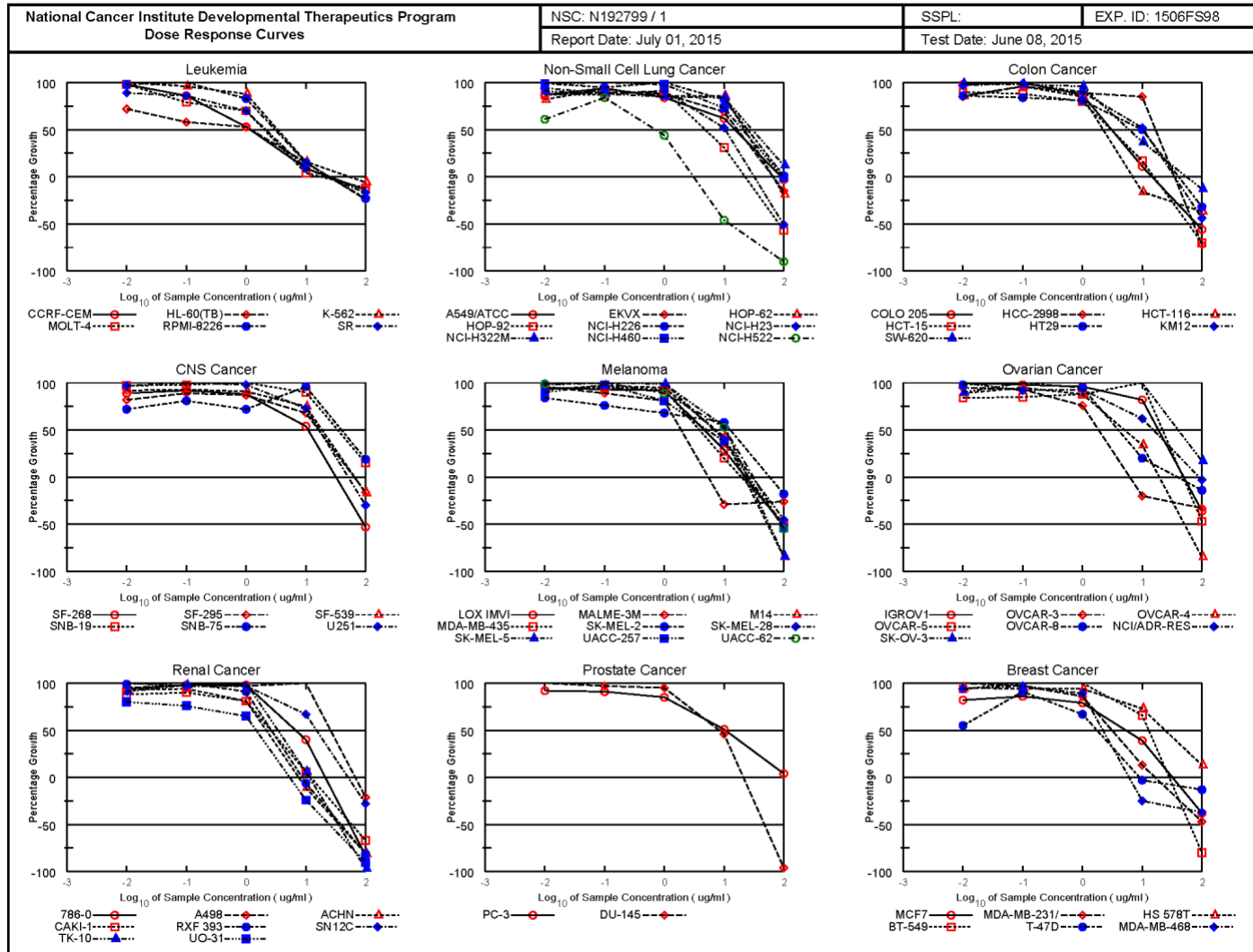


Figure S11. Dose response curves of the *Diospyros hispida* root (wood + bark) ethyl acetate extract (BR 501/N192799) against NCI-60 panels, with the highest activity against the non-small cell lung cancer NCI-H522.

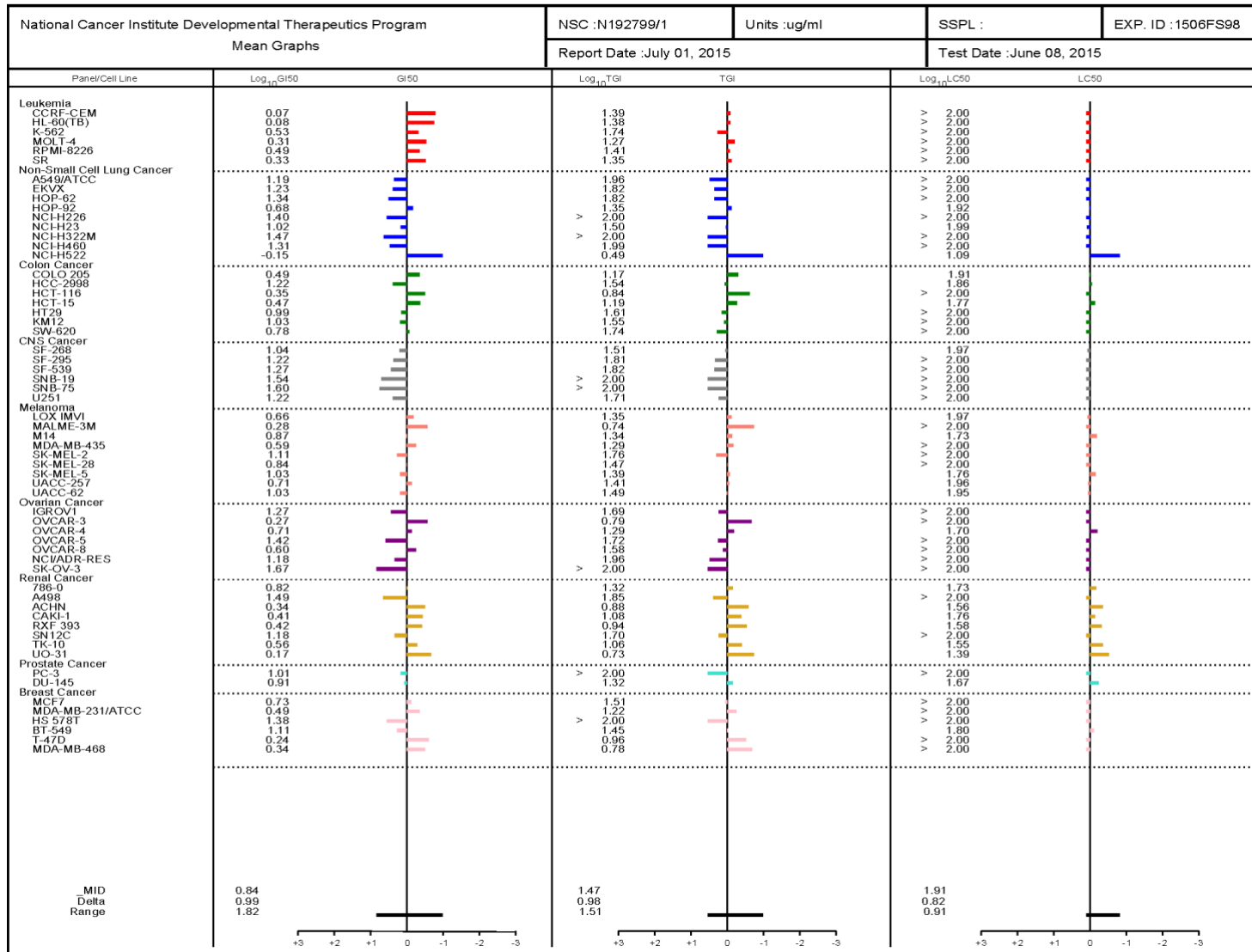


Figure S12. Mean bar graph of the *Diospyros hispida* root (wood + bark) ethyl acetate extract (BR 501/N192799) in the NCI-60 cell five-dose screen.

Sensitive cell lines project to the right of the mean and resistant cell lines project to the left.

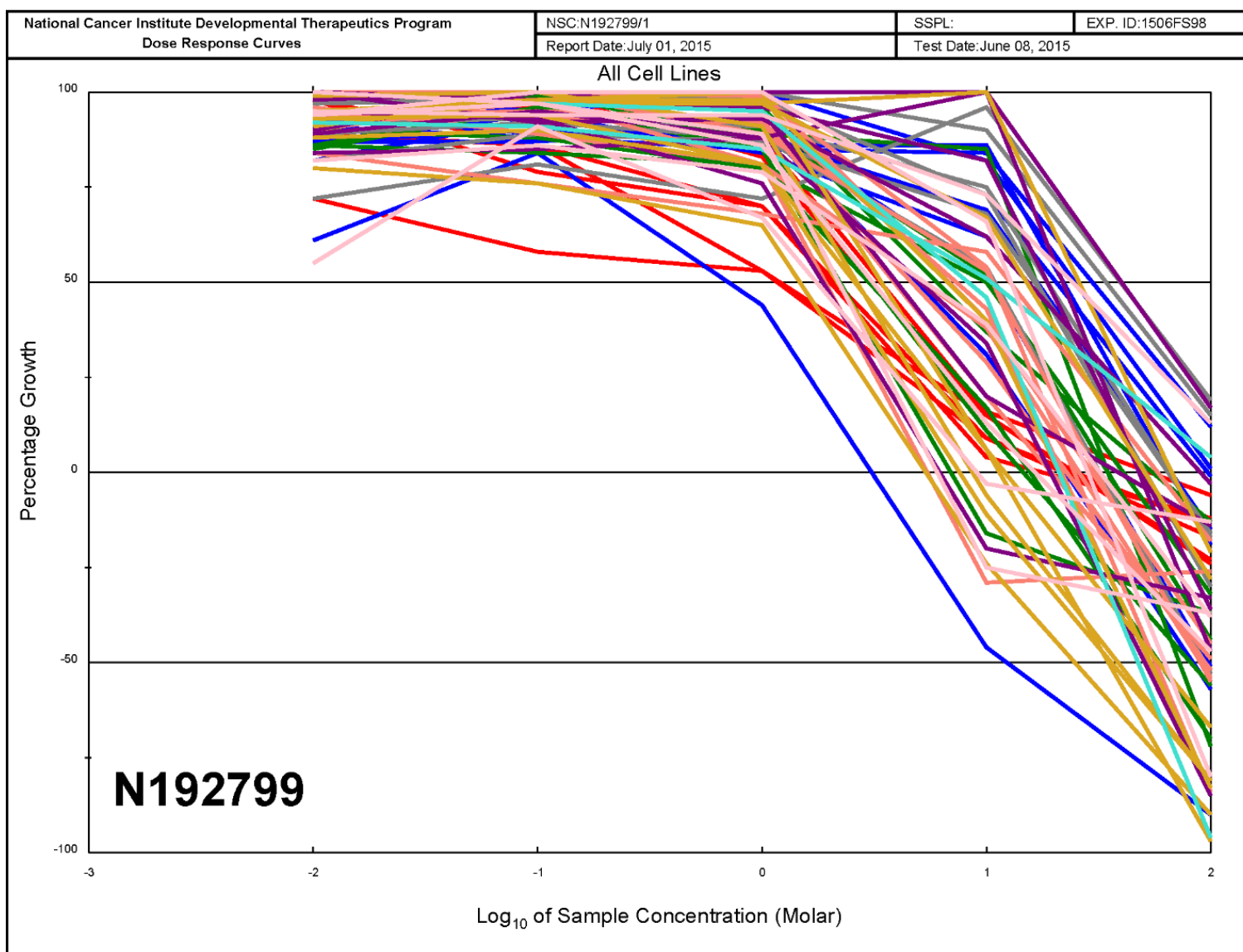


Figure S13. Composite of the NCI-60 dose response curves of the *Diospyros hispida* root (wood + bark) ethyl acetate extract (BR 501/N192799) with higher activity against the non-small cell lung cancer NCI-H522.

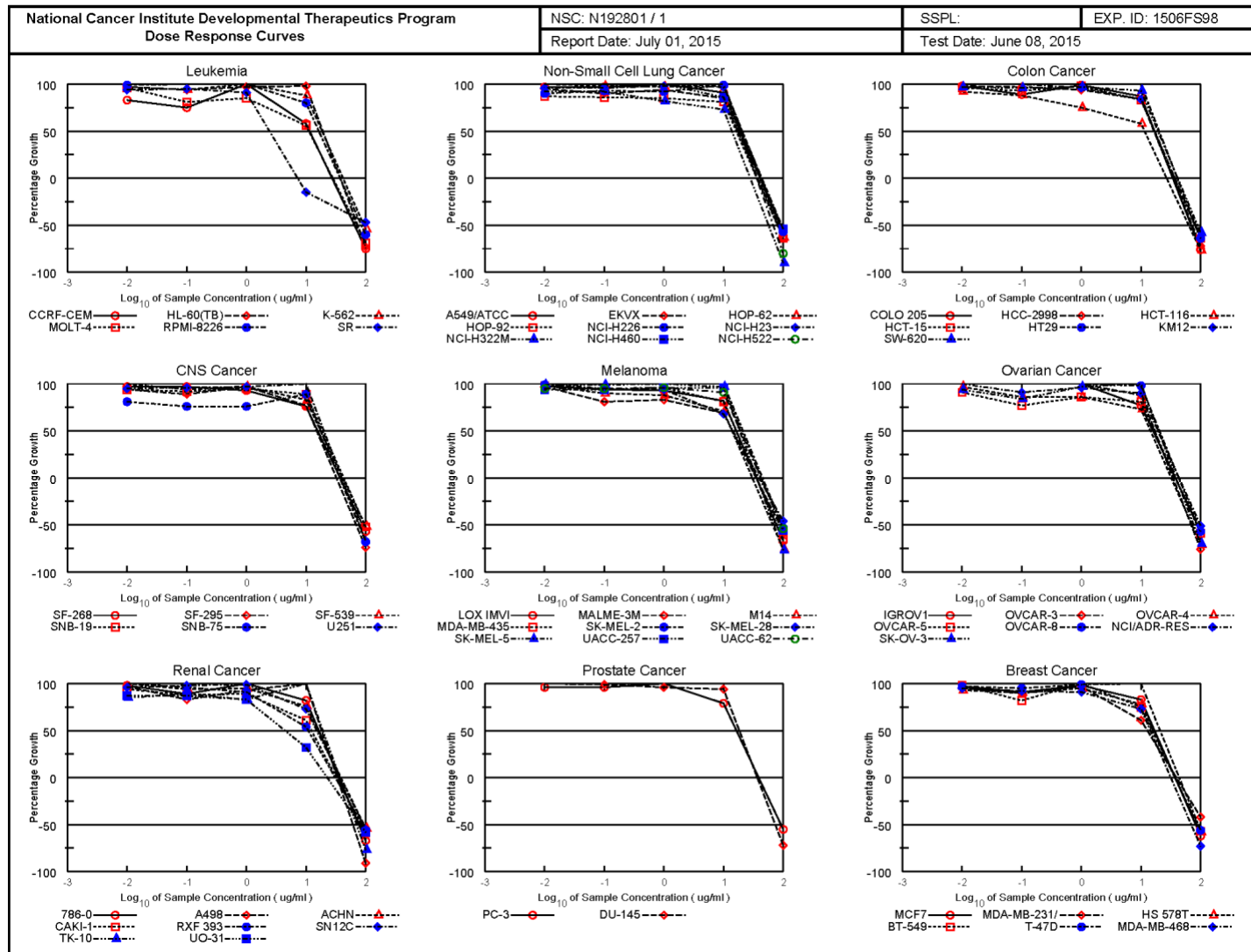
D. *Rapanea guianensis*

Figure S14. Dose response curves of the *Rapanea guianensis* root wood ethanol extract (BR 627/N192801) against NCI-60 panels, with the highest activity against the leukemia SR cell line.

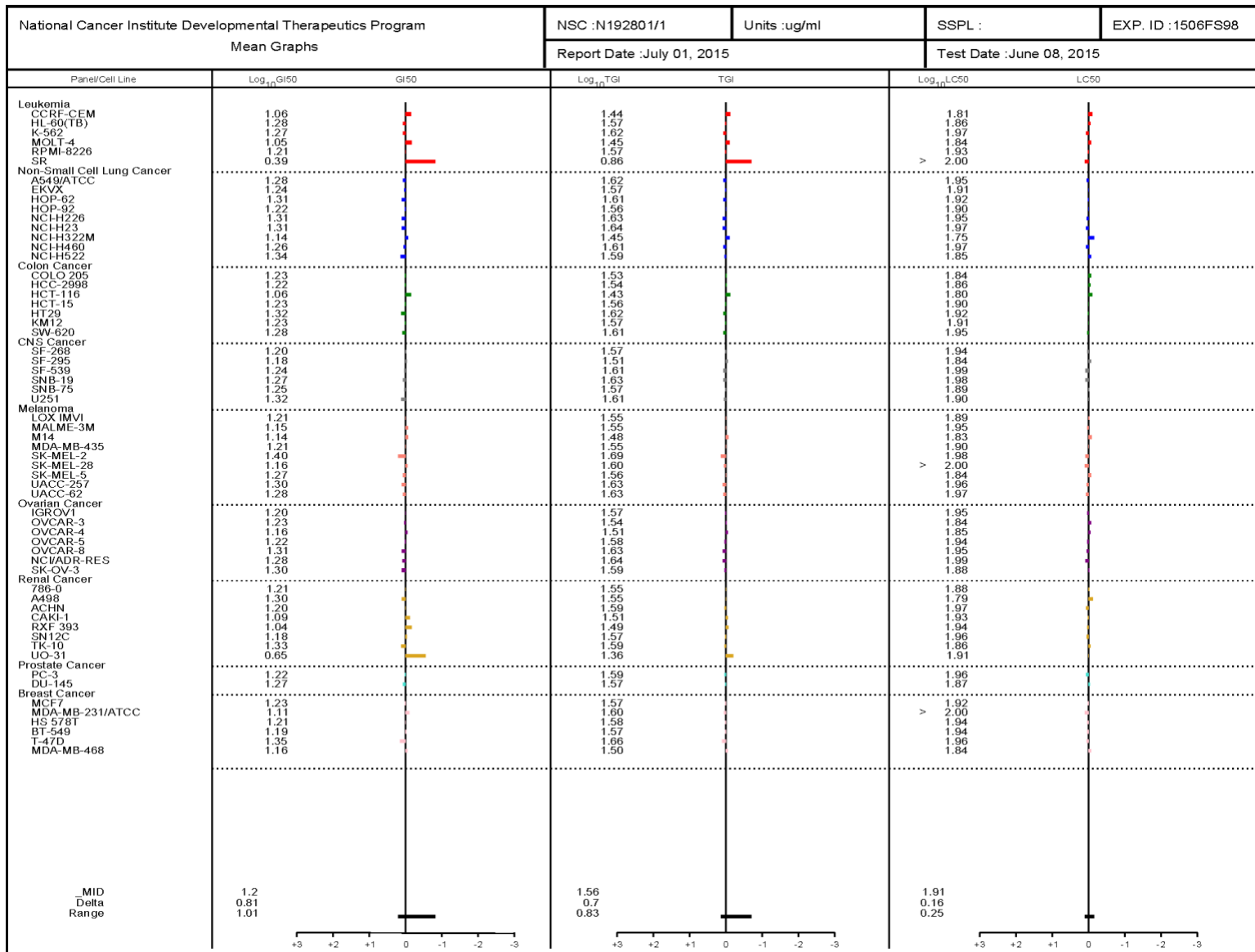


Figure S15. Mean bar graph of the *Rapanea guianensis* root wood ethanol extract (BR 627/N192801) in the NCI-60 cell five-dose screen.

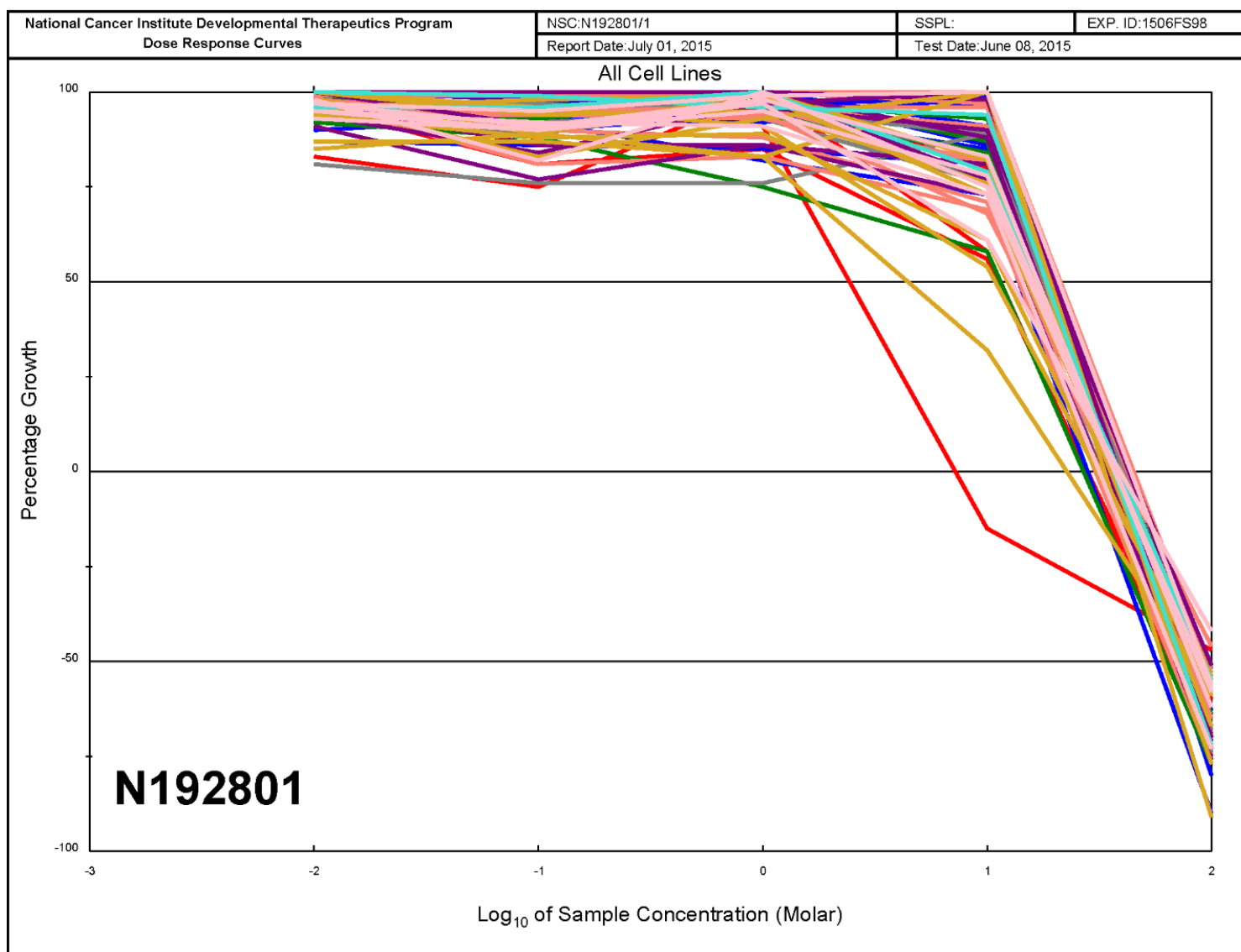


Figure S16. Composite of the NCI-60 dose response curves of the *Rapanea guianensis* root wood ethanol extract (BR 627/N192801) with higher activity against the leukemia SR cell line.

