

# Heterocyclic Iminoquinones and Quinones from National Cancer Institute (USA) COMPARE Analysis

Naemah Haji <sup>1‡</sup>, Masoma Faizi <sup>1‡</sup>, Panayiotis A. Koutentis <sup>2</sup>, Michael P. Carty <sup>3</sup> and Fawaz Aldabbagh <sup>1\*</sup>

<sup>1</sup> Department of Pharmacy, School of Life Sciences, Pharmacy and Chemistry, Kingston University, Penrhyn Road, Kingston upon Thames, KT1 2EE, UK

<sup>2</sup> Department of Chemistry, University of Cyprus, PO Box 20537, 1678 Nicosia, Cyprus

<sup>3</sup> School of Biological and Chemical Sciences, National University of Ireland Galway, University Road, H91 TK33 Galway, Ireland

‡ Equal contributions

\* Correspondence: F.Aldabbagh@kingston.ac.uk

## Supplementary Materials

Correlation of DPIQ (NSC753790) to NQO1	Figure S1
Correlation of DPIQ (NSC753790) to <b>3a</b> (NSC84167)	Figure S2
Correlation of <b>3a</b> (NSC84167) to NQO1	Figure S3
Correlation of DPIQ (NSC753790) to <b>4</b> (NSC94945)	Figure S4
Correlation of <b>4</b> (NSC94945) to NQO1	Figure S5
Correlation of <b>5a</b> (NSC768093) to Pleurotin (NSC401005)	Figure S6
Correlation of <b>5b</b> (NSC780813) to Pleurotin (NSC401005)	Figure S7
Correlation of <b>5a</b> (NSC768093) to <b>5b</b> (NSC780813)	Figure S8
Correlation of <b>5c</b> (NSC780816) to Pleurotin (NSC401005)	Figure S9
Correlation of <b>5a</b> (NSC768093) to <b>5c</b> (NSC780816)	Figure S10
Correlation of <b>5d</b> (NSC780815) to Pleurotin (NSC401005)	Figure S11
Correlation of <b>5a</b> (NSC768093) to <b>5d</b> (NSC780815)	Figure S12
Correlation of DPIQ (NSC753790) to <b>7</b> (NSC643735)	Figure S13
Correlation of <b>7</b> (NSC643735) to NQO1	Figure S14
Correlation of DPIQ (NSC753790) to <b>8a</b> (NSC795222)	Figure S15
Correlation of <b>8a</b> (NSC795222) to NQO1	Figure S16
Correlation of DPIQ (NSC753790) to <b>9a</b> (NSC291094)	Figure S17
Correlation of <b>9a</b> (NSC291094) to NQO1	Figure S18
Correlation of DPIQ (NSC753790) to <b>10a</b> (NSC798710)	Figure S19
Correlation of <b>10a</b> (NSC798710) to NQO1	Figure S20
Correlation of DPIQ (NSC753790) to <b>10b</b> (NSC798709)	Figure S21
Correlation of <b>10b</b> (NSC798709) to NQO1	Figure S22
Correlation of DPIQ (NSC753790) to <b>11b</b> (NSC750104)	Figure S23
Correlation of <b>11b</b> (NSC750104) to NQO1	Figure S24
Correlation of DPIQ (NSC753790) to <b>12</b> (NSC647943)	Figure S25
Correlation of <b>12</b> (NSC647943) to NQO1	Figure S26
Correlation of <b>5a</b> (NSC768093) to <b>13a</b> (NSC787555)	Figure S27
Correlation of <b>13a</b> (NSC787555) to Pleurotin (NSC401005)	Figure S28
Correlation of <b>5a</b> (NSC768093) to <b>13b</b> (NSC787553)	Figure S29
Correlation of <b>13b</b> (NSC787553) to Pleurotin (NSC401005)	Figure S30
Correlation of <b>5a</b> (NSC768093) to <b>13c</b> (NSC787554)	Figure S31
Correlation of <b>13c</b> (NSC787554) to Pleurotin (NSC401005)	Figure S32
Correlation of <b>5a</b> (NSC768093) to <b>13d</b> (NSC791347)	Figure S33
Correlation of <b>13d</b> (NSC791347) to Pleurotin (NSC401005)	Figure S34
Correlation of <b>5a</b> (NSC768093) to <b>14a</b> (NSC92937)	Figure S35
Correlation of <b>14a</b> (NSC92937) to Pleurotin (NSC401005)	Figure S36
Correlation of <b>5a</b> (NSC768093) to <b>14b</b> (NSC668844)	Figure S37
Correlation of <b>14b</b> (NSC668844) to Pleurotin (NSC401005)	Figure S38

Correlation of <b>5a</b> (NSC768093) to <b>14c</b> (NSC661222)	<i>Figure S39</i>
Correlation of <b>14c</b> (NSC661222) to Pleurotin (NSC401005)	<i>Figure S40</i>
Correlation of <b>5a</b> (NSC768093) to <b>14d</b> (NSC645330)	<i>Figure S41</i>
Correlation of <b>14d</b> (NSC645330) to Pleurotin (NSC401005)	<i>Figure S42</i>
Correlation of <b>5a</b> (NSC768093) to <b>14e</b> (NSC661221)	<i>Figure S43</i>
Correlation of <b>14e</b> (NSC661221) to Pleurotin (NSC401005)	<i>Figure S44</i>
Correlation of <b>5a</b> (NSC768093) to <b>14f</b> (NSC641396)	<i>Figure S45</i>
Correlation of <b>14f</b> (NSC641396) to Pleurotin (NSC401005)	<i>Figure S46</i>
Correlation of <b>5a</b> (NSC768093) to Kalafungin (NSC137443)	<i>Figure S47</i>
Correlation of Kalafungin (NSC137443) to Pleurotin (NSC401005)	<i>Figure S48</i>
Correlation of <b>5a</b> (NSC768093) to Nanomycin A (NSC267461)	<i>Figure S49</i>
Correlation of Nanomycin A (NSC267461) to Pleurotin (NSC401005)	<i>Figure S50</i>
Correlation of <b>5a</b> (NSC768093) to <b>15a</b> (NSC641401)	<i>Figure S51</i>
Correlation of <b>15a</b> (NSC641401) to Pleurotin (NSC401005)	<i>Figure S52</i>
Correlation of <b>5a</b> (NSC768093) to Discorhabdin C (NSC626162)	<i>Figure S53</i>
Correlation of Discorhabdin C (NSC626162) to Pleurotin (NSC401005)	<i>Figure S54</i>
Correlation of <b>5a</b> (NSC768093) to <b>9b</b> (NSC682995)	<i>Figure S55</i>
Correlation of <b>9b</b> (NSC682995) to Pleurotin (NSC401005)	<i>Figure S56</i>
Correlation of <b>5a</b> (NSC768093) to Melampomagnolide B (MMB) analogue (NSC801078)	<i>Figure S57</i>
Correlation of MMB analogue (NSC801078) to Pleurotin (NSC401005)	<i>Figure S58</i>
Correlation of NQO1 to <b>19</b> (NSC409304)	<i>Figure S59</i>
Correlation of <b>19</b> (NSC409304) to DPIQ (NSC753790)	<i>Figure S60</i>
Correlation of NQO1 to <b>20</b> (NSC2785)	<i>Figure S61</i>
Correlation of <b>20</b> (NSC2785) to DPIQ (NSC753790)	<i>Figure S62</i>
Correlation of NQO1 to <b>21a</b> (NSC783640)	<i>Figure S63</i>
Correlation of <b>21a</b> (NSC783640) to DPIQ (NSC753790)	<i>Figure S64</i>
Correlation of NQO1 to <b>21b</b> (NSC783641)	<i>Figure S65</i>
Correlation of <b>21b</b> (NSC783641) to DPIQ (NSC753790)	<i>Figure S66</i>
Correlation of NQO1 to <b>5a</b> (NSC768093)	<i>Figure S67</i>
Correlation of NQO1 to <b>5b</b> (NSC780813)	<i>Figure S68</i>
Correlation of NQO1 to Pleurotin (NSC401005)	<i>Figure S69</i>
Correlation of NQO1 to <b>14b</b> (NSC668844)	<i>Figure S70</i>
Correlation of NQO1 to Kalafungin (NSC137443)	<i>Figure S71</i>
Correlation of NQO1 to Discorhabdin C (NSC626162)	<i>Figure S72</i>
Correlation of TrxR to <b>5a</b> (NSC768093)	<i>Figure S73</i>
Correlation of TrxR to <b>5b</b> (NSC780813)	<i>Figure S74</i>
Correlation of TrxR to Pleurotin (NSC401005)	<i>Figure S75</i>
Correlation of TrxR to <b>14b</b> (NSC668844)	<i>Figure S76</i>
Correlation of TrxR to Kalafungin (NSC137443)	<i>Figure S77</i>
Correlation of TrxR to Discorhabdin C (NSC626162)	<i>Figure S78</i>
Correlation of TrxR to DPIQ (NSC753790)	<i>Figure S79</i>
Correlation of TrxR to <b>3a</b> (NSC84167)	<i>Figure S80</i>
Correlation of TrxR to <b>4</b> (NSC94945)	<i>Figure S81</i>
Correlation of TrxR to <b>19</b> (NSC409304)	<i>Figure S82</i>

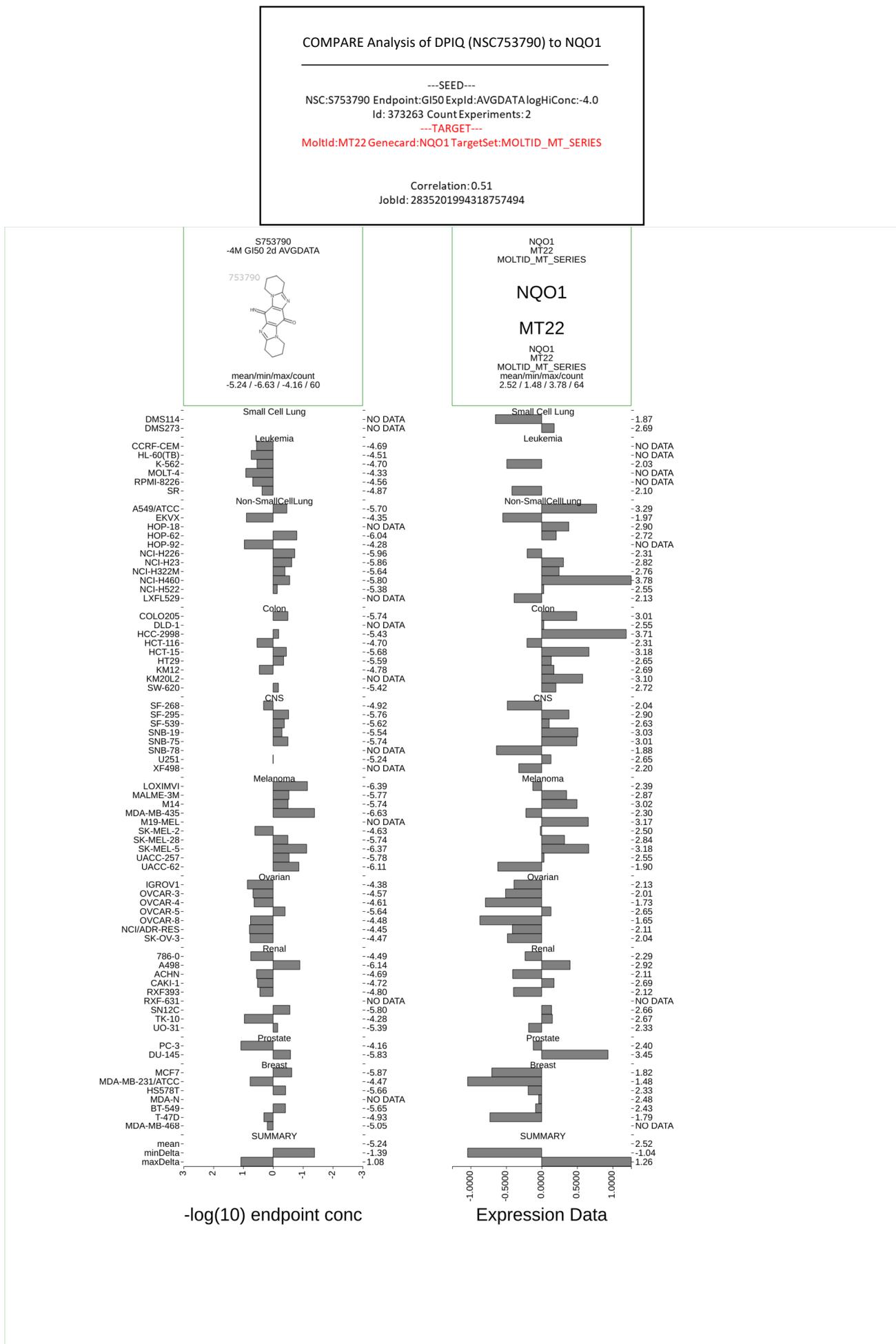


Figure S1

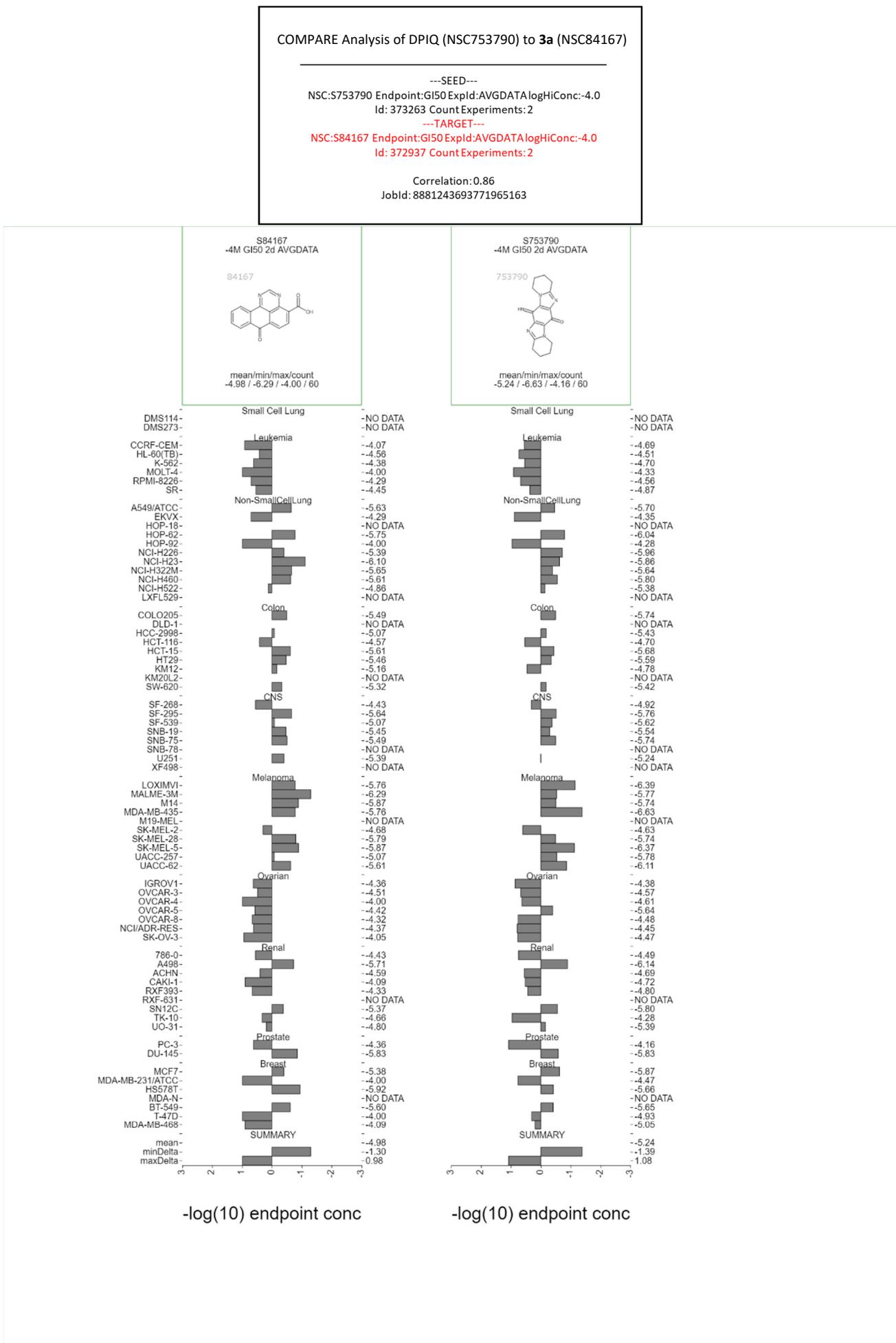


Figure S2

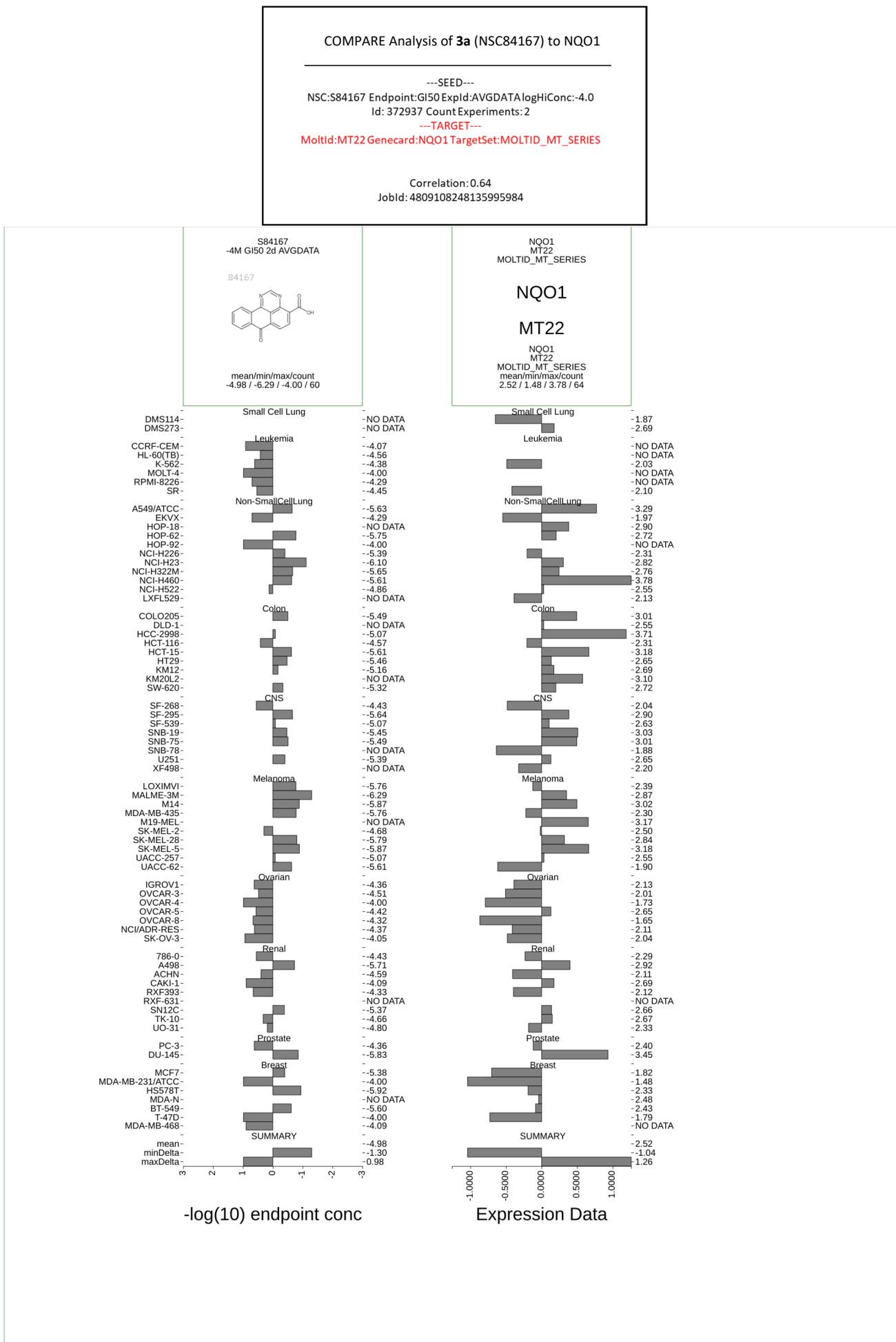


Figure S3

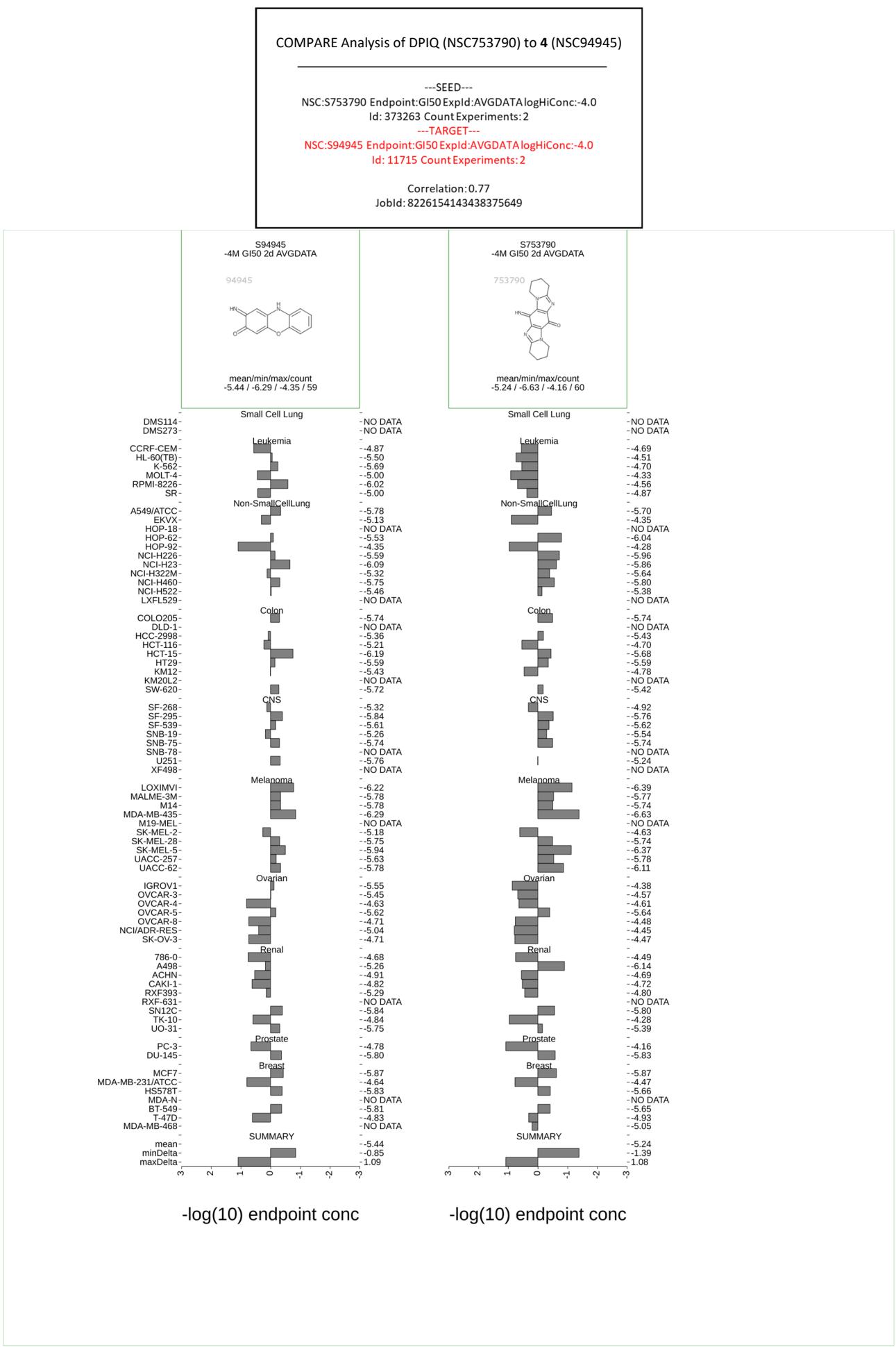


Figure S4

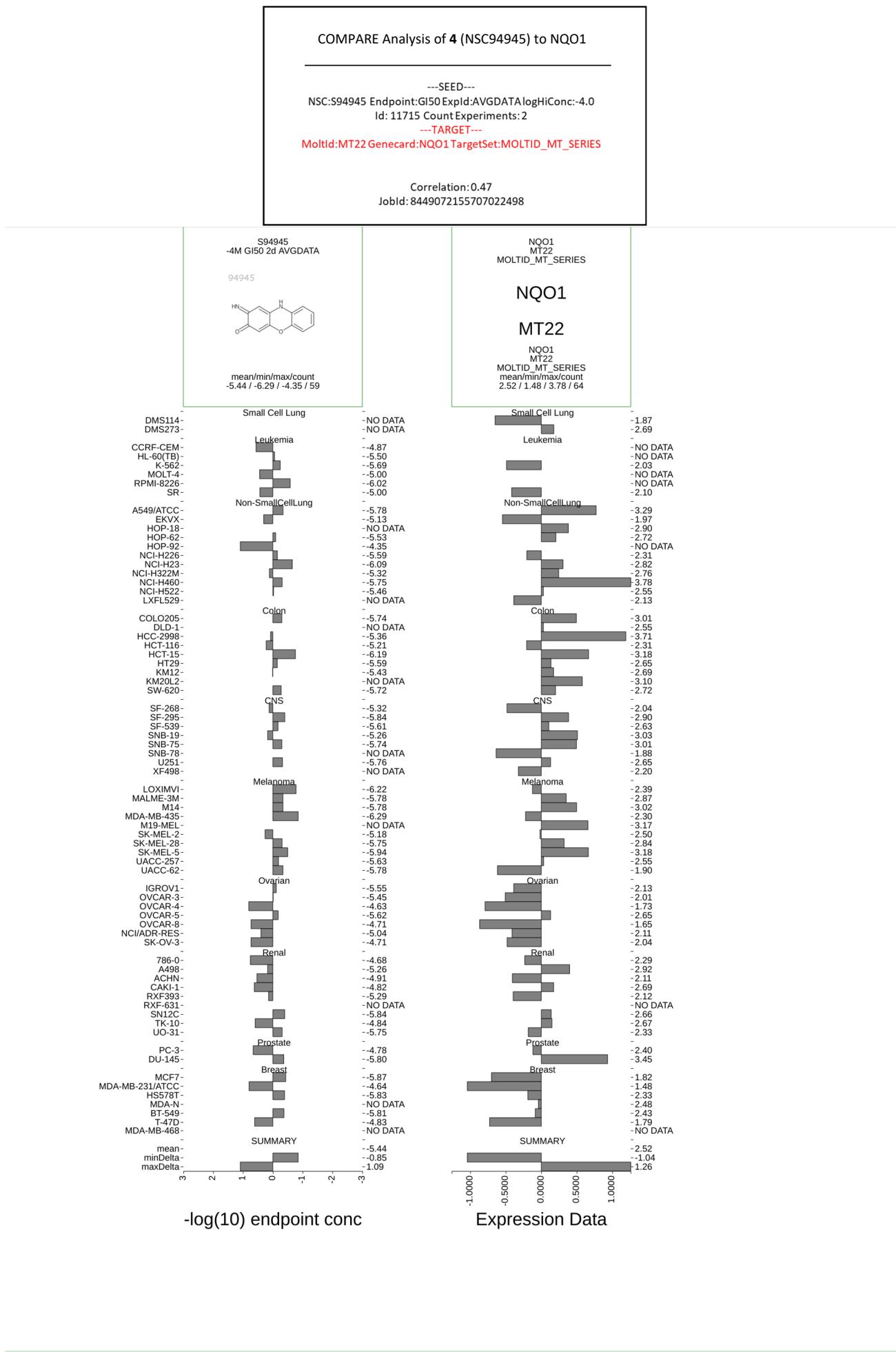


Figure S5

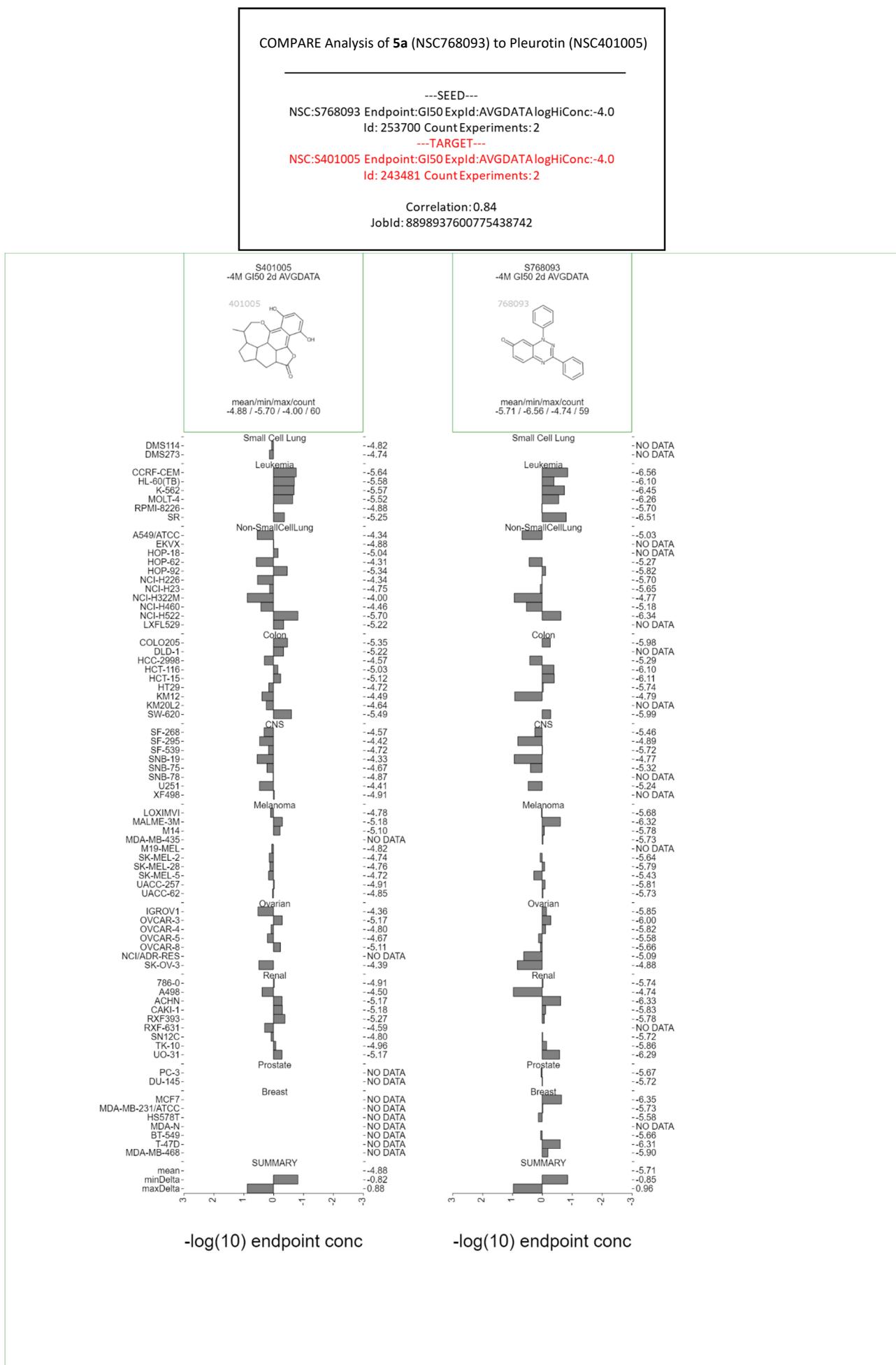


Figure S6

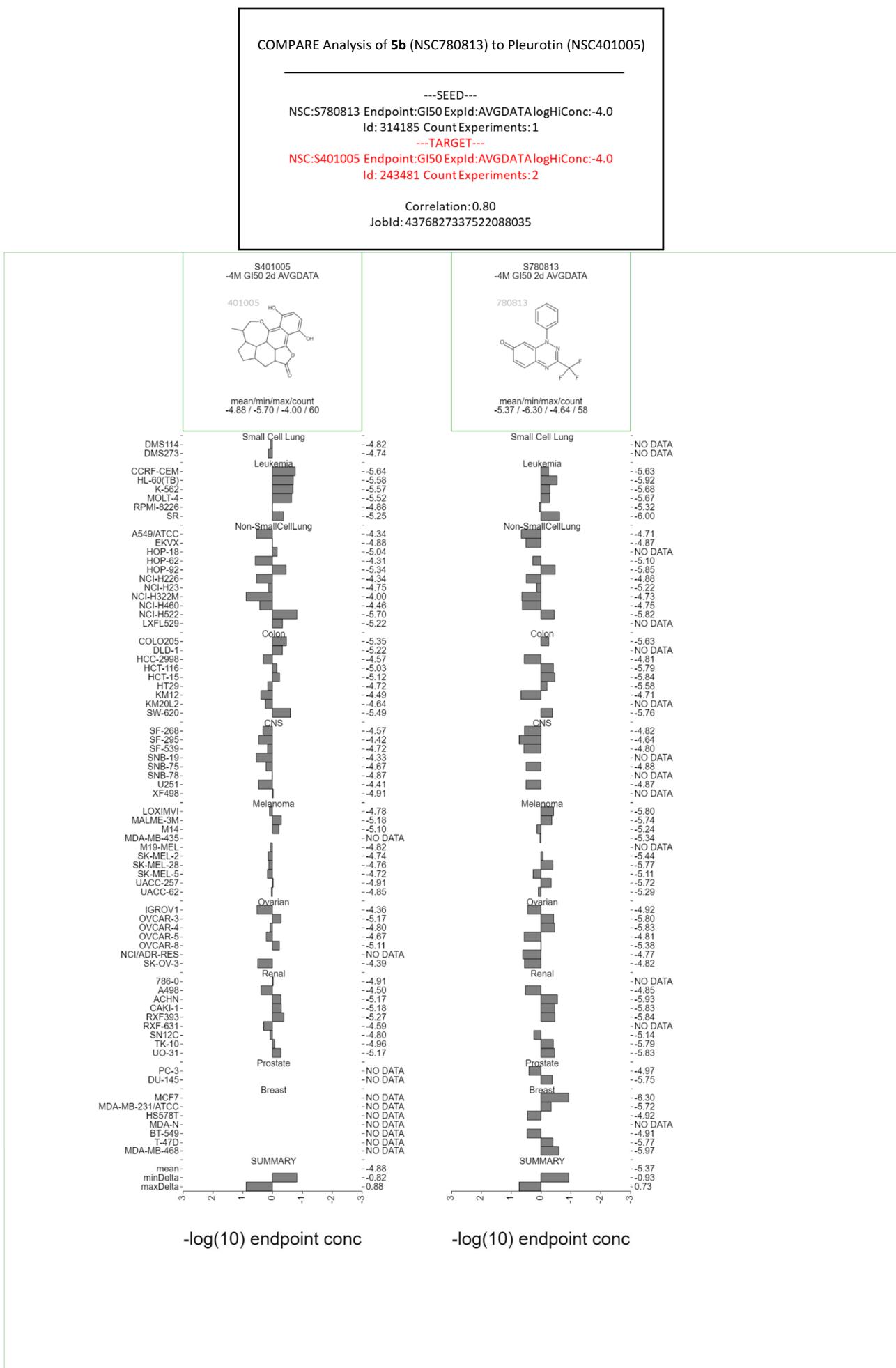


Figure S7

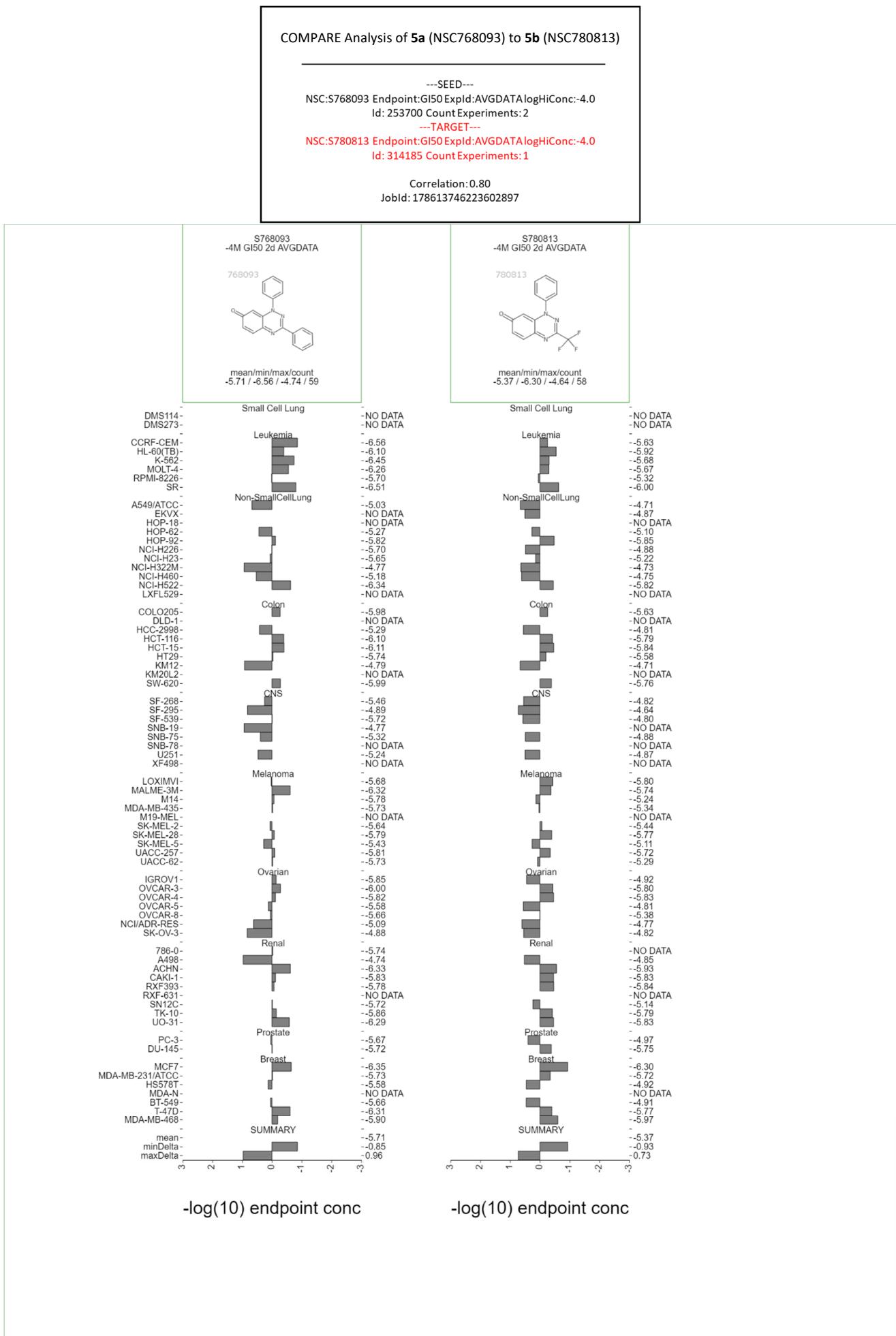


Figure S8

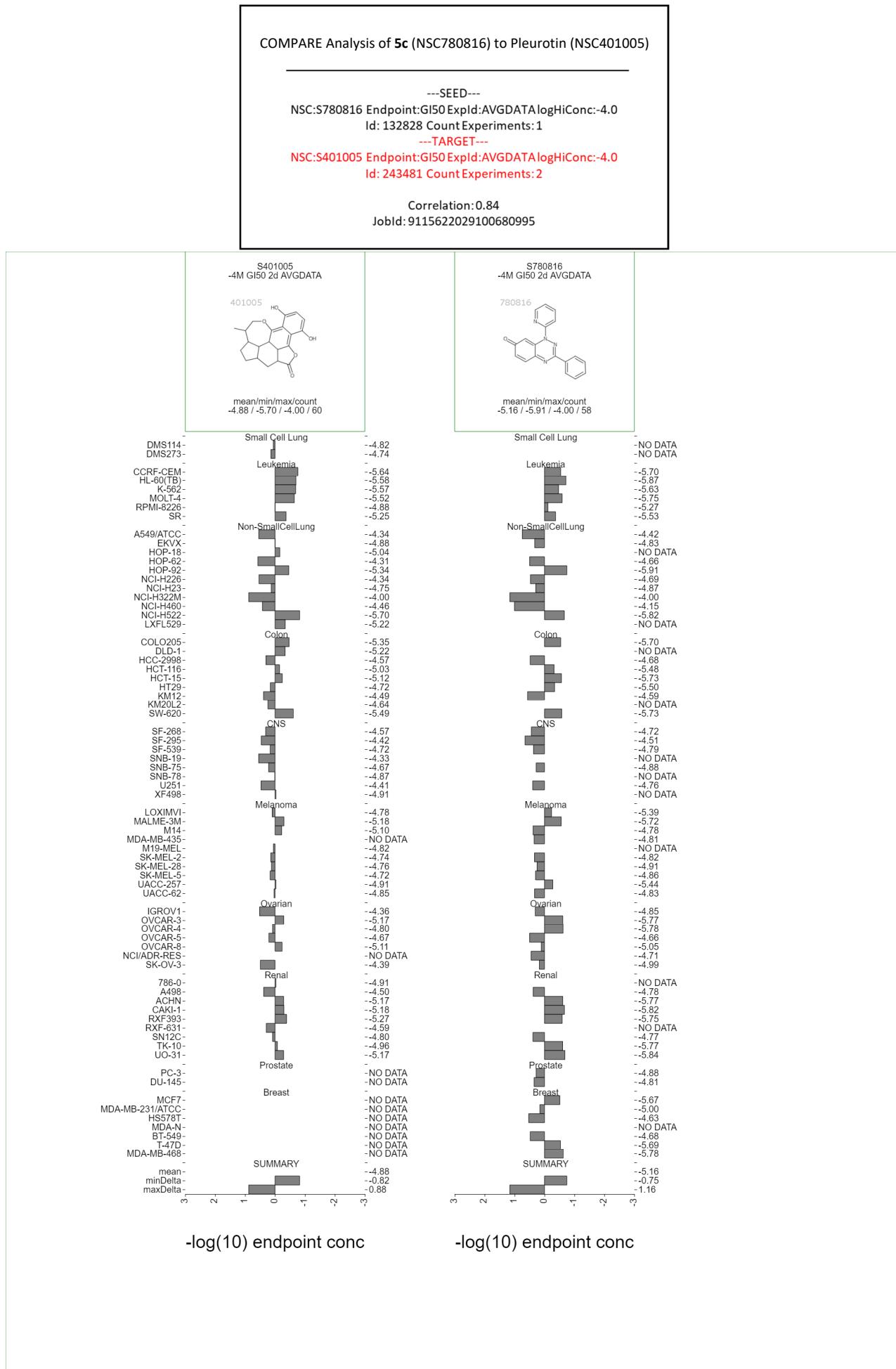


Figure S9

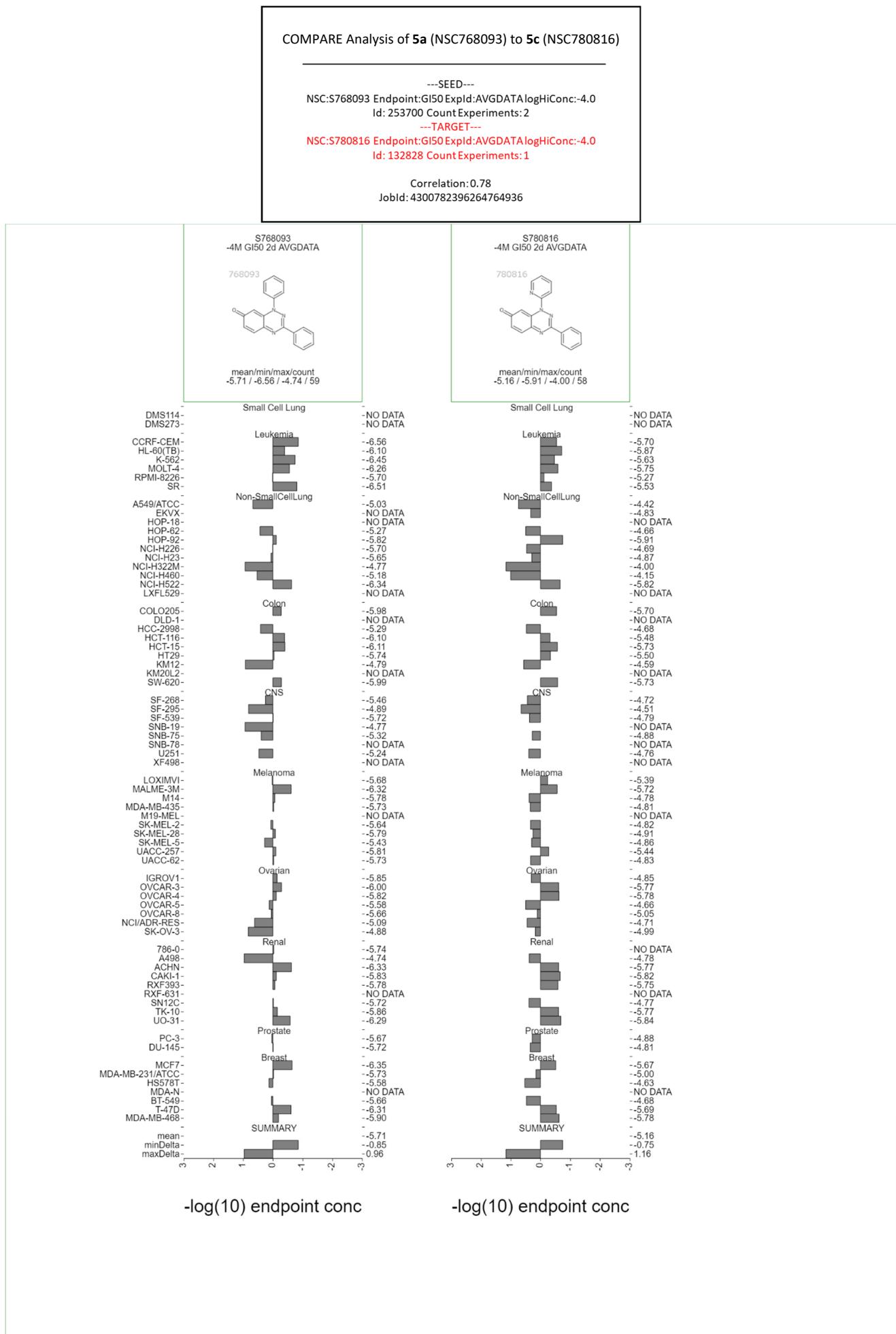


Figure S10

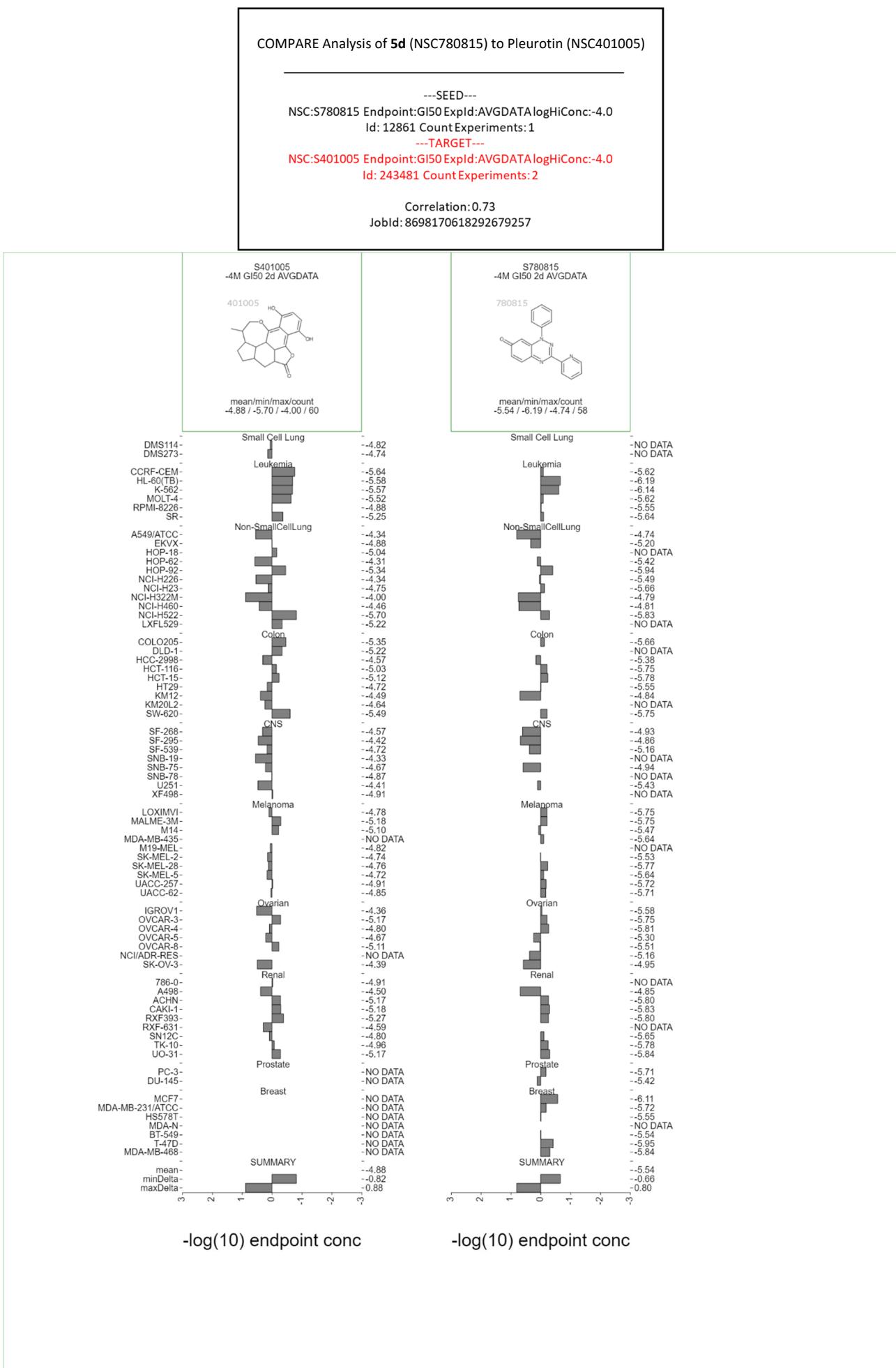


Figure S11

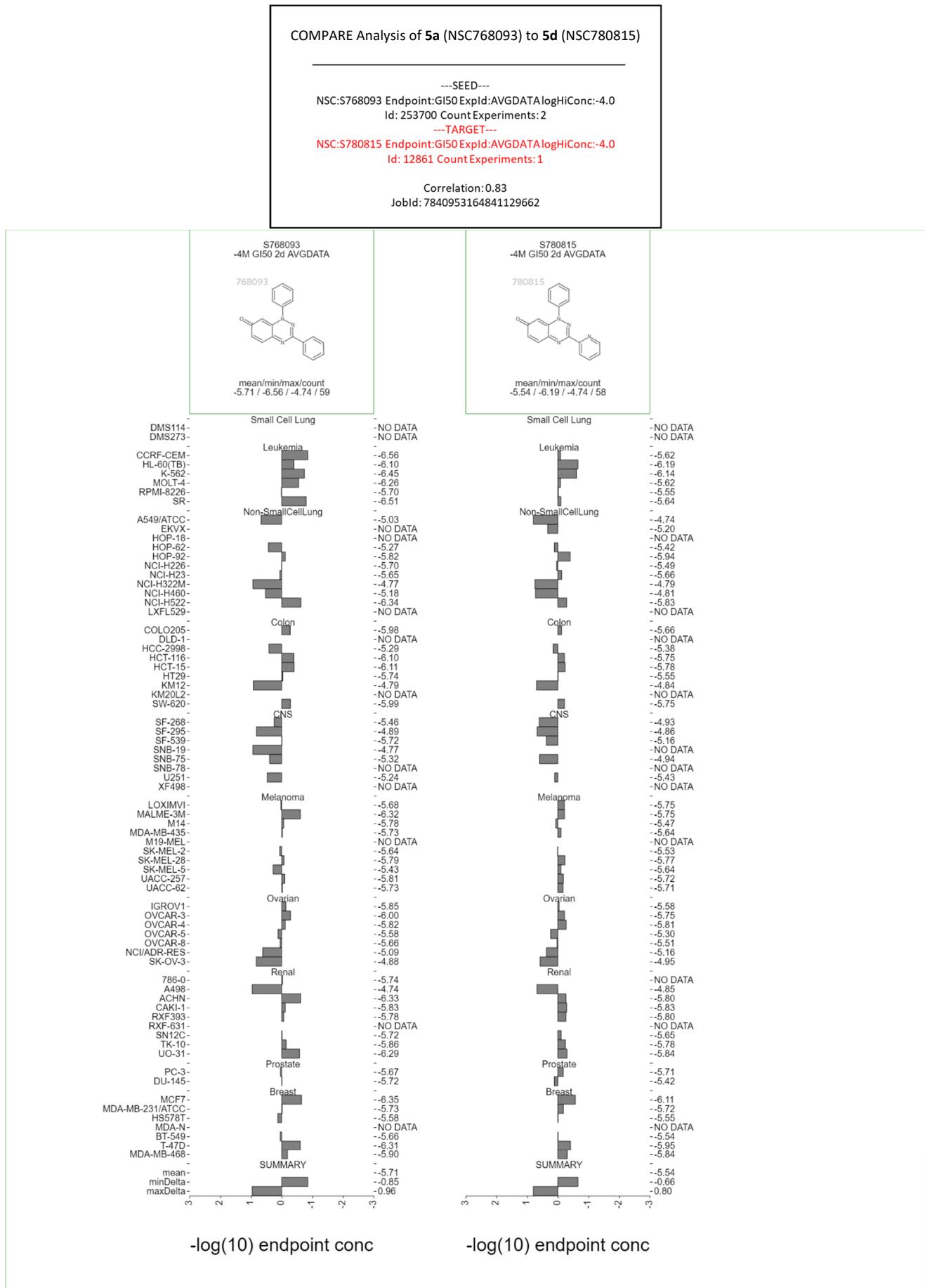


Figure S12

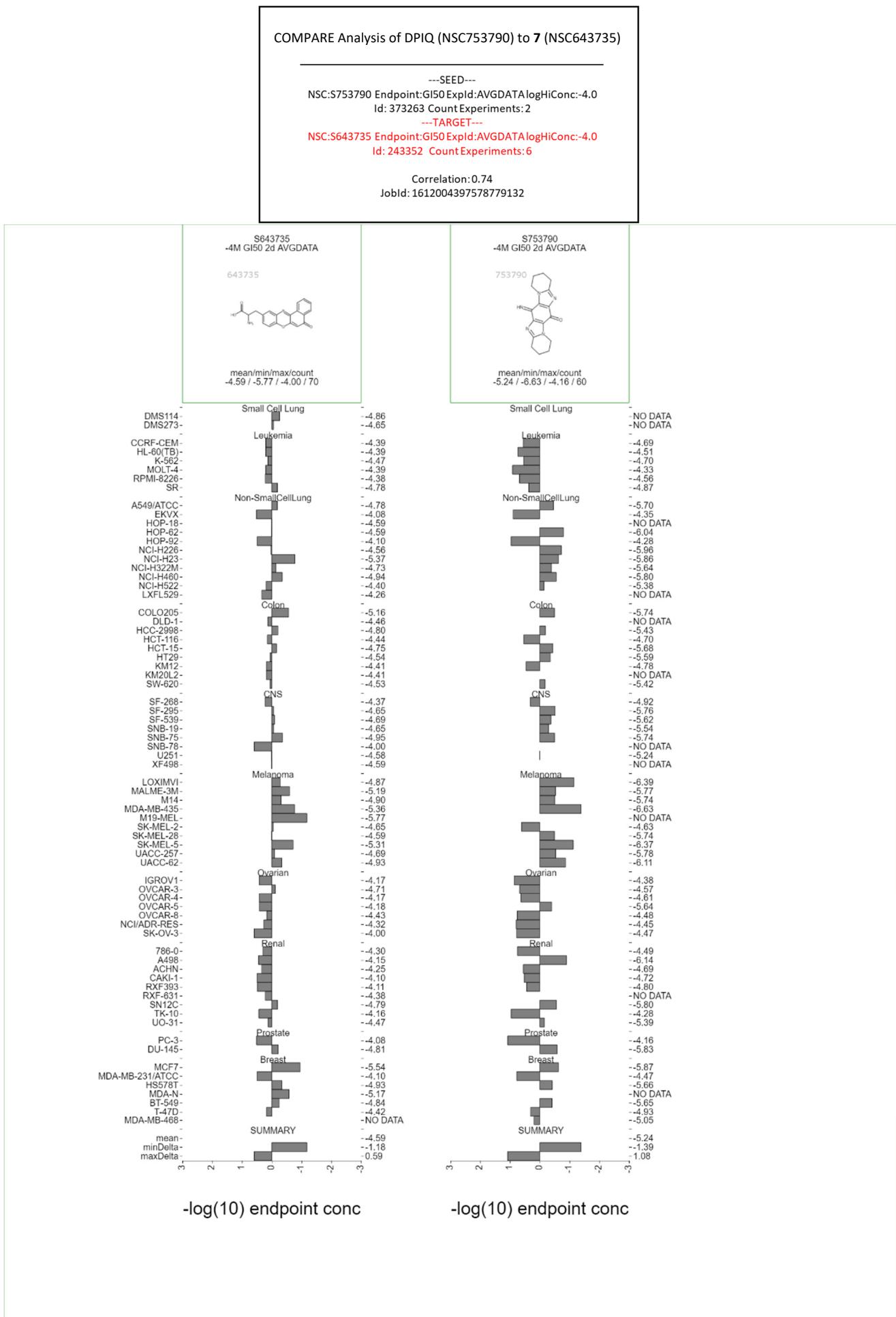


Figure S13

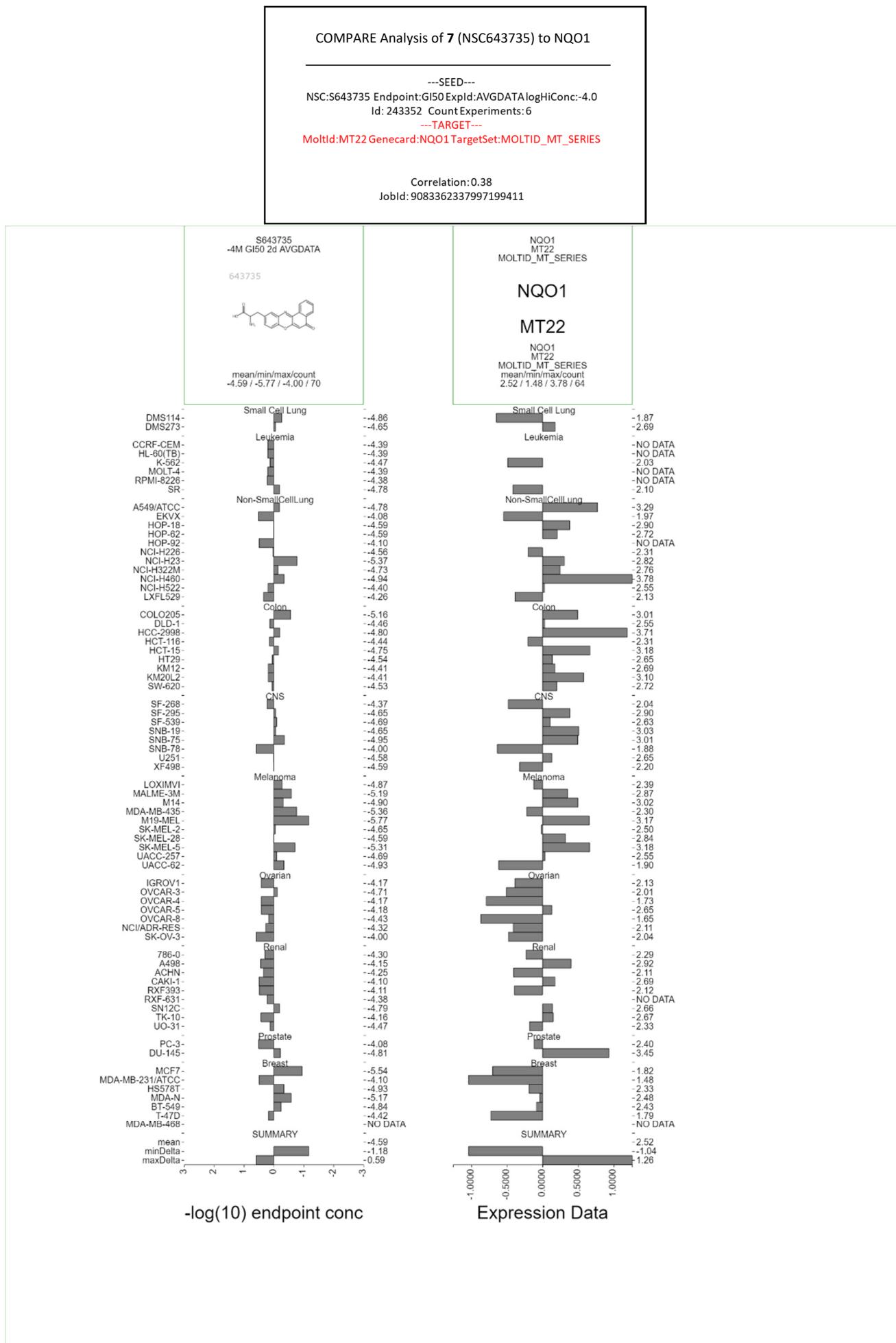


Figure S14