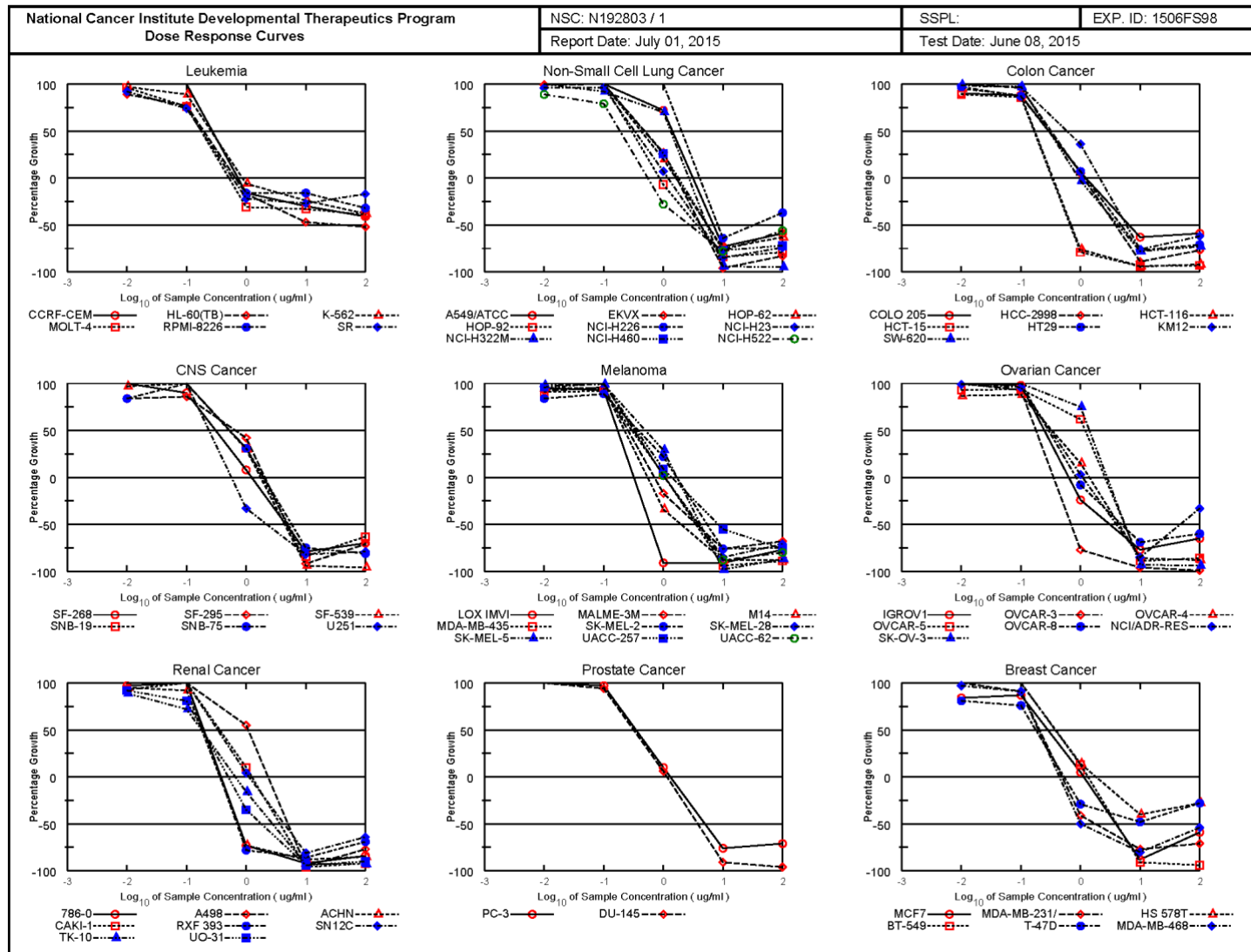
E. *Salacia crassifolia*

Figure S17. Dose response curves of the *Salacia crassifolia* root wood hexane extract (BR 640/N192803) against NCI-60 panels, with the highest activity against the colon cancer HCT-15 cell line.

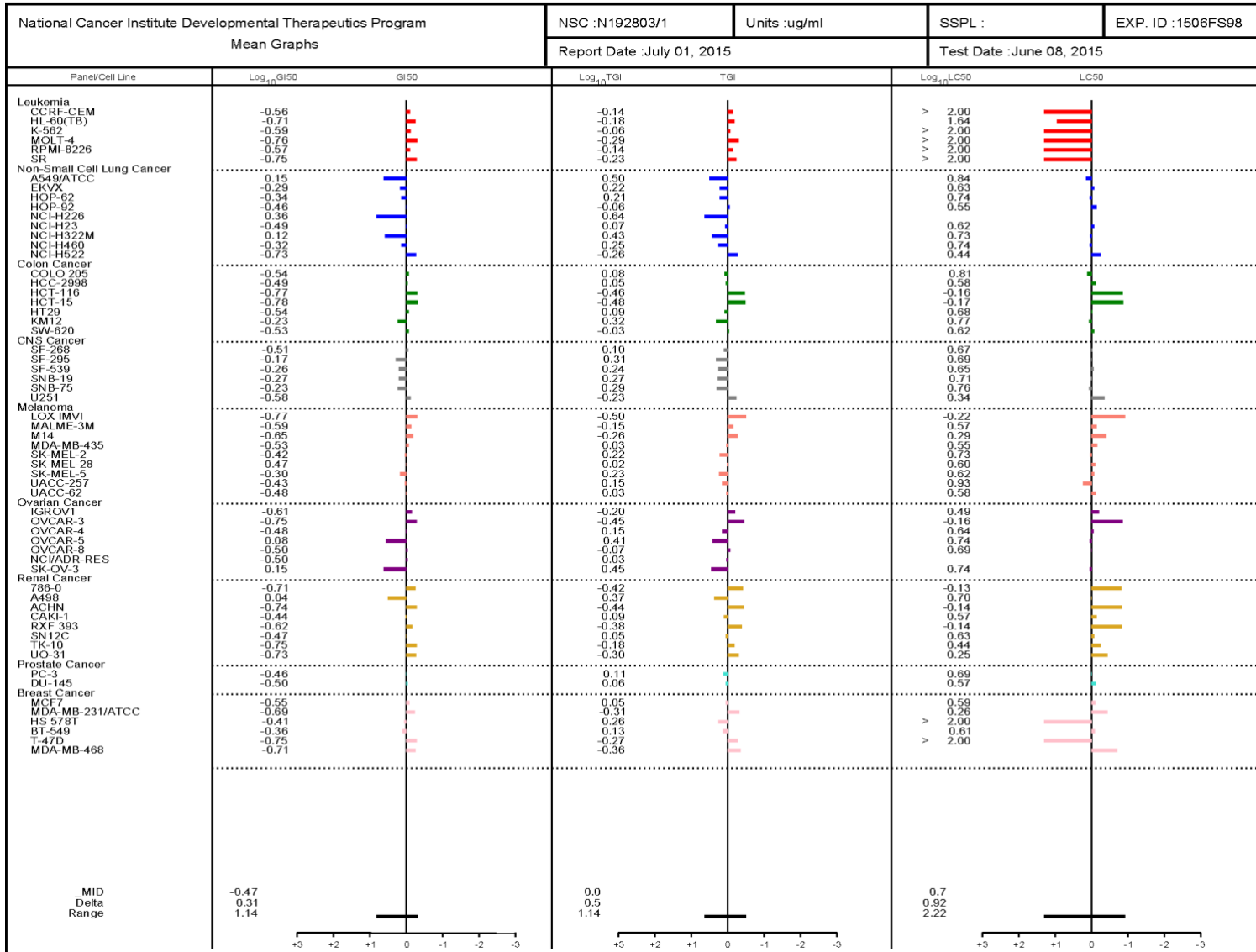


Figure S18. Cytotoxicity of the *Salacia crassifolia* root wood hexane extract (BR 640/N192803) in the NCI-60 cell five-dose screen.

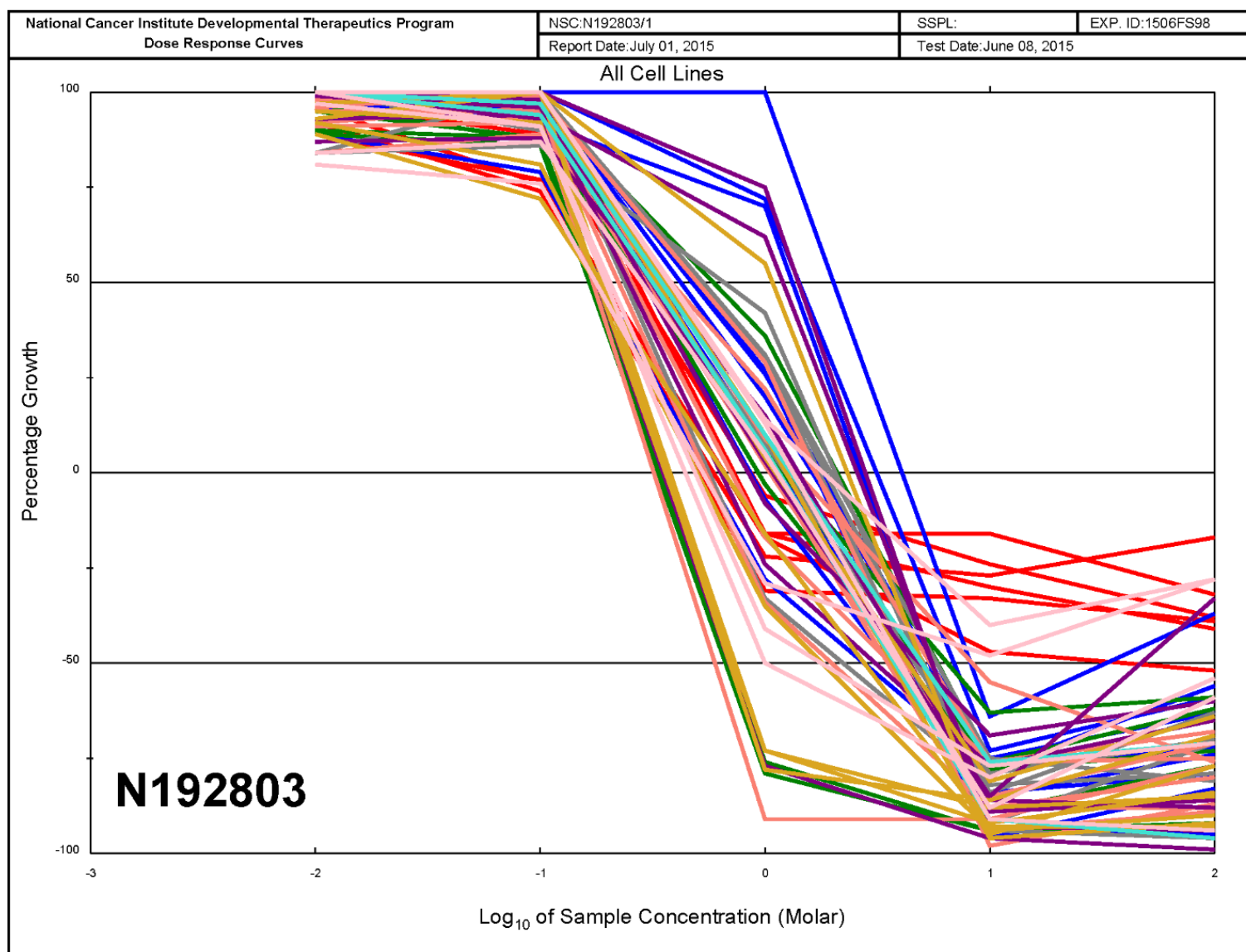


Figure S19. Composite of the NCI-60 dose response curves of the *Salacia crassifolia* root wood hexane extract (BR 640/N192803) with higher activity against the colon cancer HCT-15 cell line.

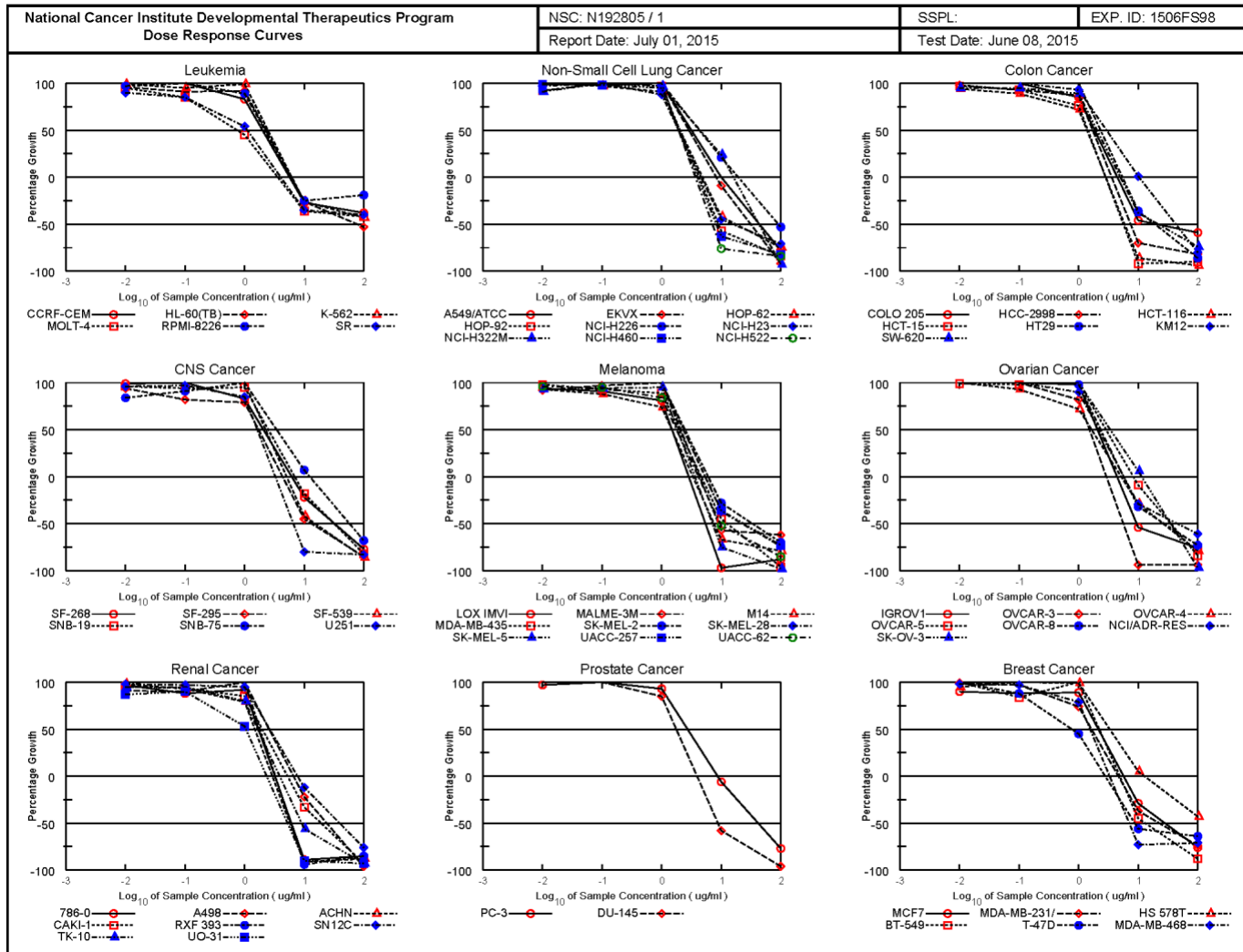
F. *Salacia elliptica*

Figure S20. Dose response curves of the *Salacia elliptica* root wood ethyl acetate extract (BR 652/N192805) against NCI-60 panels, with the highest activity against the leukemia MOLT-4 cell line.

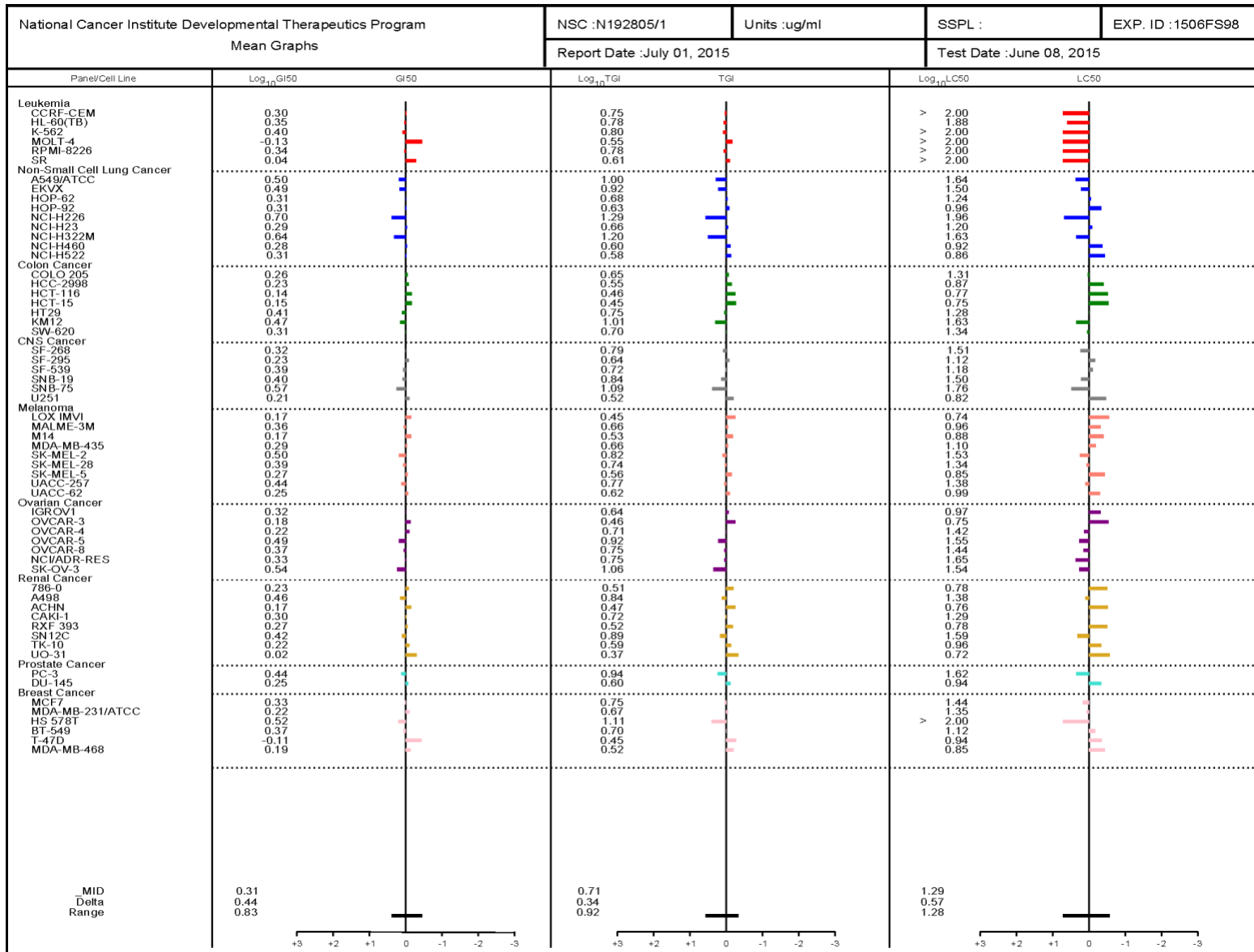


Figure S21. Mean bar graphs of the *Salacia elliptica* root wood ethyl acetate extract (BR 652/N192805) in the NCI-60 cell five-dose screen.