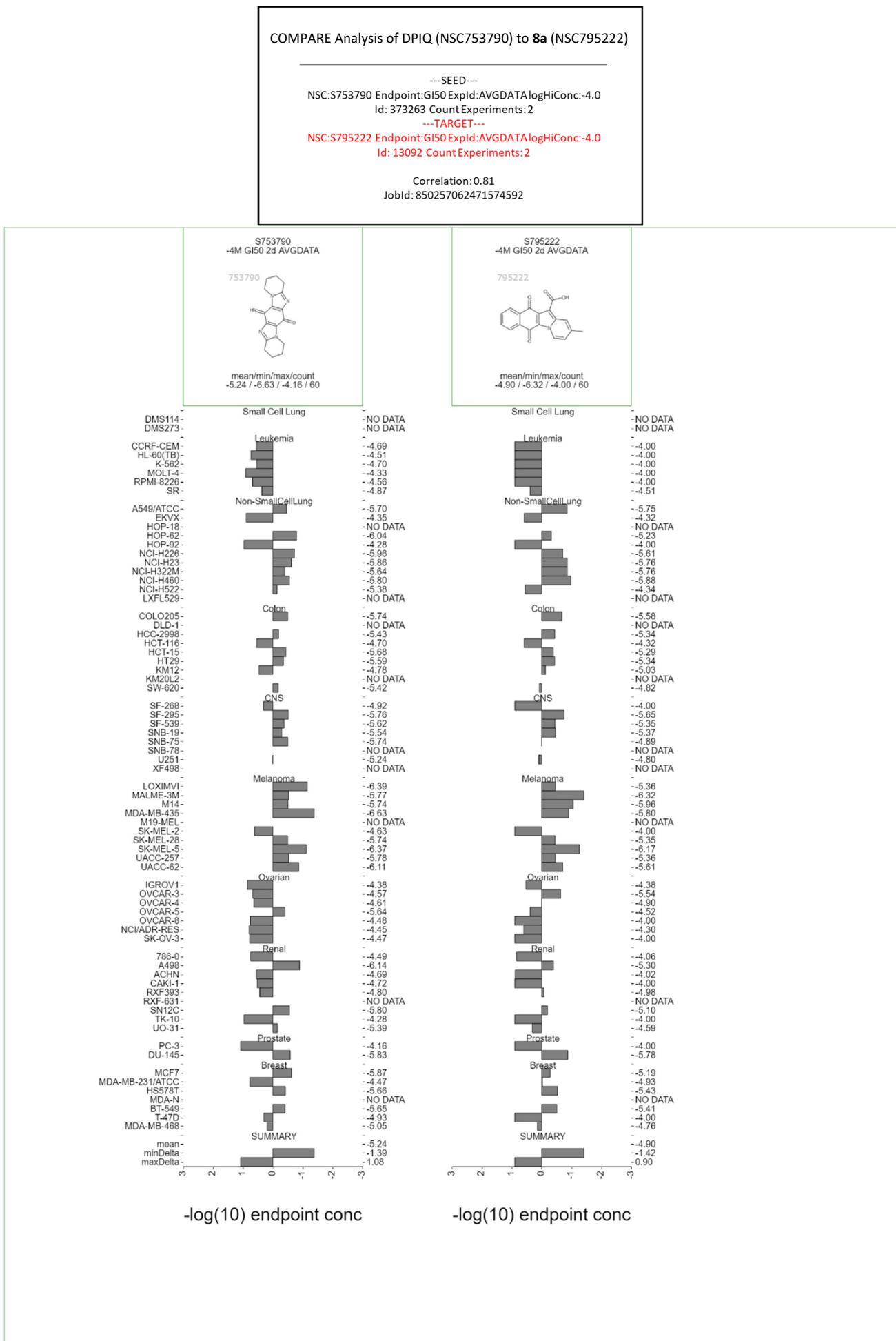


Figure S15

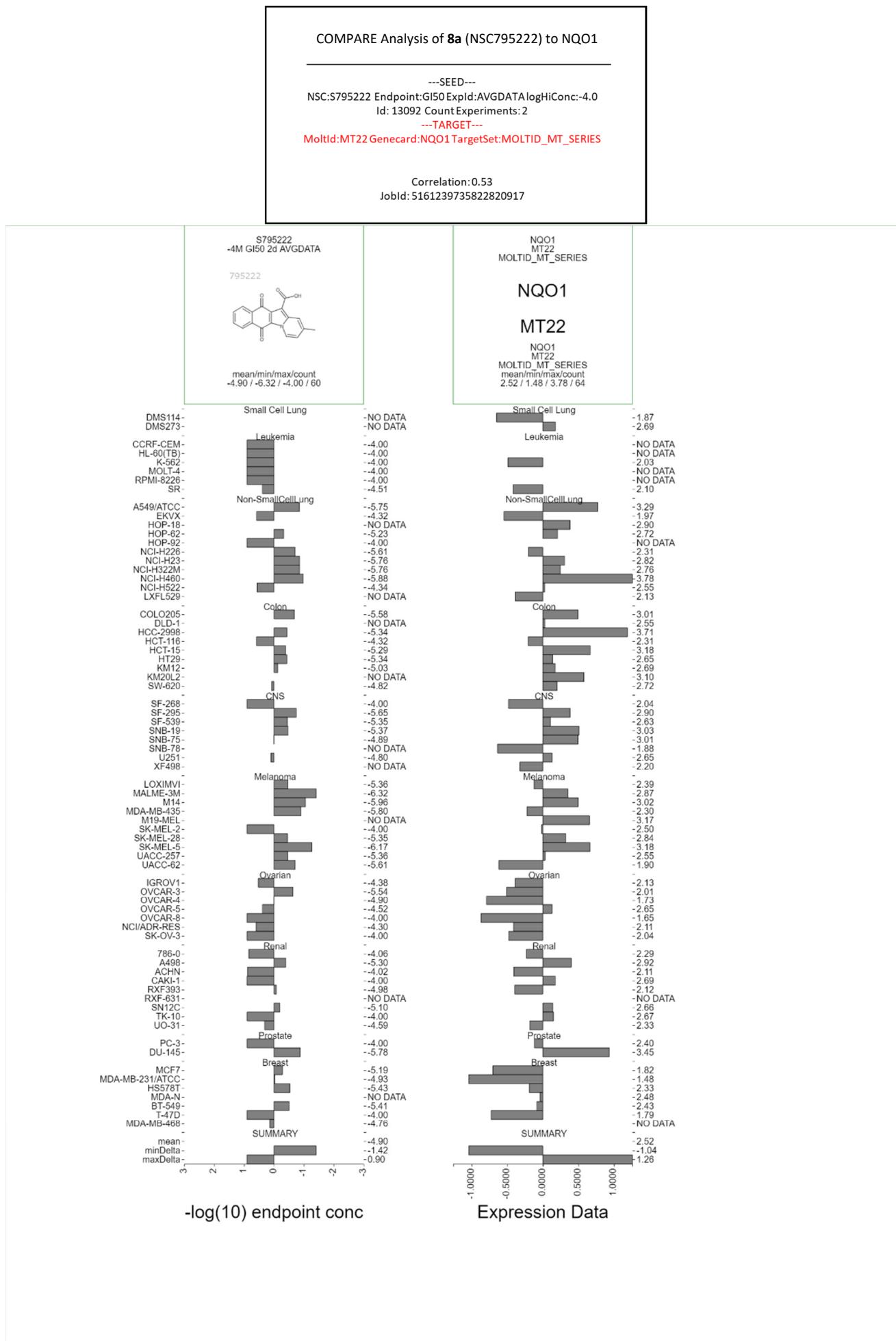


Figure S16



Figure S17

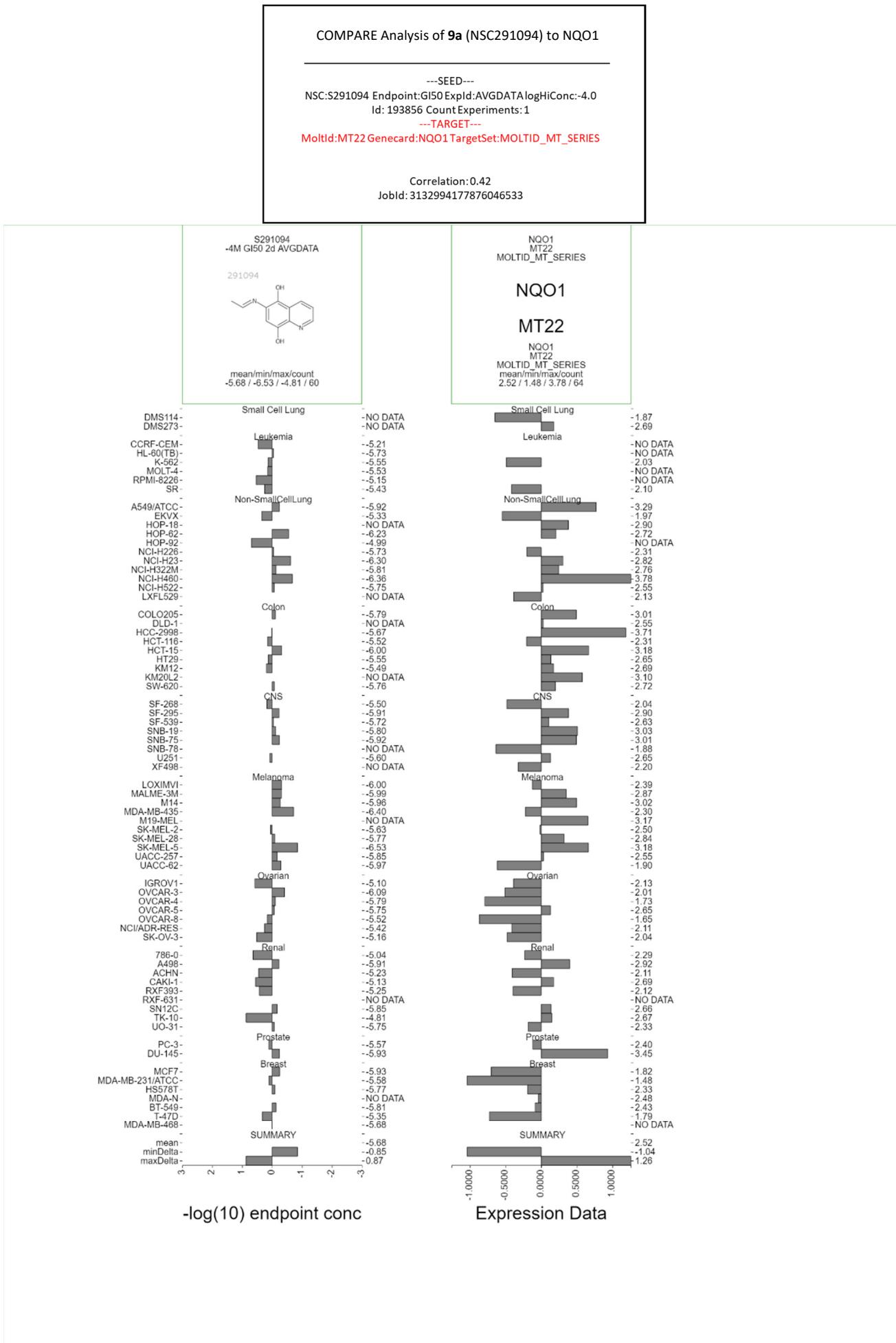


Figure S18

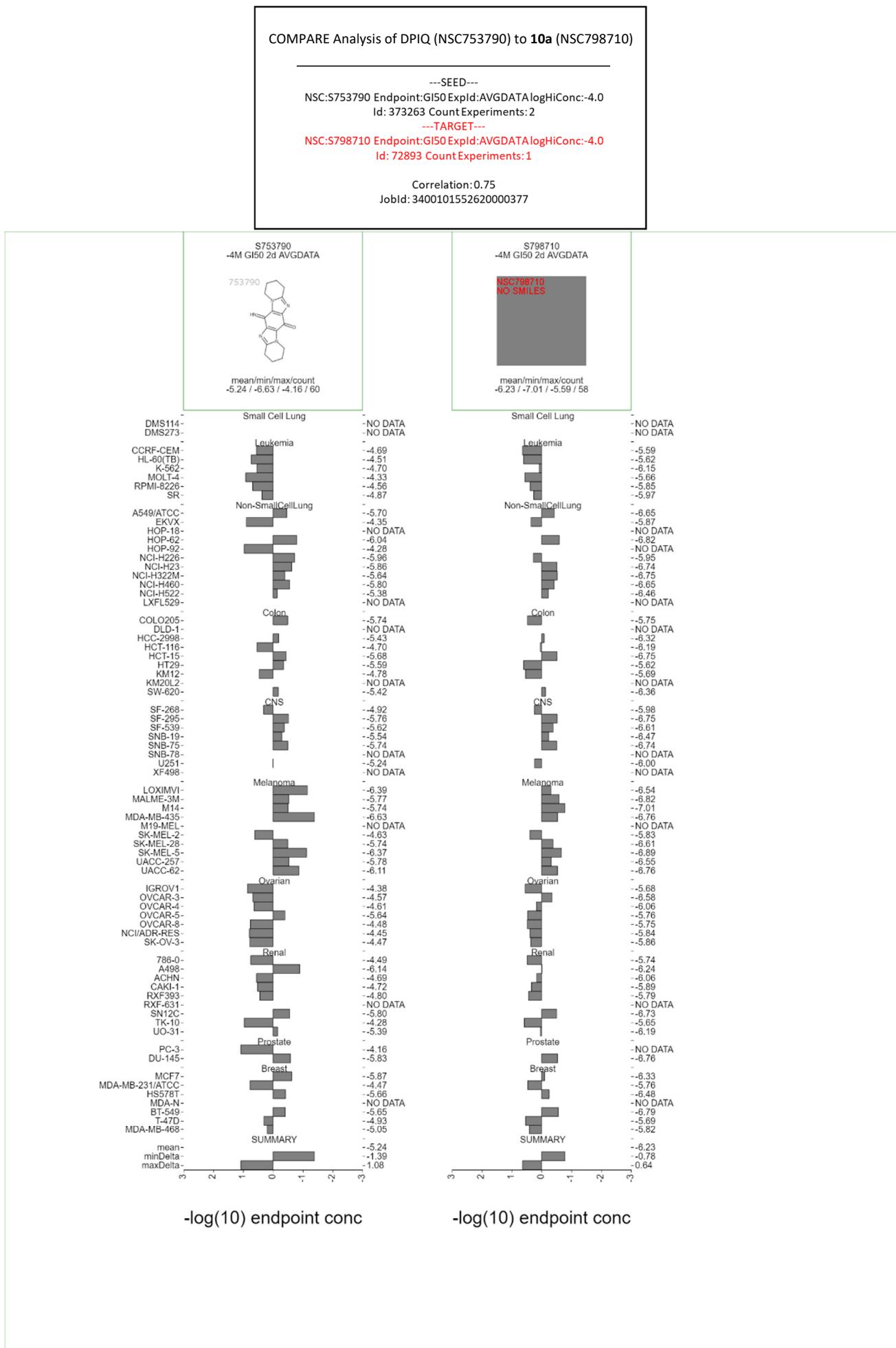


Figure S19

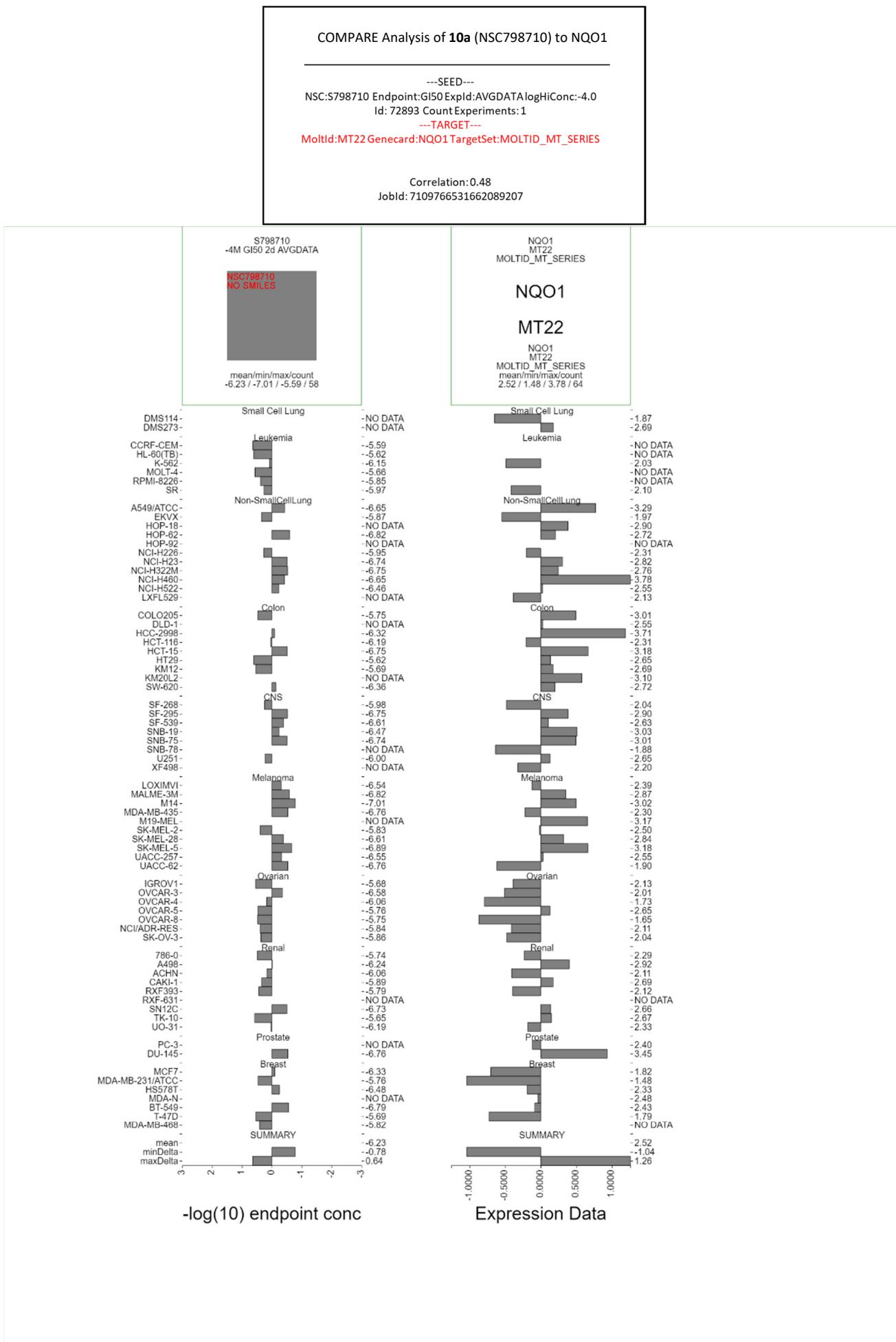


Figure S20

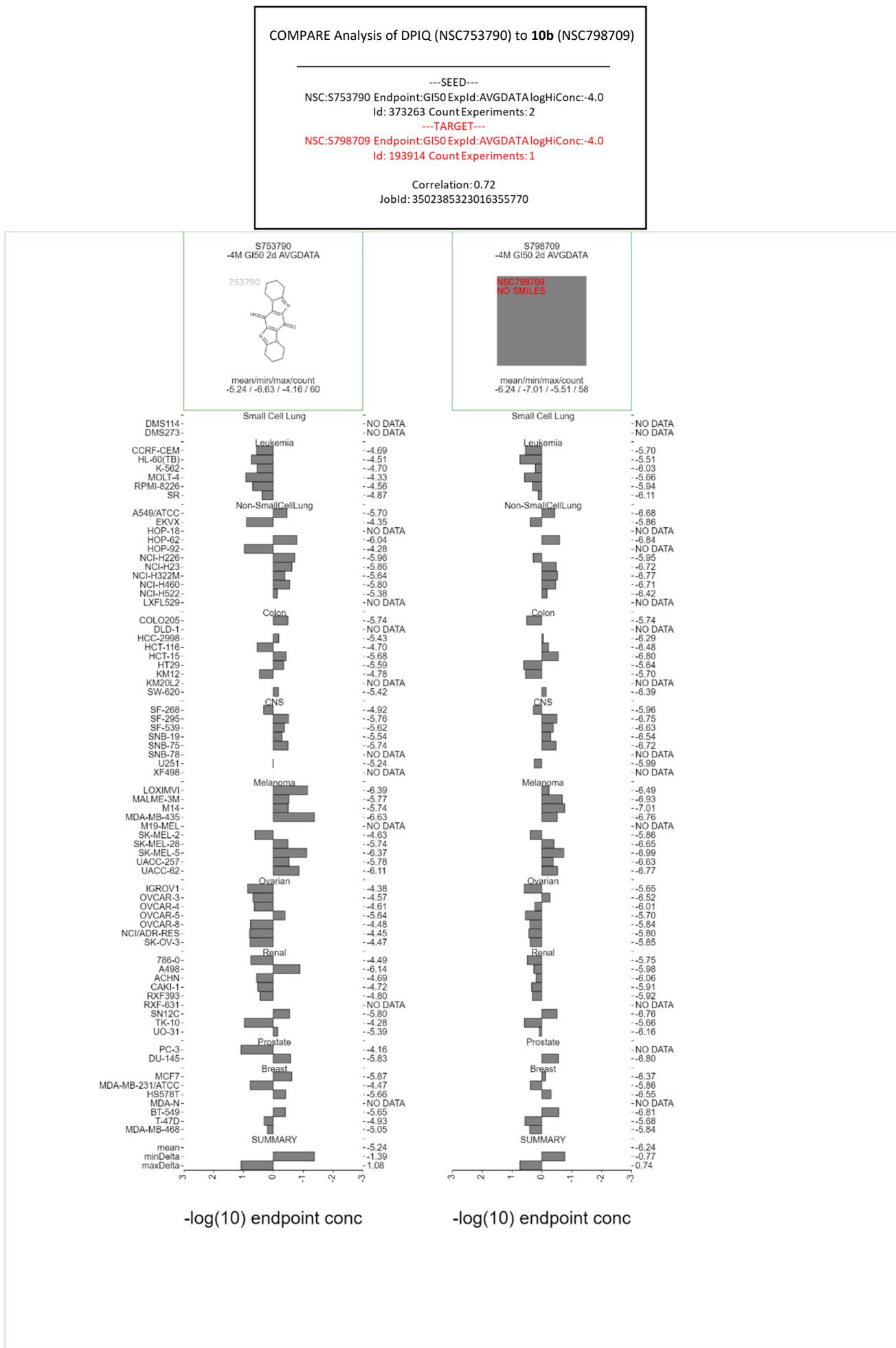


Figure S21

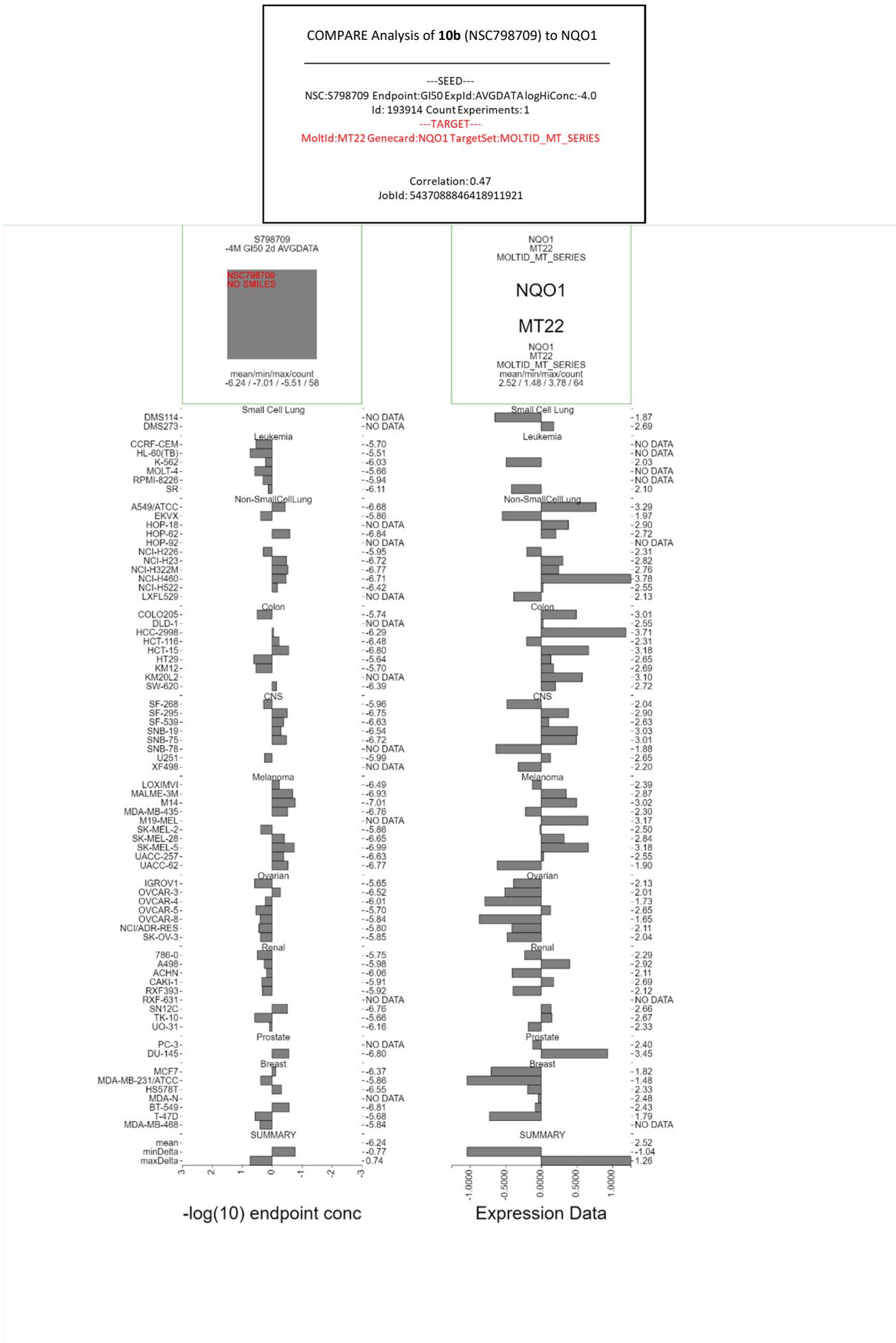


Figure S22

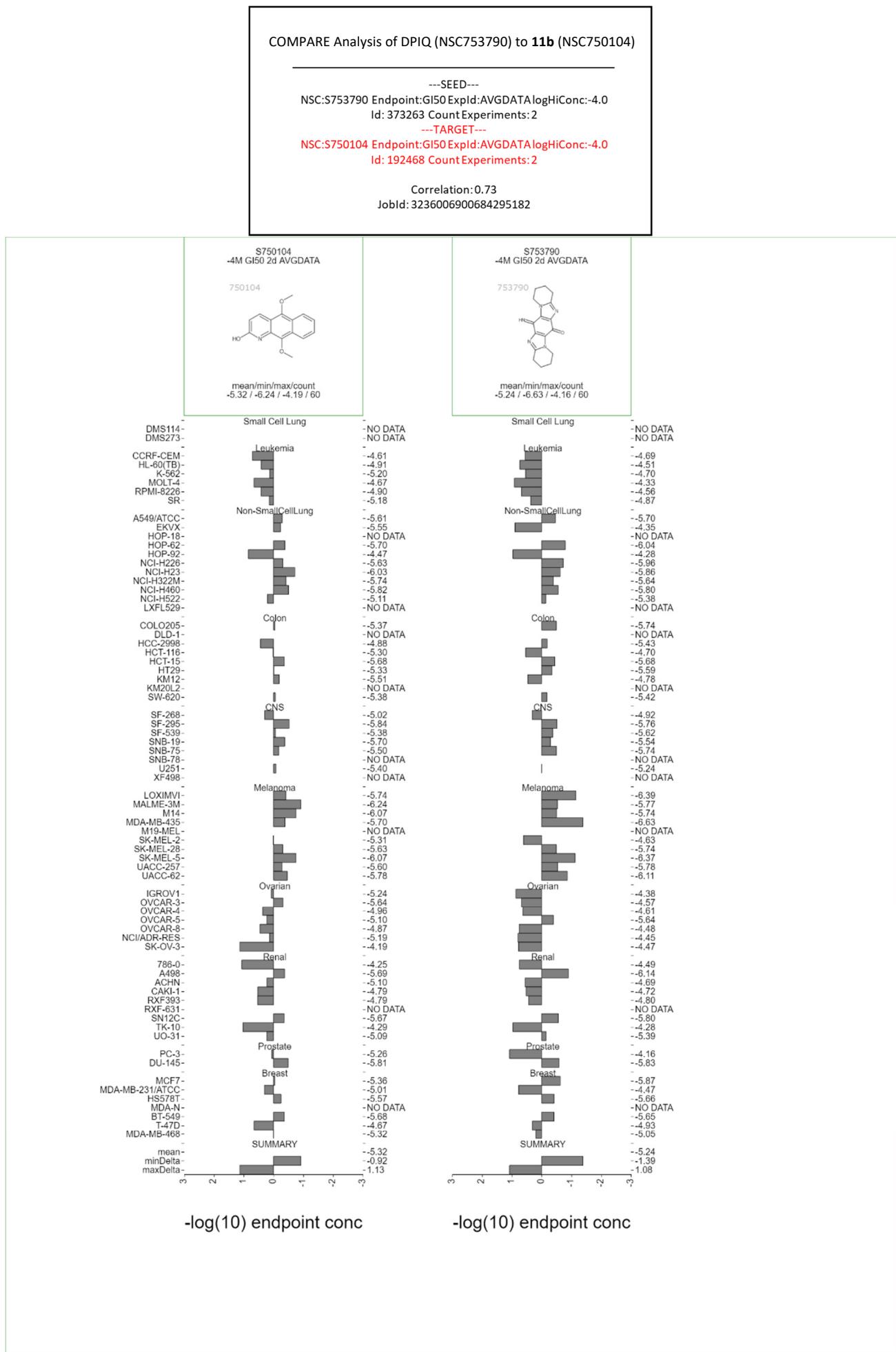


Figure S23

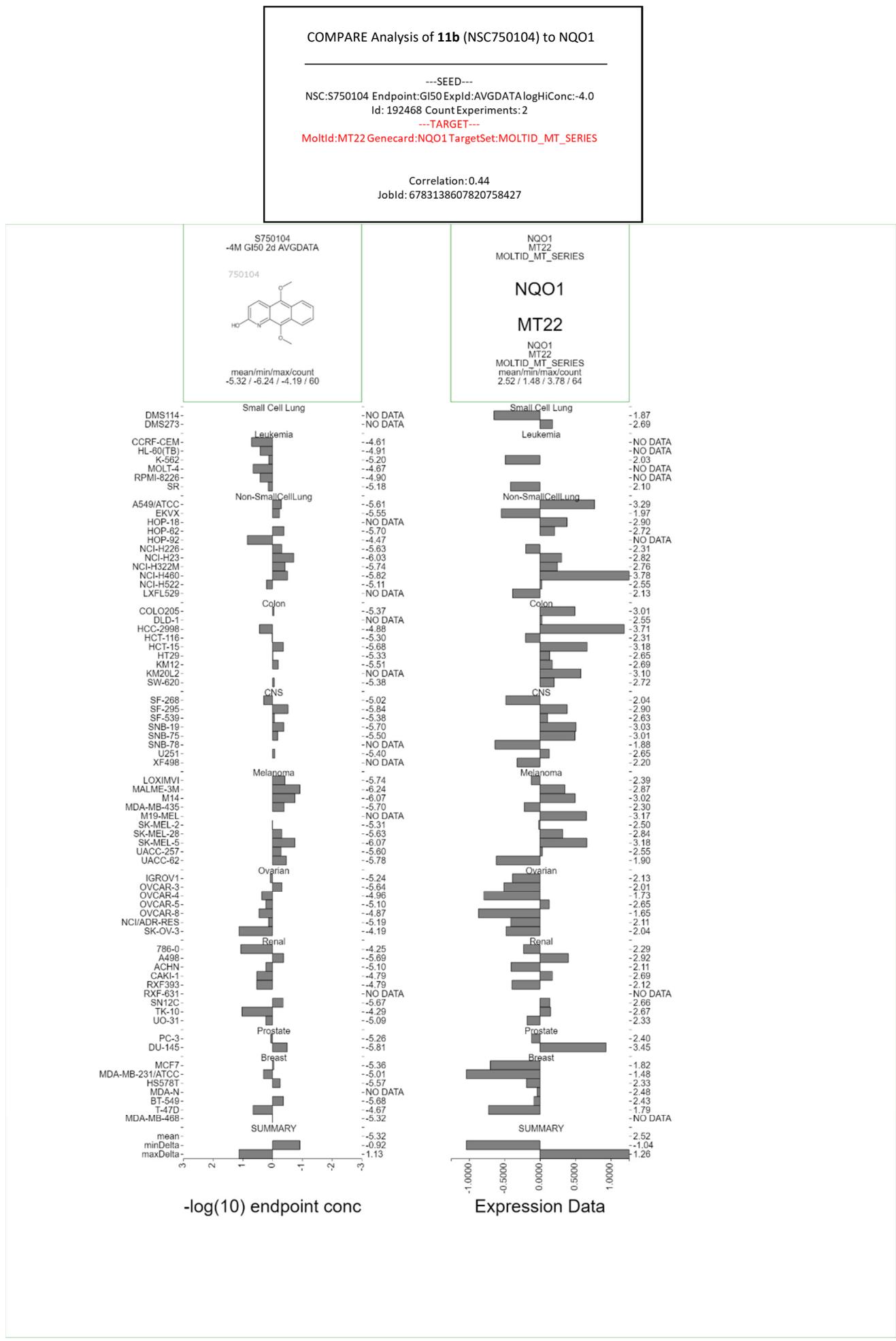


Figure S24

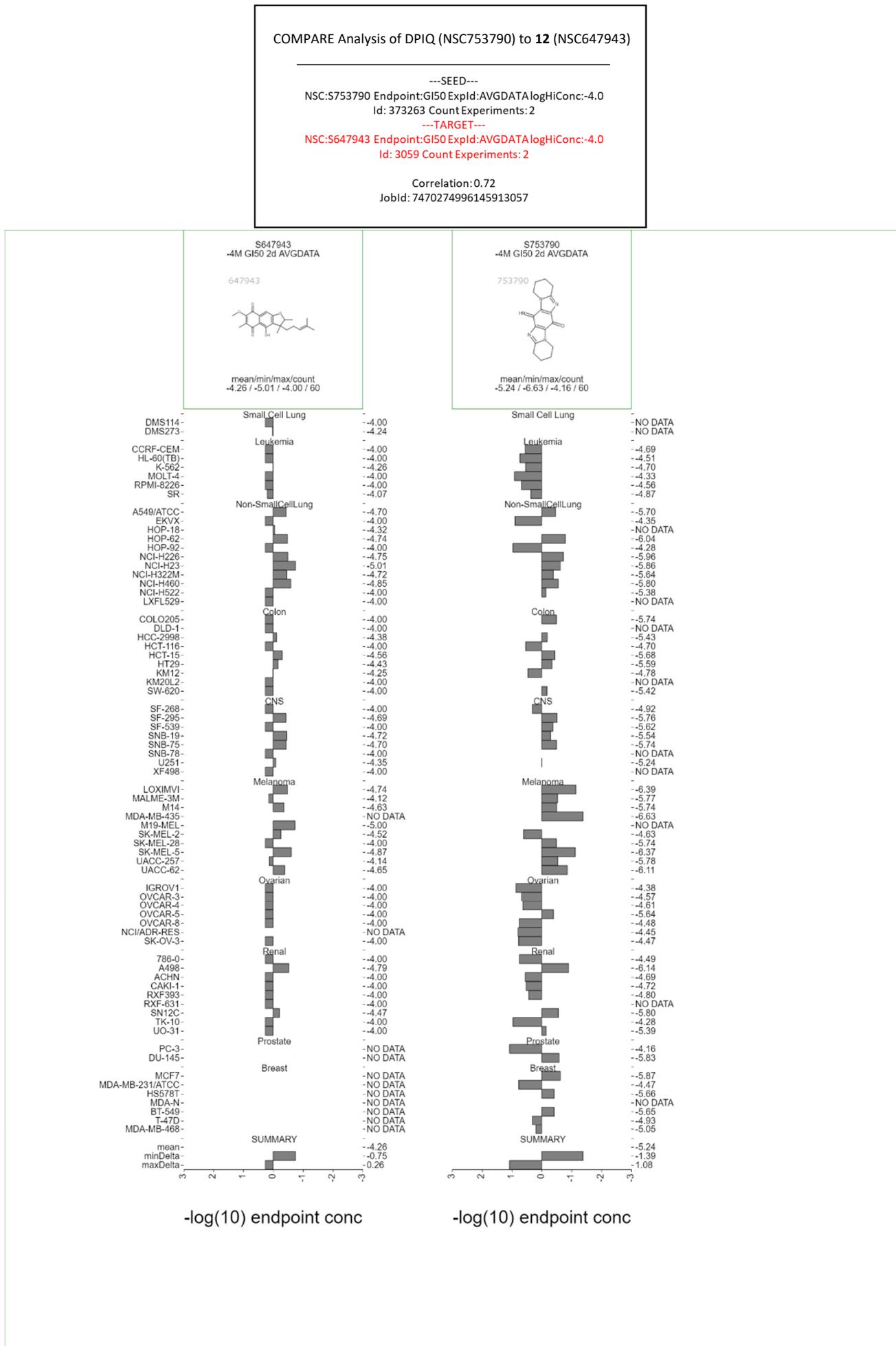


Figure S25

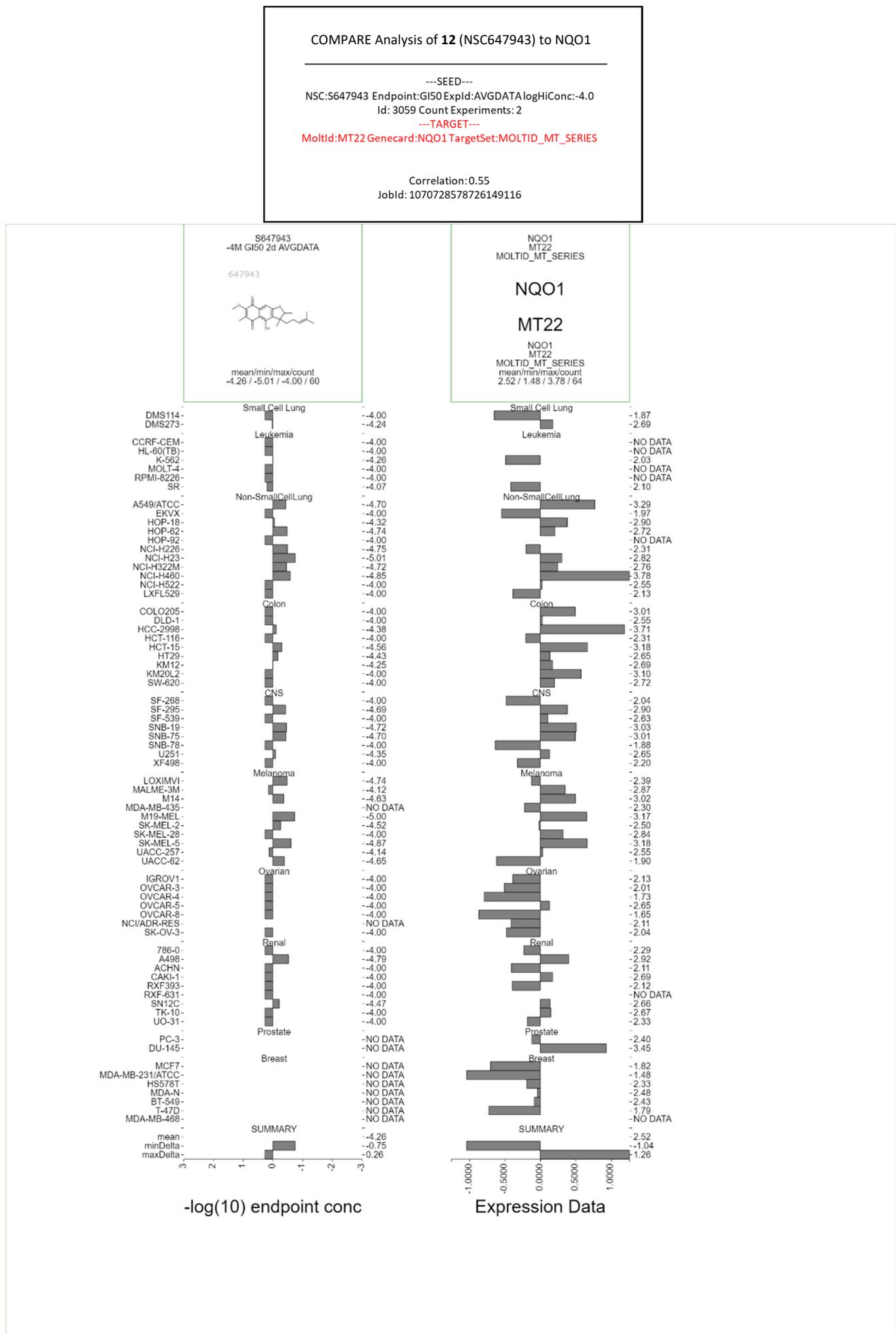


Figure S26

**COMPARE Analysis of 5a (NSC768093) to 13a (NSC787555)**

---SEED---

NSC:768093 Endpoint:GI50 Expld:AVGDATA logHiConc:-4.0  
Id: 253700 Count Experiments:2