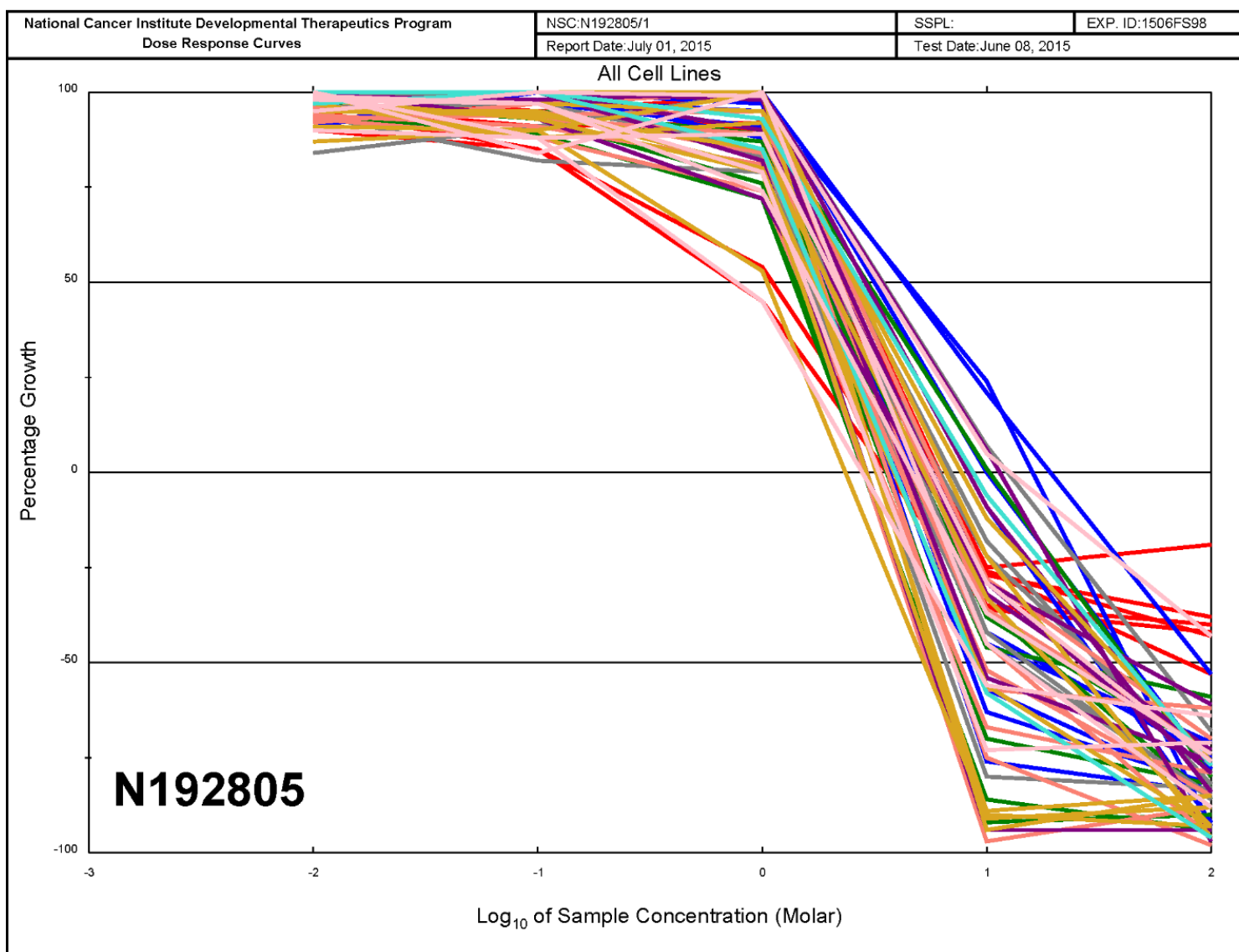


Figure S22. Composite of the NCI-60 dose response curves of the *Salacia elliptica* root wood ethyl acetate extract (BR 652/N192805) with higher activity against the leukemia MOLT-4 cell line.

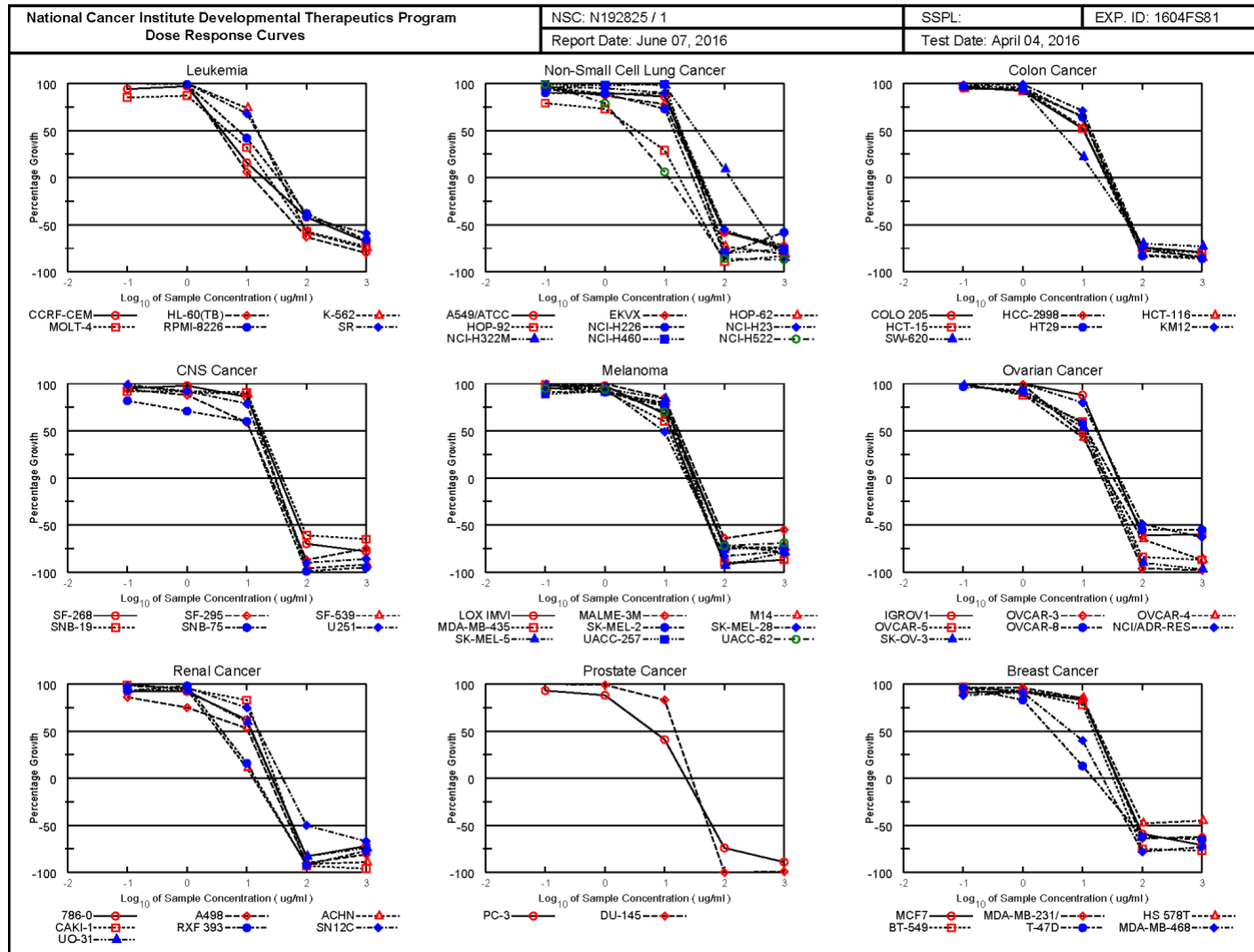
G. *Casearia sylvestris* var. *lingua*

Figure S23. Dose response curves of the *Casearia sylvestris* var. *lingua* stem wood hexane extract (BR 177/N192825) against NCI-60 panels, with the highest activity against the non-small cell lung cancer NCI-H522.

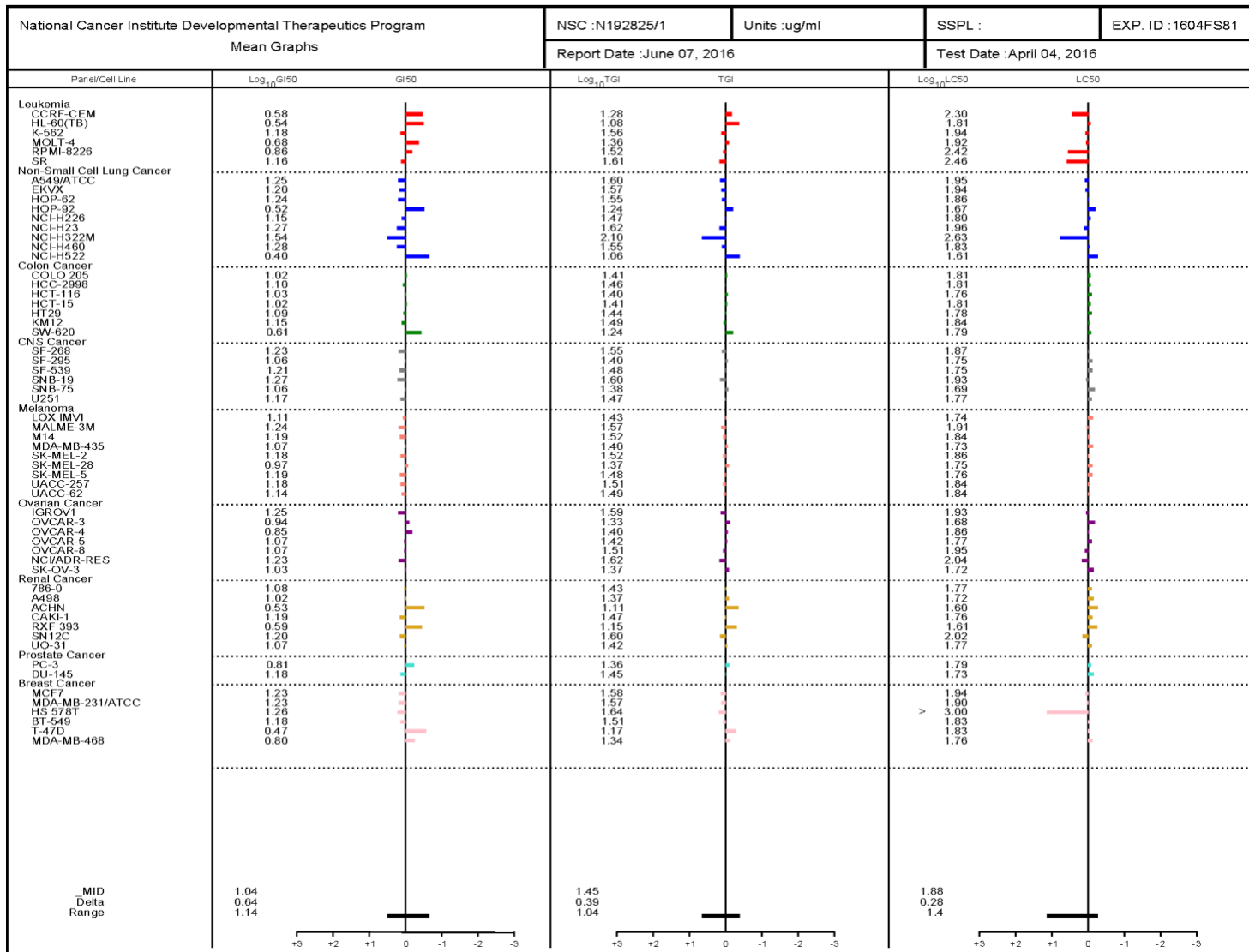


Figure S24. Mean bar graph of the *Casearia sylvestris* var. *lingua* stem wood hexane extract (BR 177/N192825) in the NCI-60 cell five-dose screen.

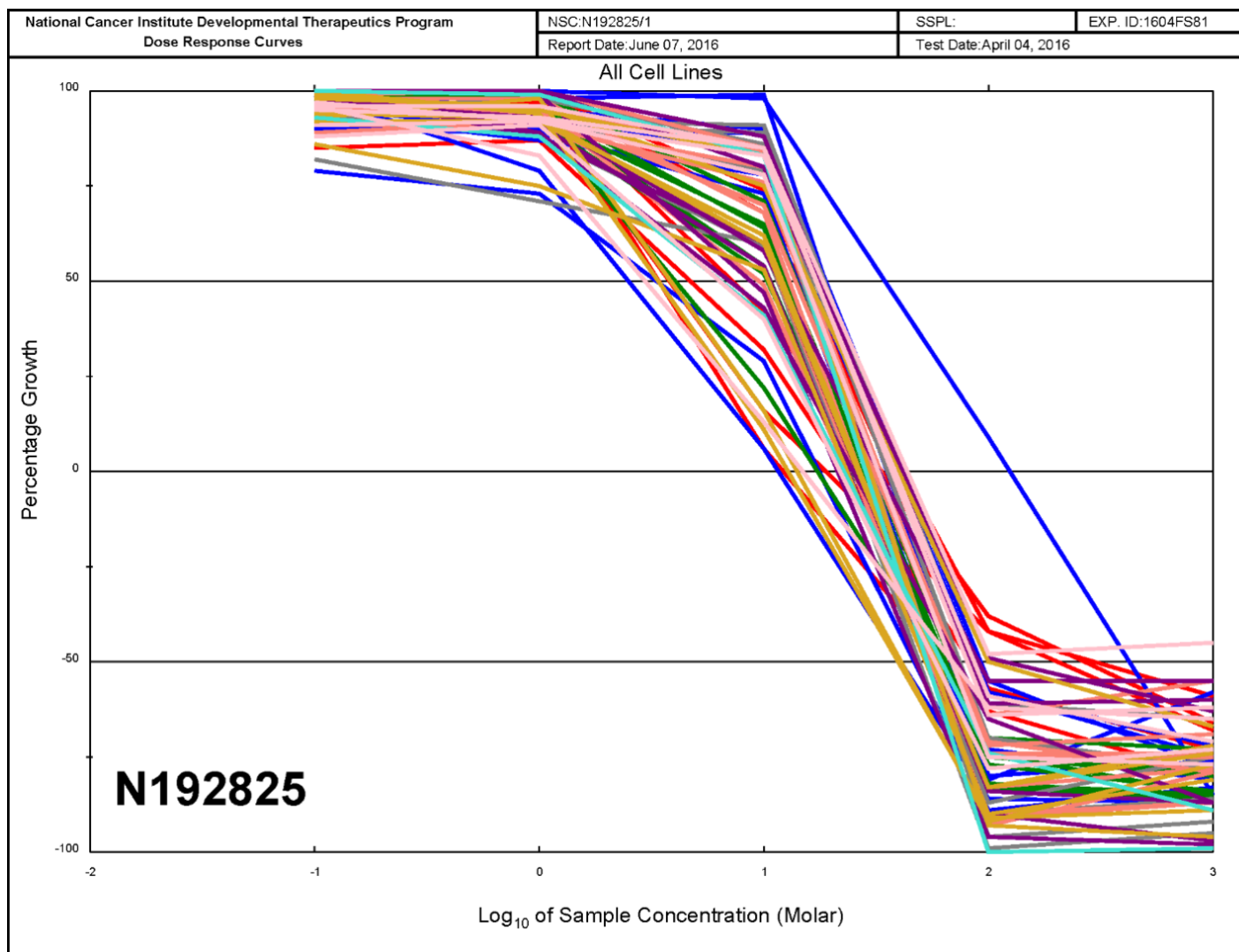


Figure S25. Composite of the NCI-60 dose response curves of the *Casearia sylvestris* var. *lingua* stem wood hexane extract (BR 177/N192825) with higher activity against the non-small cell lung cancer NCI-H522.

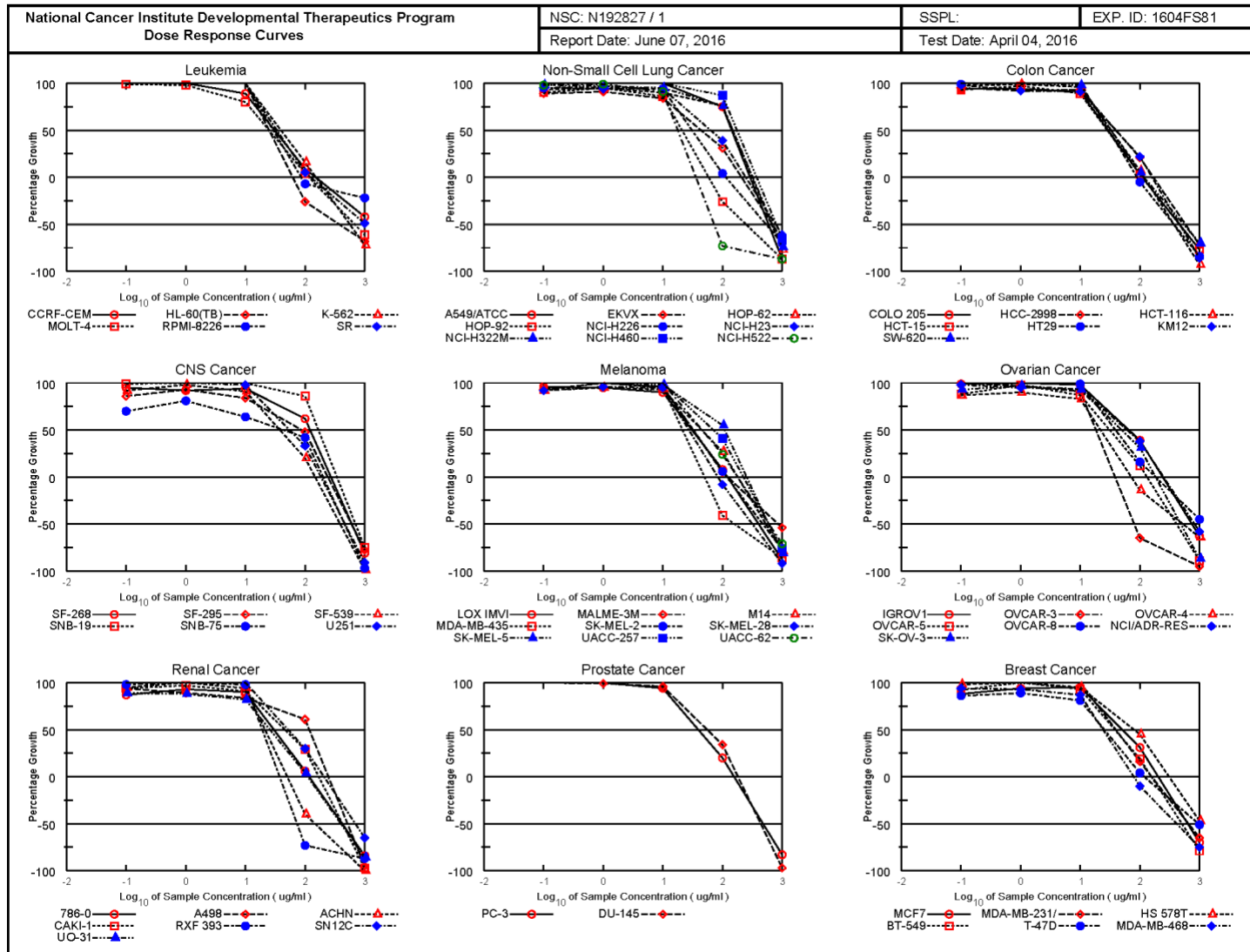
H. Cupania vernalis

Figure S26. Dose response curves of the *Cupania vernalis* leaf hexane extract (BR 193/N192827) against NCI-60 panels, with different susceptibility.

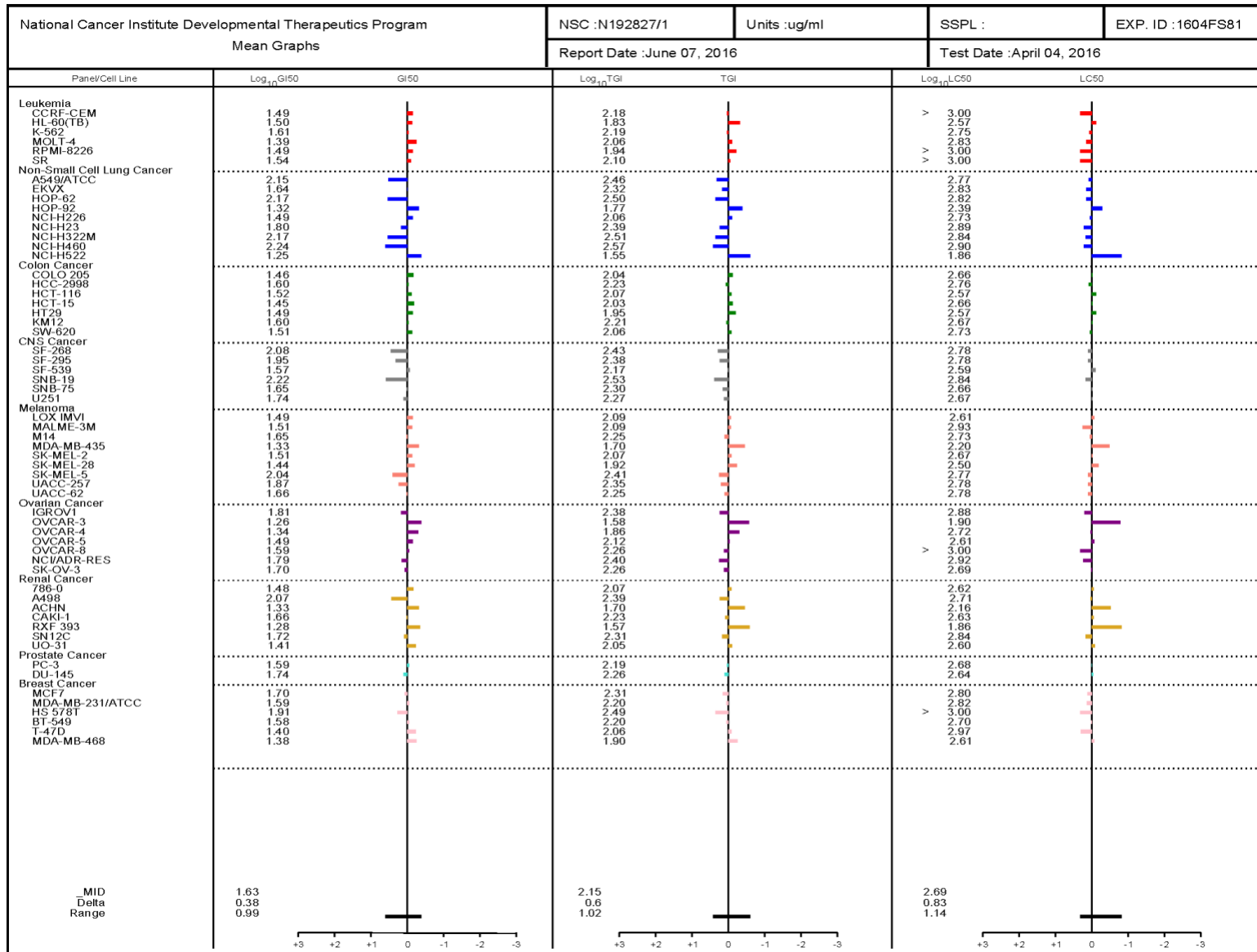


Figure S27. Mean bar graph of the *Cupania vernalis* leaf hexane extract (BR 193/N192827) in the NCI-60 cell five-dose screen.