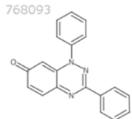
---TARGET---

NSC:787555 Endpoint:GI50 Expld:AVGDATA logHiConc:-4.0  
Id: 254082 Count Experiments:3

Correlation:0.85

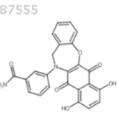
JobId: 3773562751148899517

S768093  
-4M GI50 2d AVGDATA

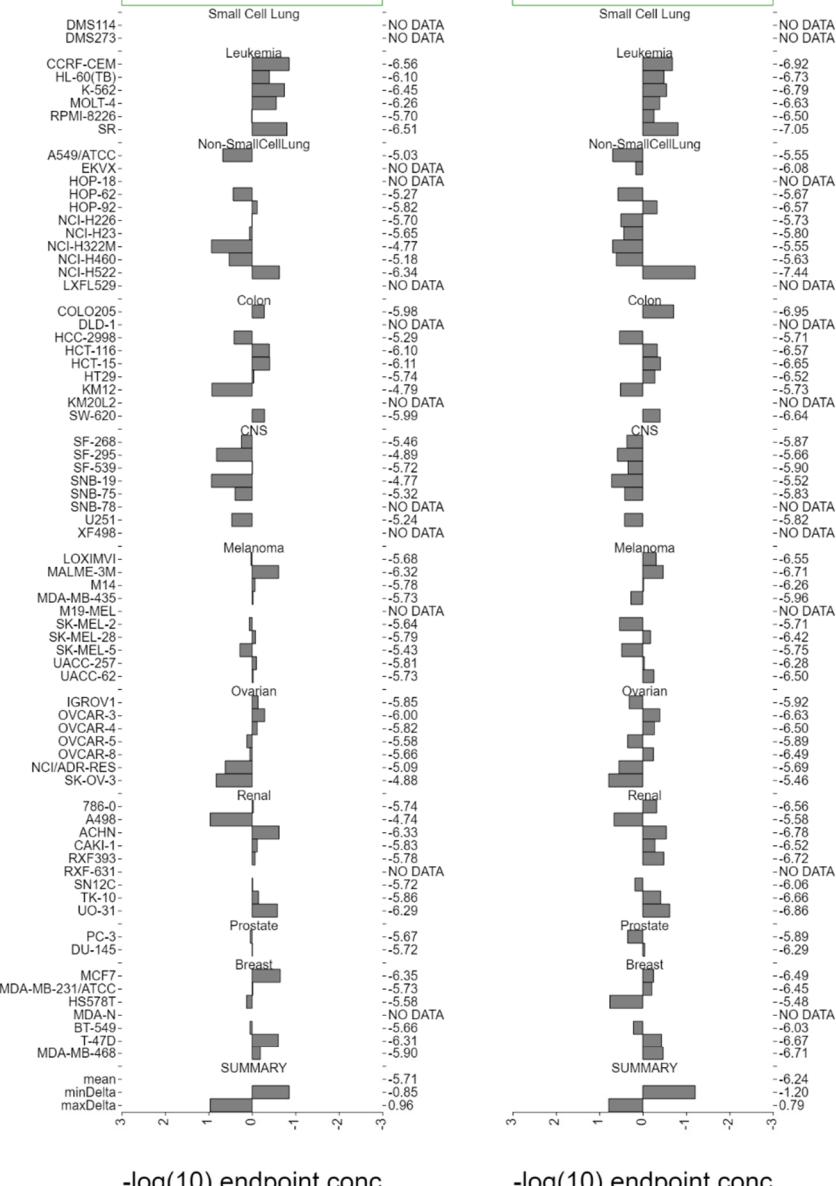


mean/min/max/count  
-5.71 / -6.56 / -4.74 / 59

S787555  
-4M GI50 2d AVGDATA



mean/min/max/count  
-6.24 / -7.44 / -5.46 / 60



-log(10) endpoint conc

-log(10) endpoint conc

Figure S27

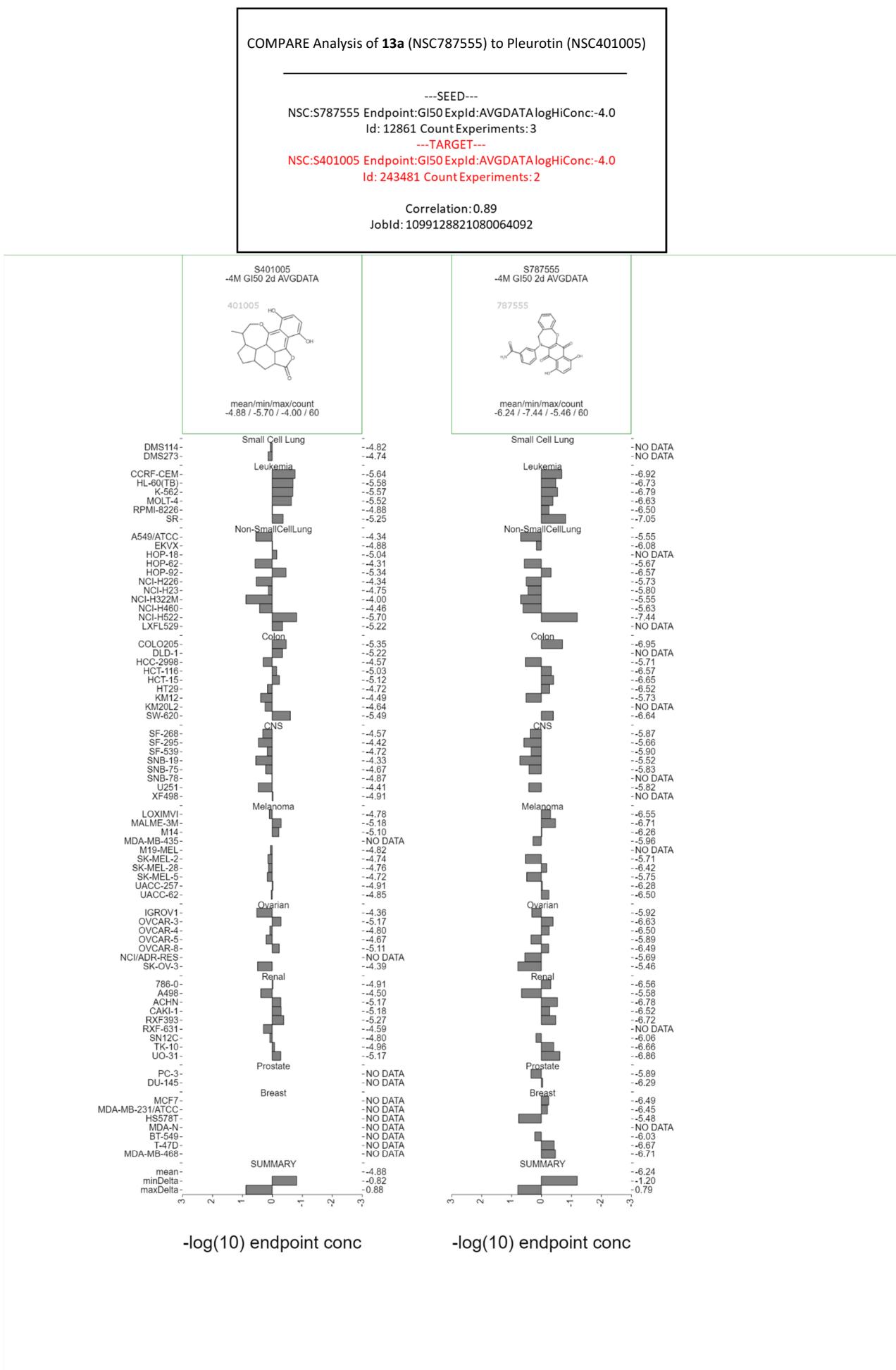


Figure S28

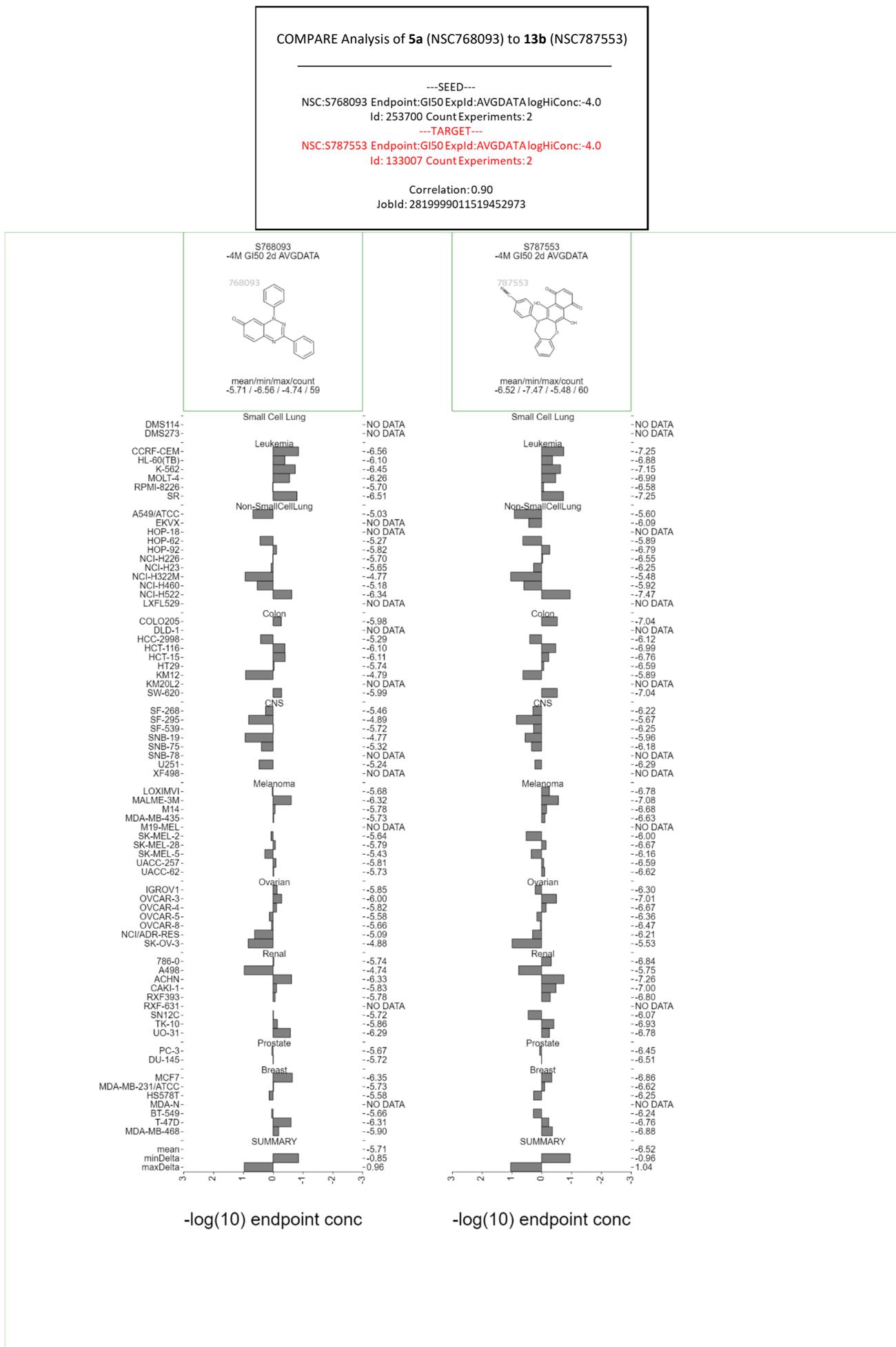


Figure S29

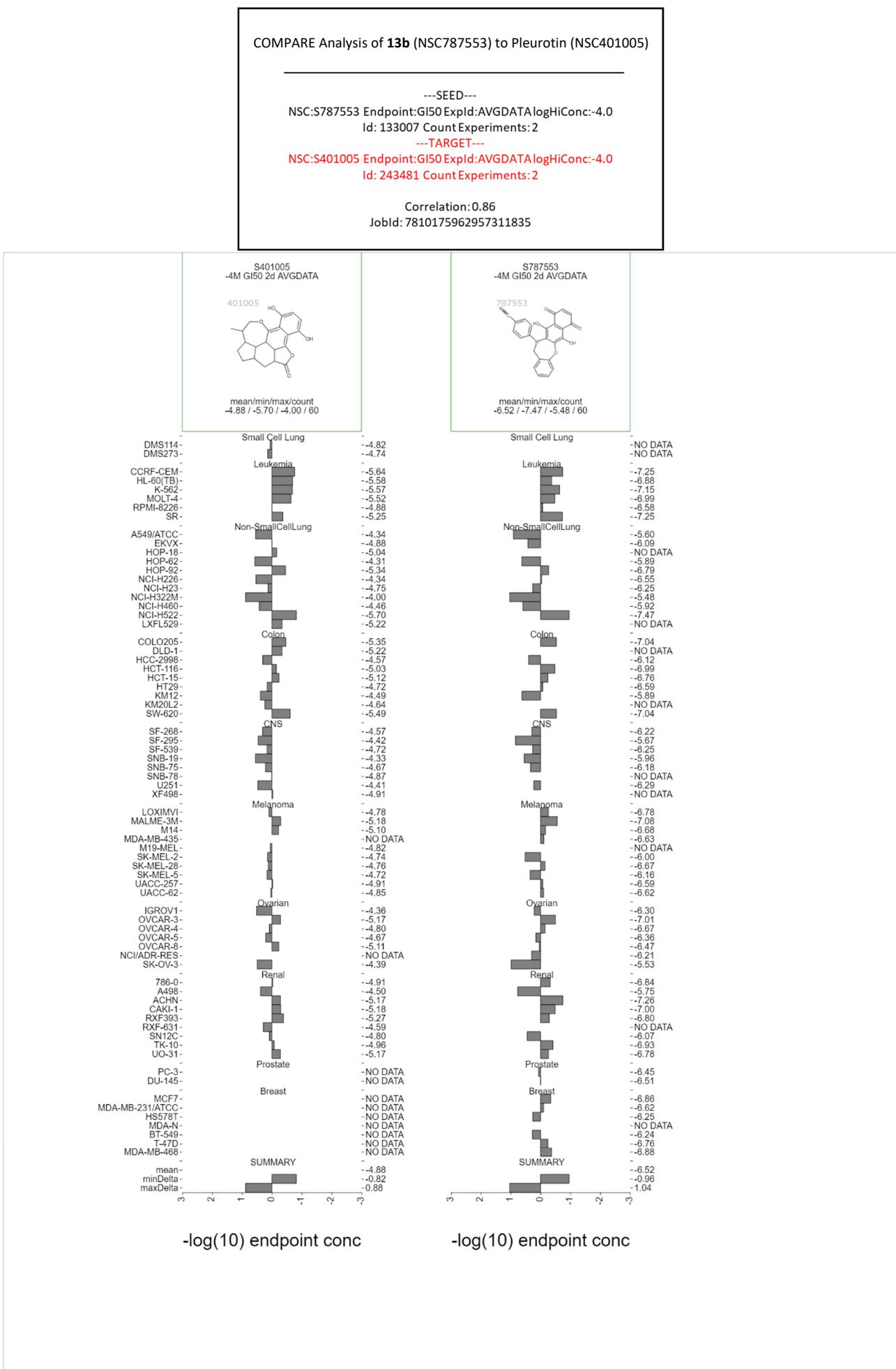


Figure S30

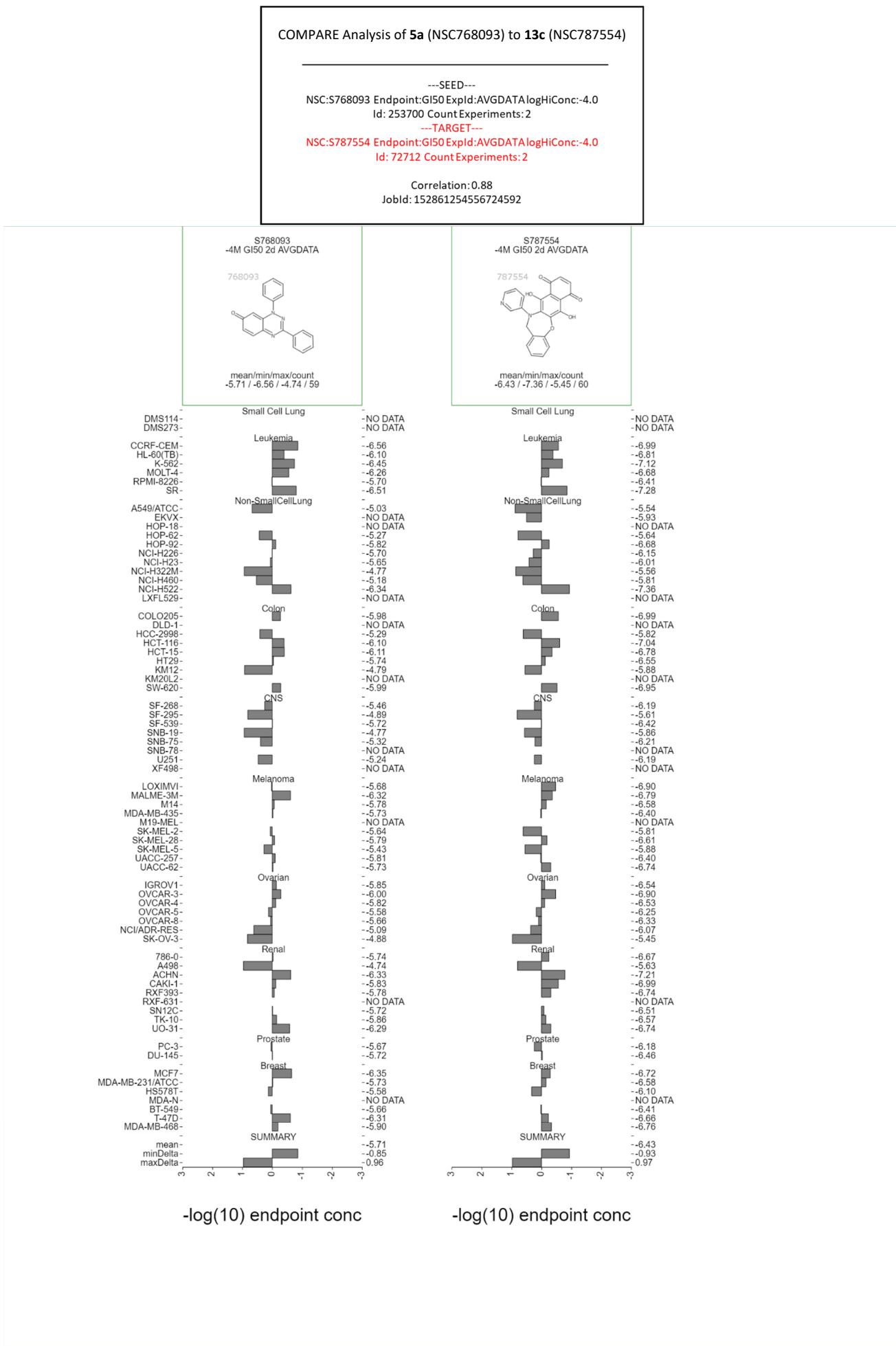


Figure S31

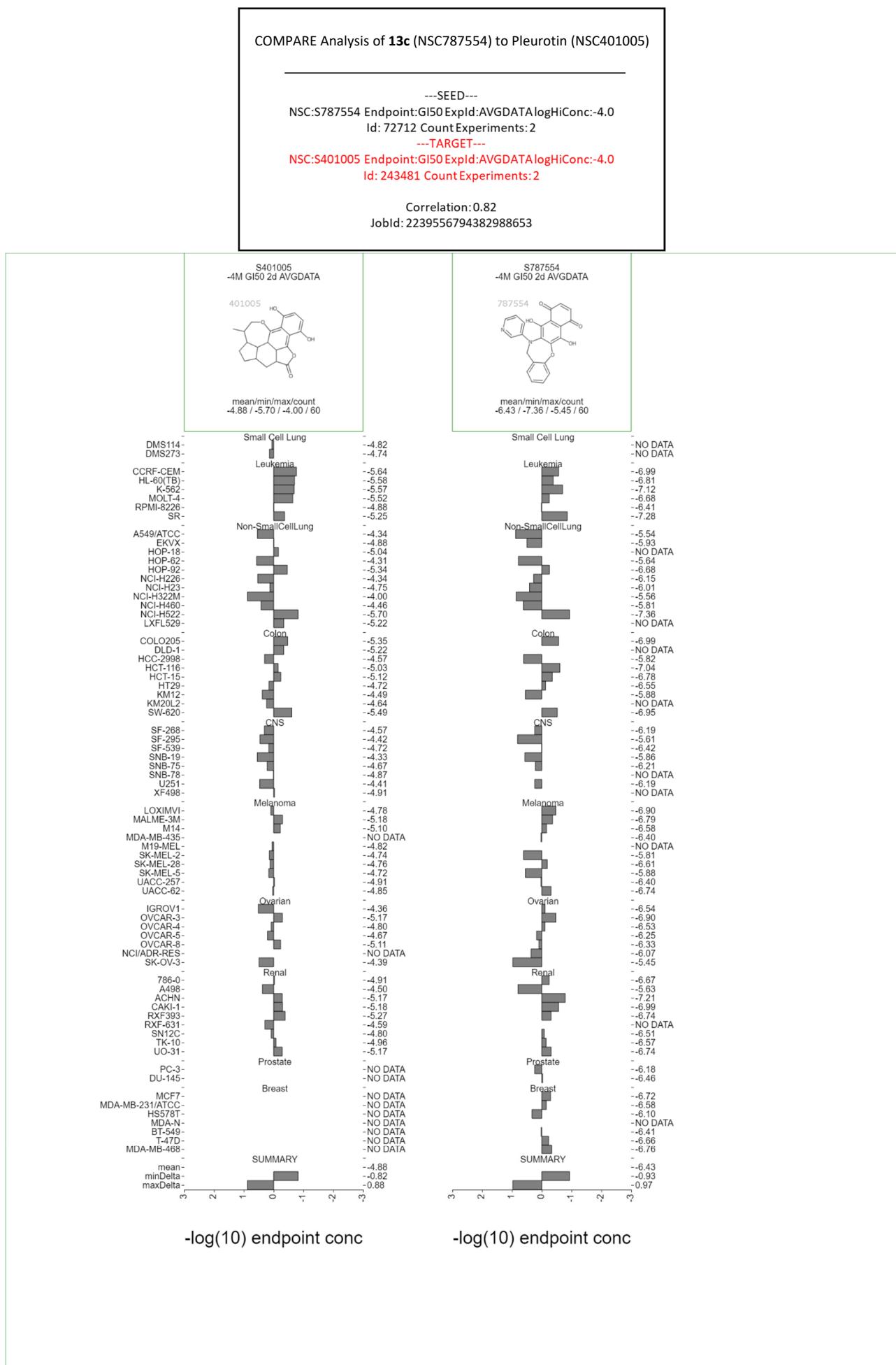


Figure S32

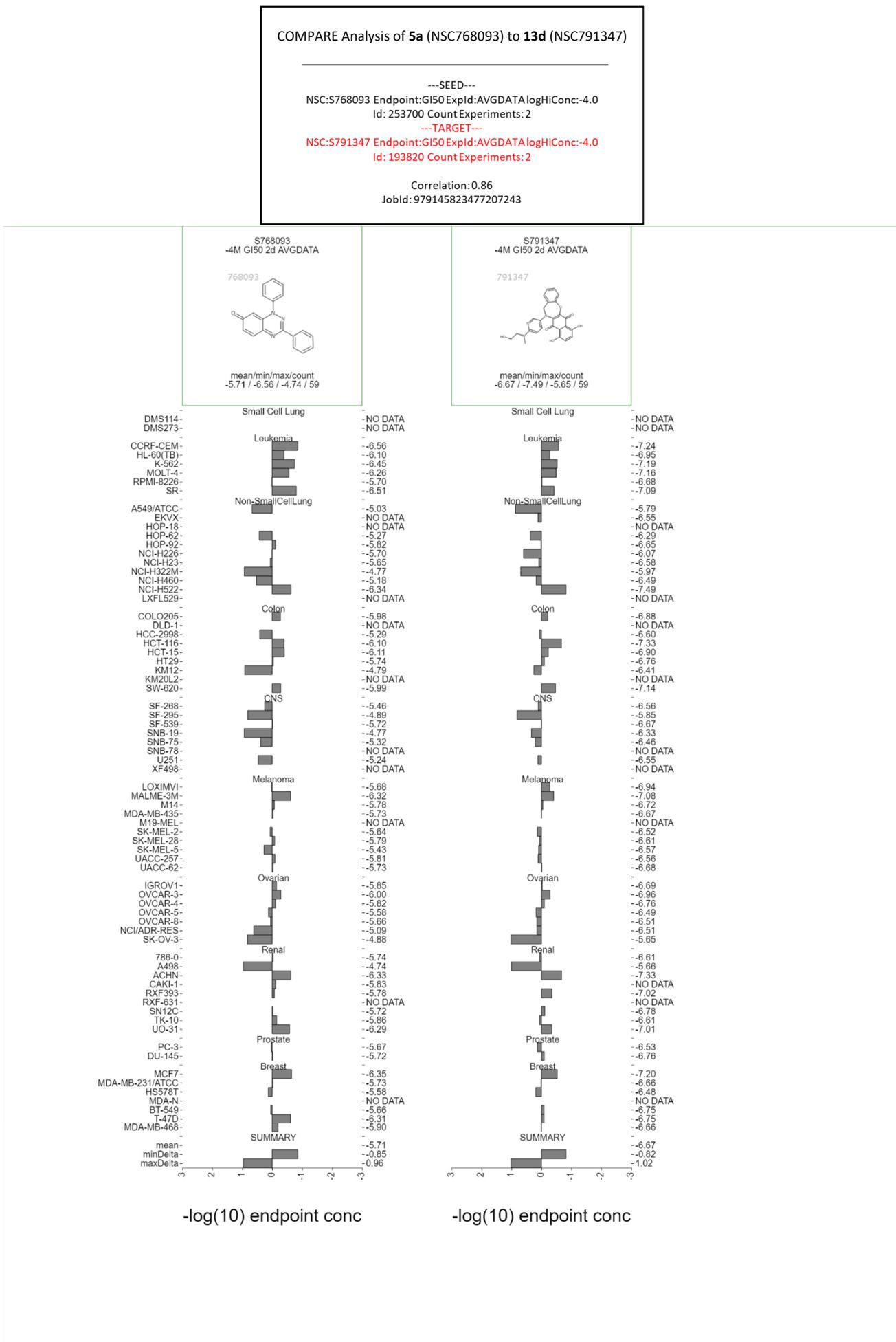


Figure S33

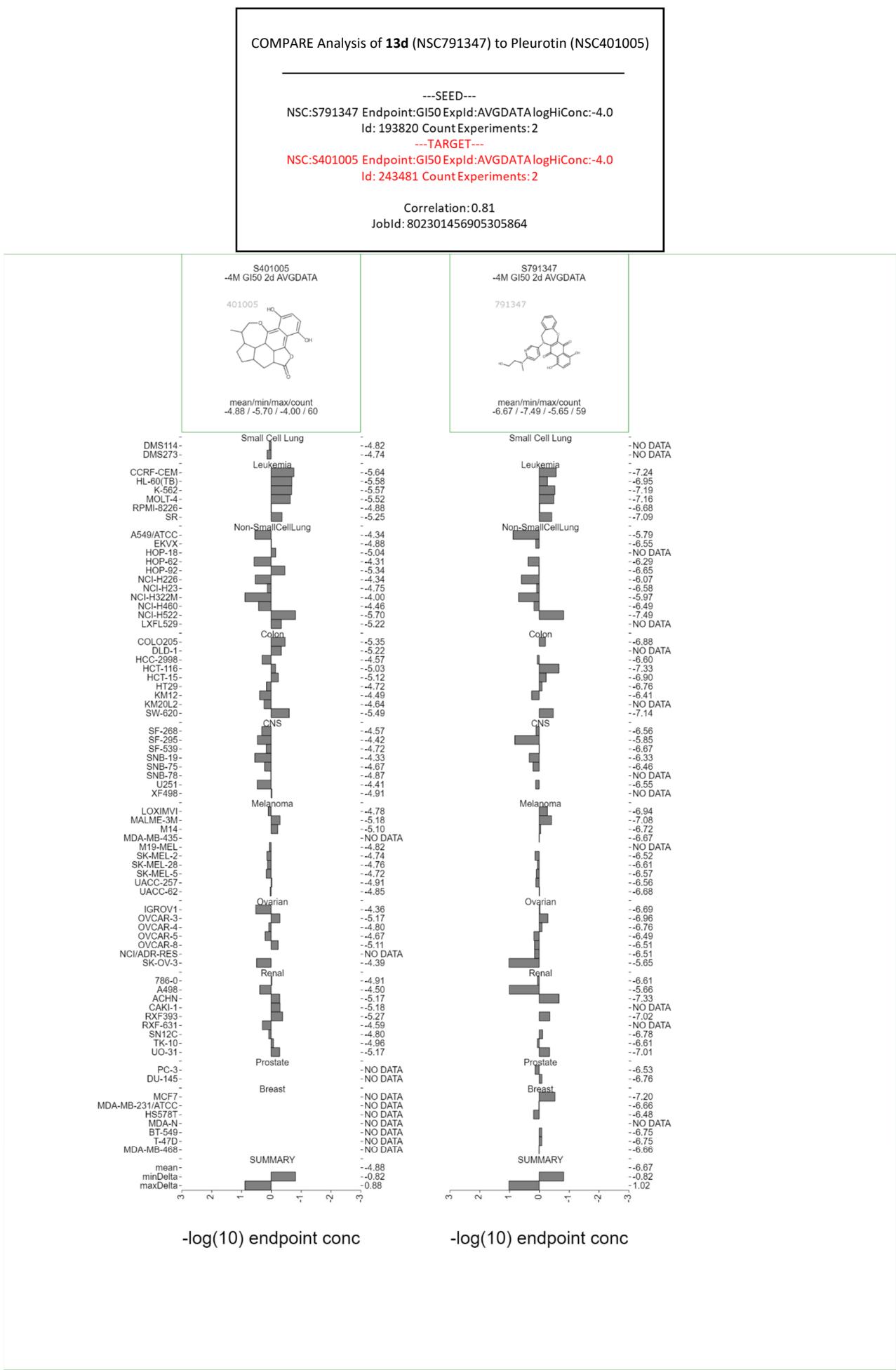


Figure S34

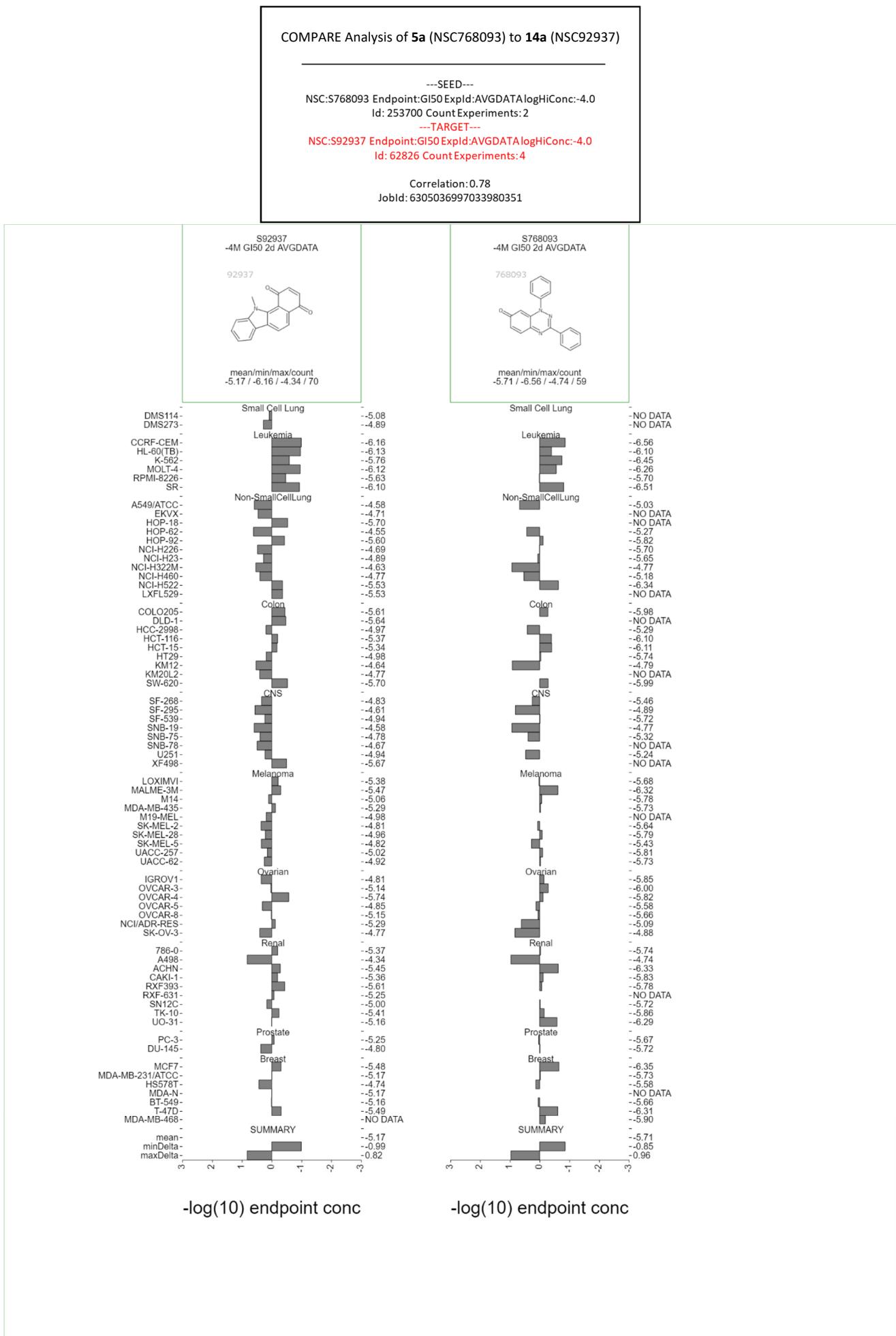


Figure S35

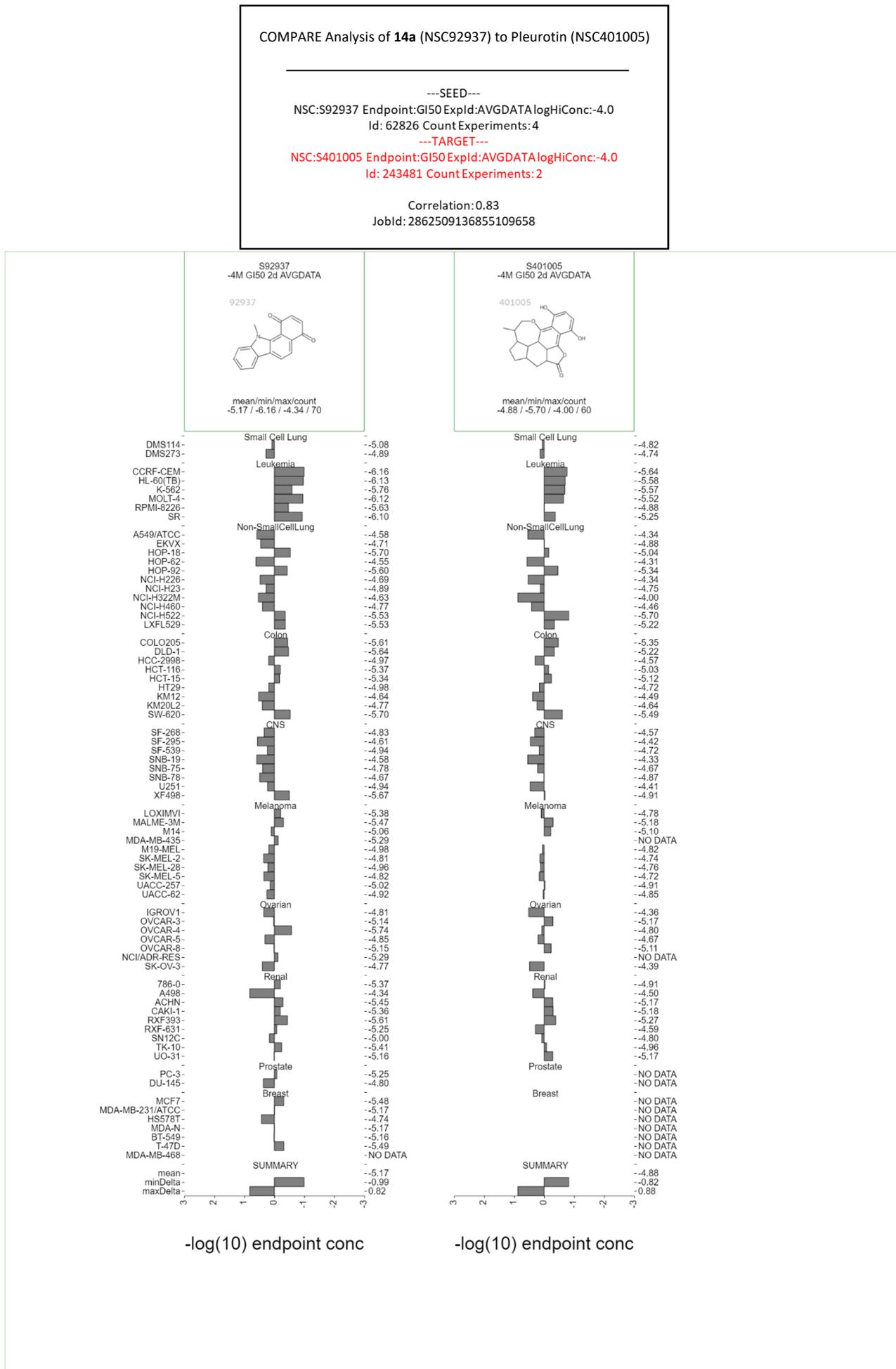


Figure S36

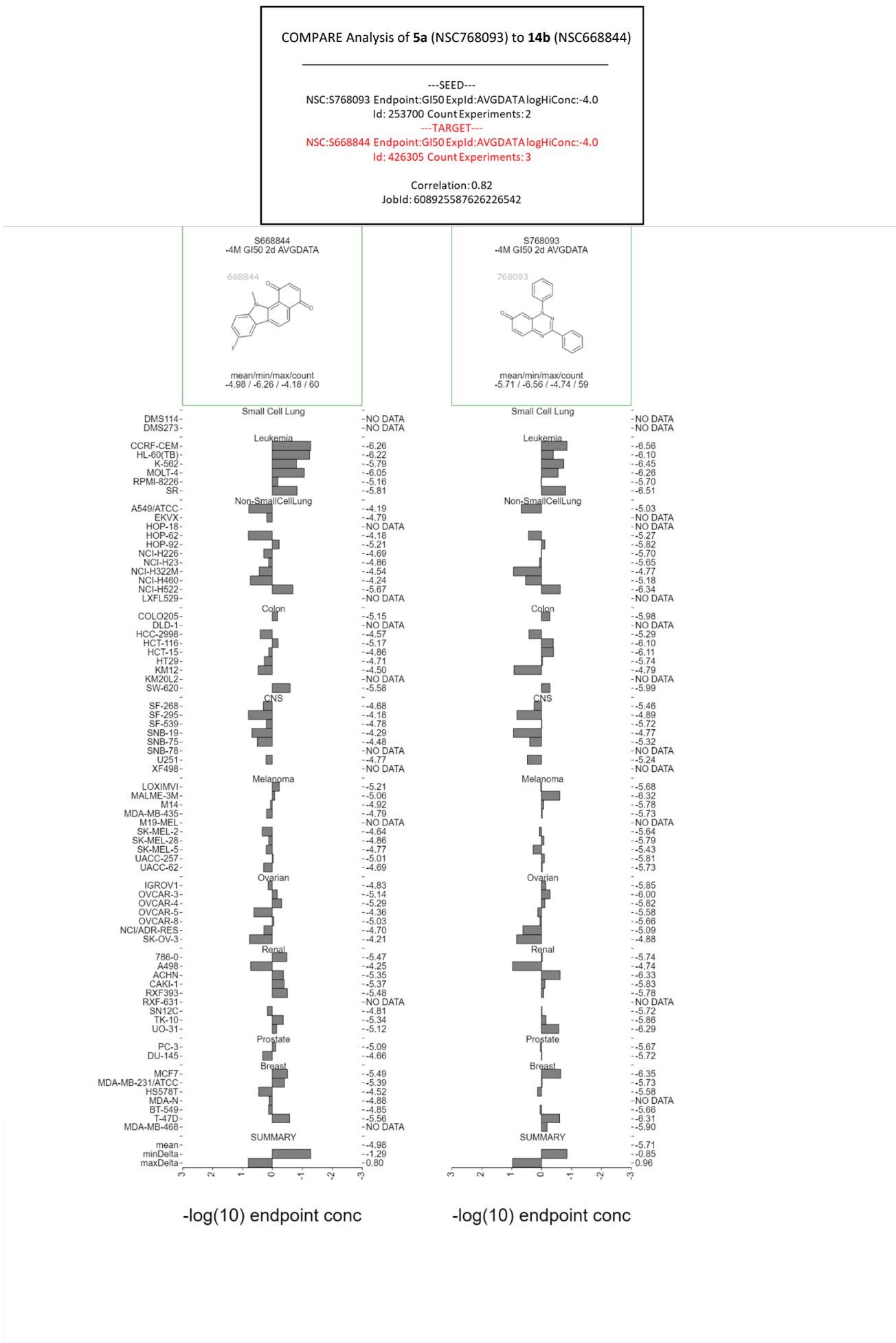


Figure S37

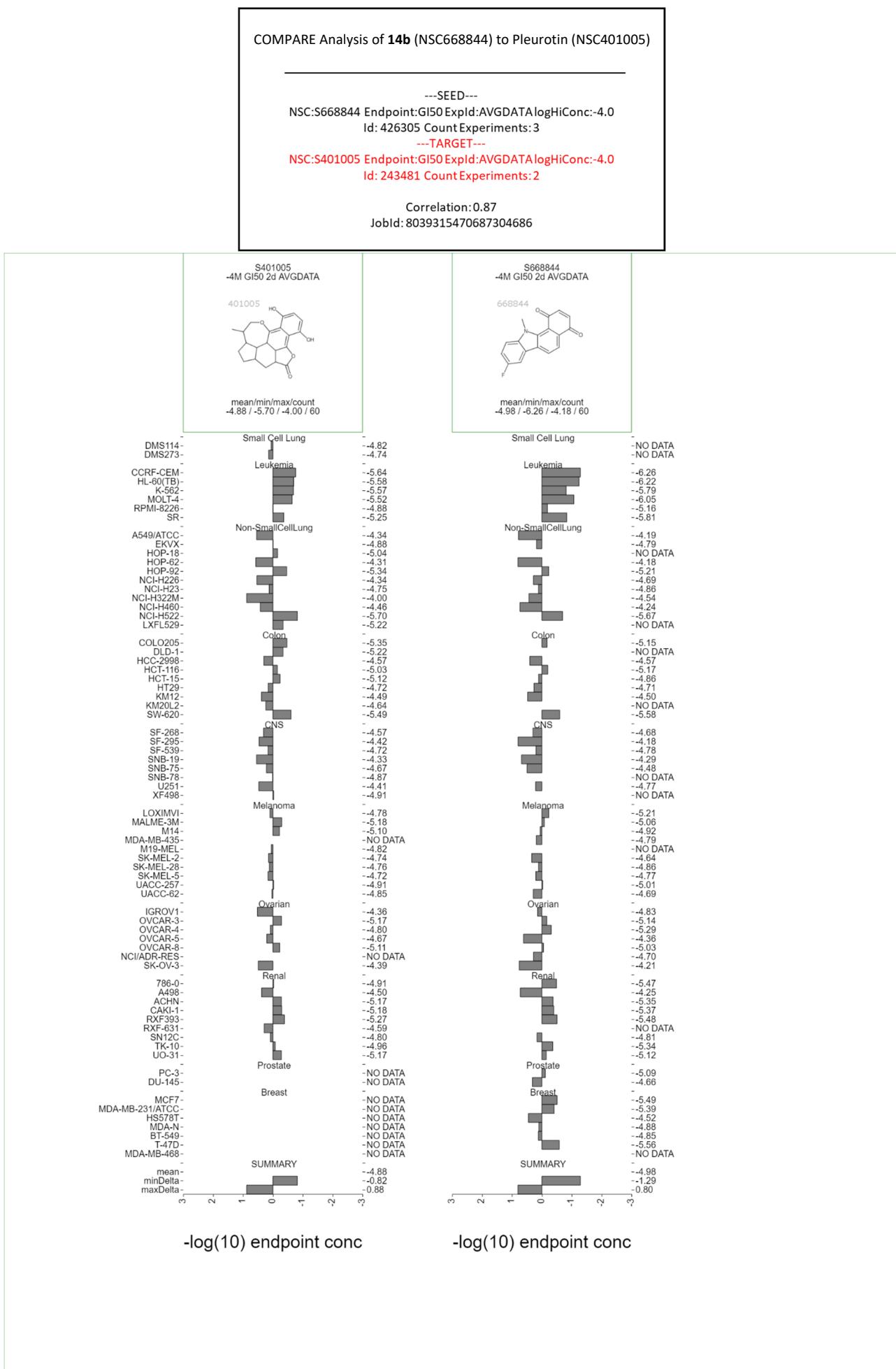


Figure S38

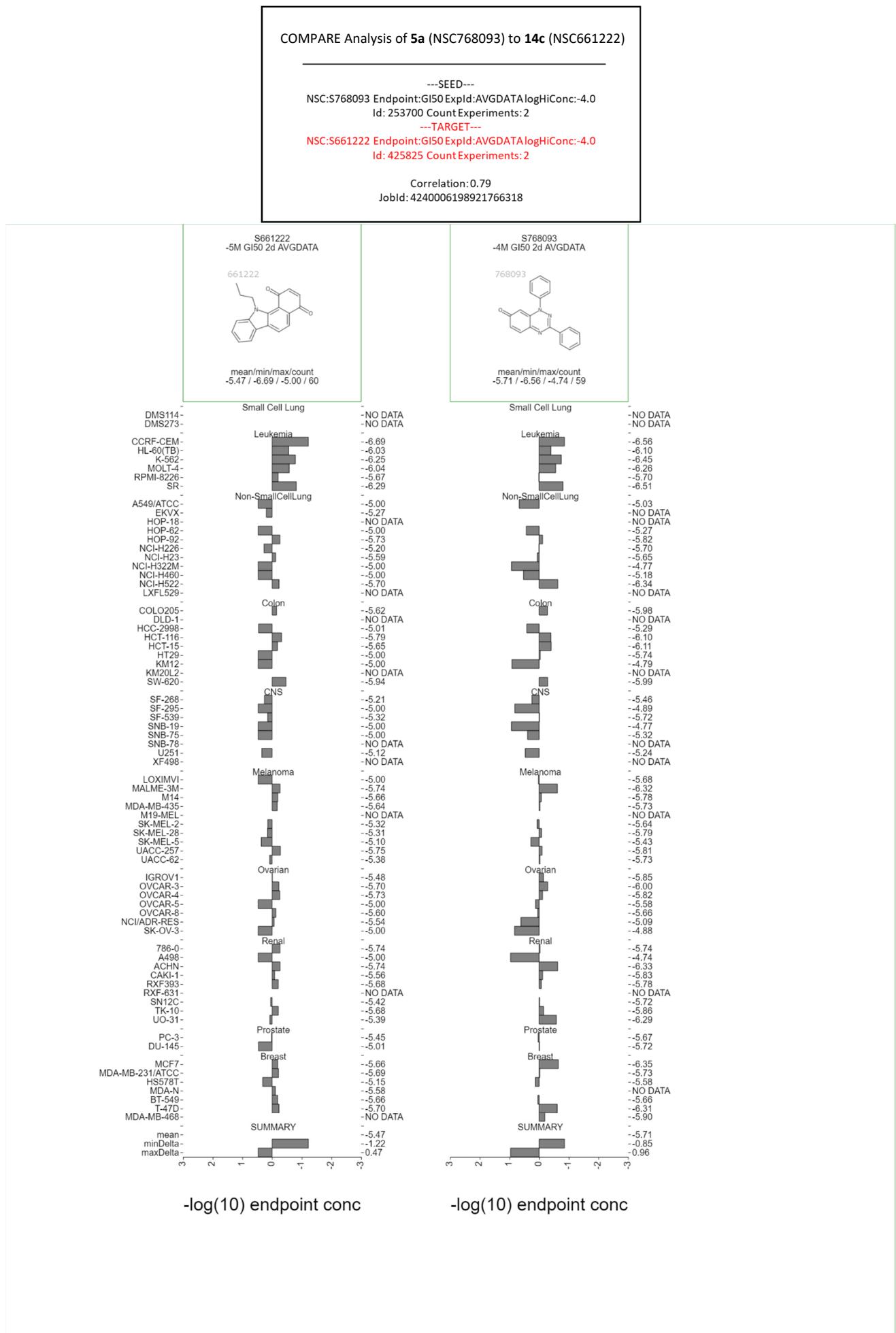