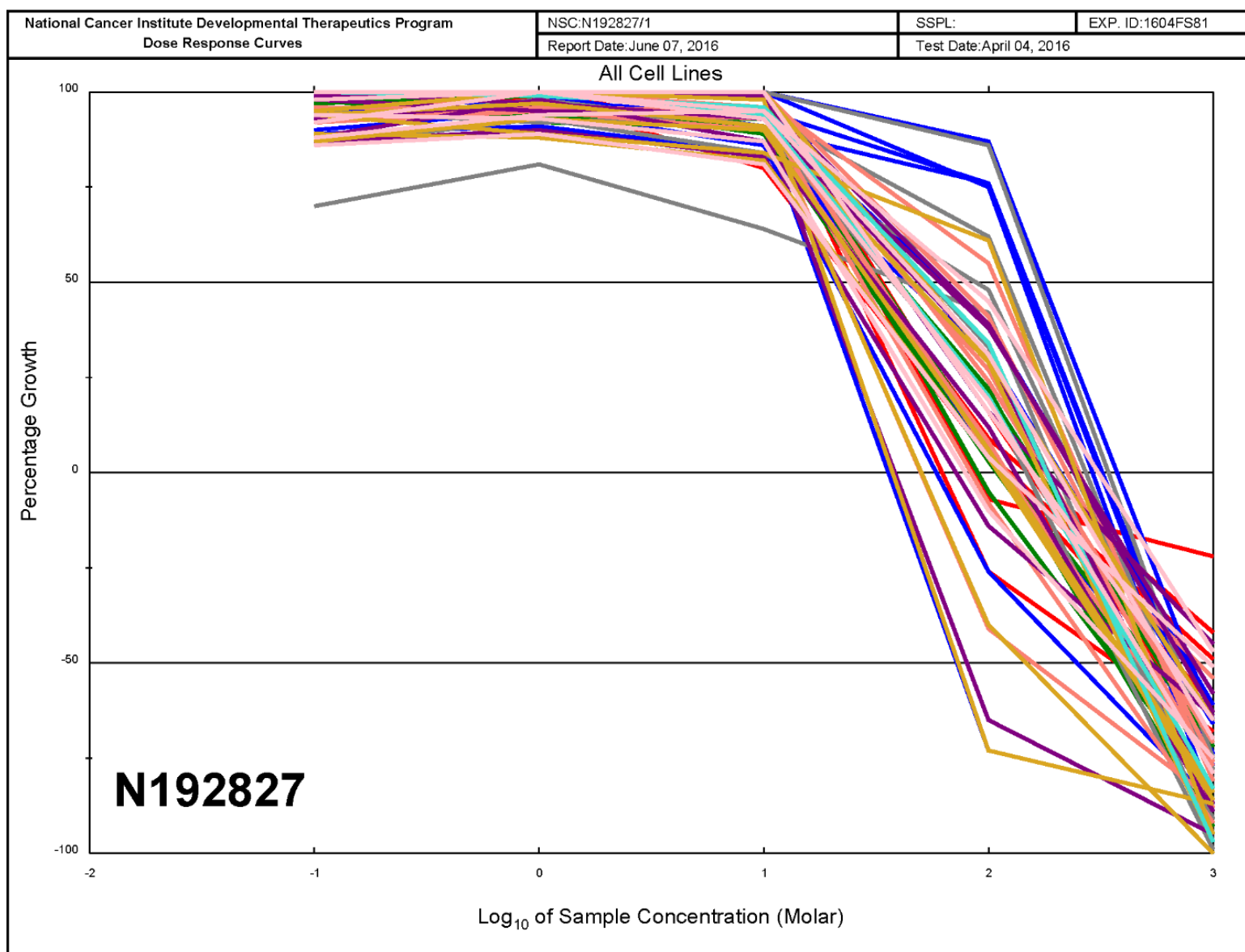


Figure S28. Composite of the NCI-60 dose response curves of the *Cupania vernalis* leaf hexane extract (BR 193/N192827).

I. *Simarouba versicolor*

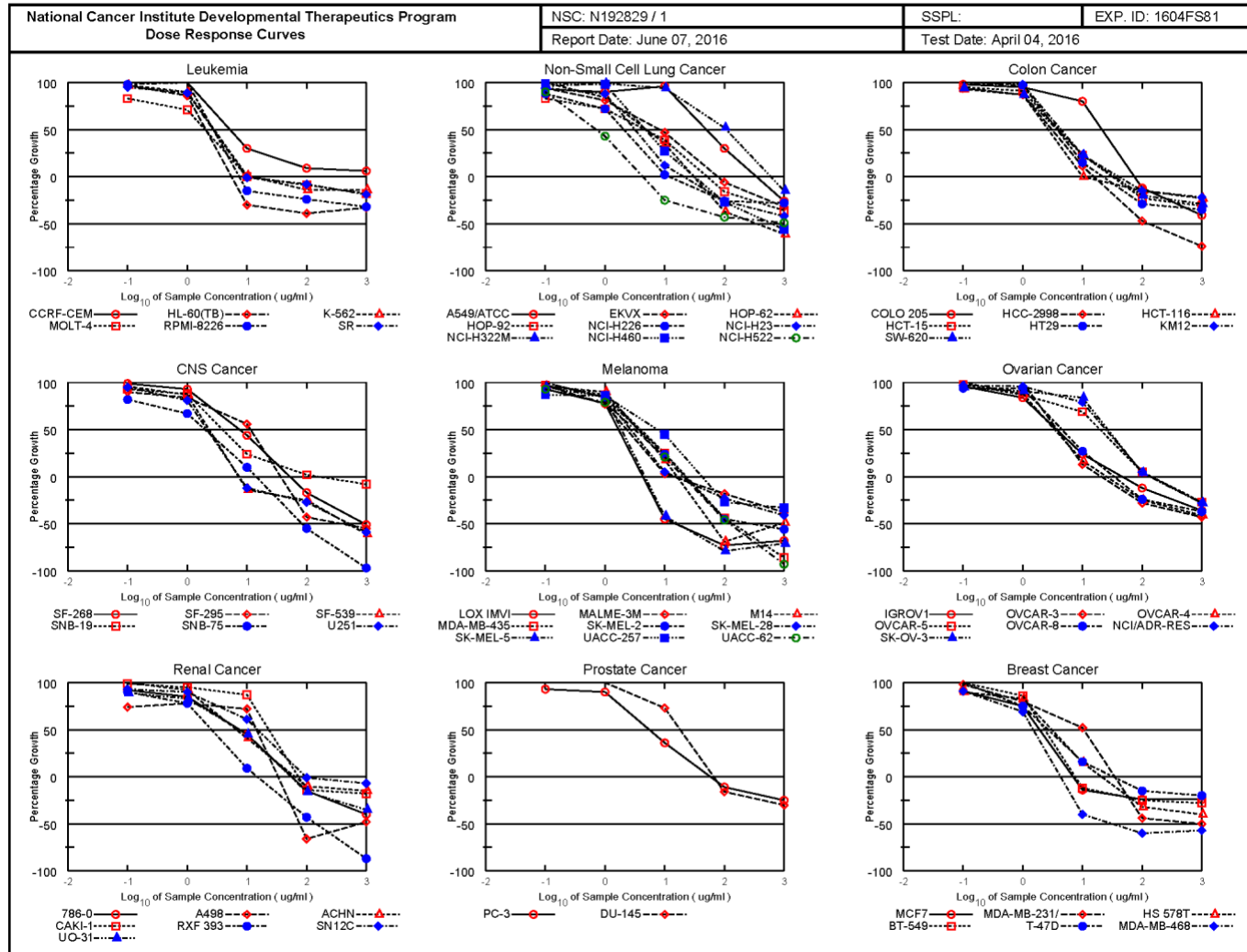


Figure S29. Dose response curves of the *Simarouba versicolor* root bark ethanol extract (BR 254/N192829) against NCI-60 panels, with the highest activity against the non-small cell lung cancer NCI-H522.

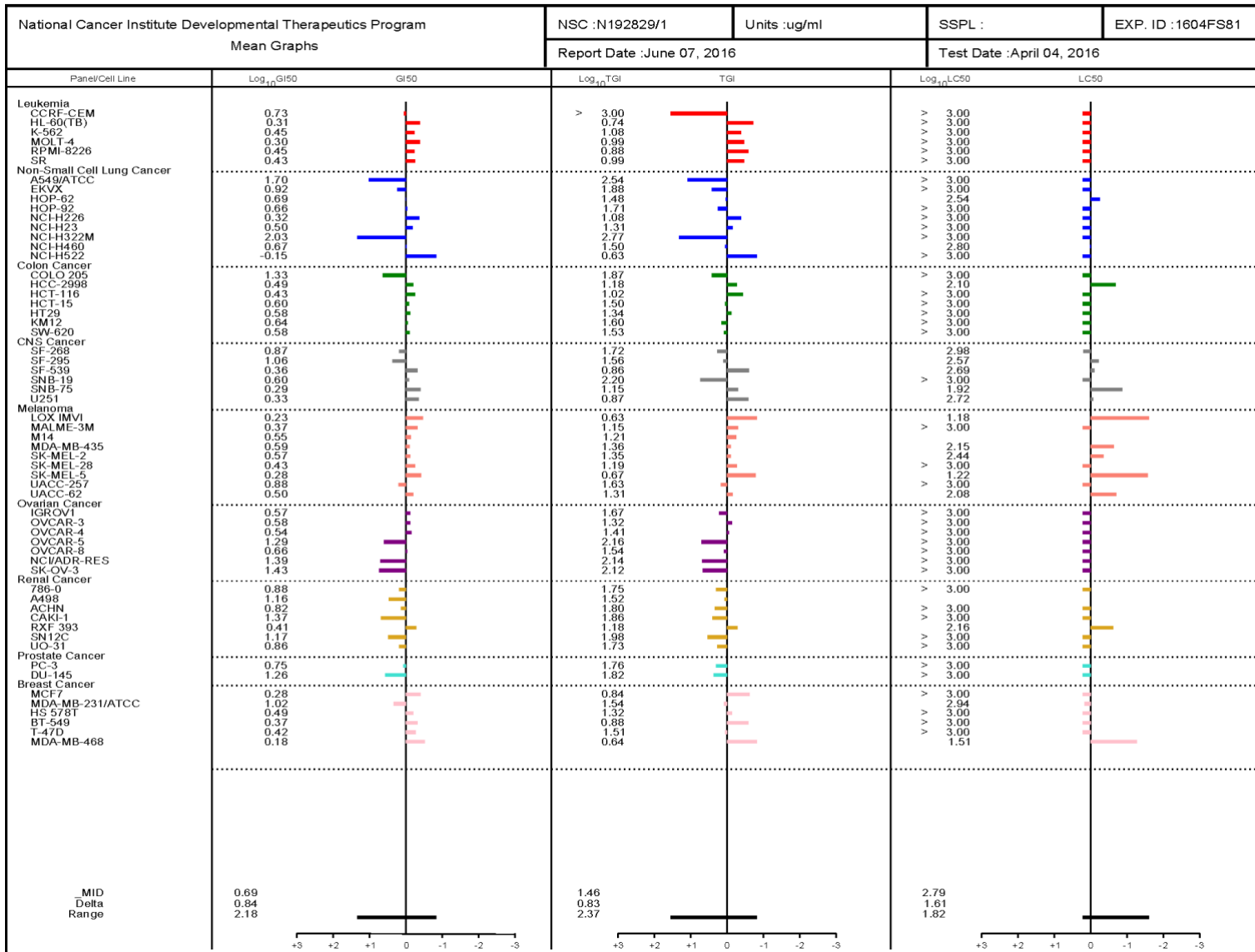


Figure S30. Mean bar graph of the *Simarouba versicolor* root bark ethanol extract (BR 254/N192829) in the NCI-60 cell five-dose screen.

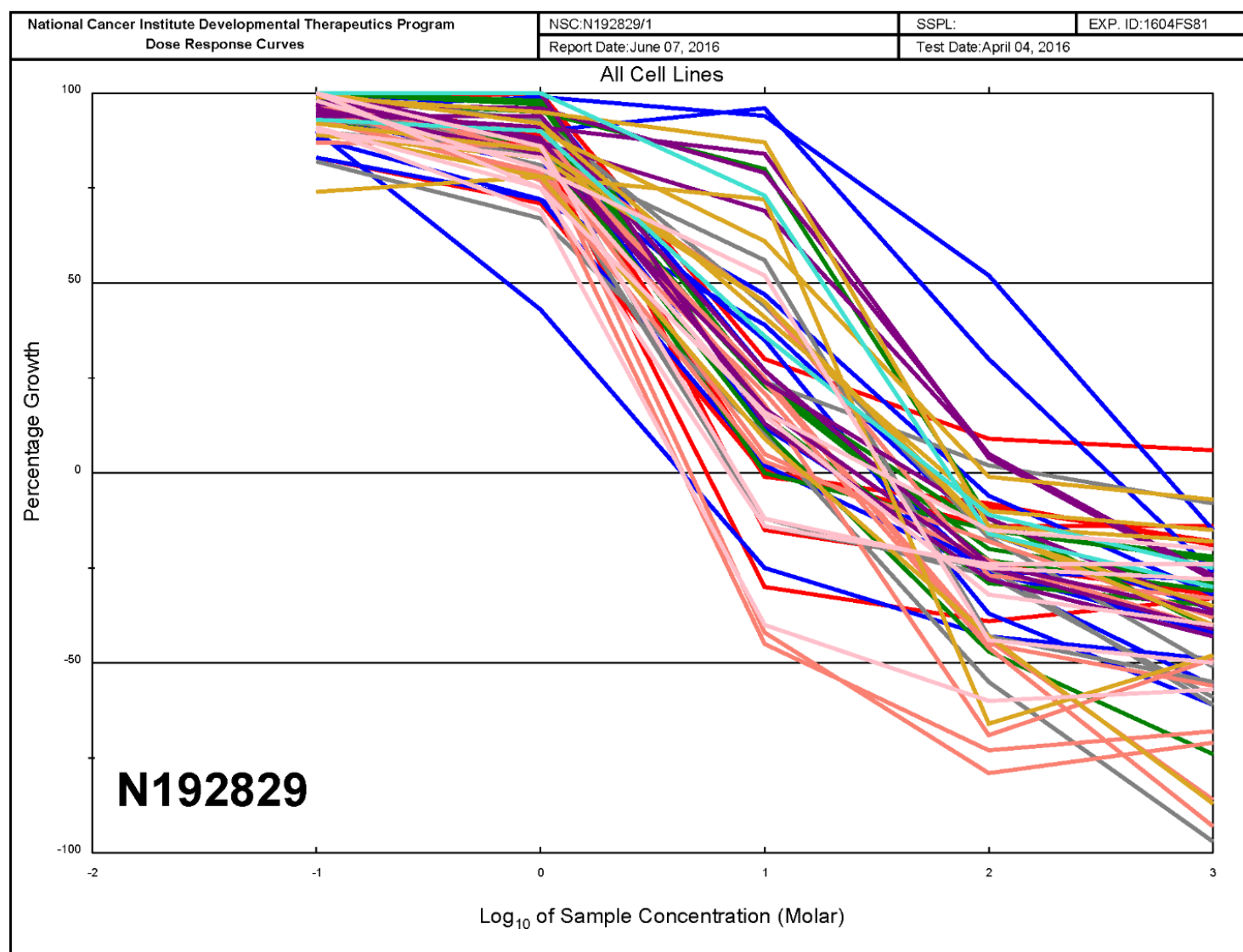


Figure S31. NCI-60 dose response curves of the *Simarouba versicolor* root bark ethanol extract (BR 254/N192829) with higher activity against the non-small cell lung cancer NCI-H522.

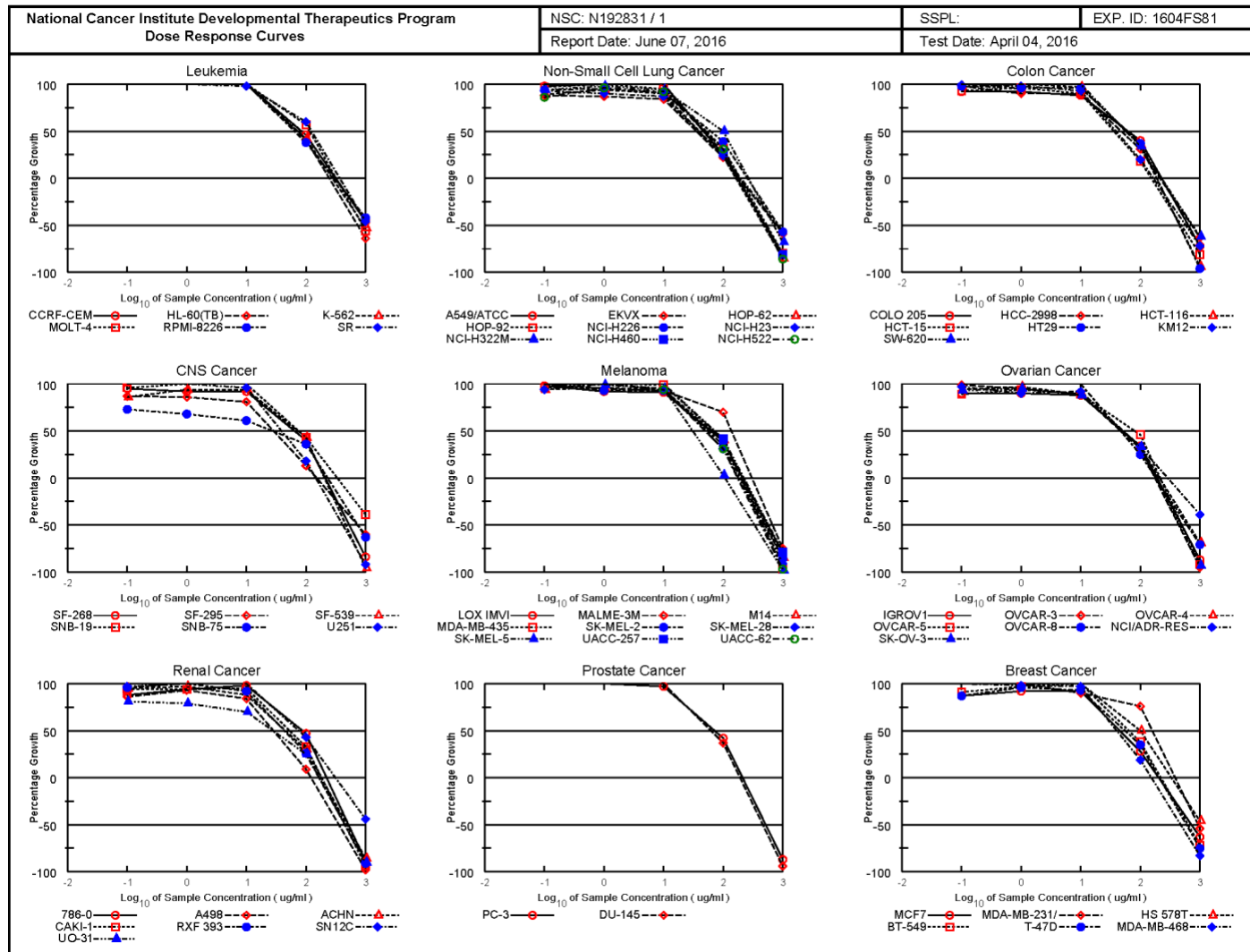
J. *Kielmeyera coriacea*

Figure S32. Dose response curves of the *Kielmeyera coriacea* stem wood hexane extract (BR 331/N192831) against NCI-60 panels, with different susceptibility.

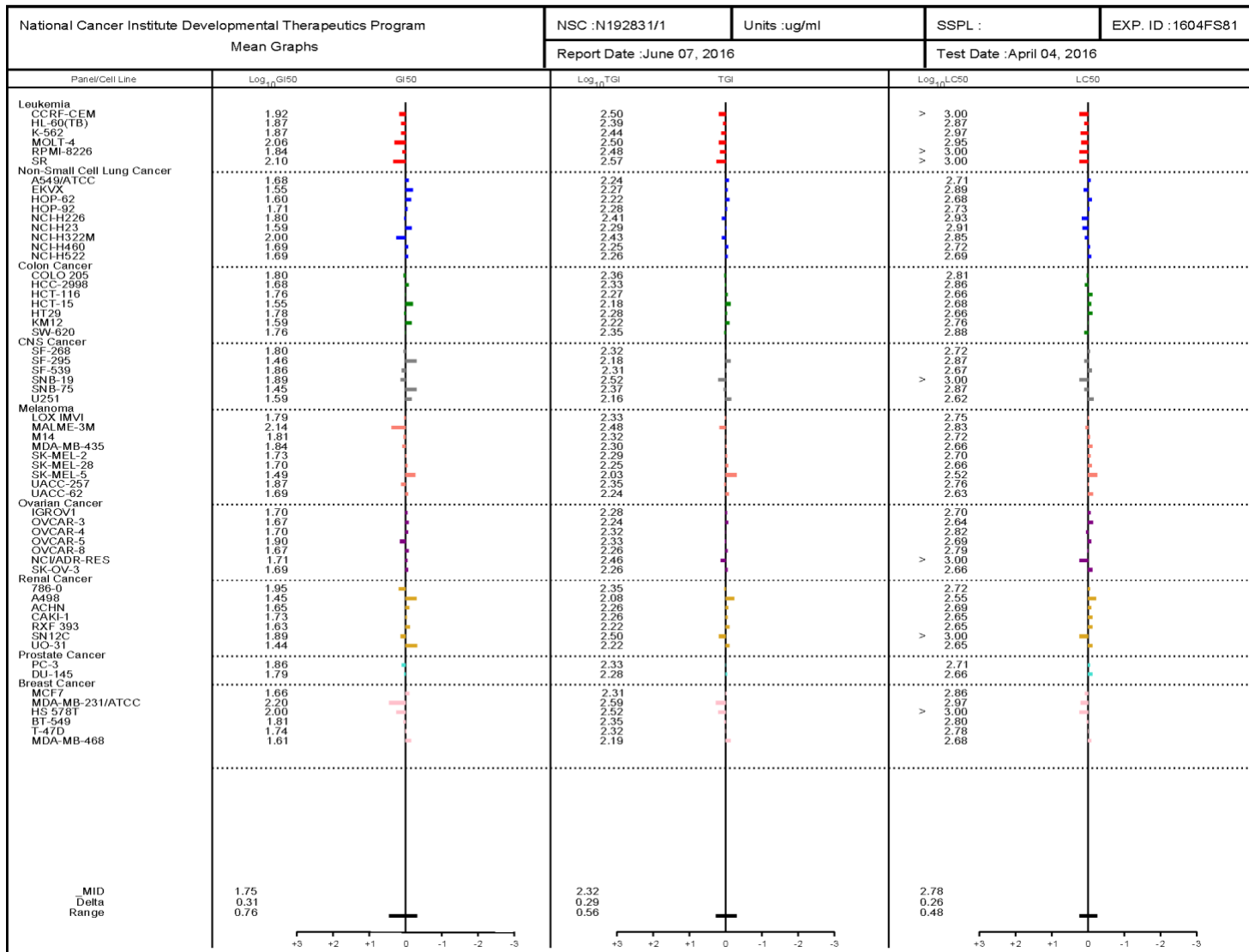


Figure S33. Mean bar graph of the *Kielmeyera coriacea* stem wood hexane extract (BR 331/N192831) in the NCI-60 cell five-dose screen.

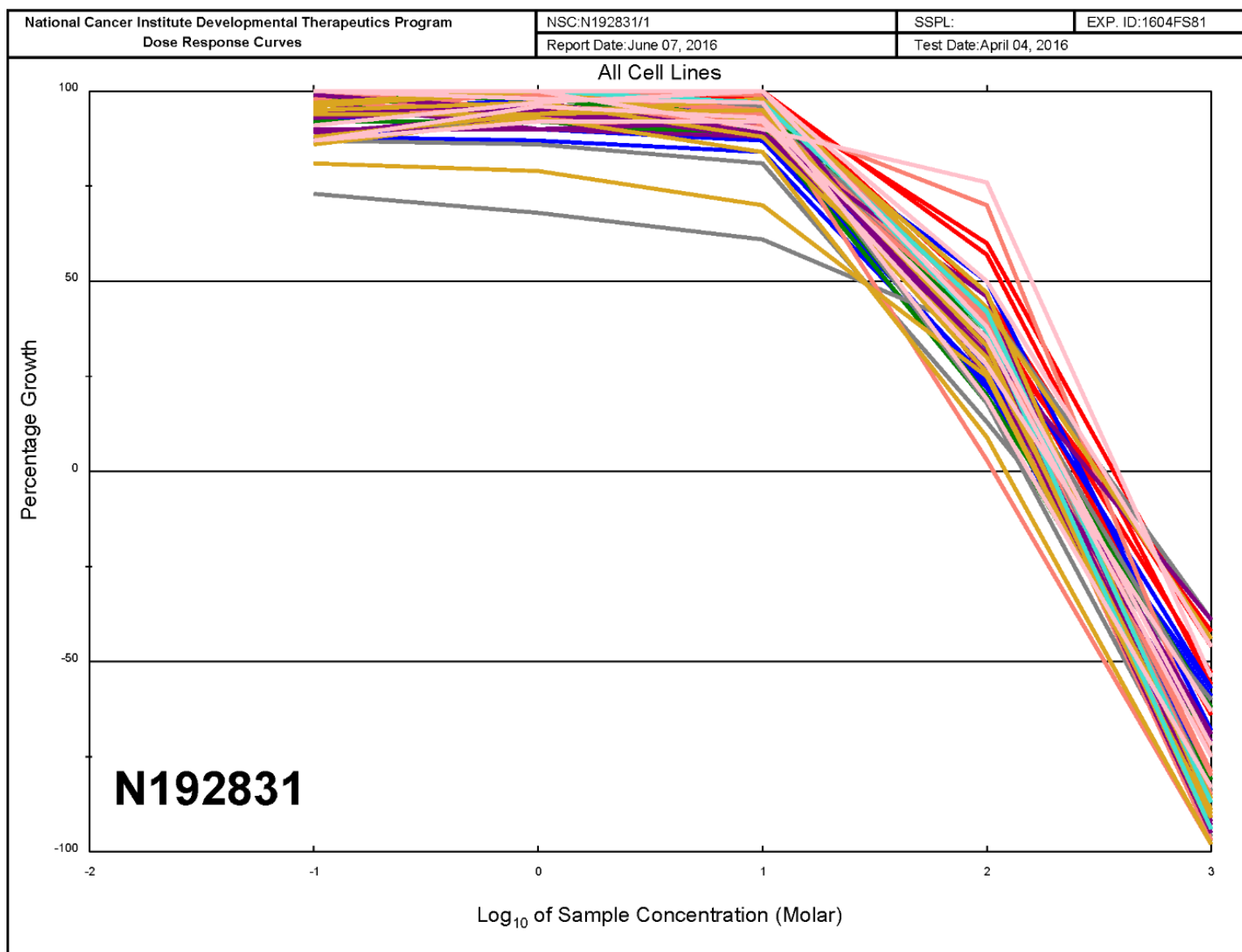


Figure S34. NCI-60 dose response curves of the *Kielmeyera coriacea* stem wood hexane extract (BR 331/N192831).

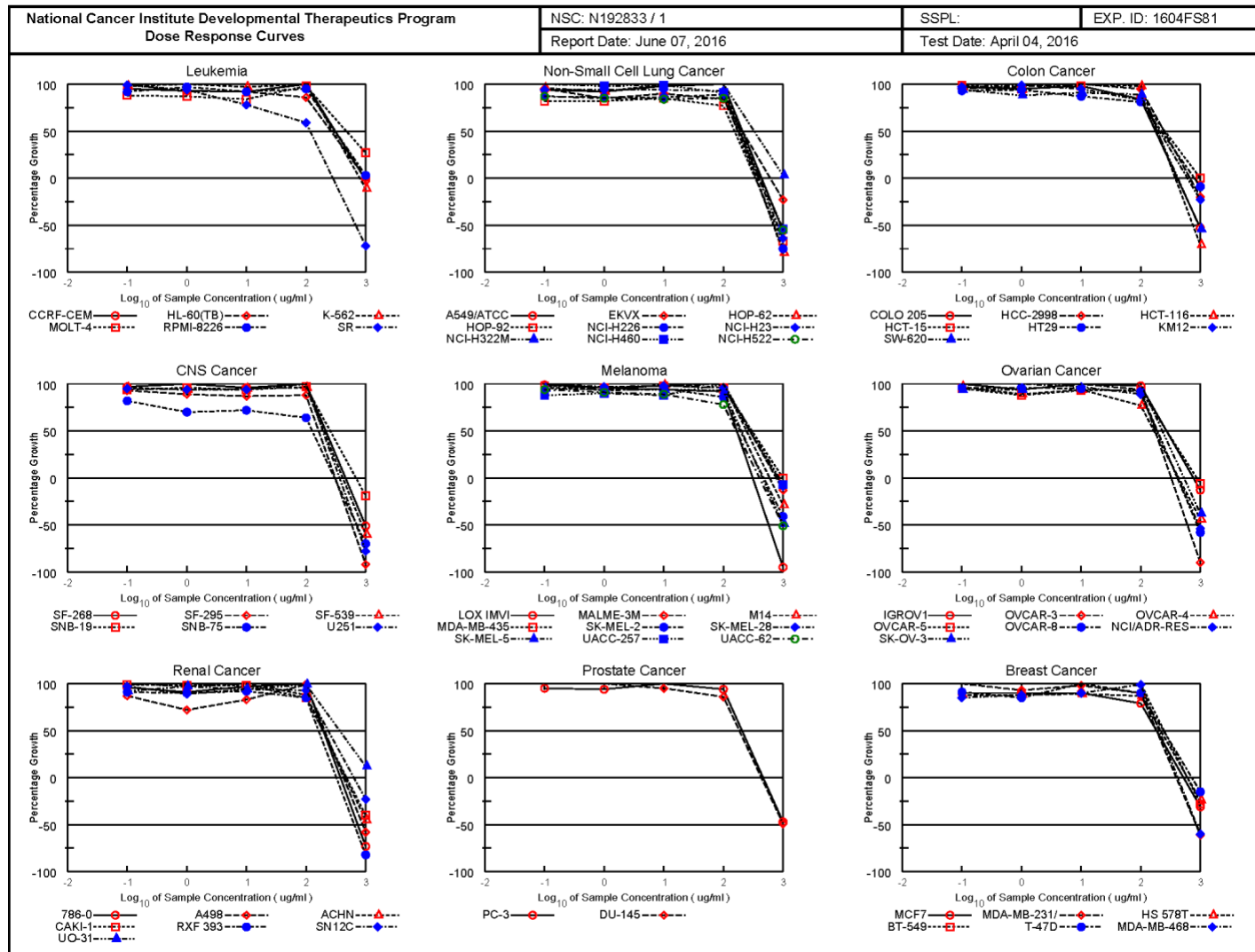
K. *Byrsonima crassa*

Figure S35. Dose response curves of the *Byrsonima crassa* root bark hexane extract (BR 411/N192833) against NCI-60 panels, with different susceptibility.

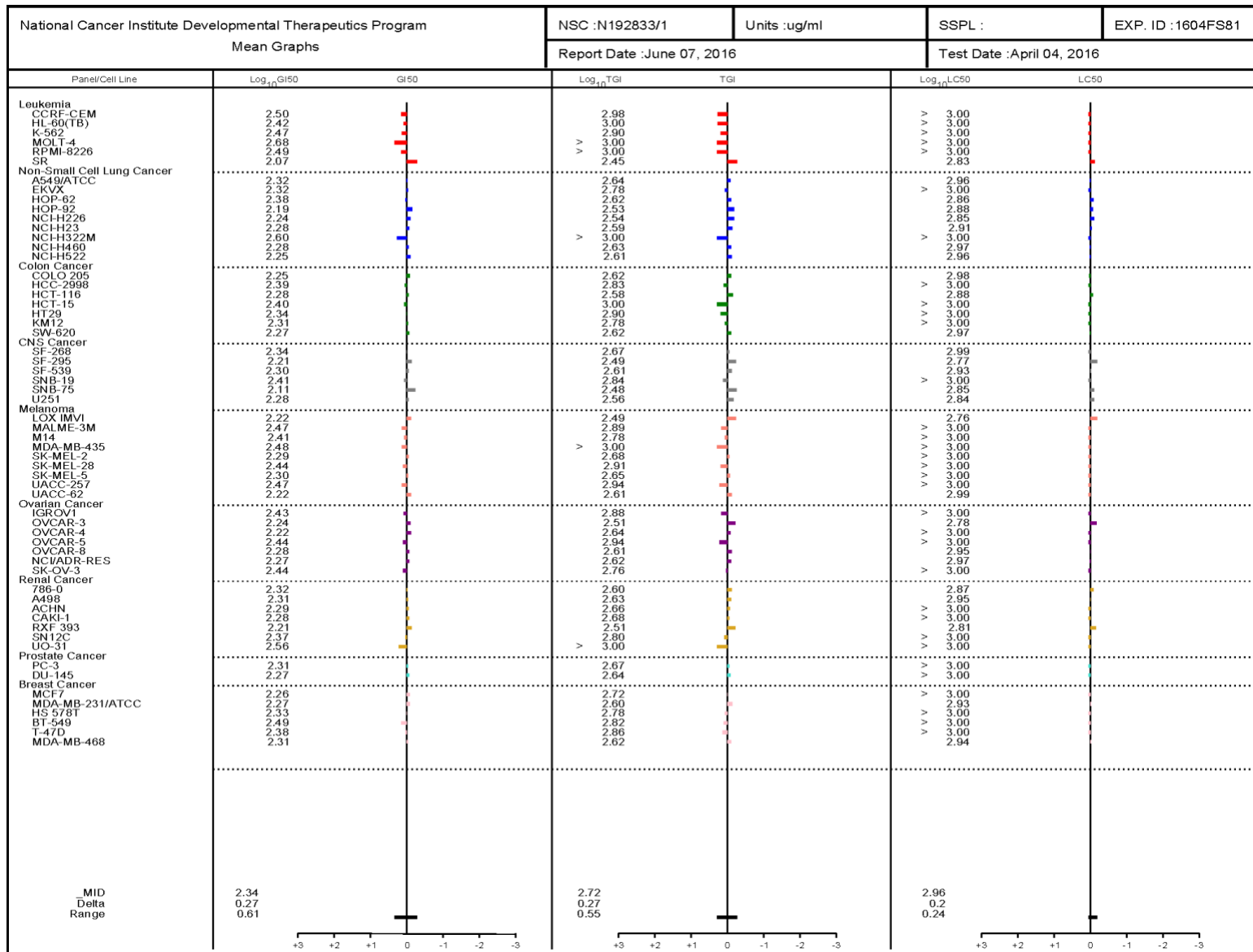


Figure S36. Mean bar graph of the *Byrsonima crassa* root bark hexane extract (BR 411/N192833) in the NCI-60 cell five-dose screen.

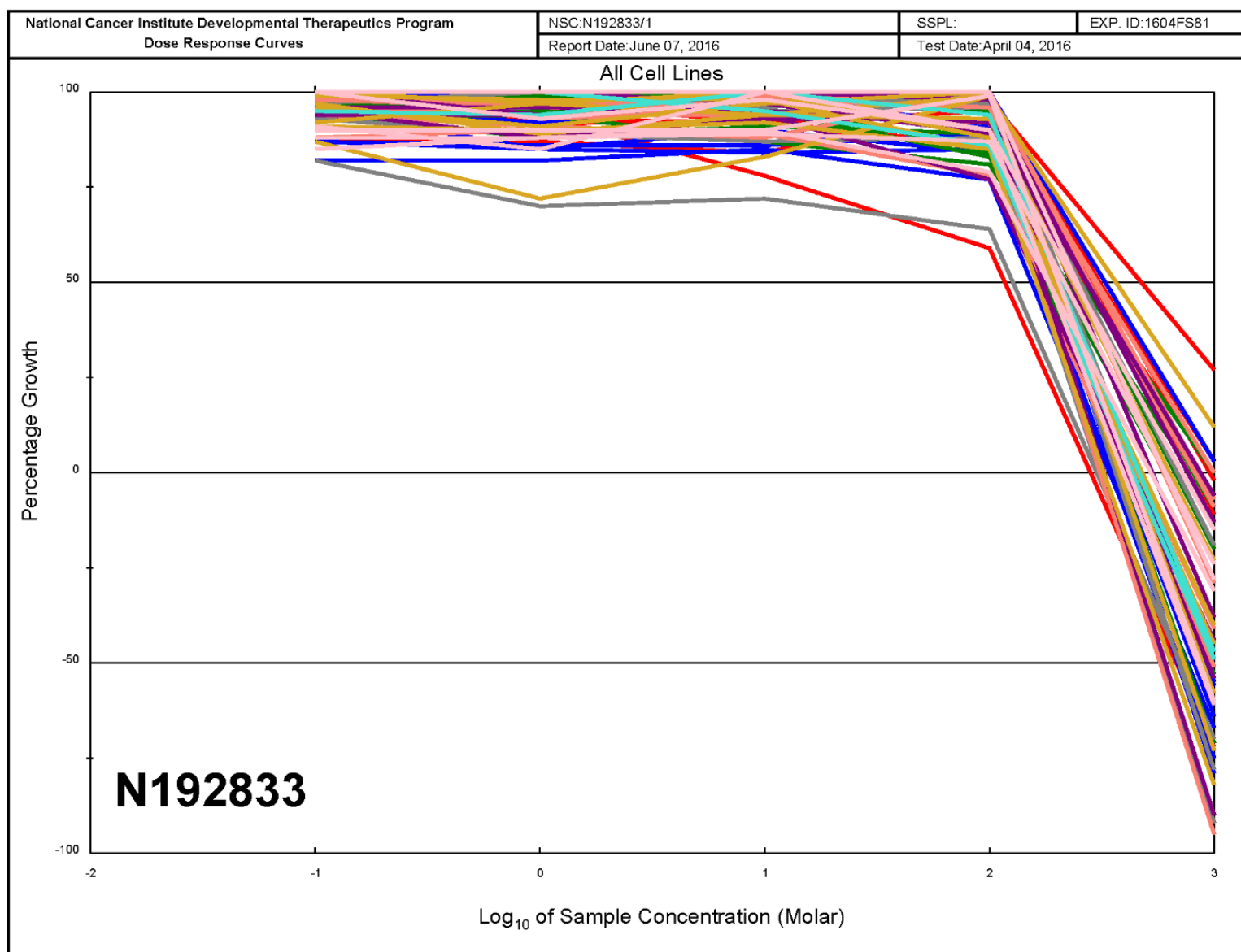


Figure S37. Composite of the NCI-60 dose response curves of the *Byrsonima crassa* root bark hexane extract (BR 411/N192833).

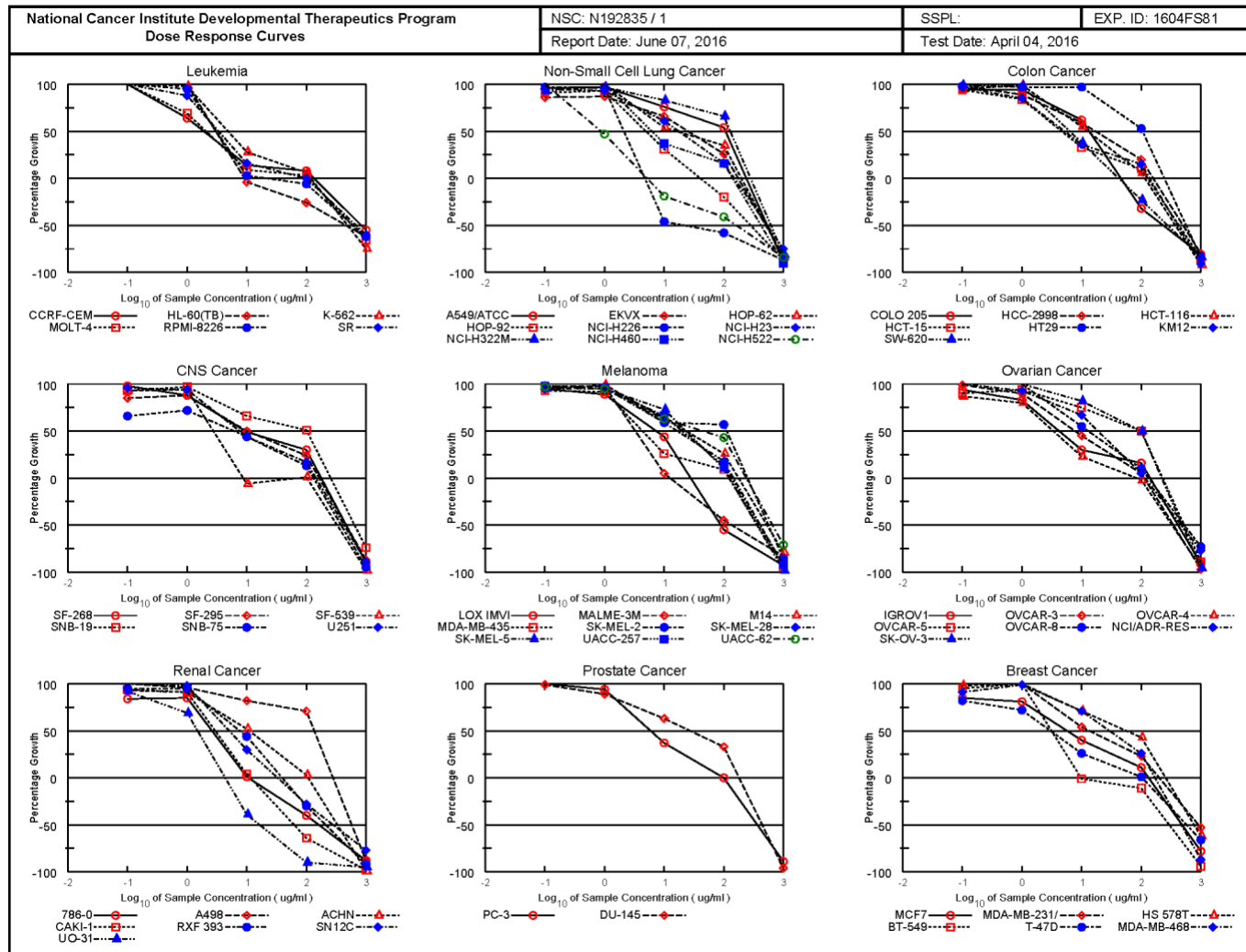
L. *Schinus terebinthifolia*

Figure S38. Dose response curves of the *Schinus terebinthifolia* leaf dichloromethane extract (BR 436/N192835) against NCI-60 panels, with the highest activity against the non-small cell lung cancer NCI-H522.