Figure S39

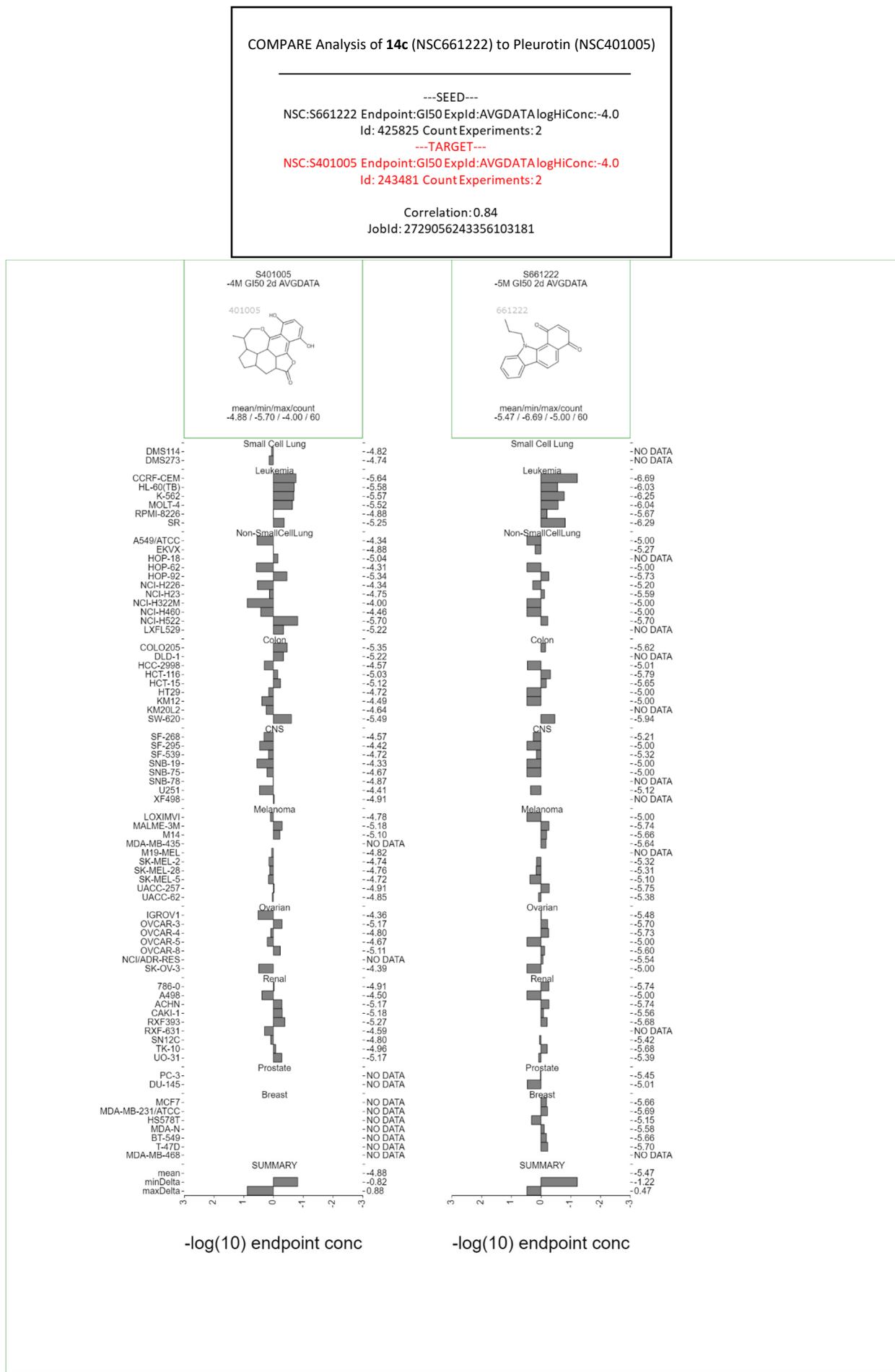


Figure S40

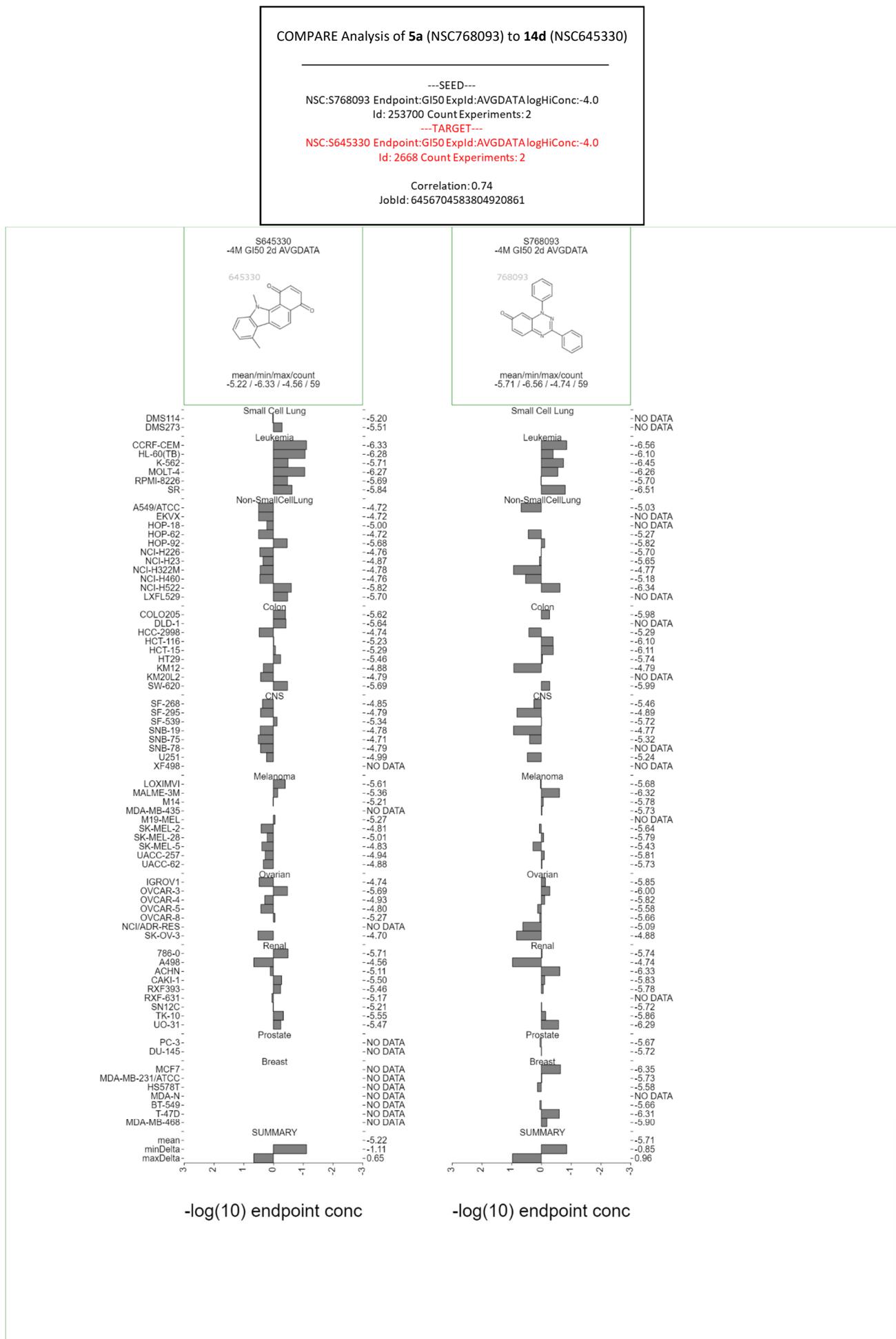


Figure S41

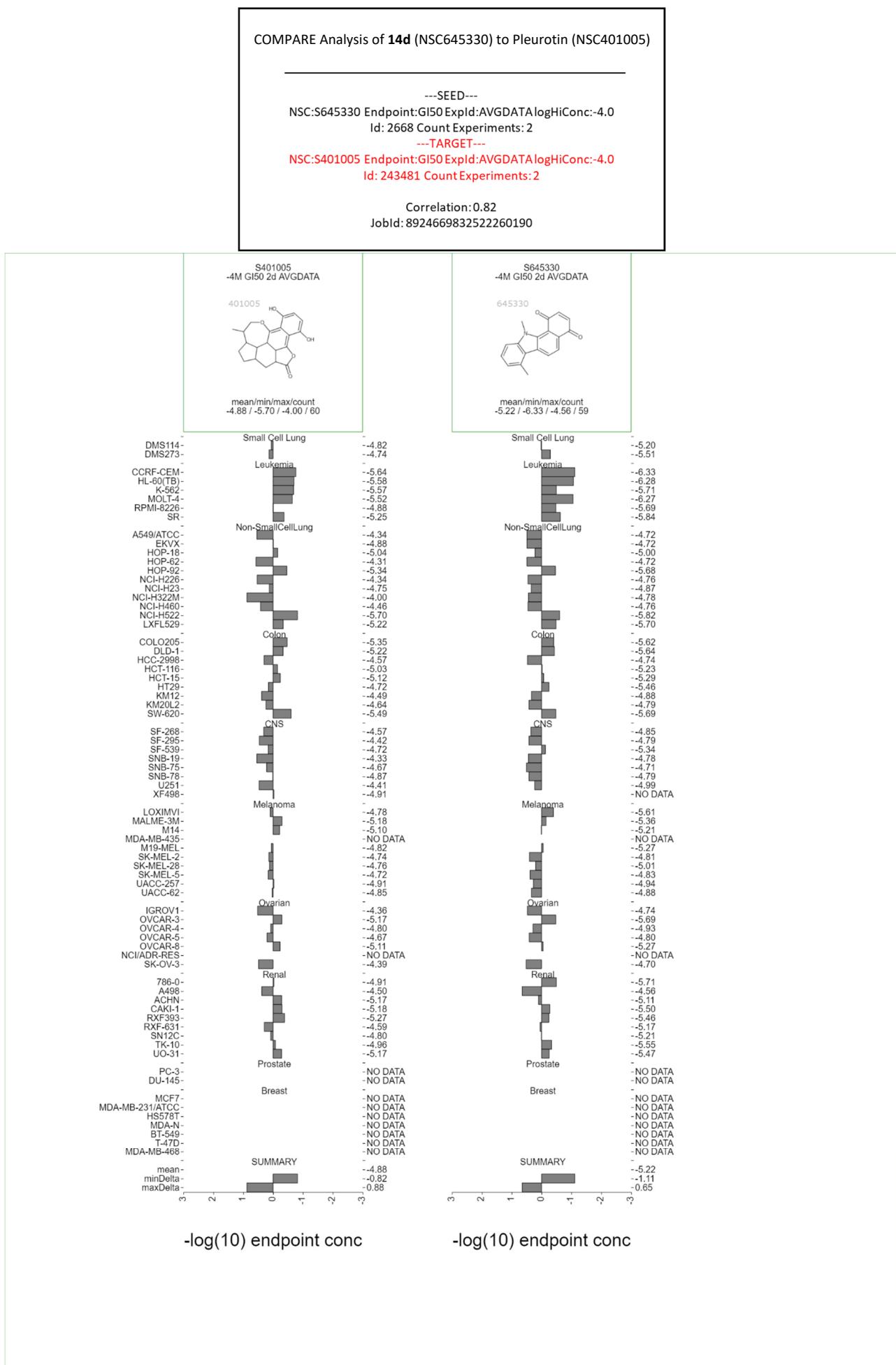


Figure S42

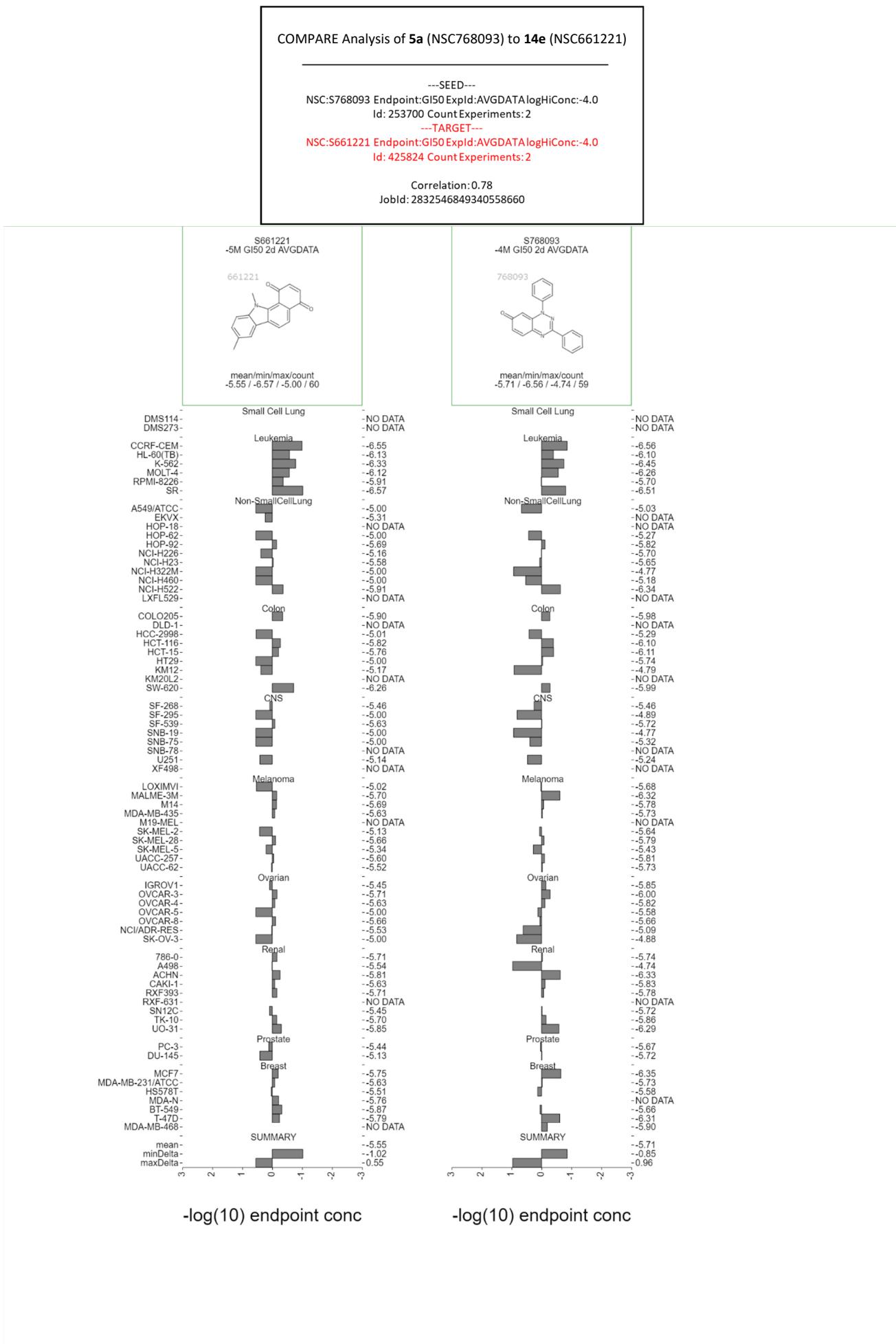


Figure S43

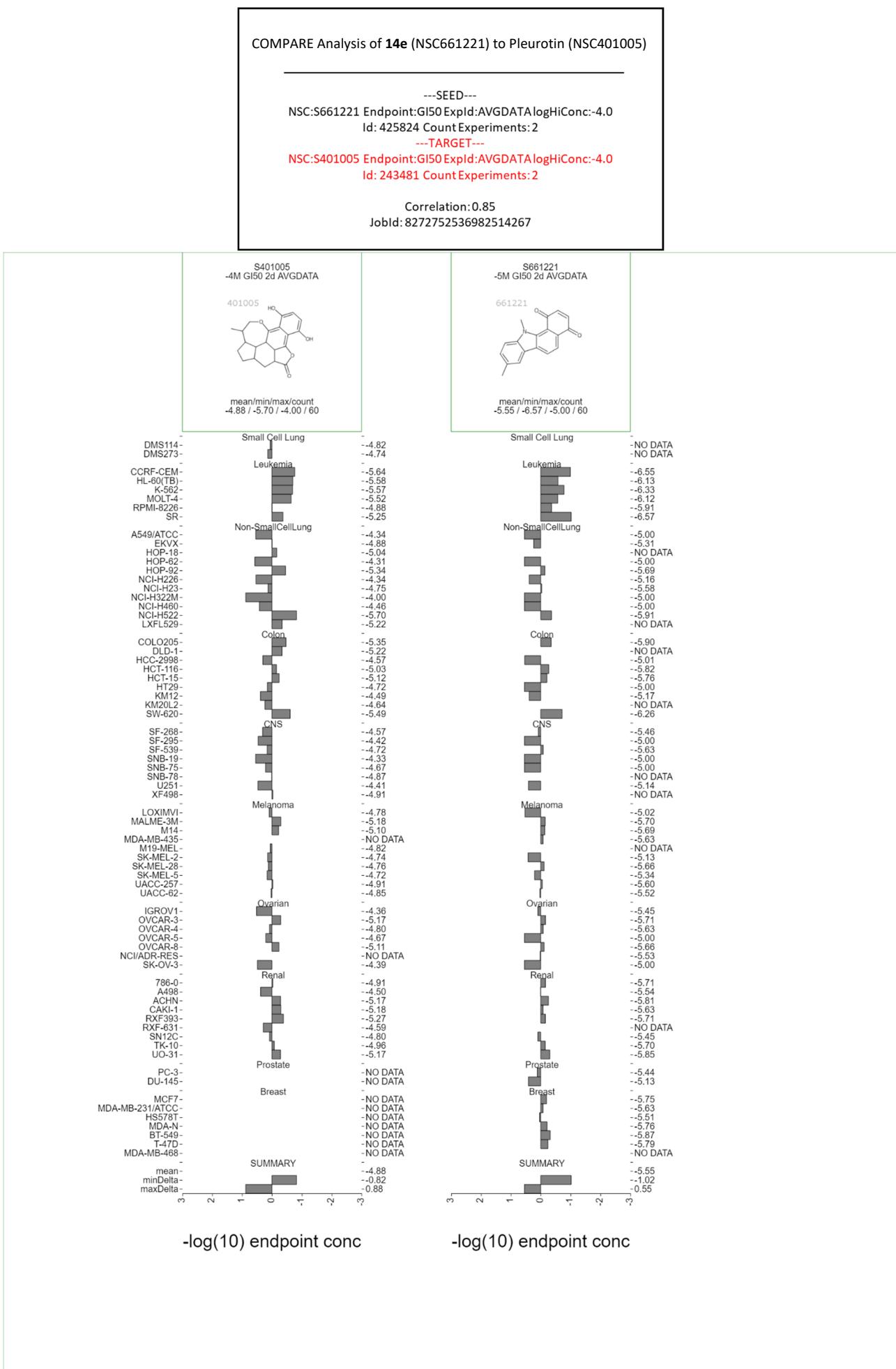


Figure S44

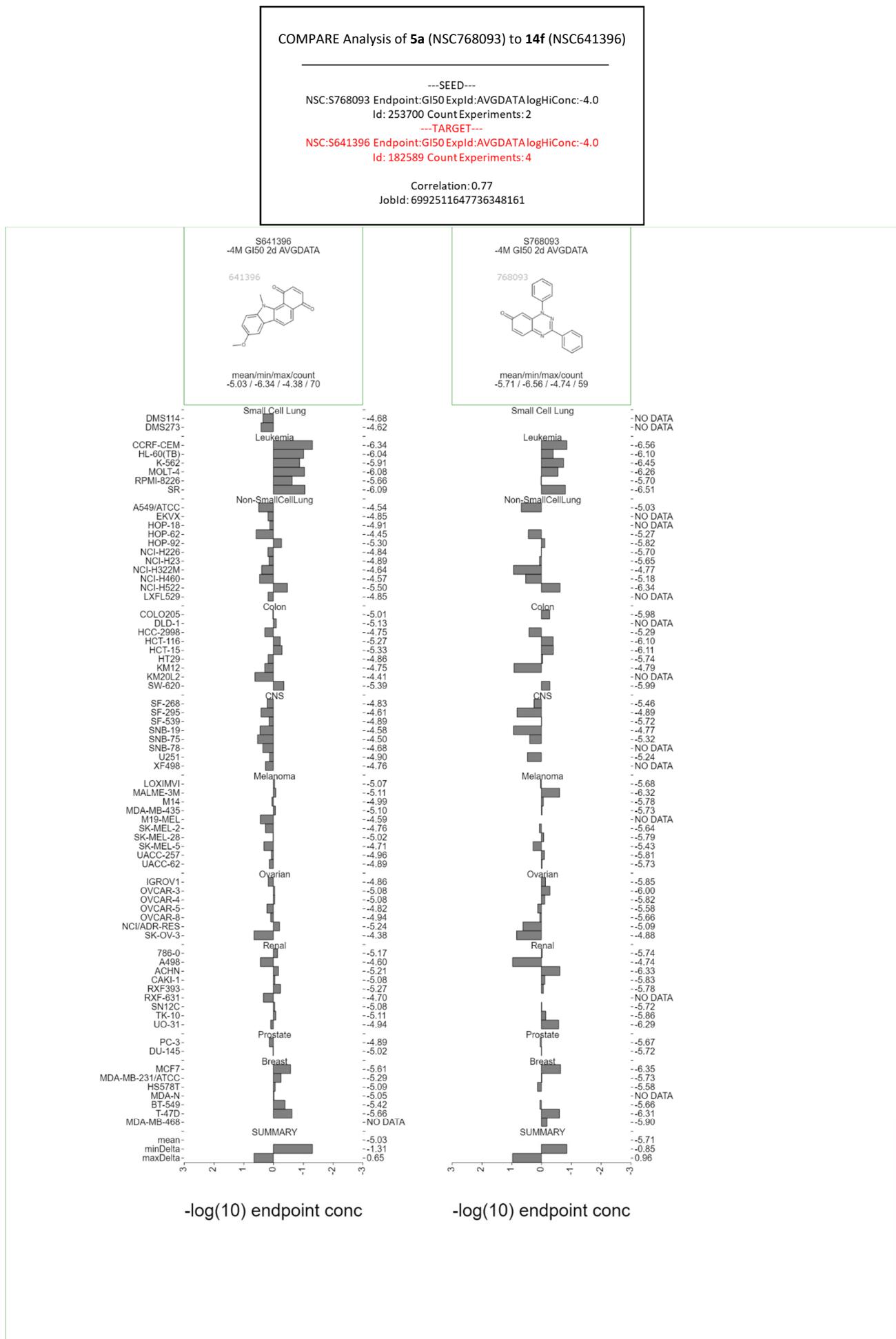


Figure S45

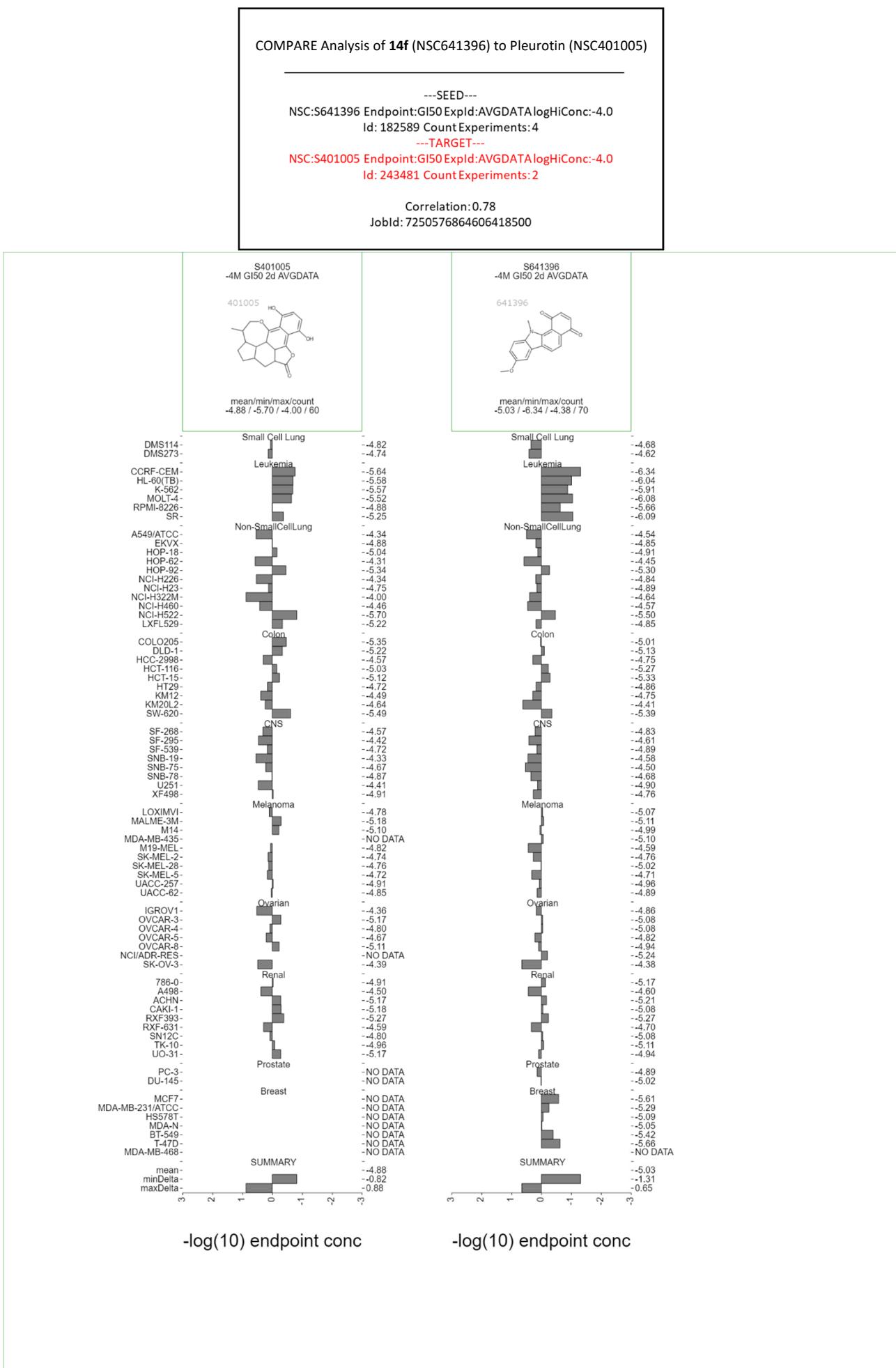


Figure S46

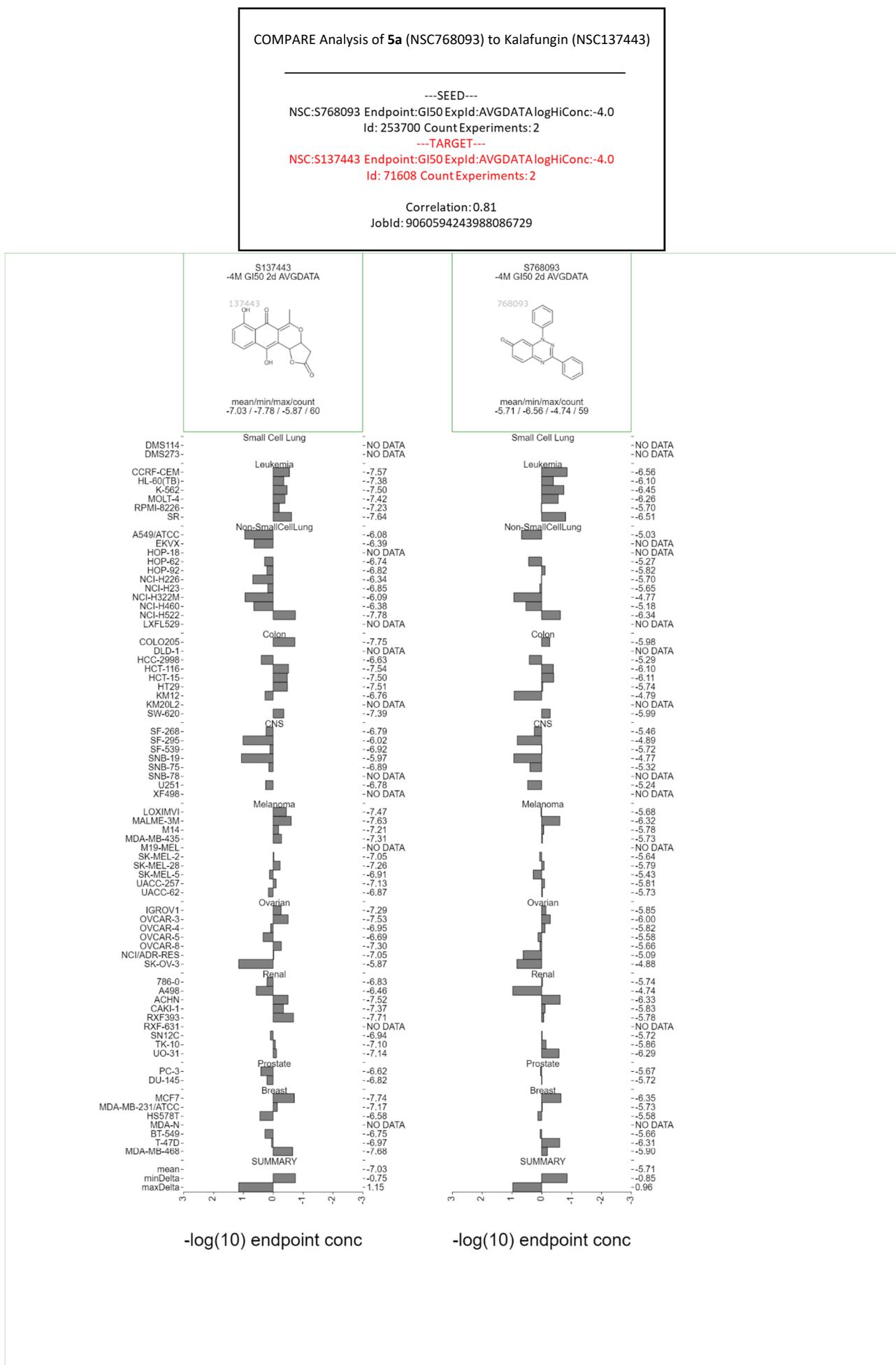


Figure S47

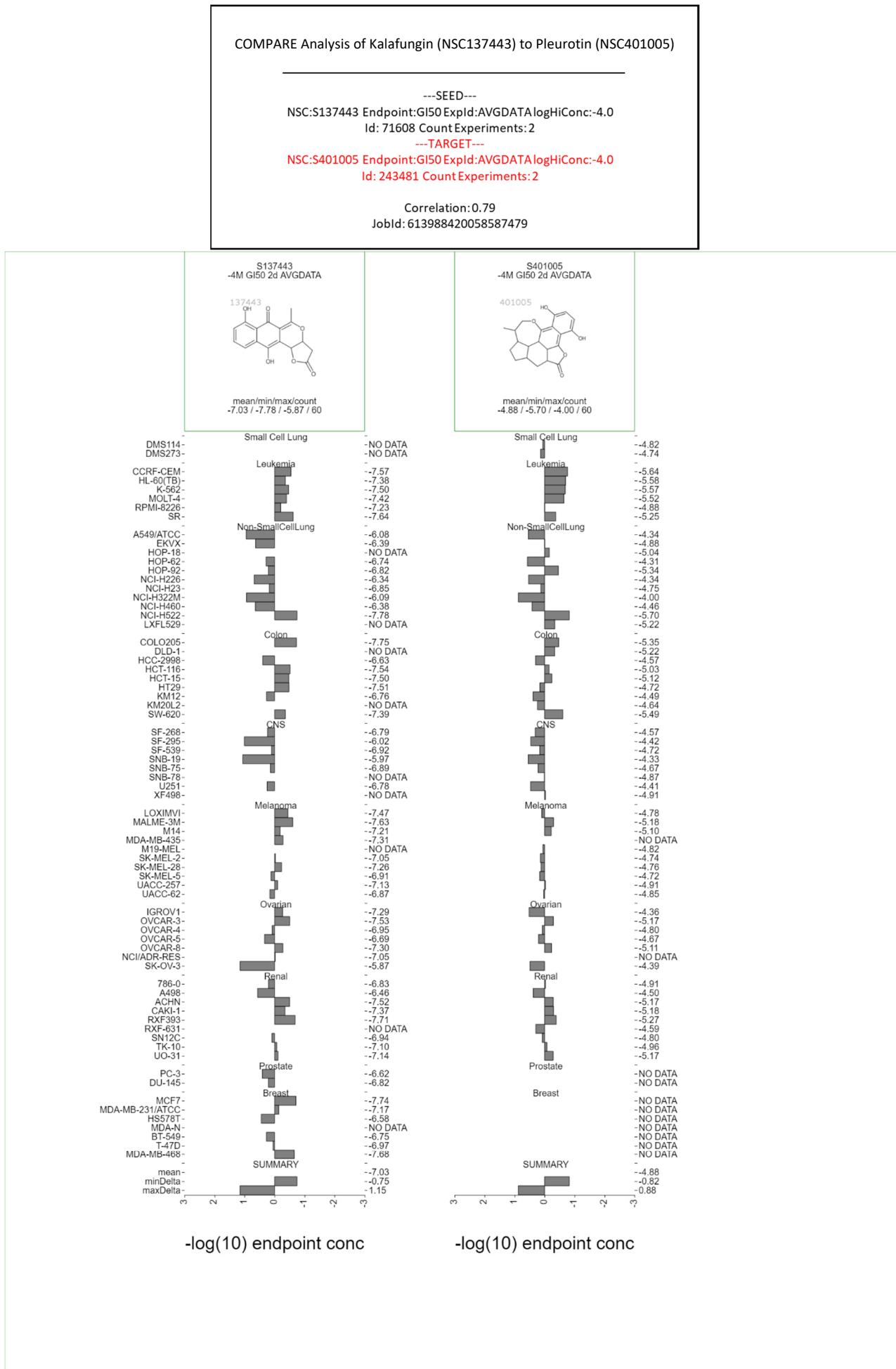


Figure S48

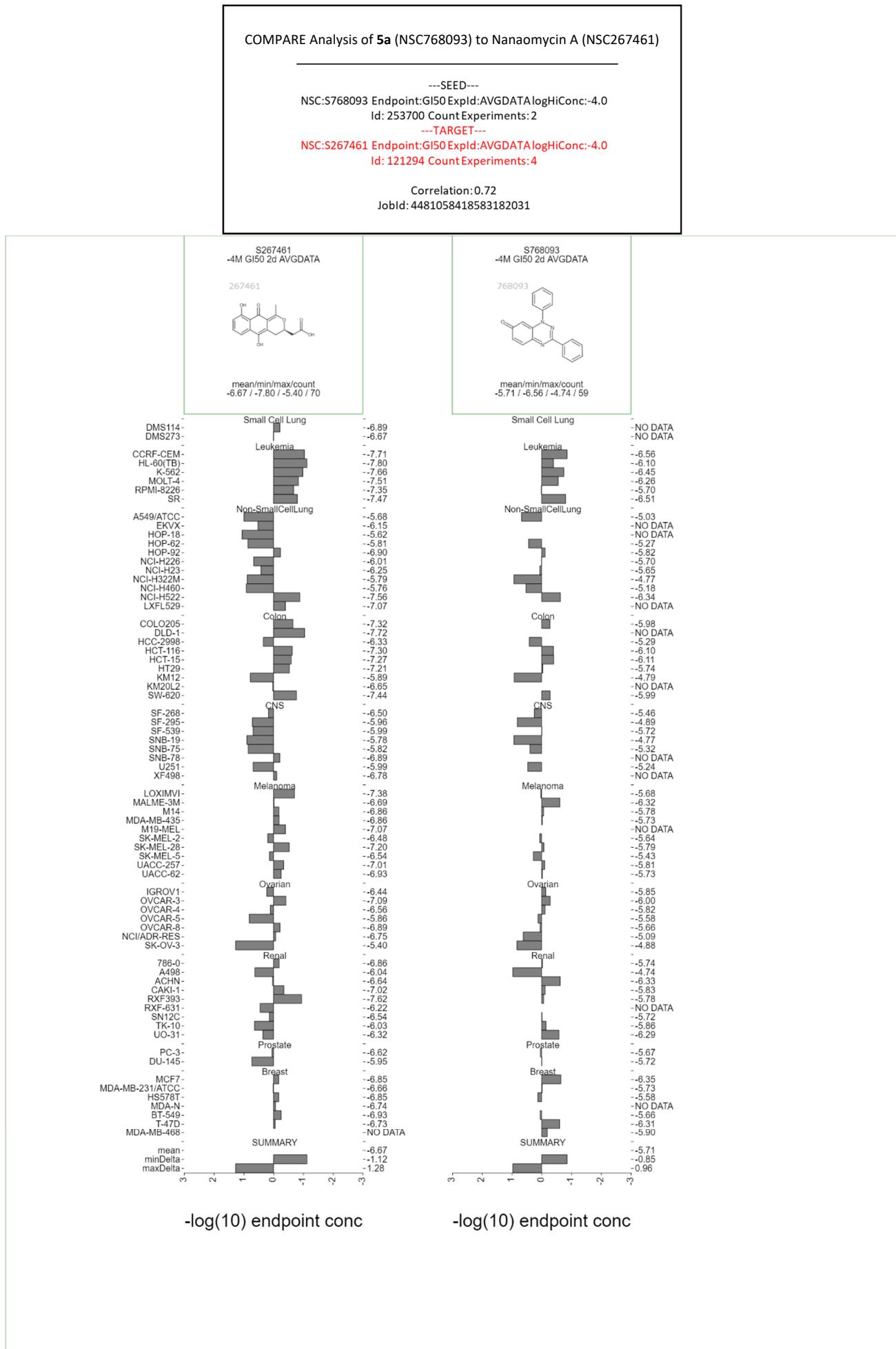


Figure S49

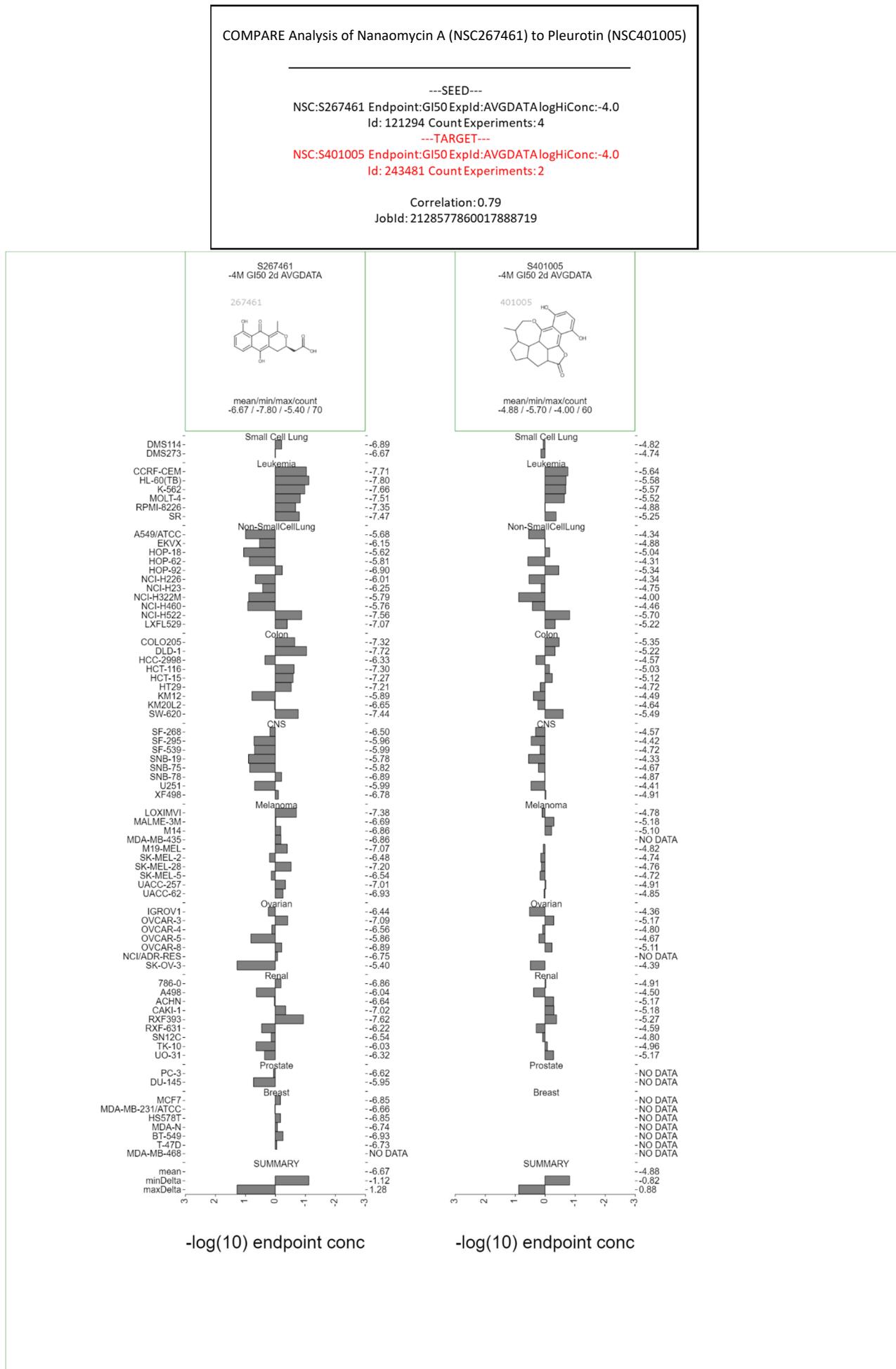


Figure S50

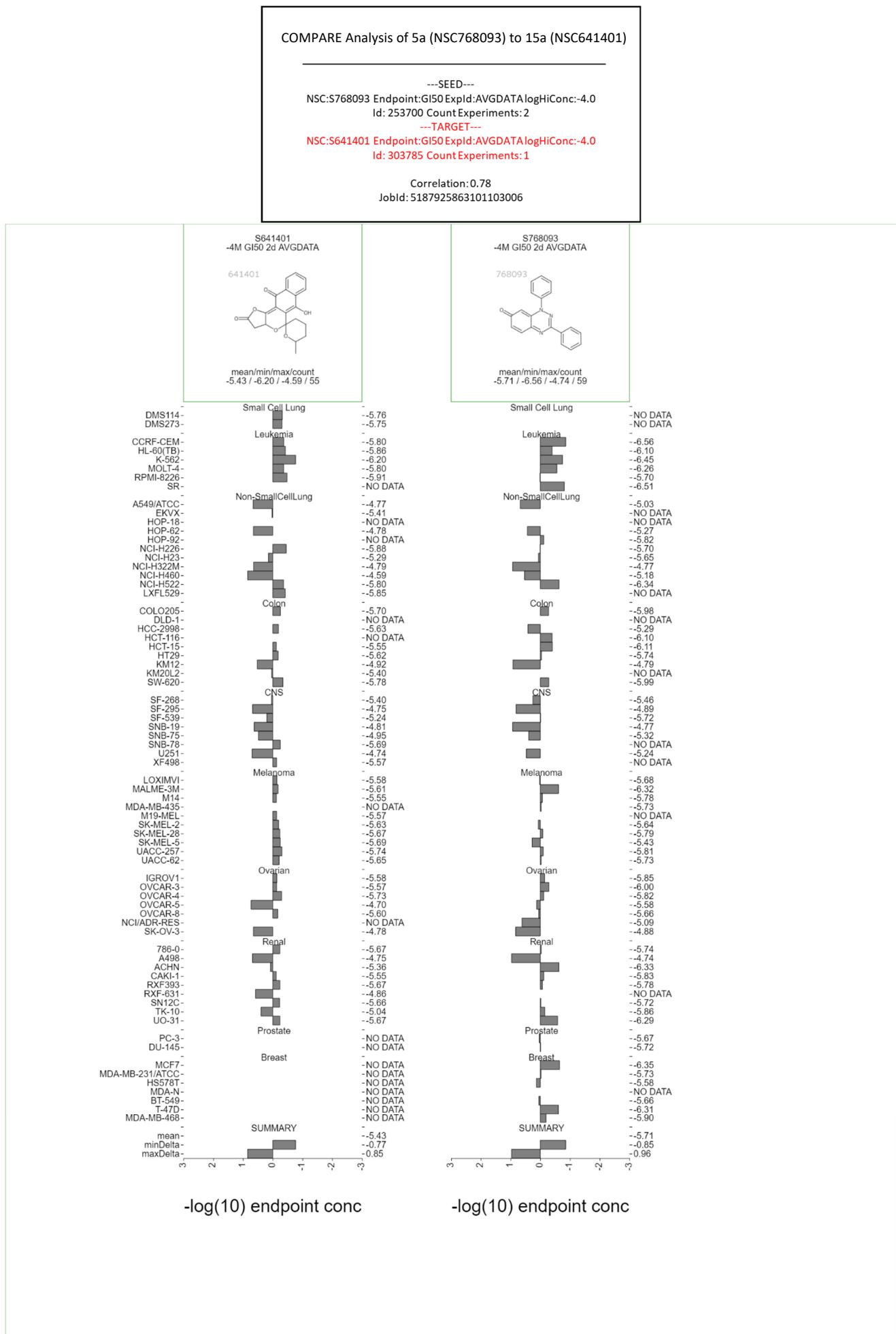


Figure S51

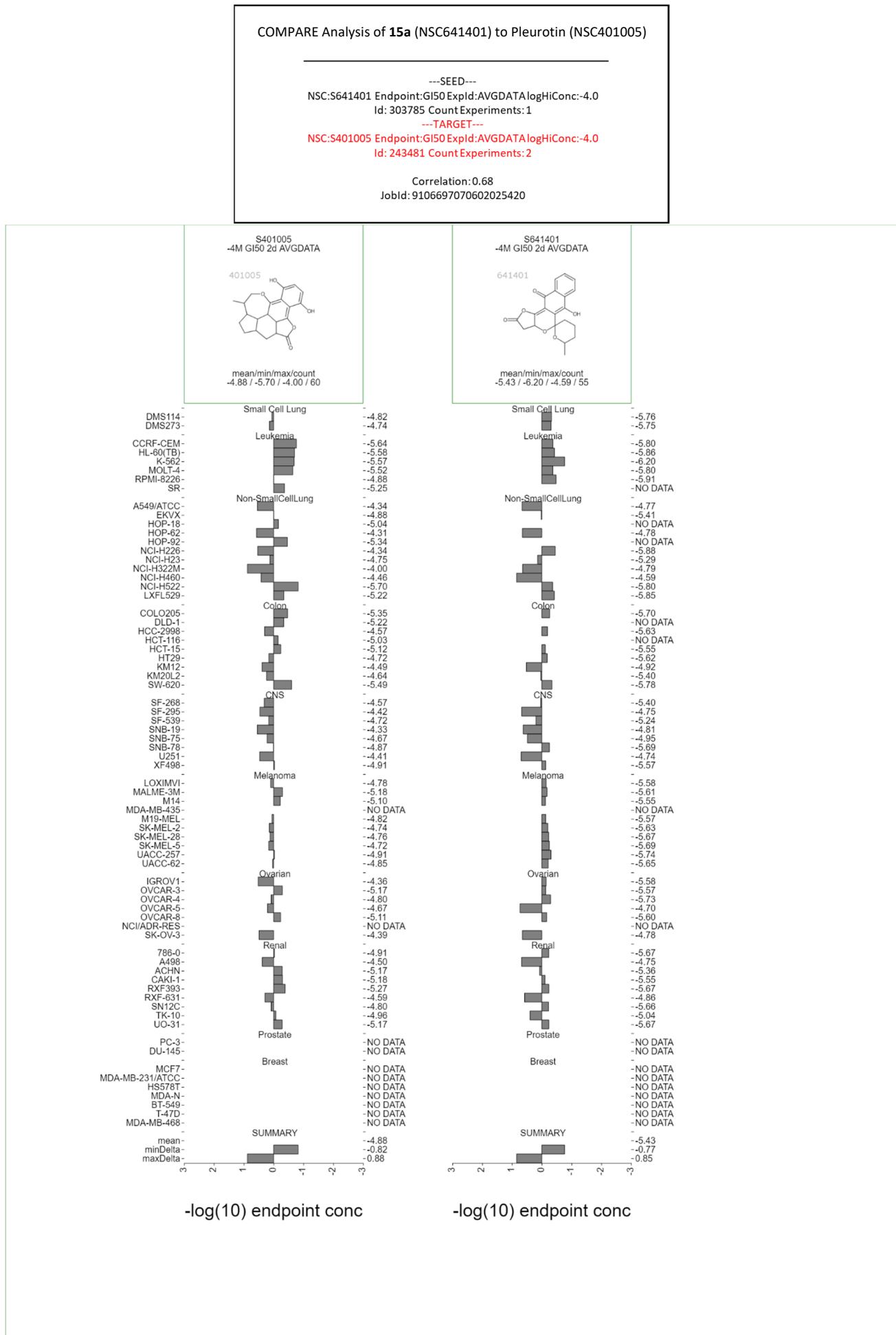


Figure S52

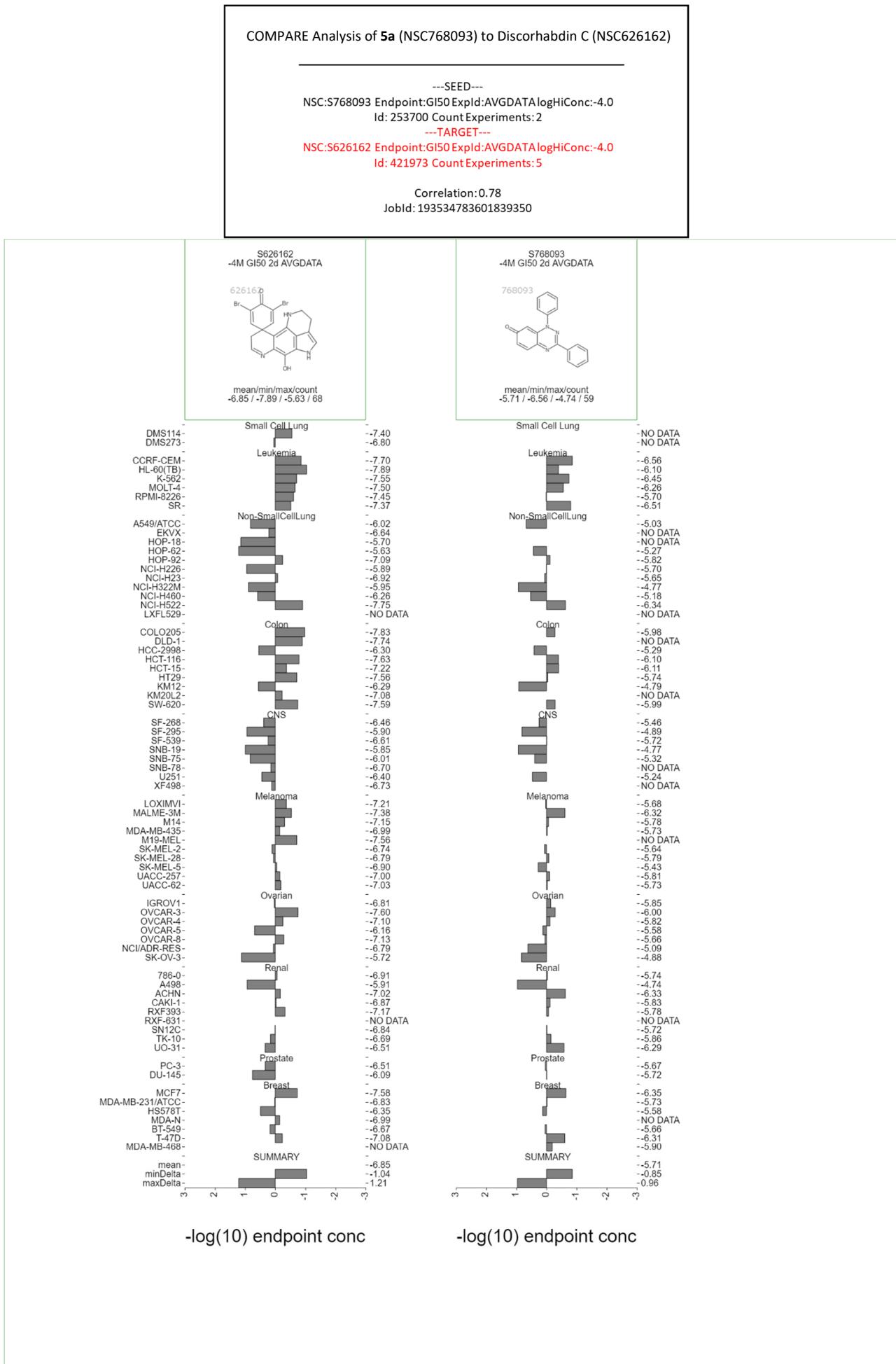


Figure S53

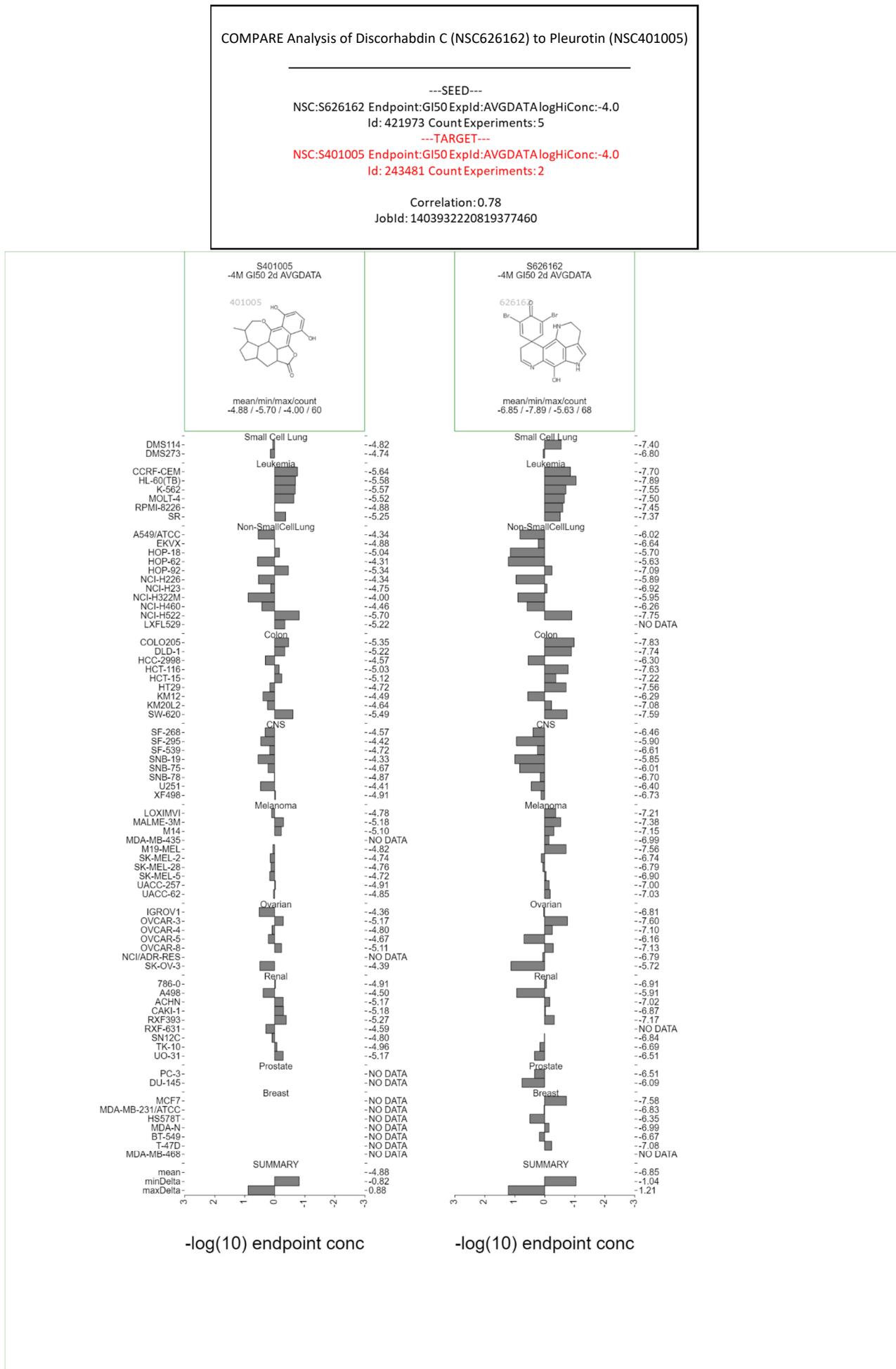


Figure S54

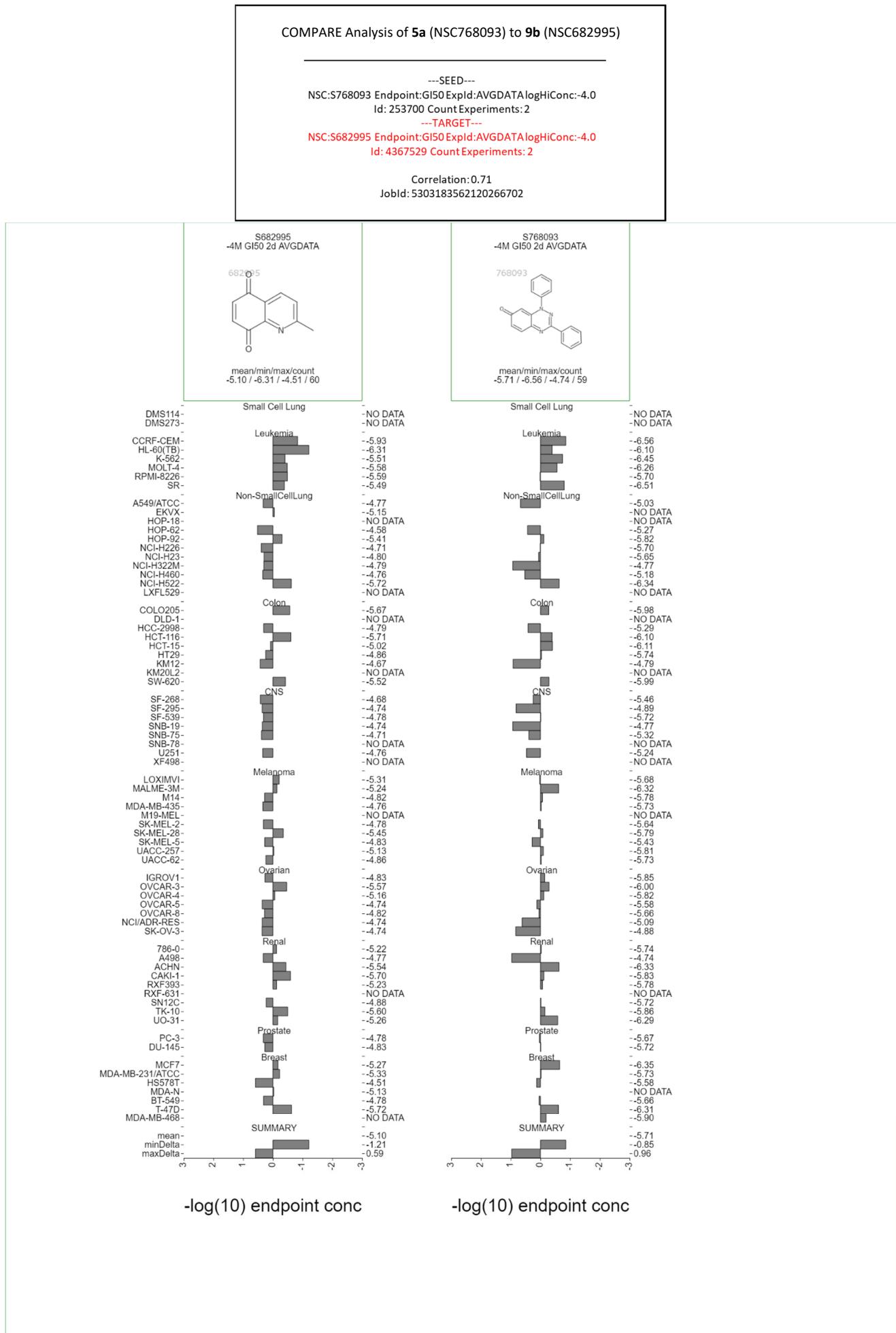


Figure S55

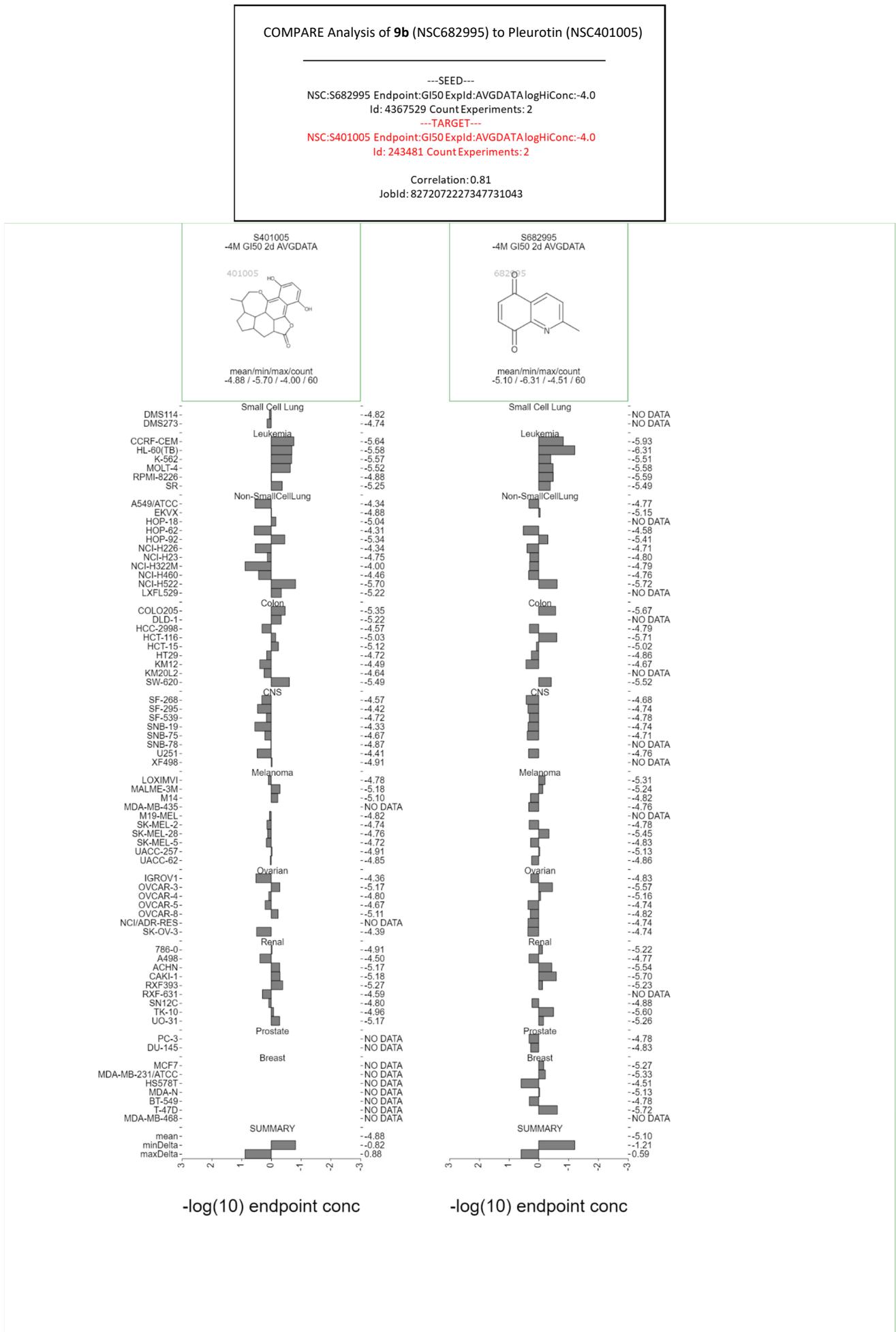


Figure S56

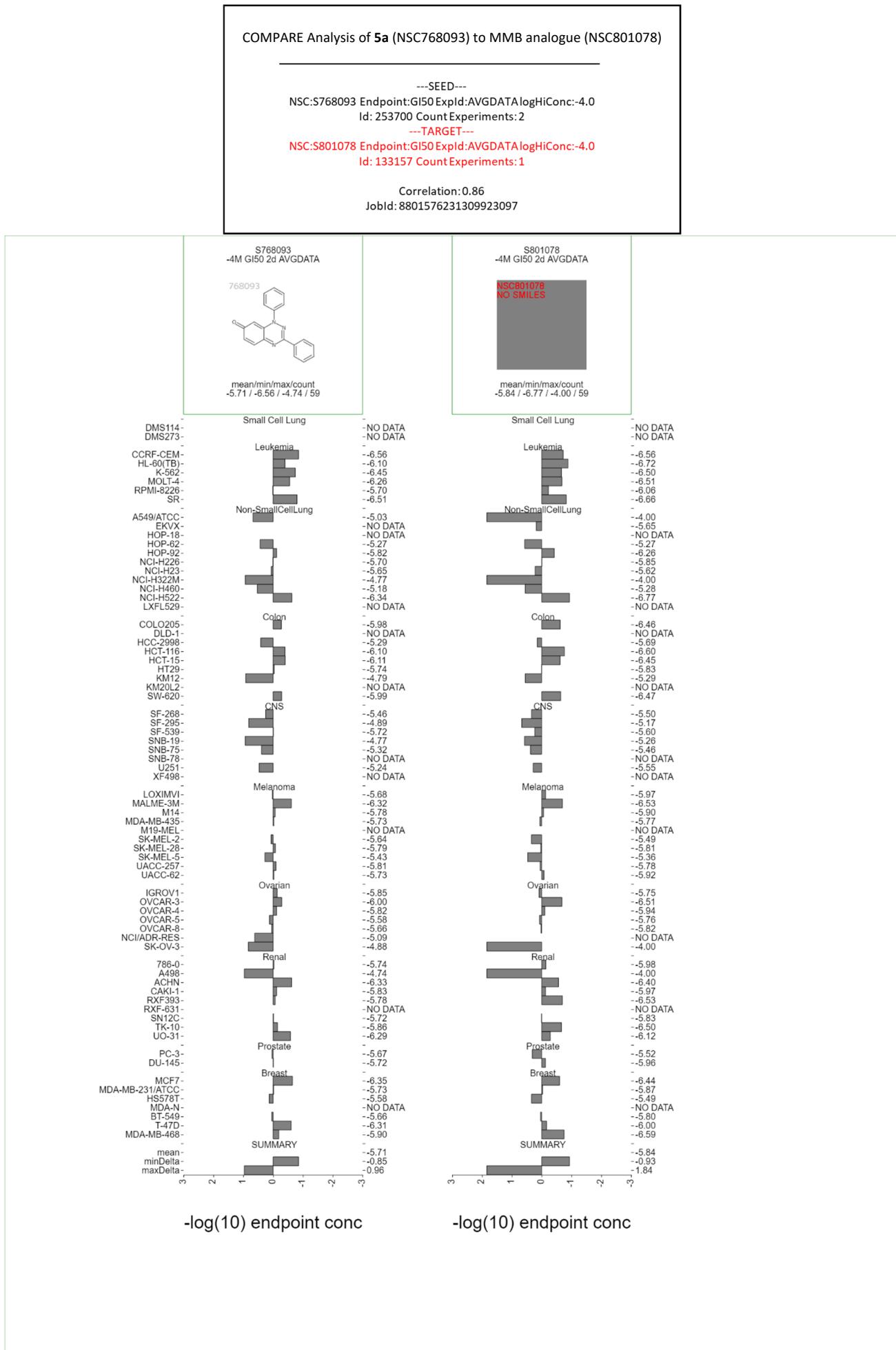


Figure S57

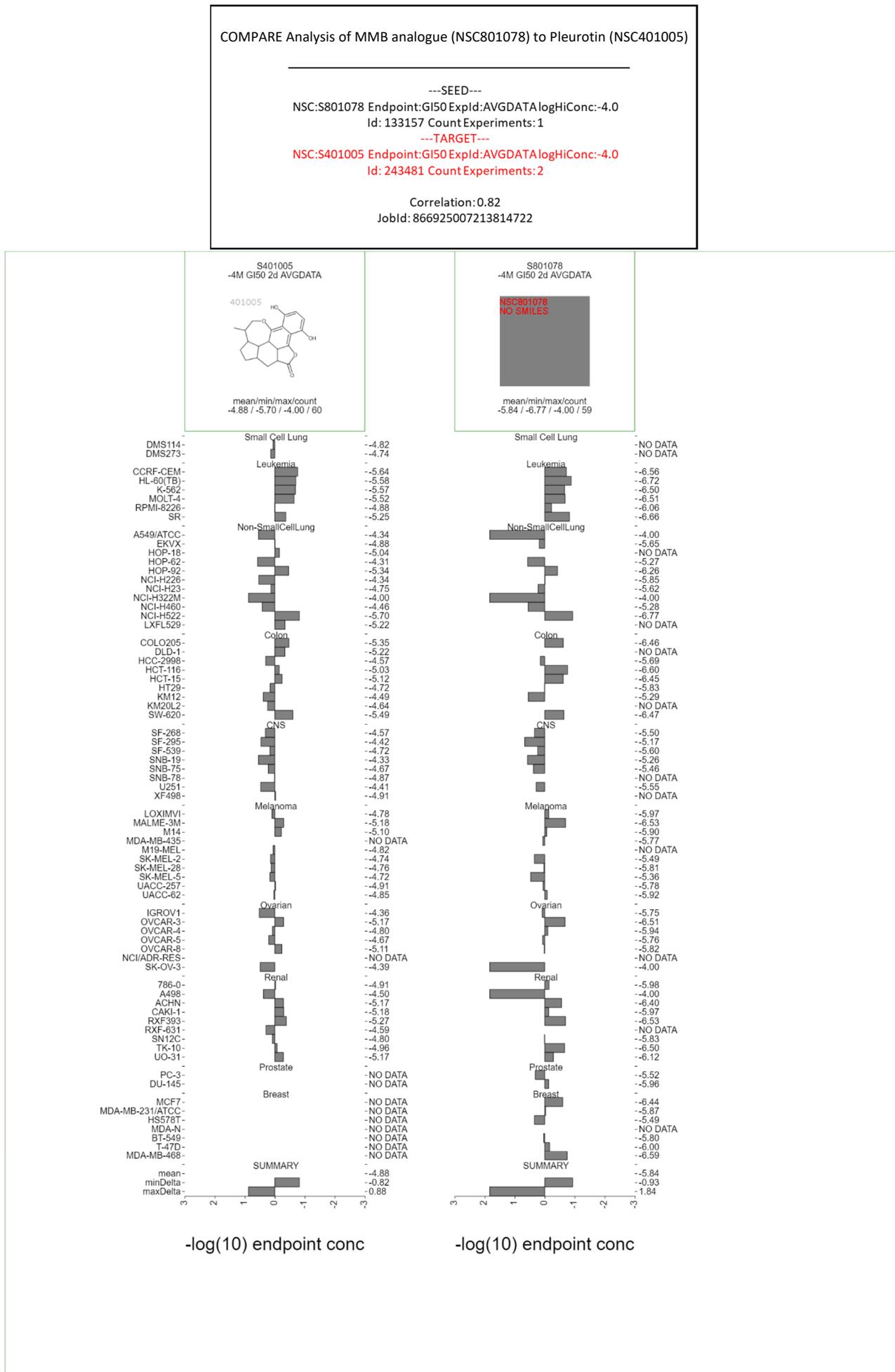


Figure S58

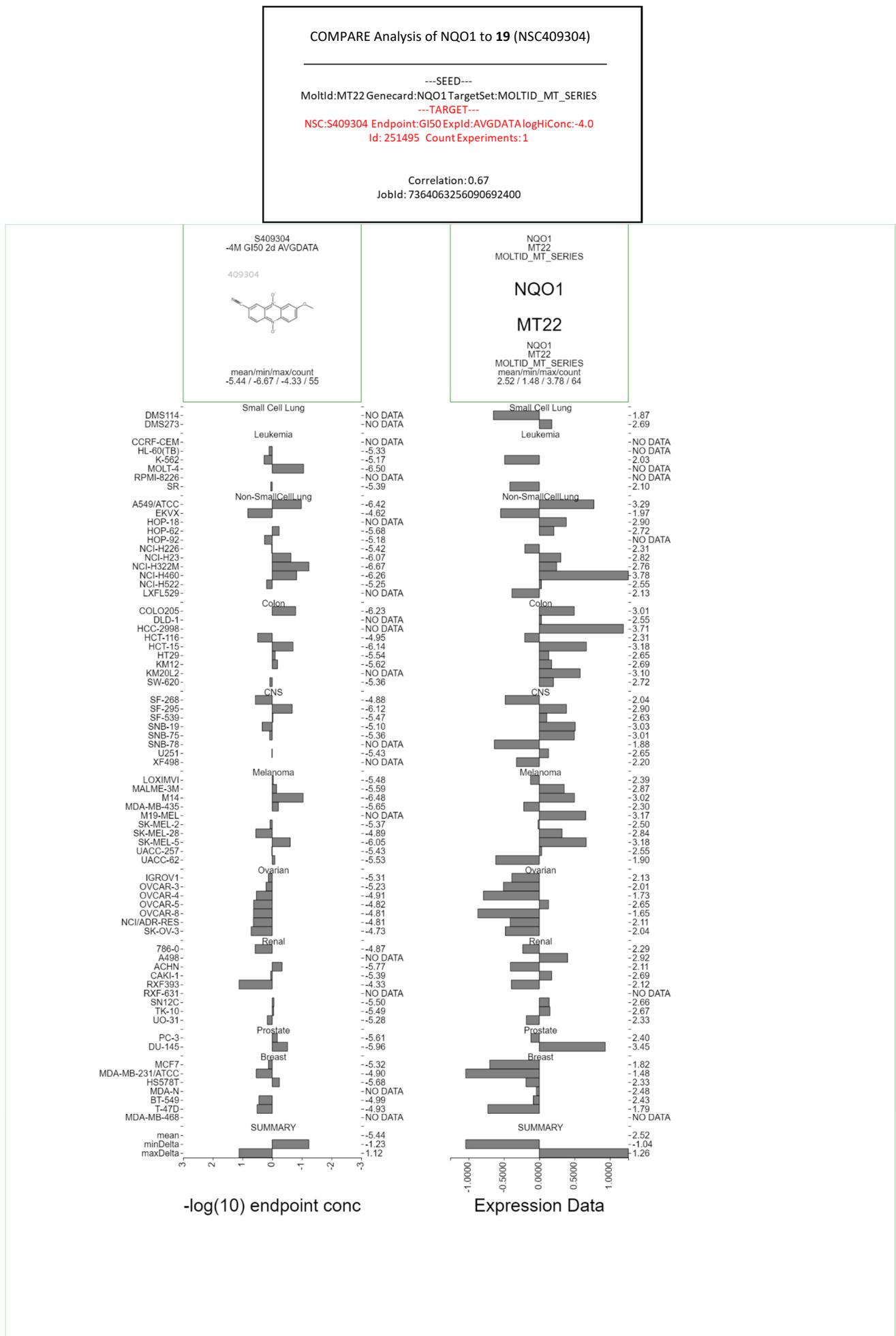


Figure S59

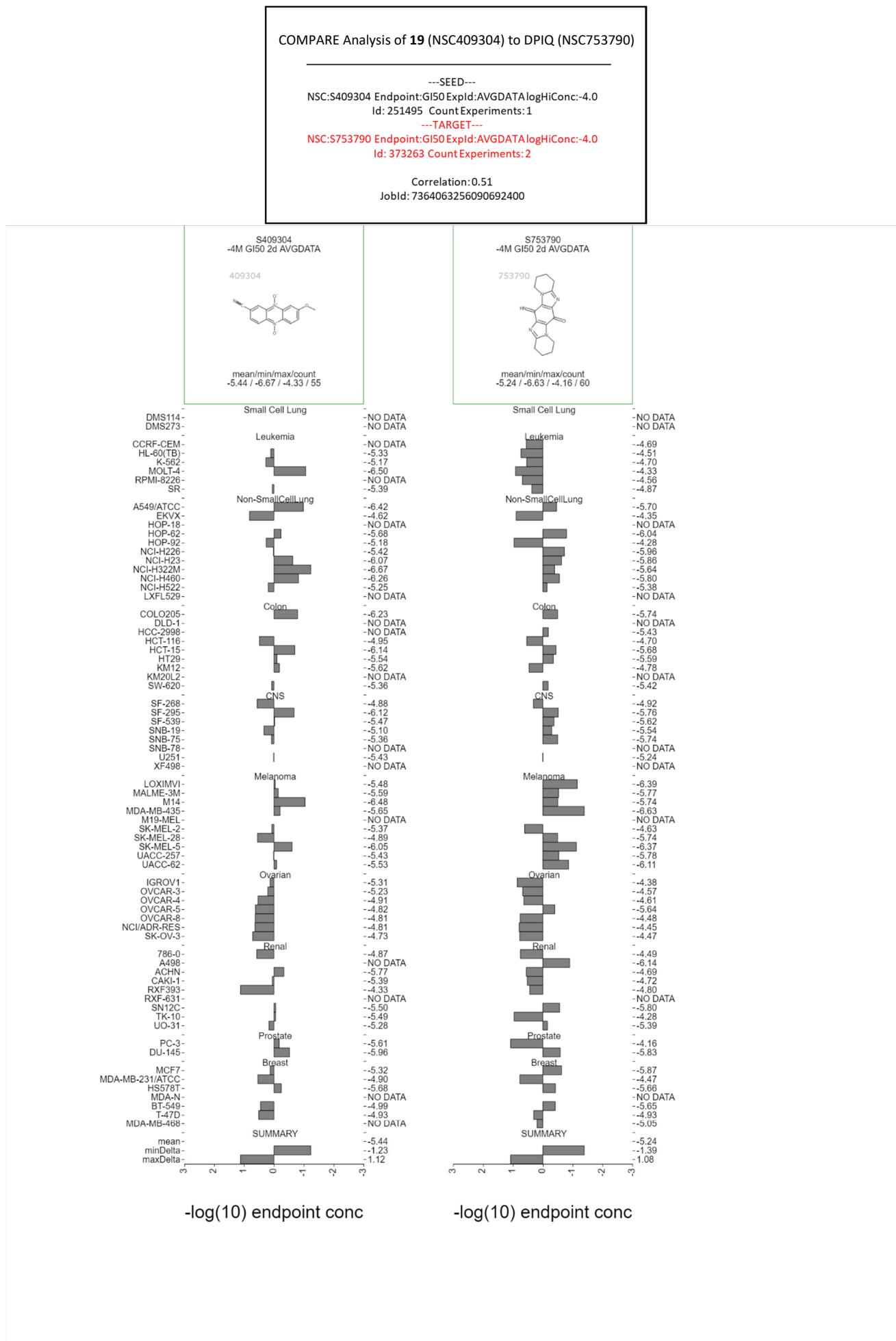