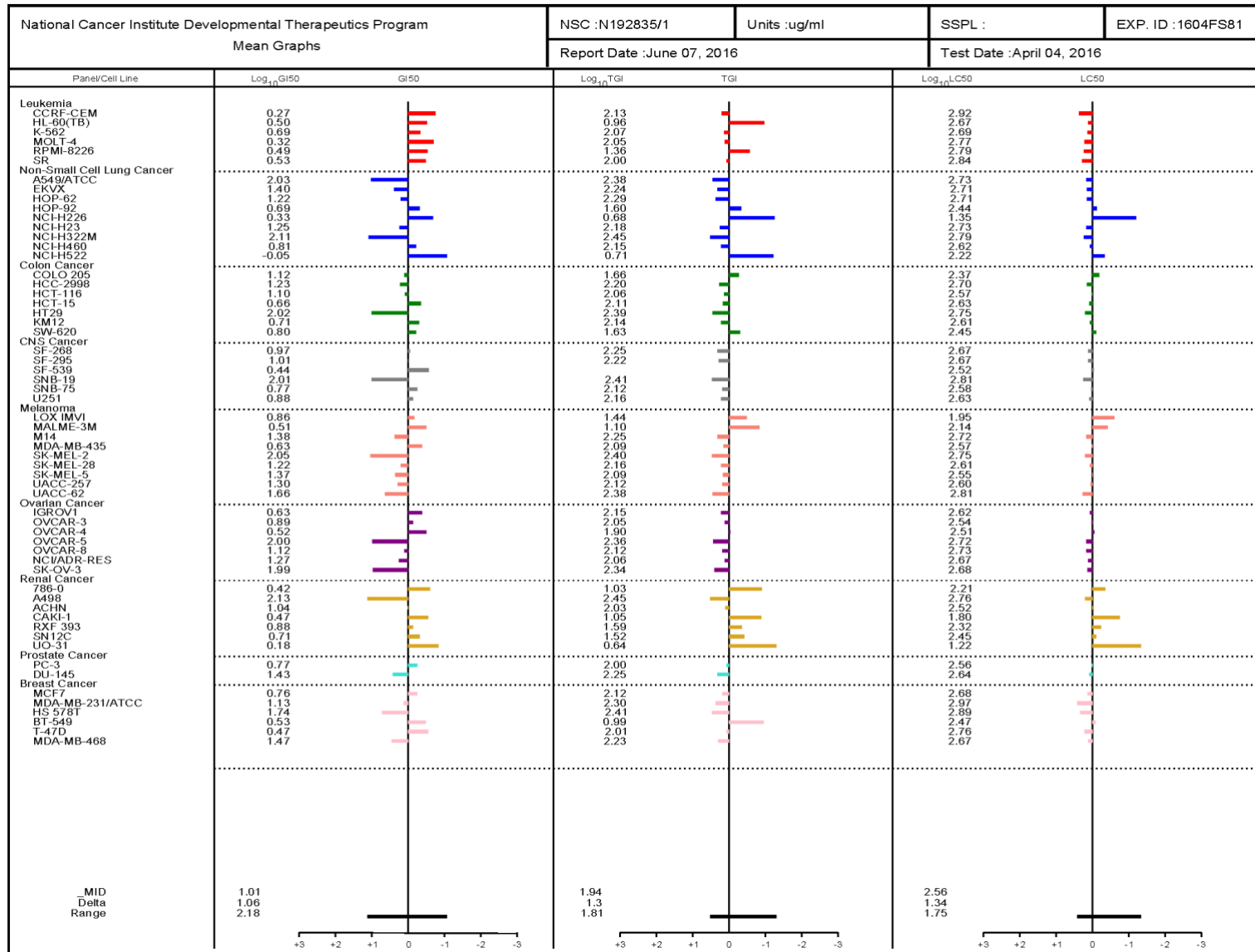


Figure S39. Mean bar graph of the *Schinus terebinthifolia* leaf dichloromethane extract (BR 436/N192835) in the NCI-60 cell five-dose screen.

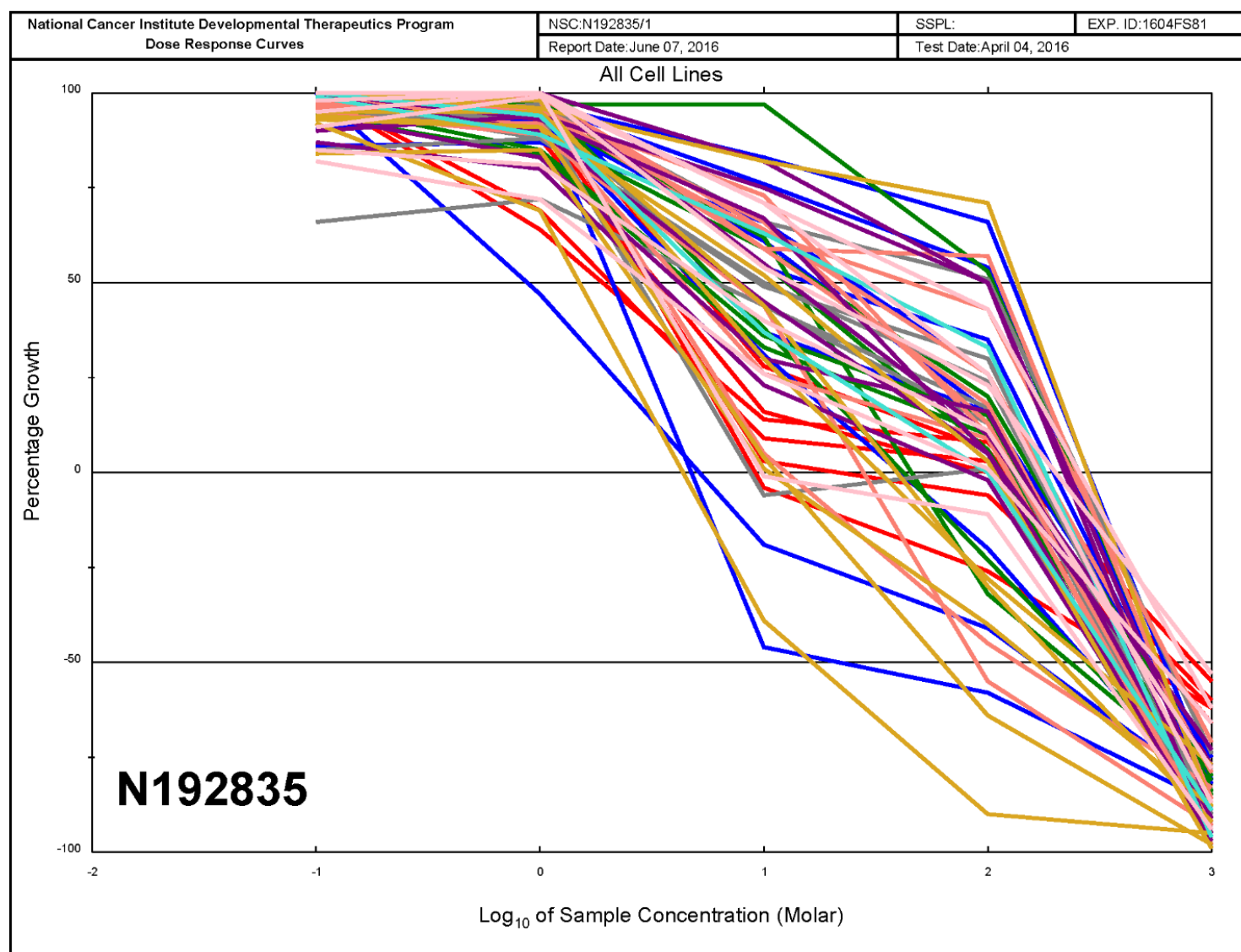


Figure S40. Composite of the NCI-60 dose response curves of the *Schinus terebinthifolia* leaf dichloromethane extract (BR 436/N192835) with higher activity against the non-small cell lung cancer NCI-H522.

M. Enterolobium gummiferum

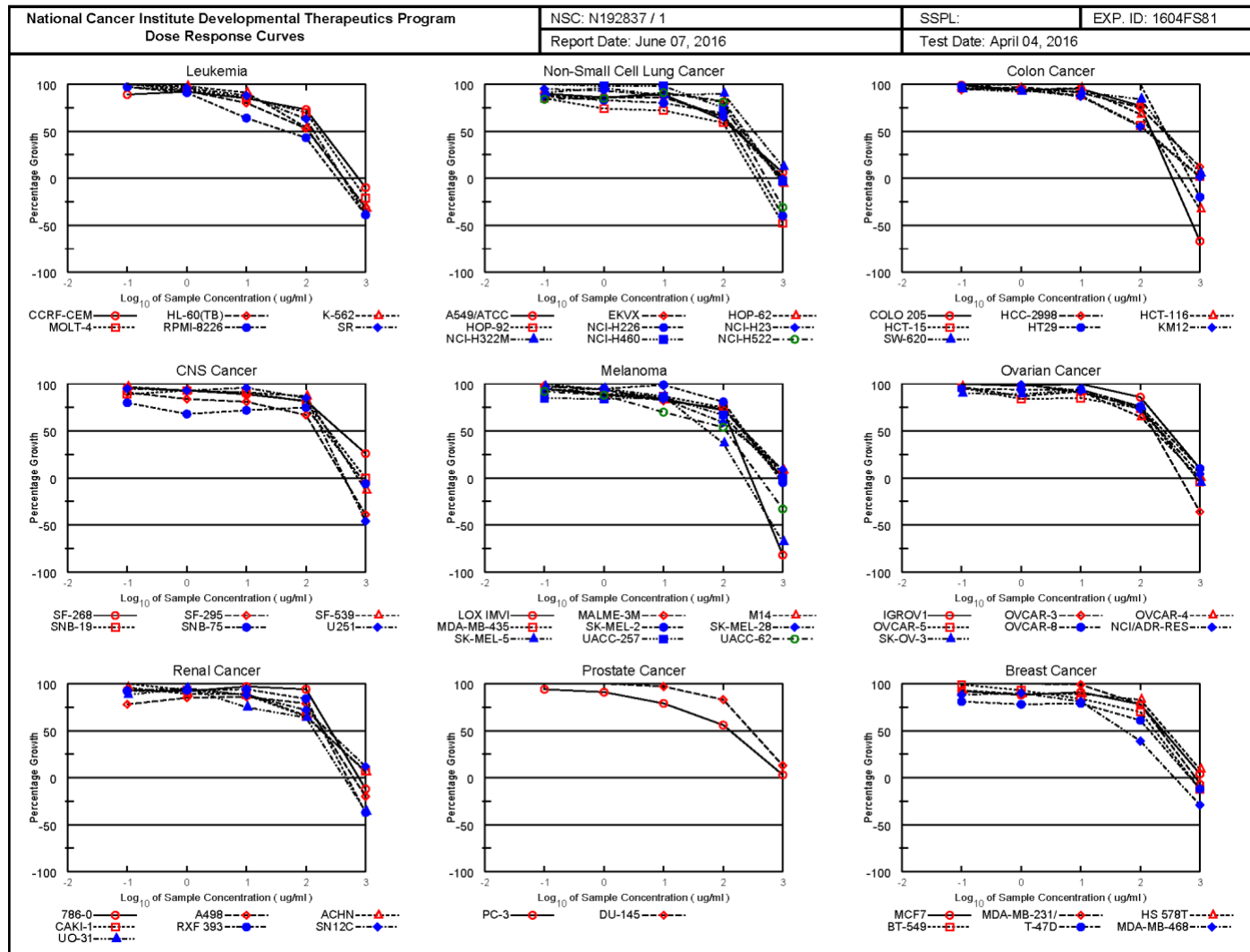


Figure S41. Dose response curves of the *Enterolobium gummiferum* stem bark hexane extract (BR 469/N192837) against 9 cell panels with different susceptibility.

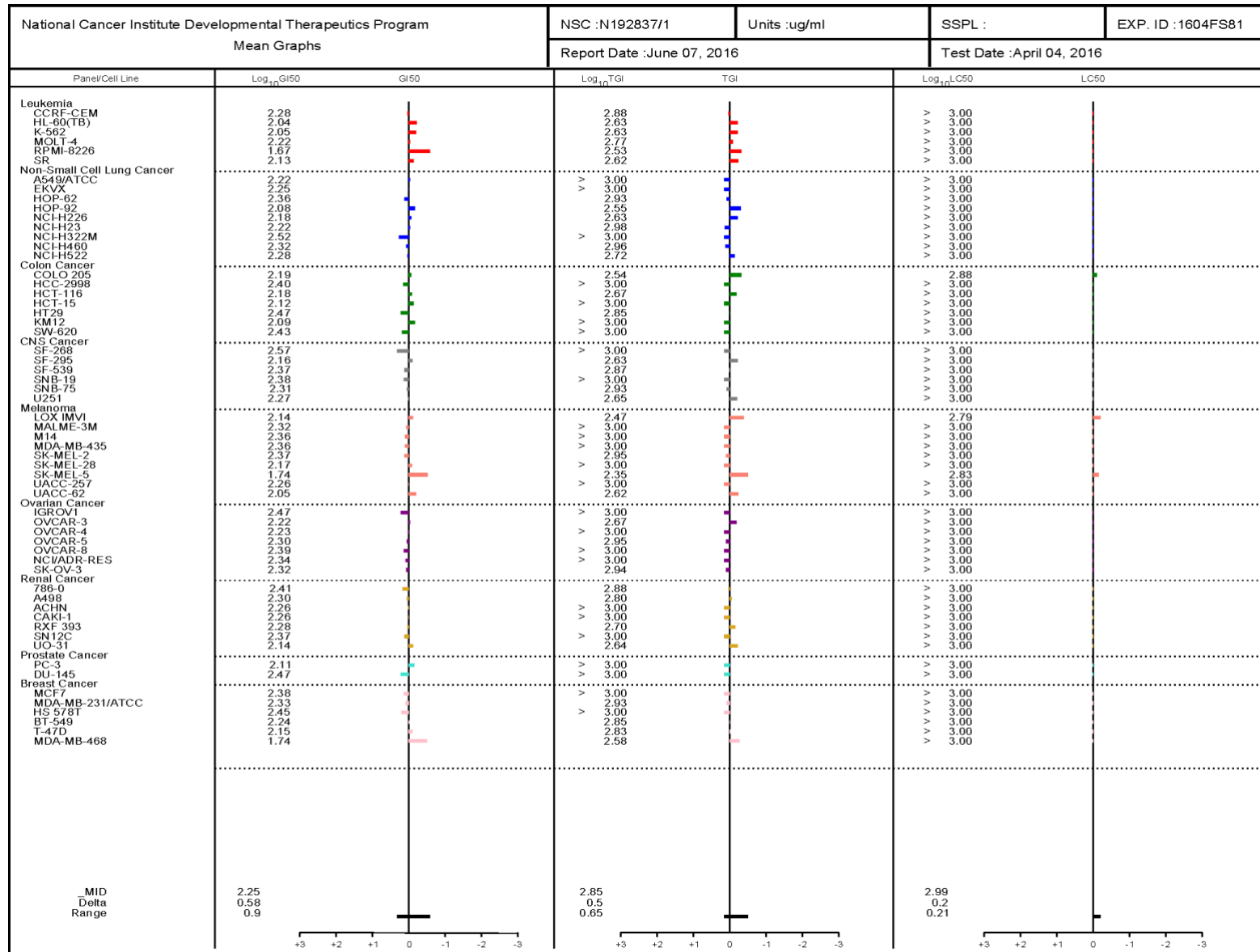


Figure S42. Mean bar graph of the *Enterolobium gummiferum* stem bark hexane extract (BR 469/N192837) in the NCI-60 cell five-dose screen.

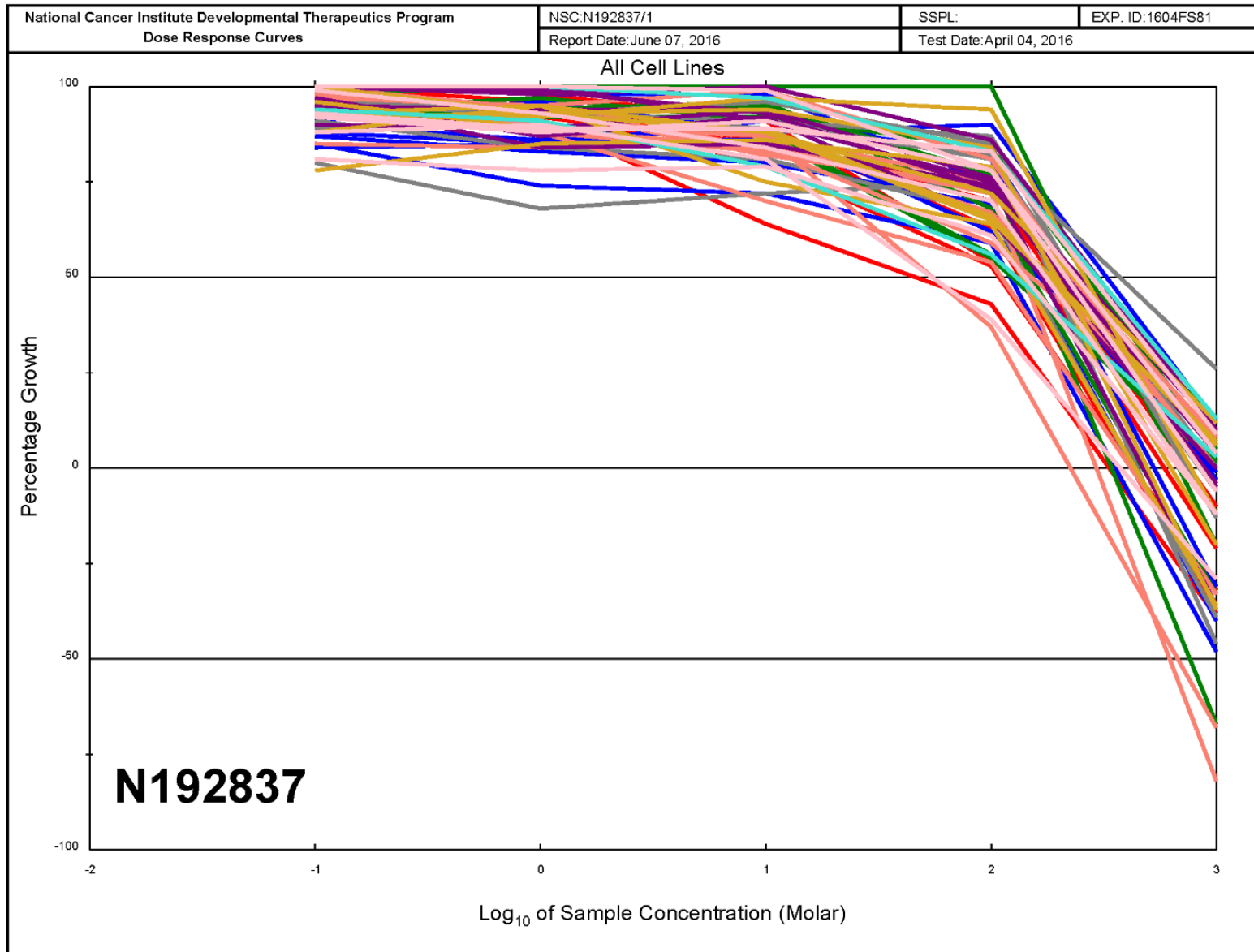


Figure S43. Composite of the NCI-60 dose response curves of the *Enterolobium gummiferum* stem bark hexane extract (BR 469/N192837).

N. Plathymenia reticulata

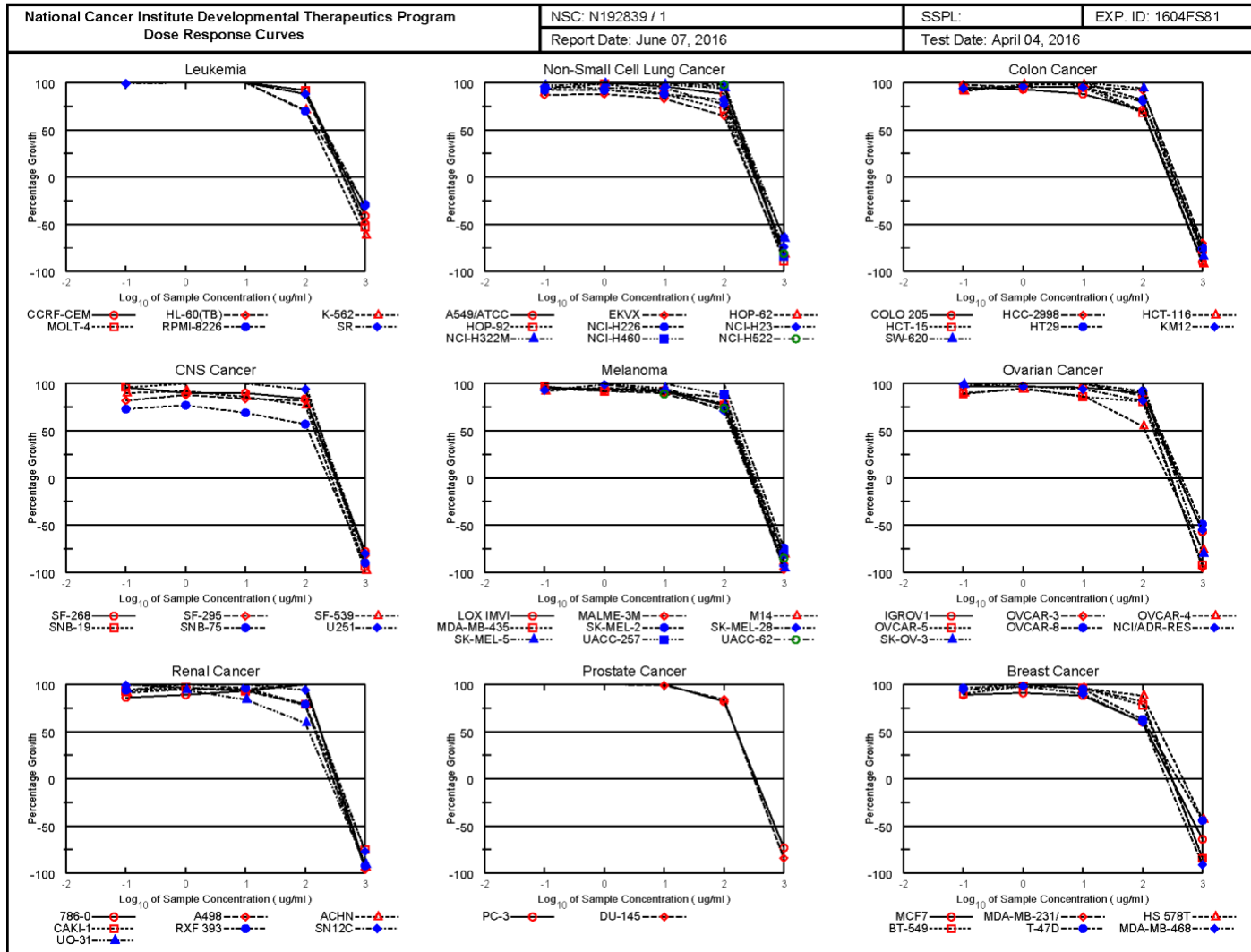


Figure S44. Dose response curves of the *Plathymenia reticulata* root wood hexan extract (BR 489/N192839) against 9 cell panels with different susceptibility.

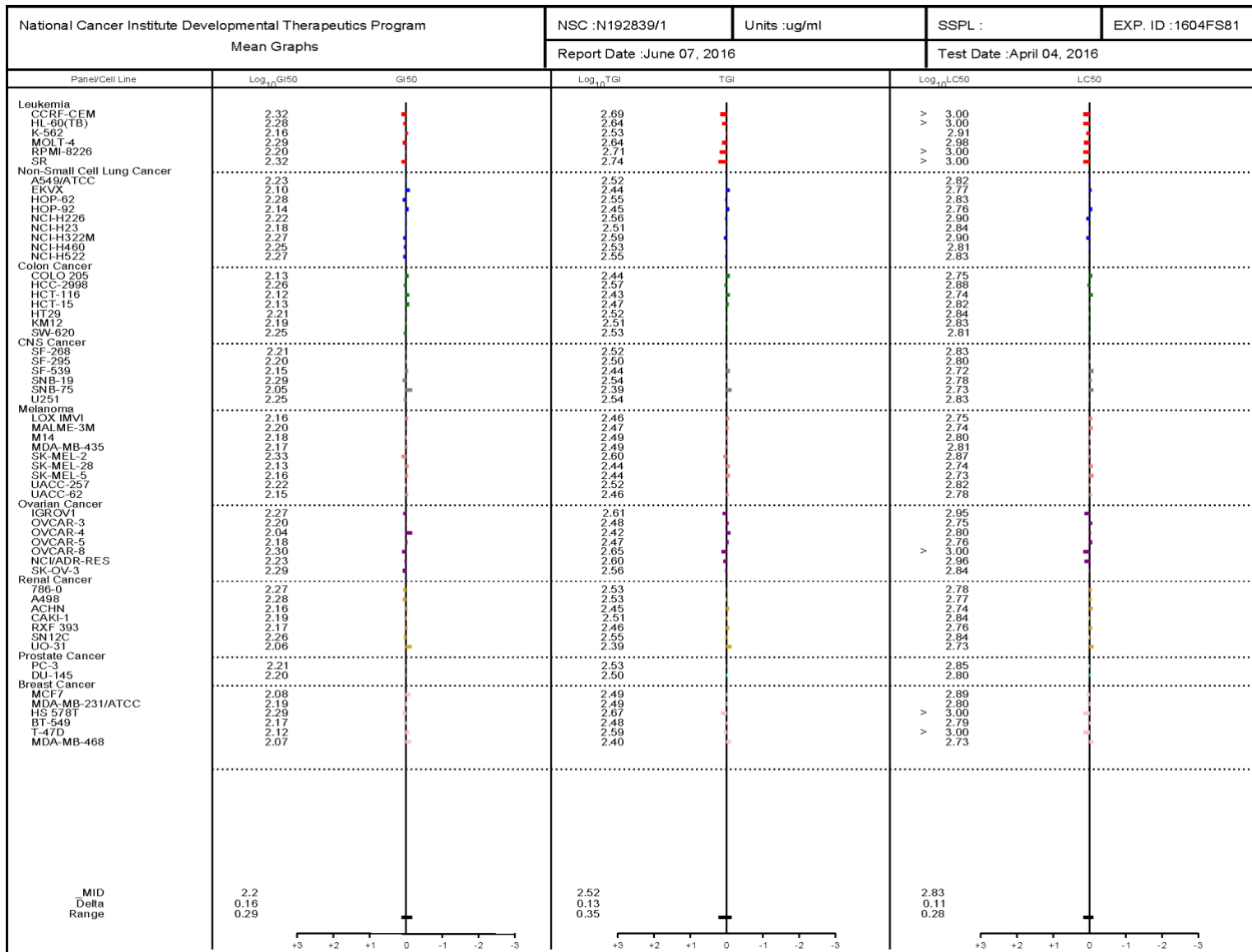


Figure S45. Mean bar graph of the *Plathymenia reticulata* root wood hexane extract (BR 489/N192839) in the NCI-60 cell five-dose screen.

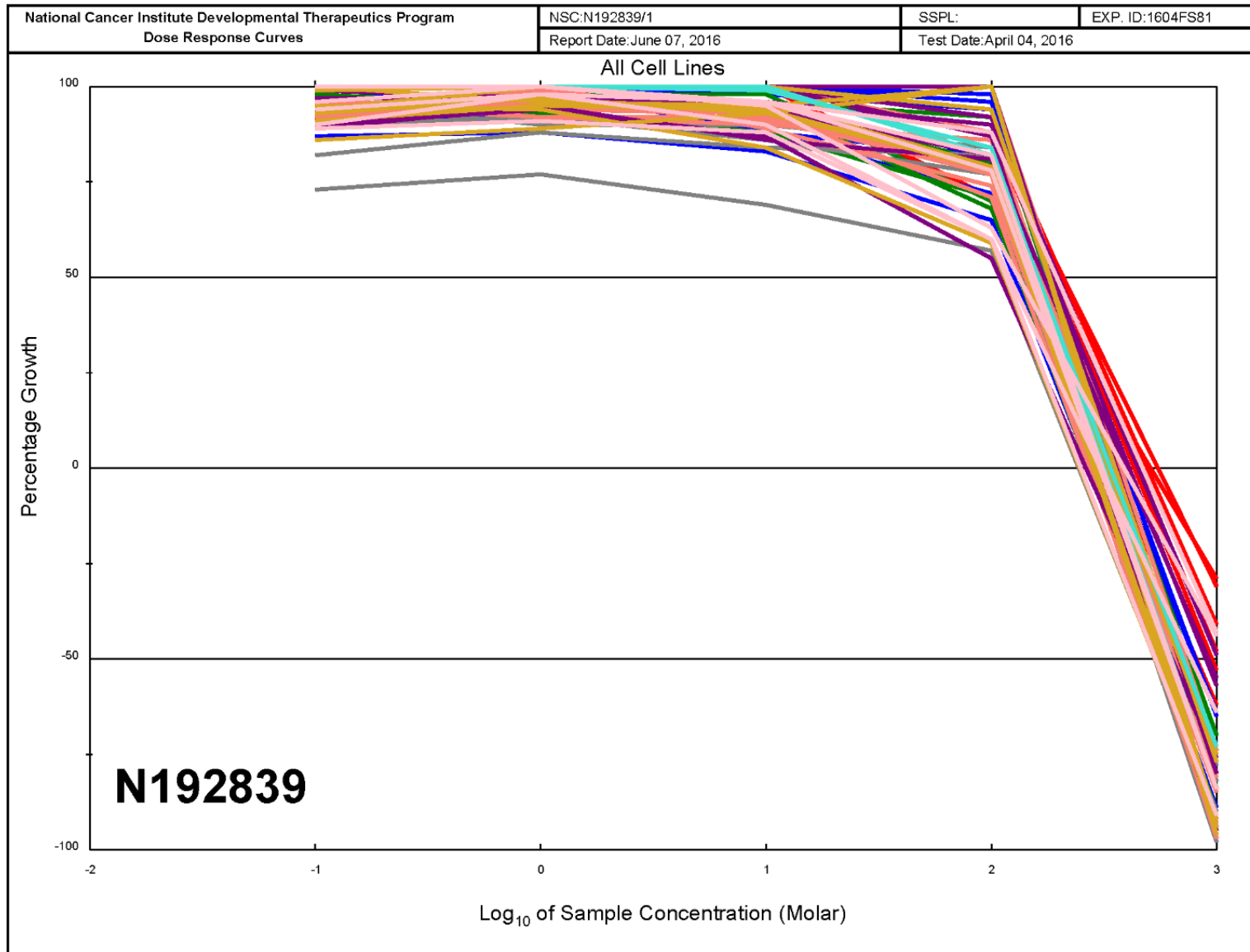


Figure S46. Composite of the NCI-60 dose response curves of the *Plathymenia reticulata* root wood hexane extract (BR 489/N192839).

O. Psidium laruotteanum

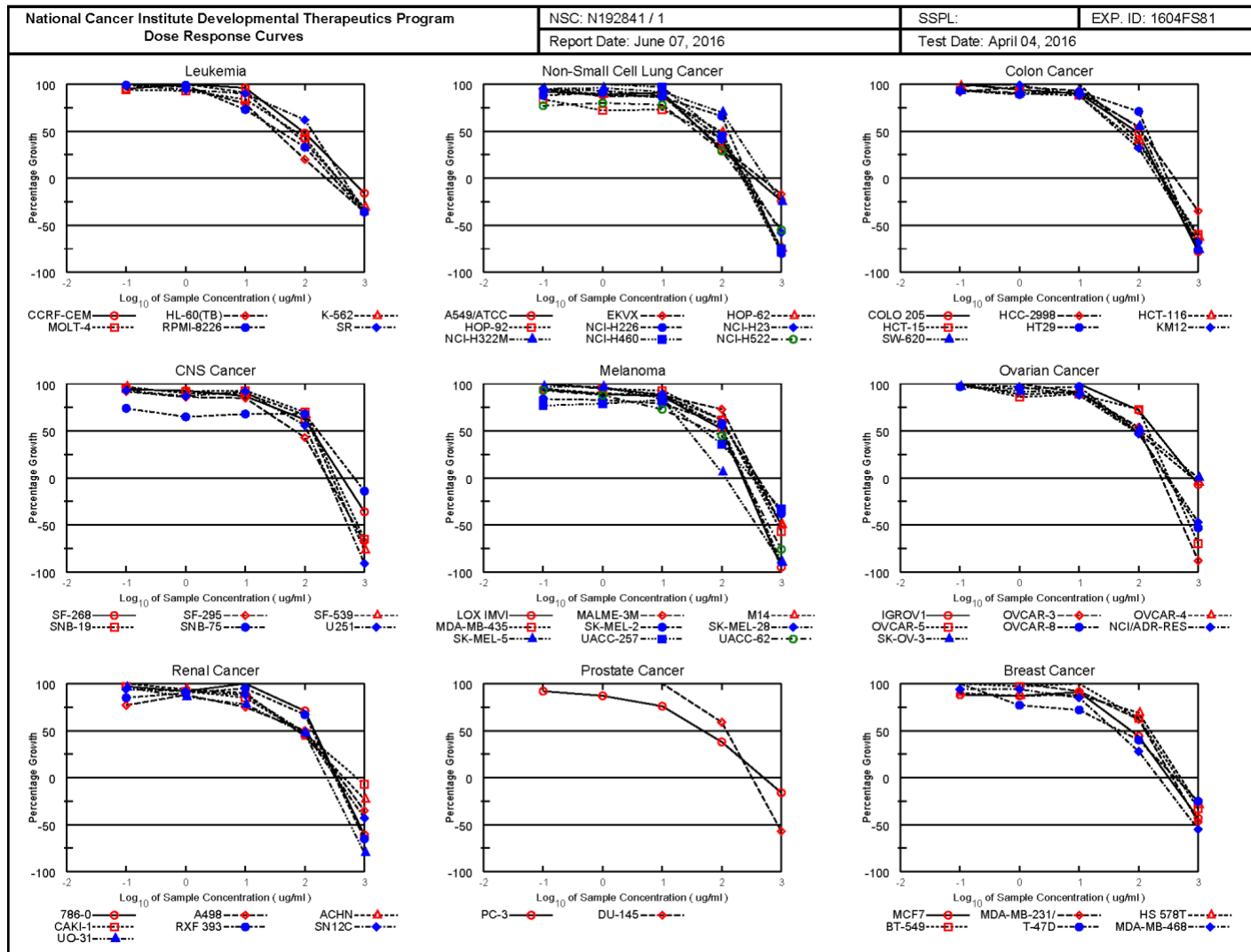


Figure S47. Dose response curves of the *Psidium laruotteanum* stem bark hexane extract (BR 549/N192841) against 9 cell panels with different susceptibility.

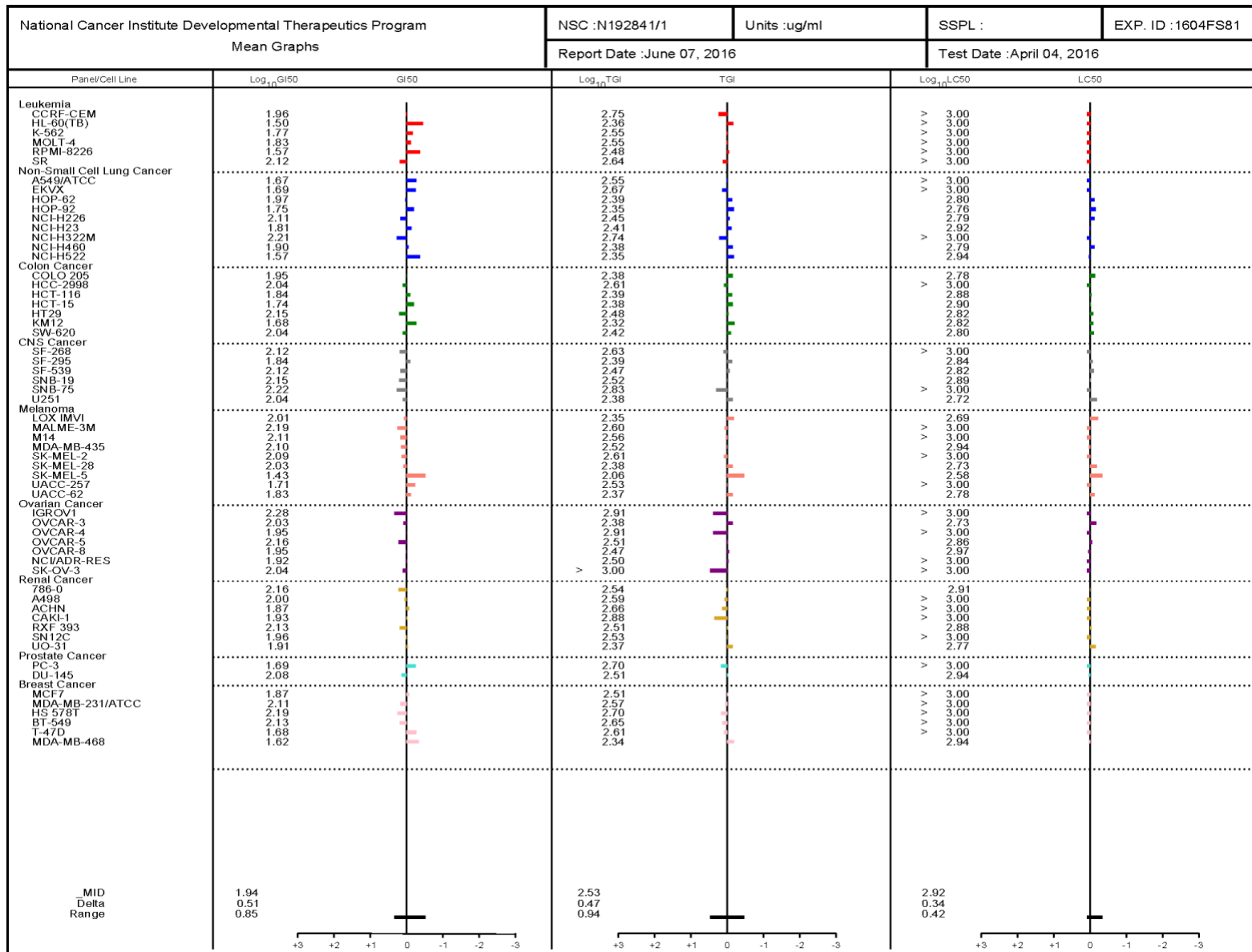


Figure S48. Mean bar graph of the *Psidium laruotteanum* stem bark hexane extract (BR 549/N192841) in the NCI-60 cell five-dose screen.

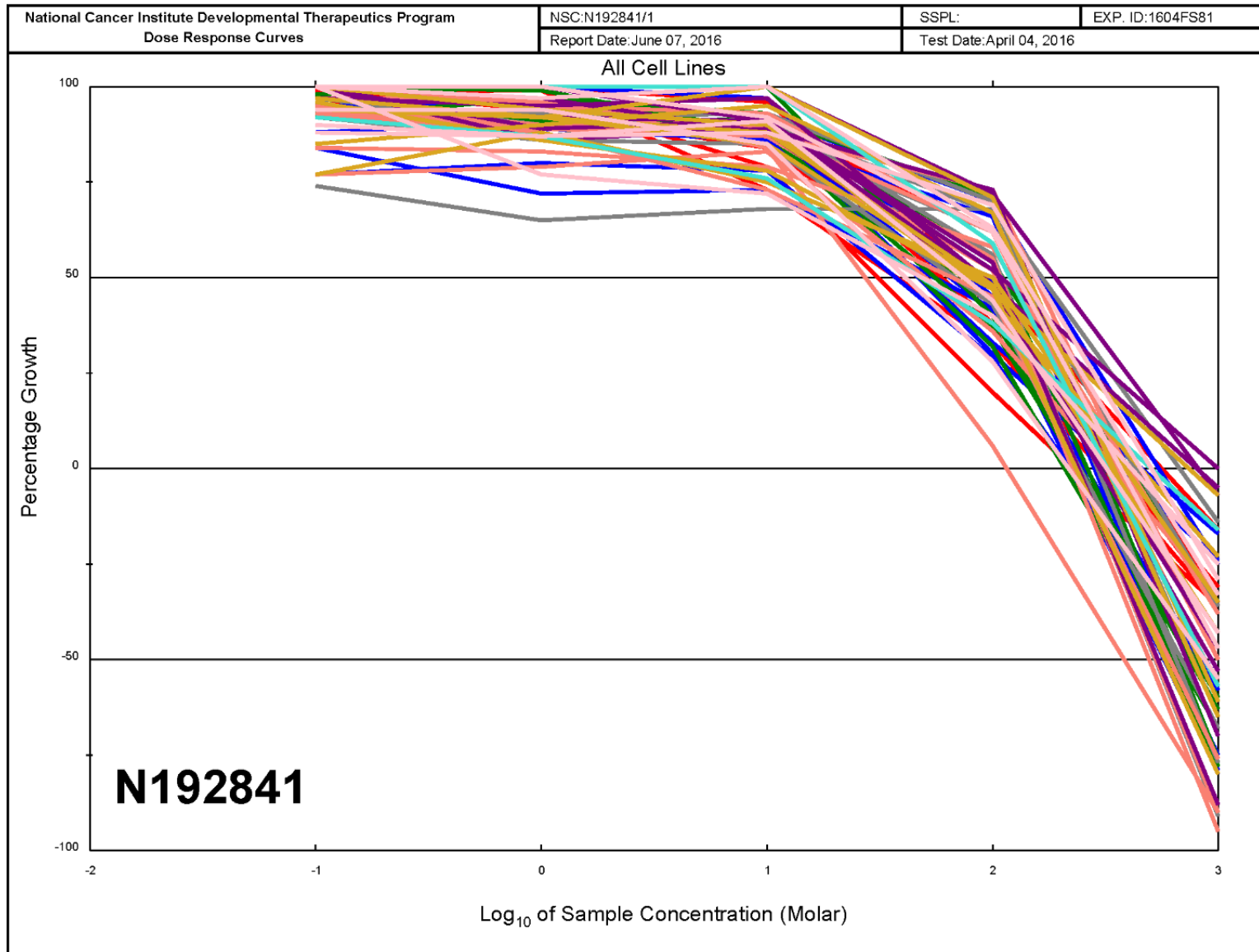


Figure S49. Composite of the NCI-60 dose response curves of the *Psidium laruotteanum* stem bark hexane extract (BR 549/N192841).

P. Lippia rotundifolia

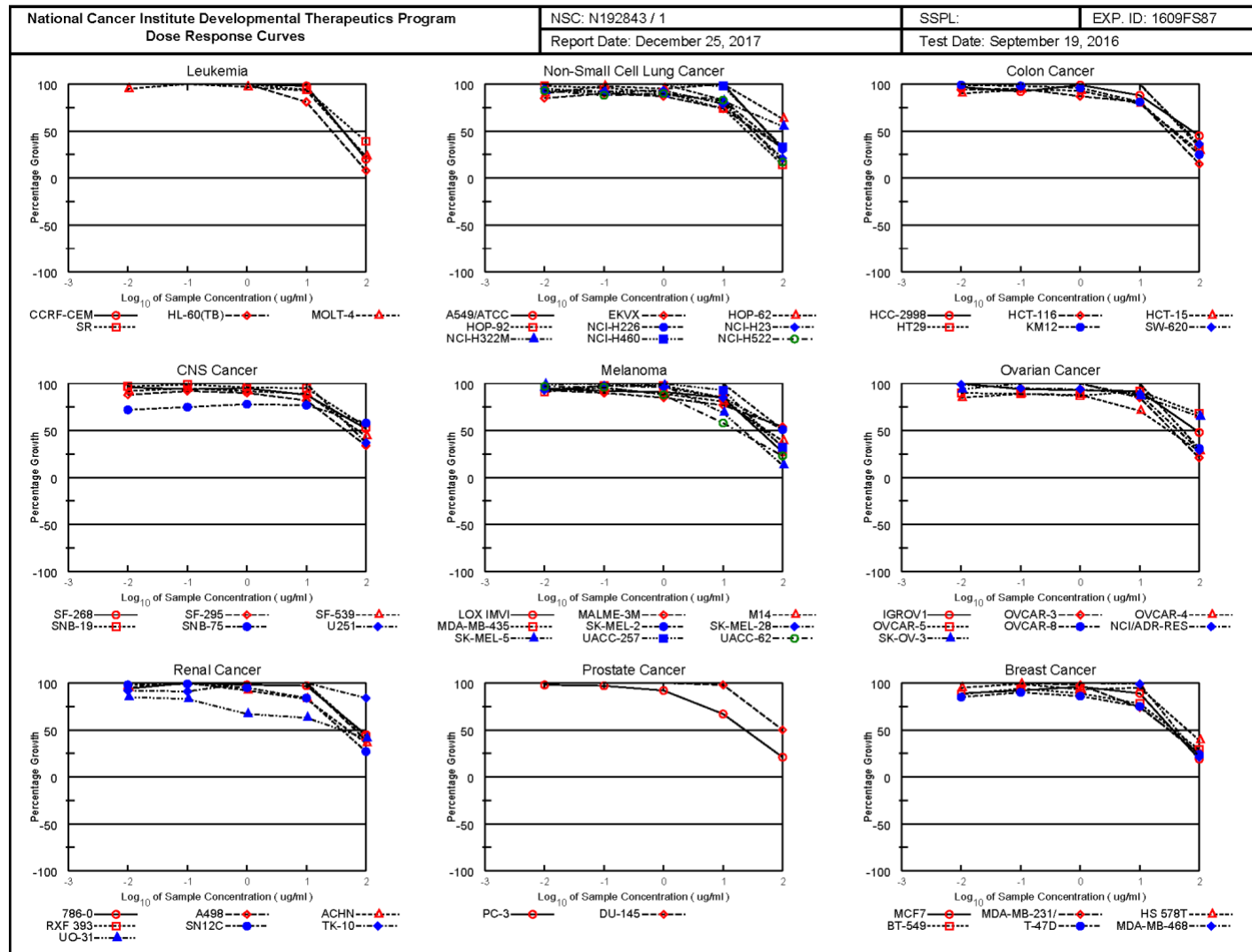


Figure S50. Dose response curves of the *Lippia rotundifolia* stem wood ethyl acetate extract (BR 660/N192843) against 9 cell panels with different susceptibility.

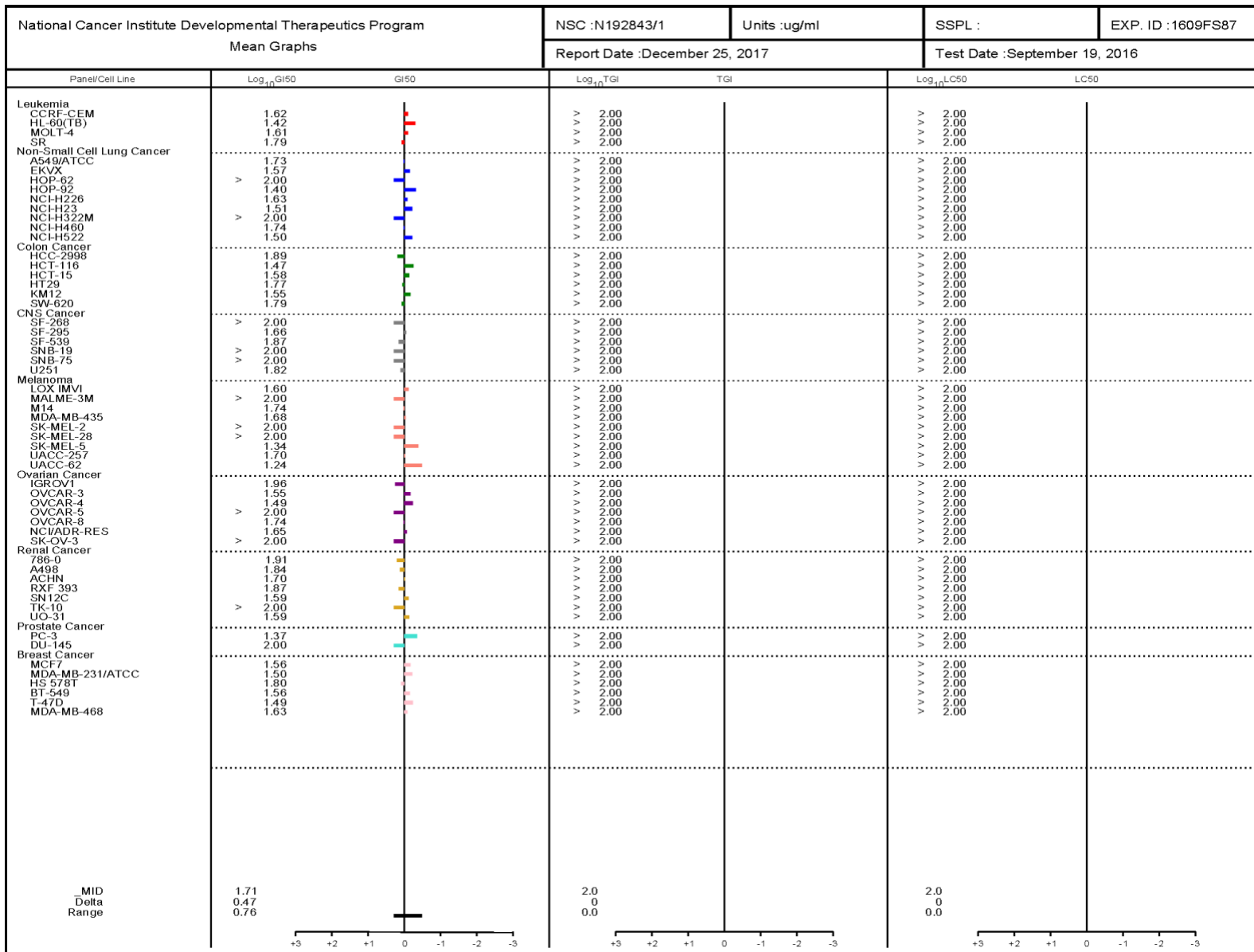


Figure S51. Mean bar graph of the *Lippia rotundifolia* stem wood ethyl acetate extract (BR 660/N192843) in the NCI-60 cell five-dose screen.

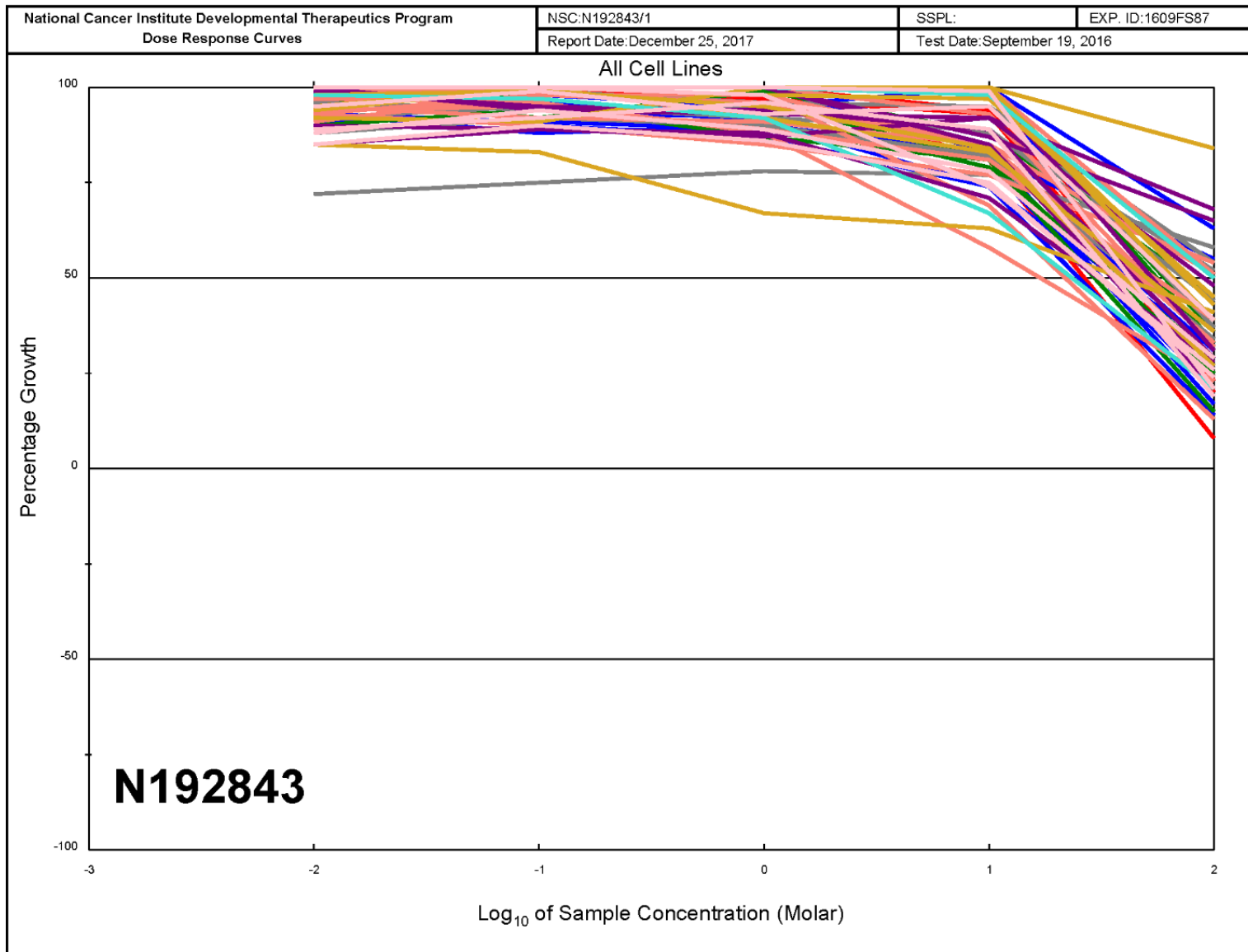


Figure S52. Composite of the NCI-60 dose response curves of the *Lippia rotundifolia* stem wood ethyl acetate extract (BR 660/N192843).

Q. Connarus suberosus

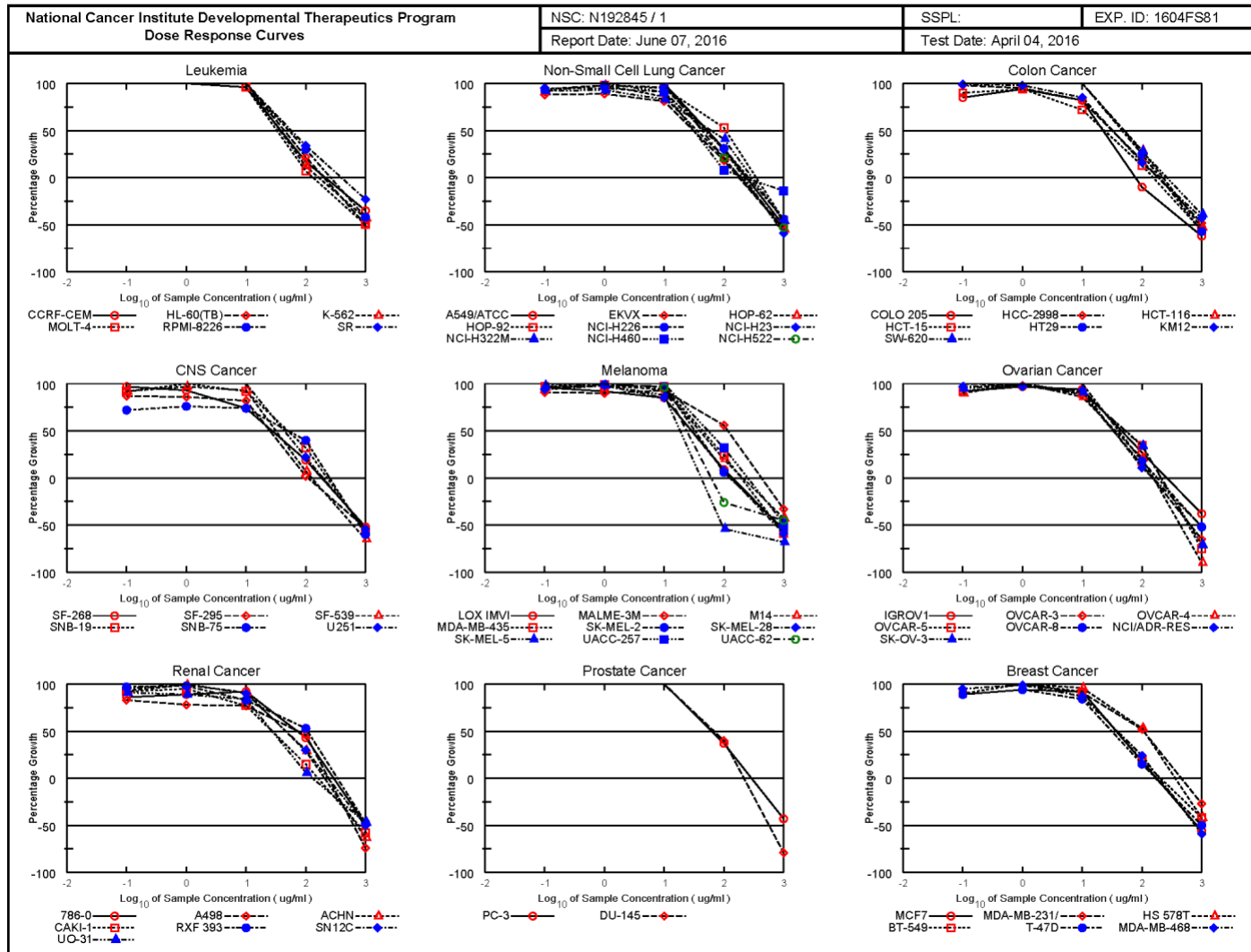


Figure S53. Dose response curves of the *Connarus suberosus* root wood ethyl acetate extract (BR 693/N192845) against 9 cell panels with different susceptibility.

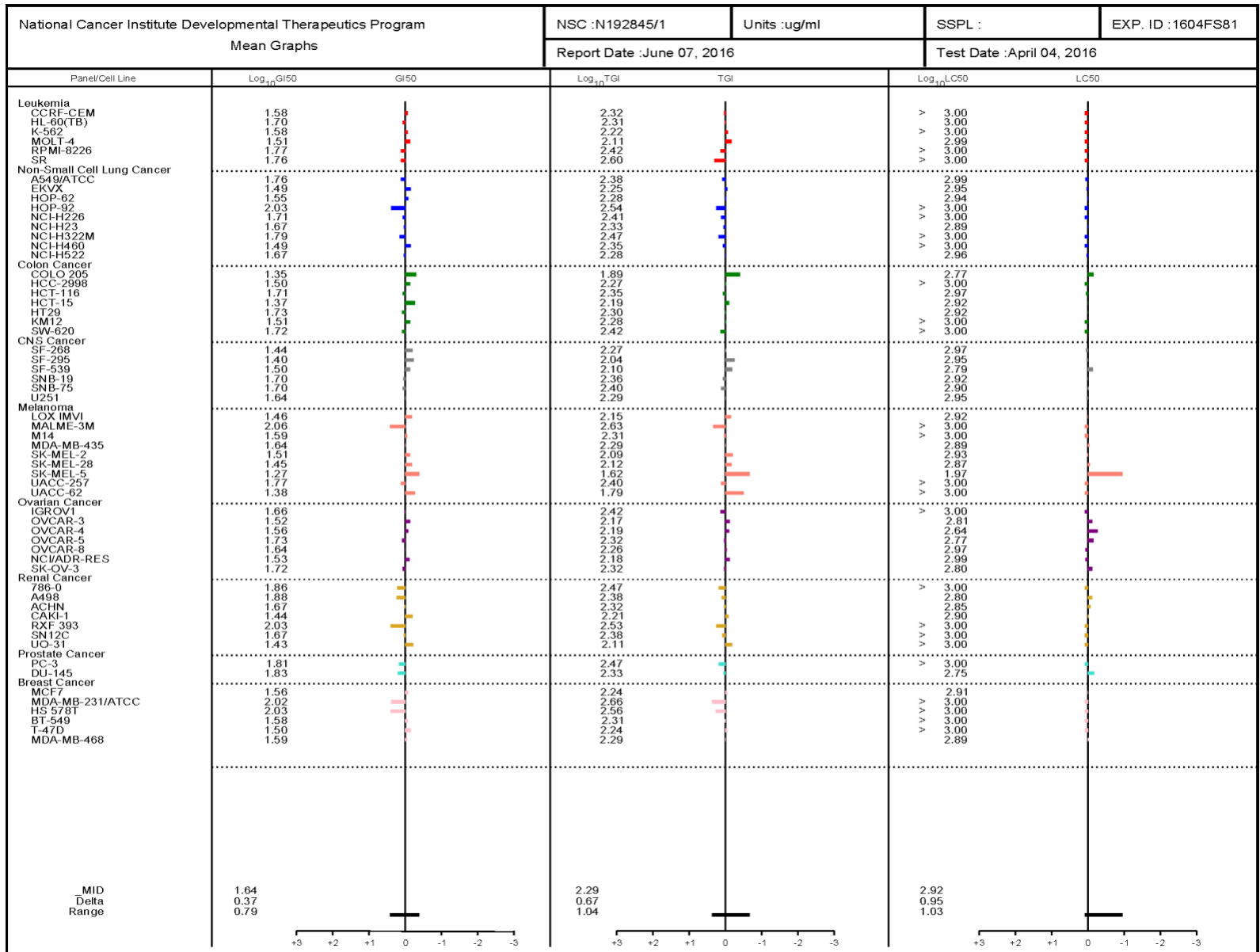


Figure S54. Mean bar graph of the *Connarus suberosus* root wood ethyl acetate extract (BR 693/N192845) in the NCI-60 cell five-dose screen.

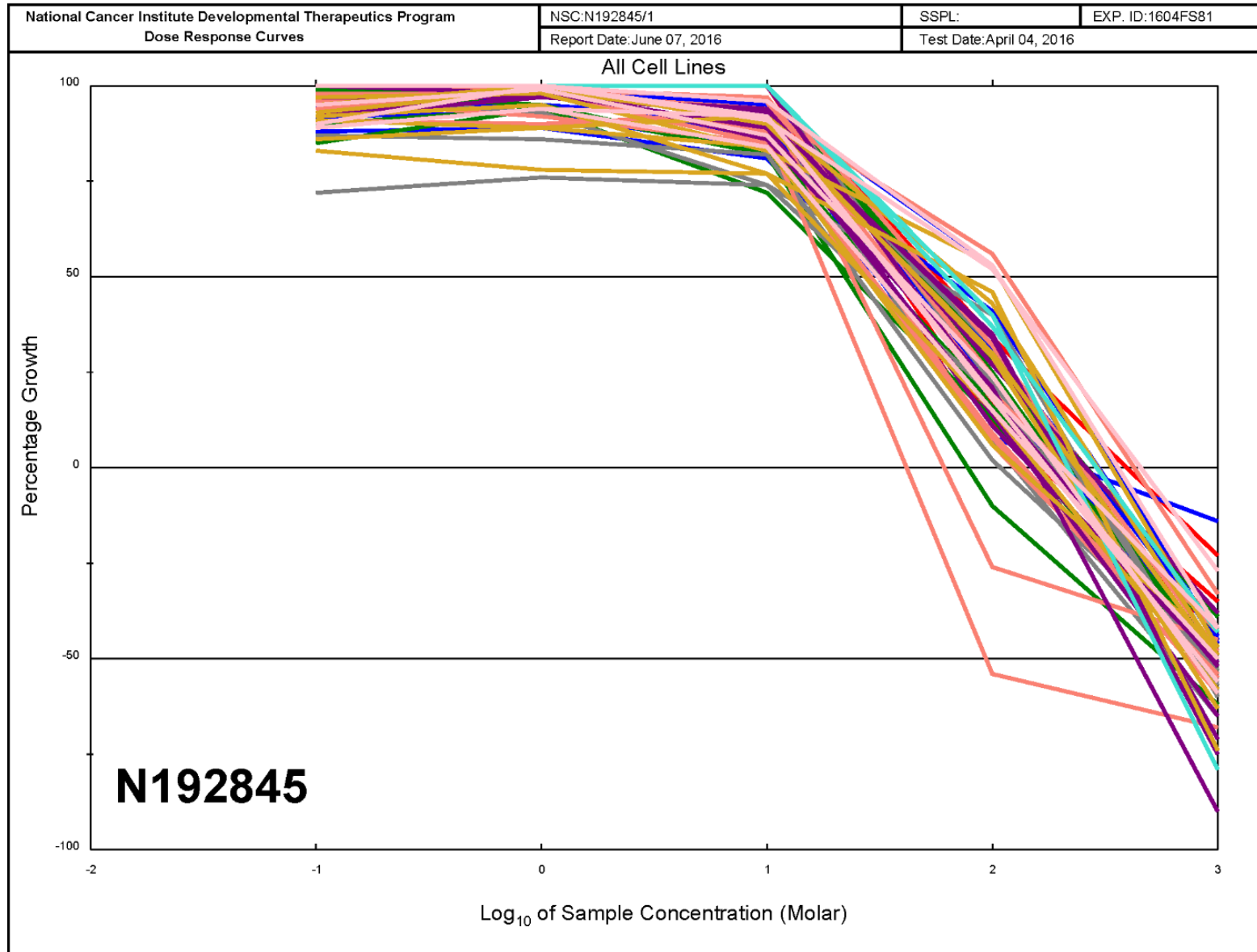


Figure S55. Composite of the NCI-60 dose response curves of the *Connarus suberosus* root wood ethyl acetate extract (BR 693/N192845).

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