Figure S60

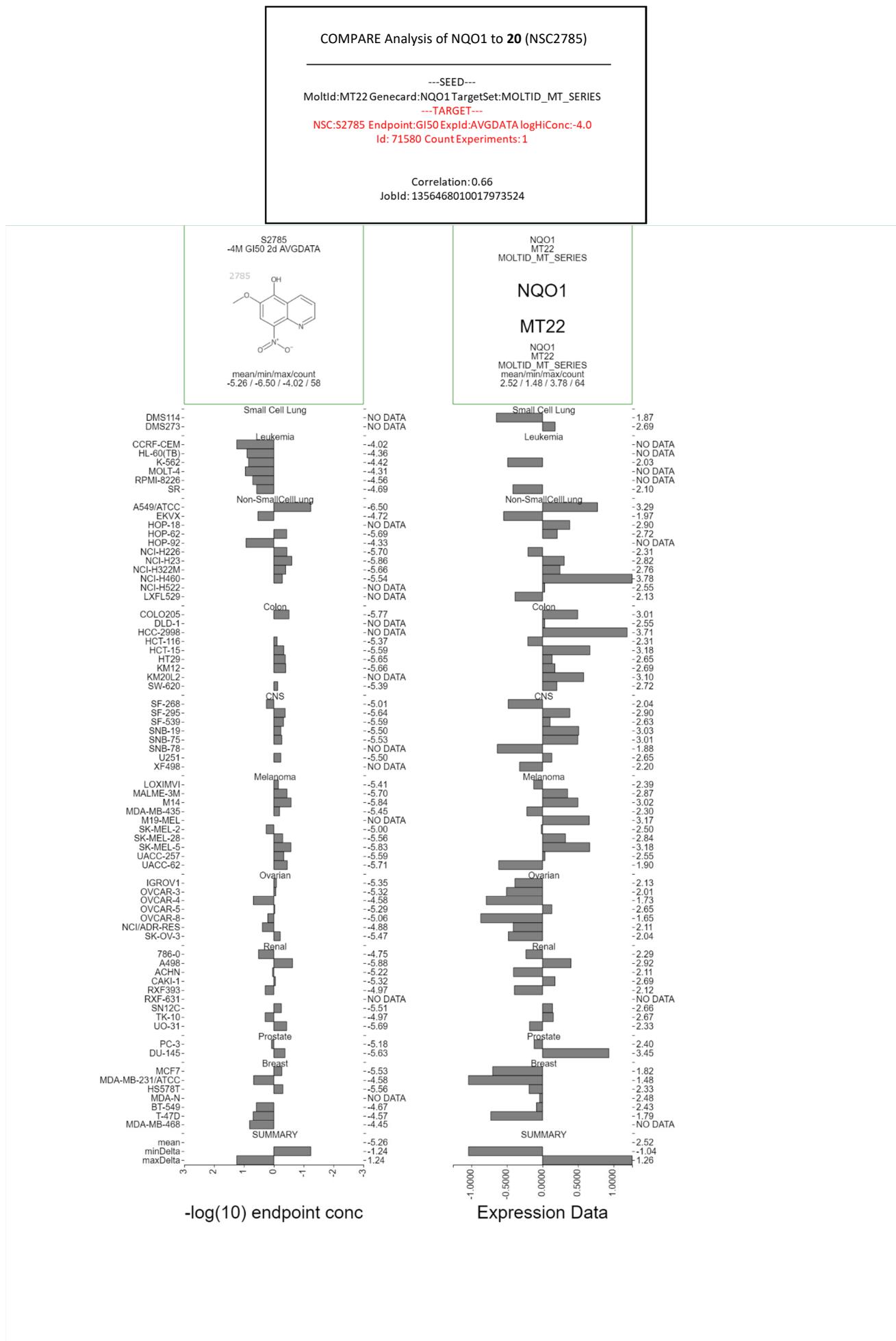


Figure S61

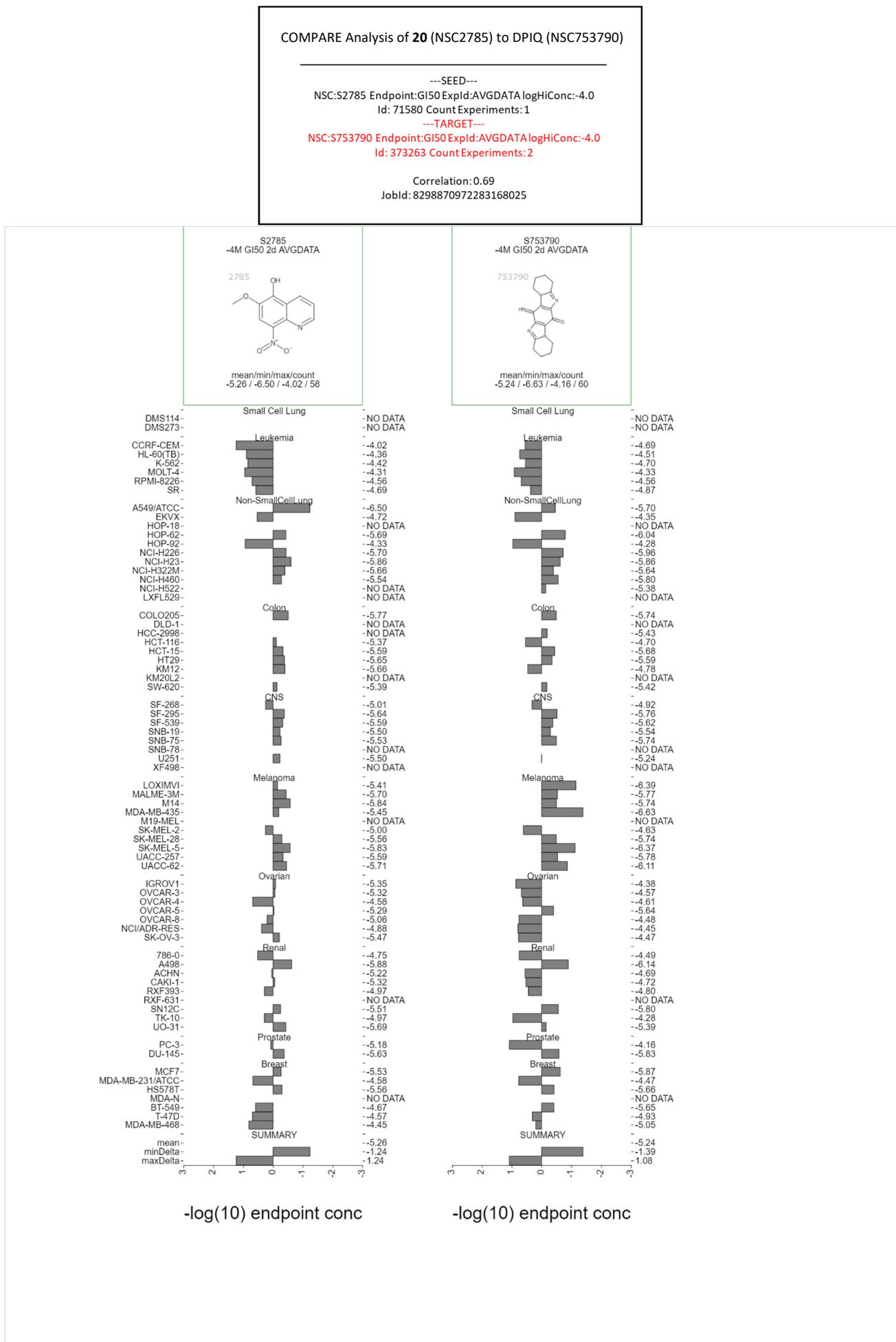


Figure S62

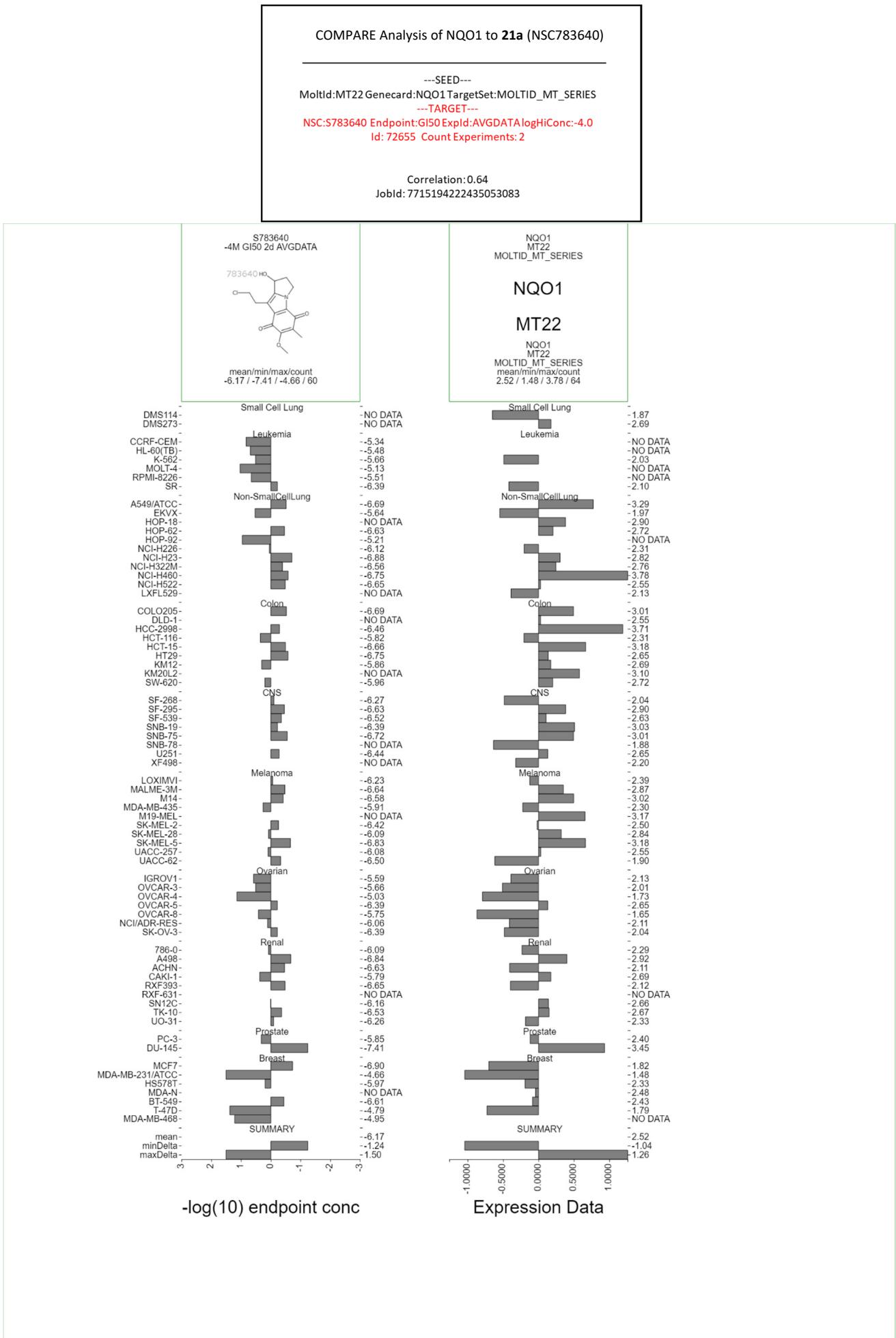


Figure S63

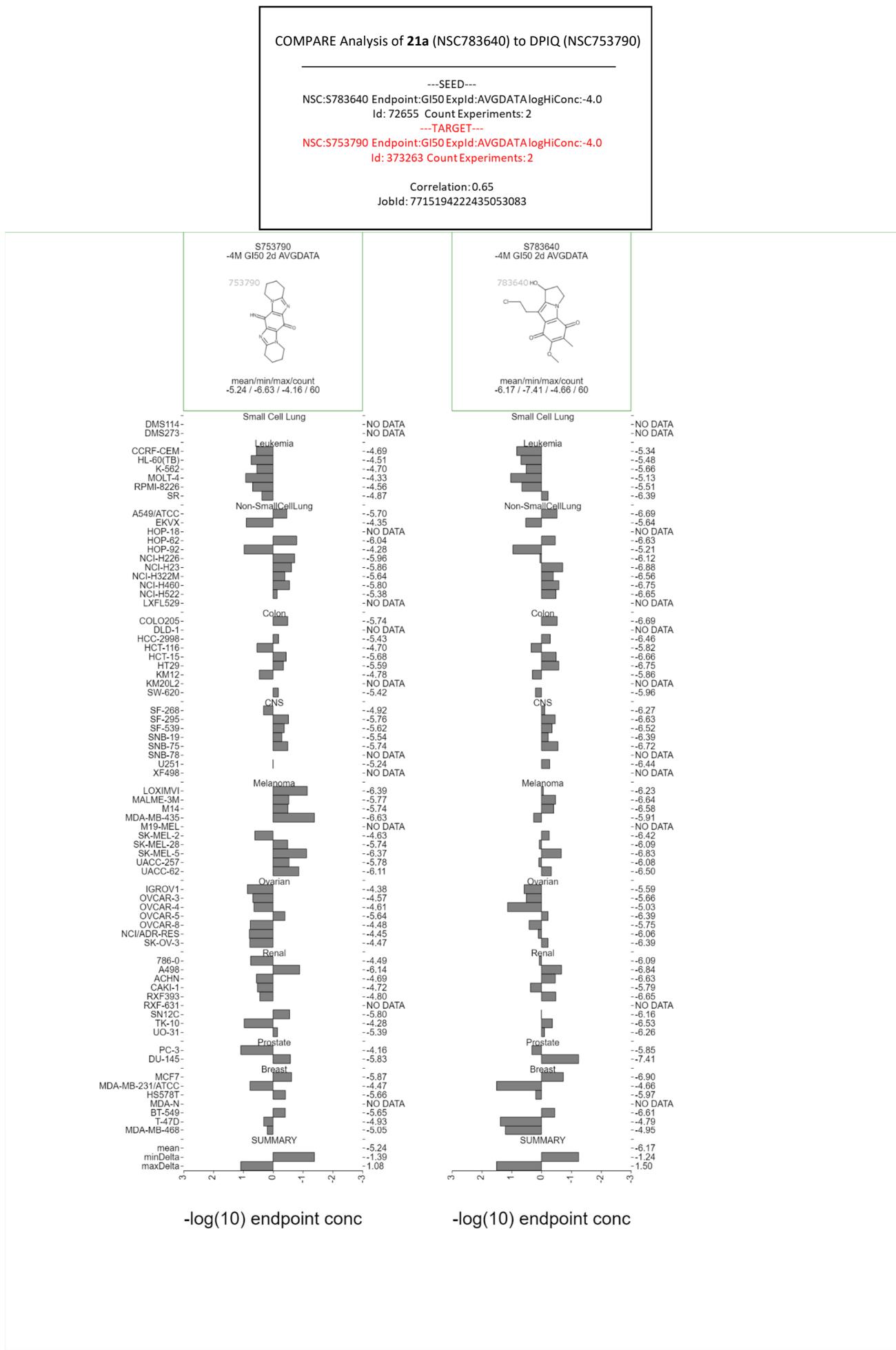


Figure S64

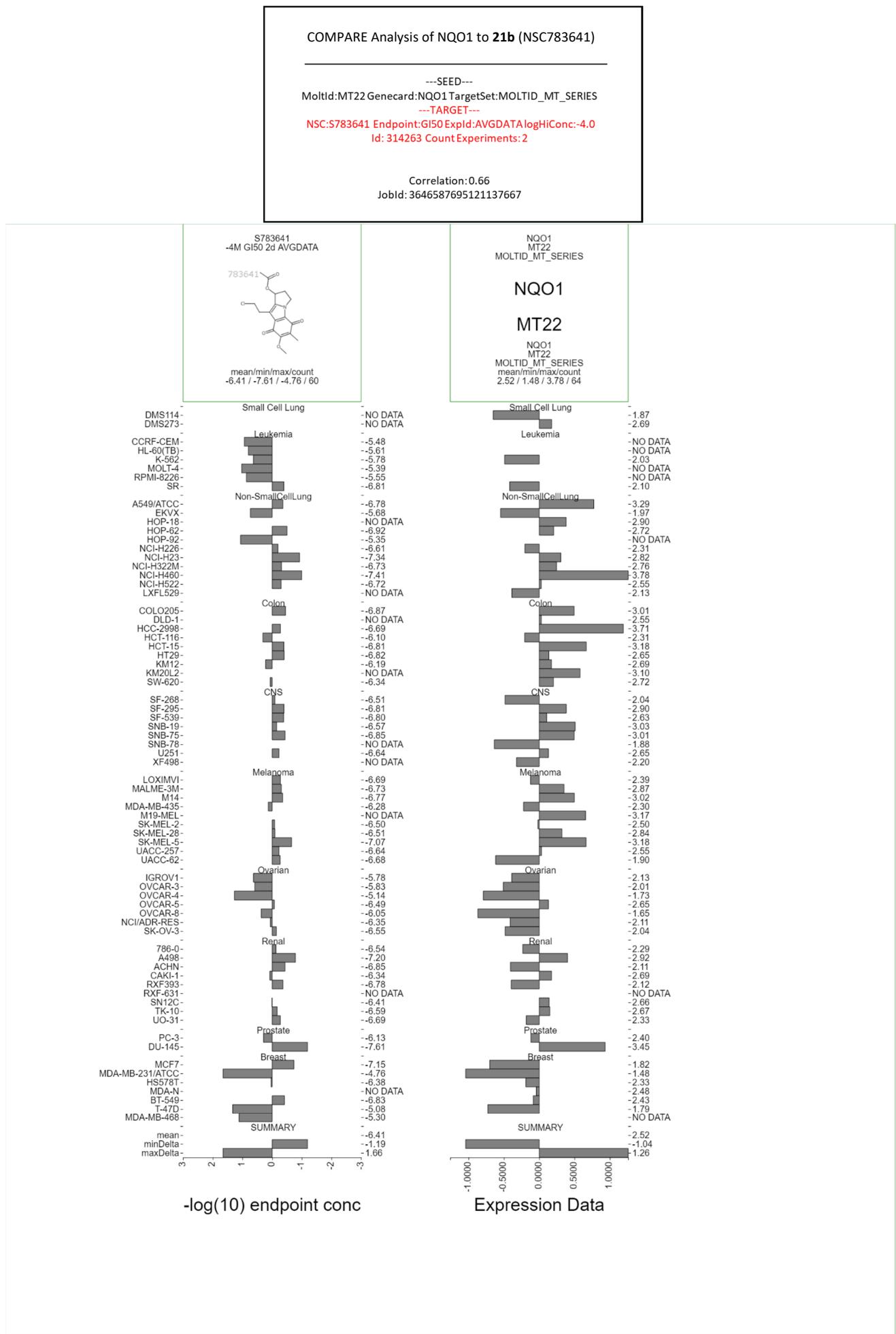


Figure S65

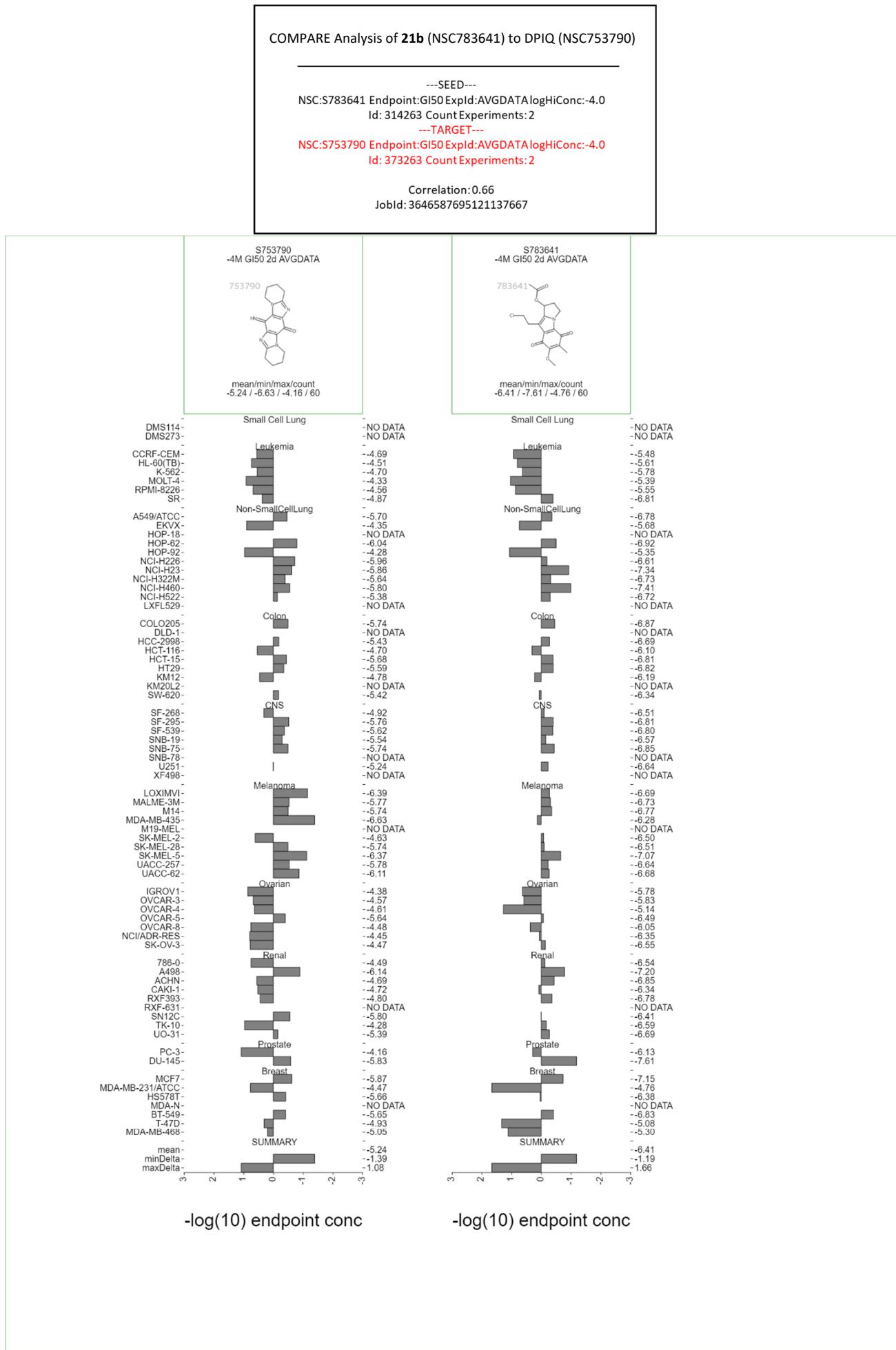


Figure S66

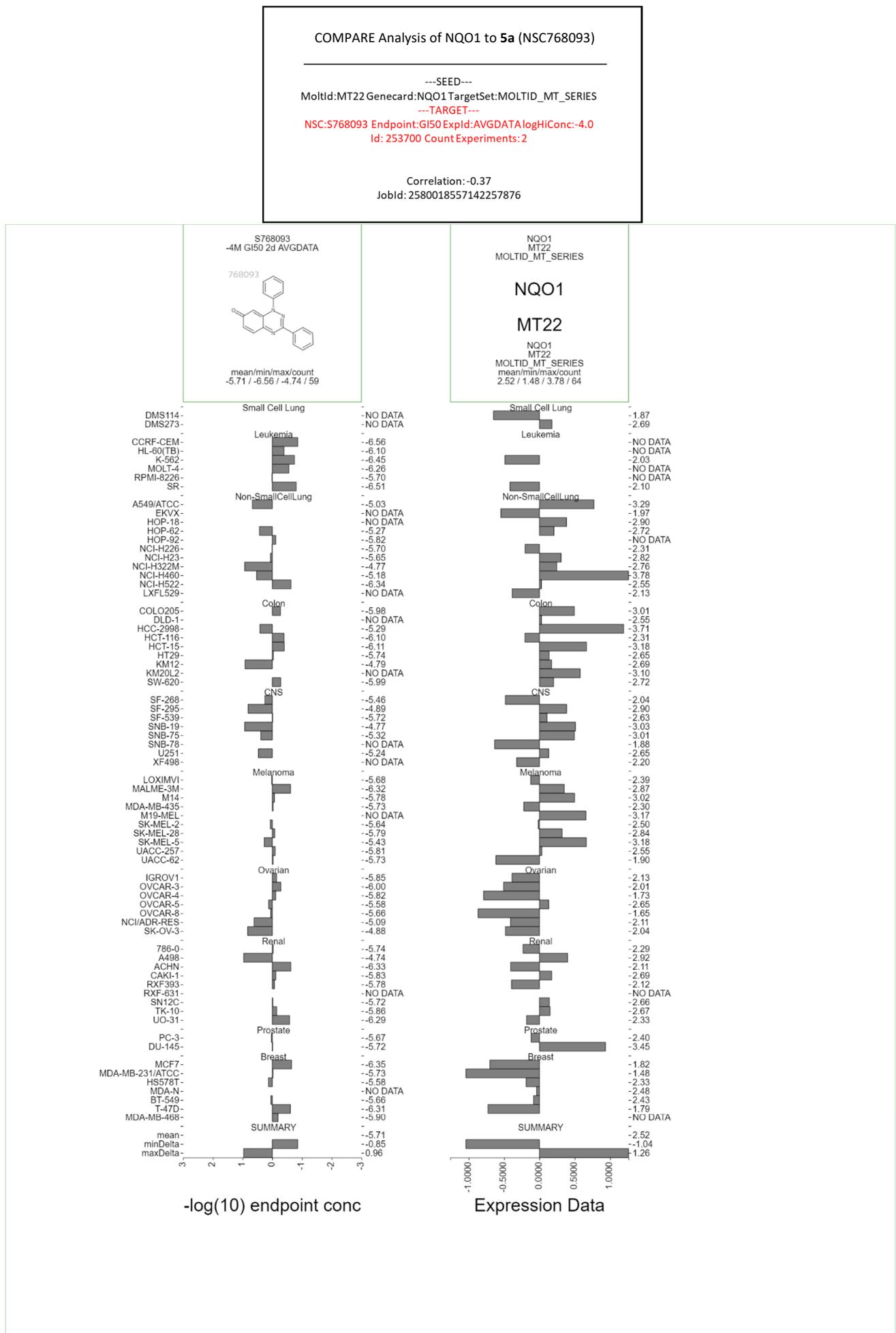


Figure S67

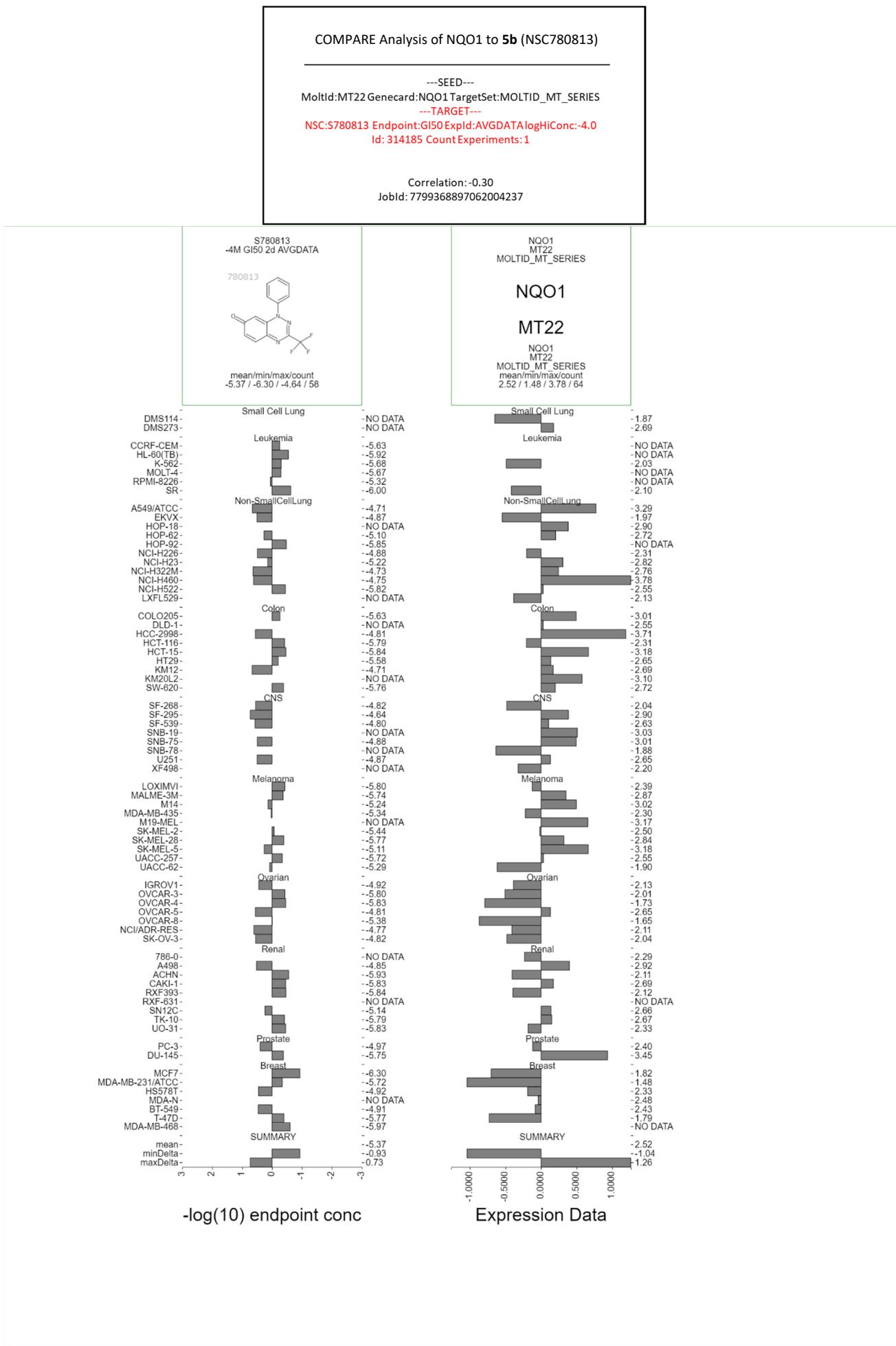


Figure S68

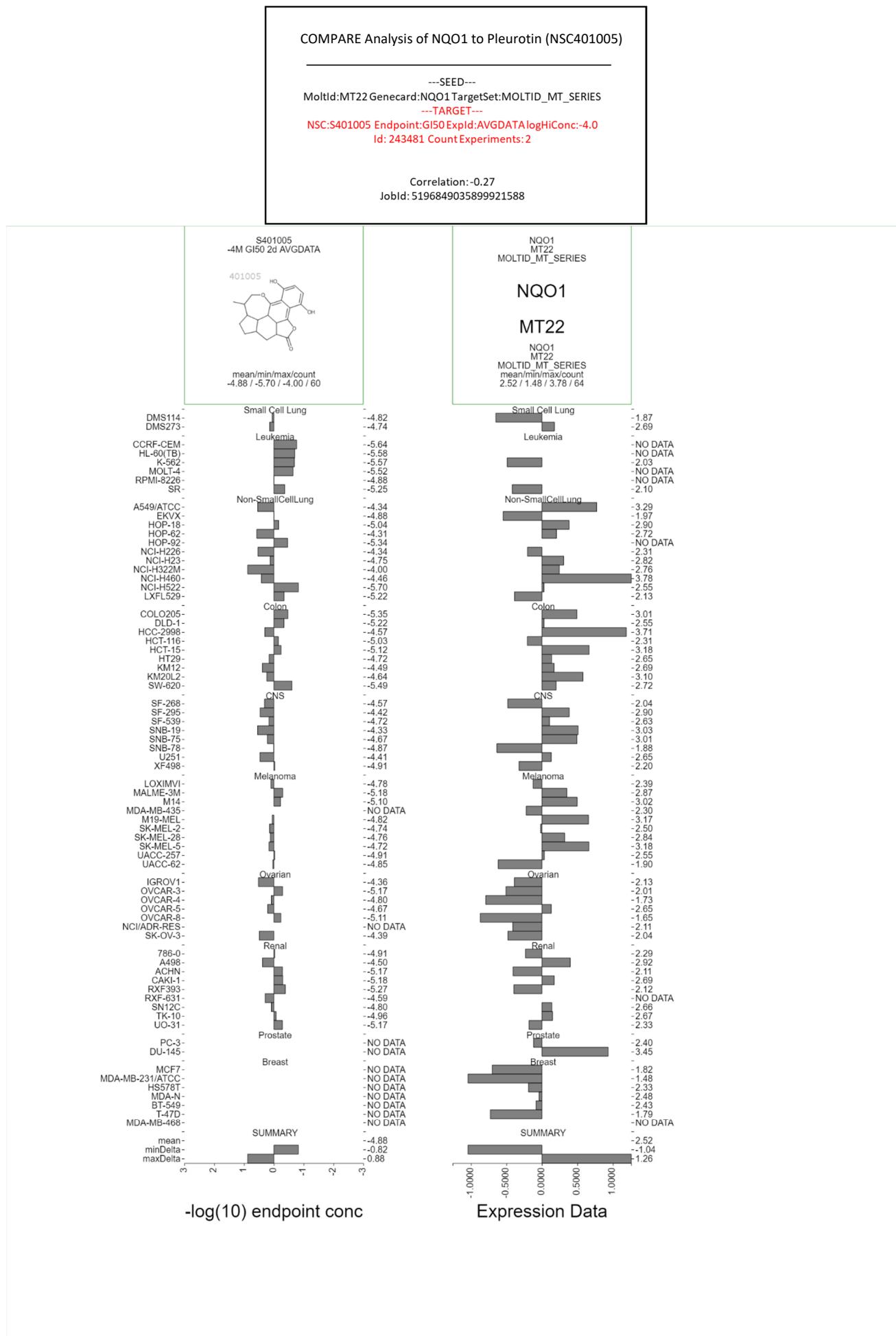


Figure S69

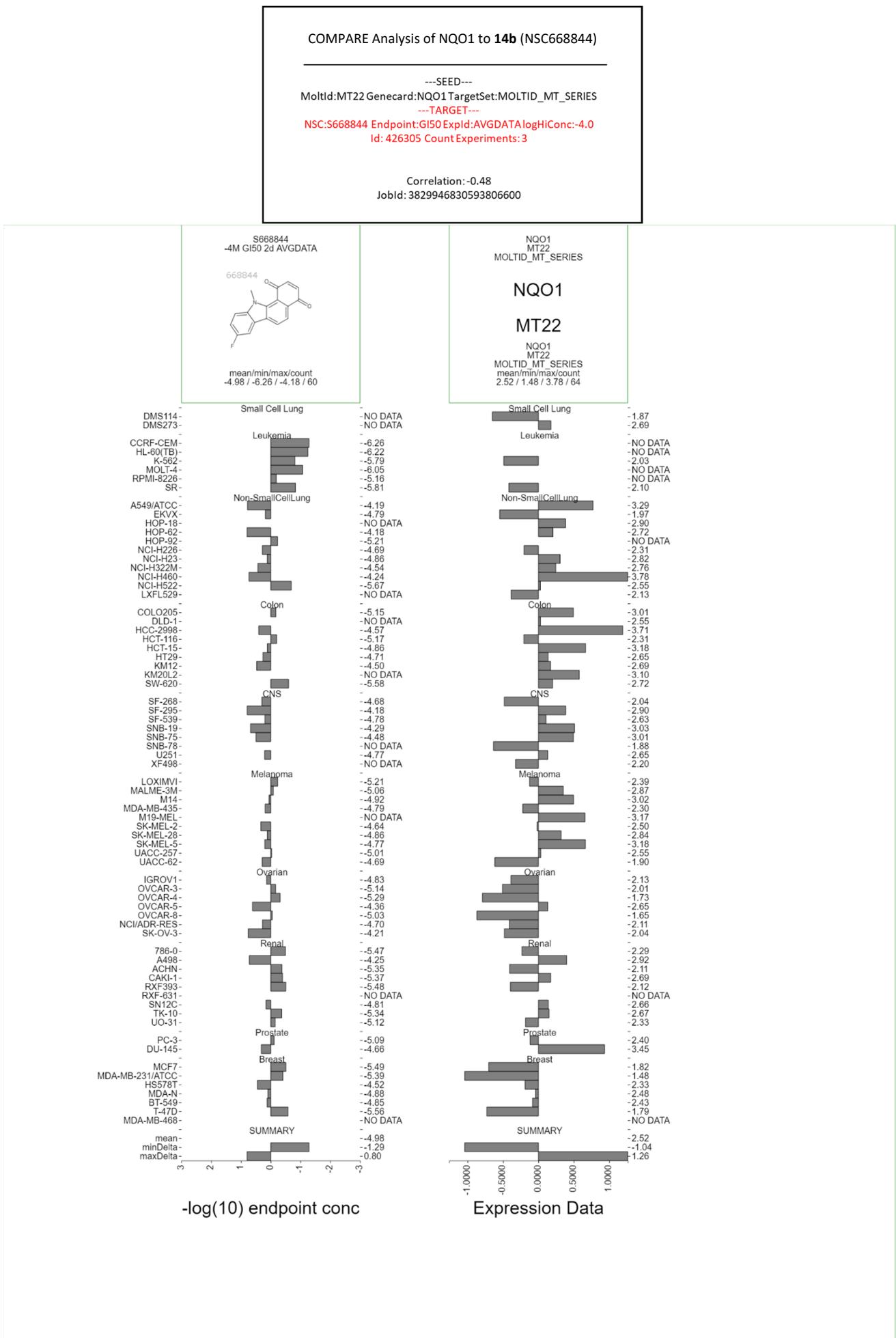


Figure S70

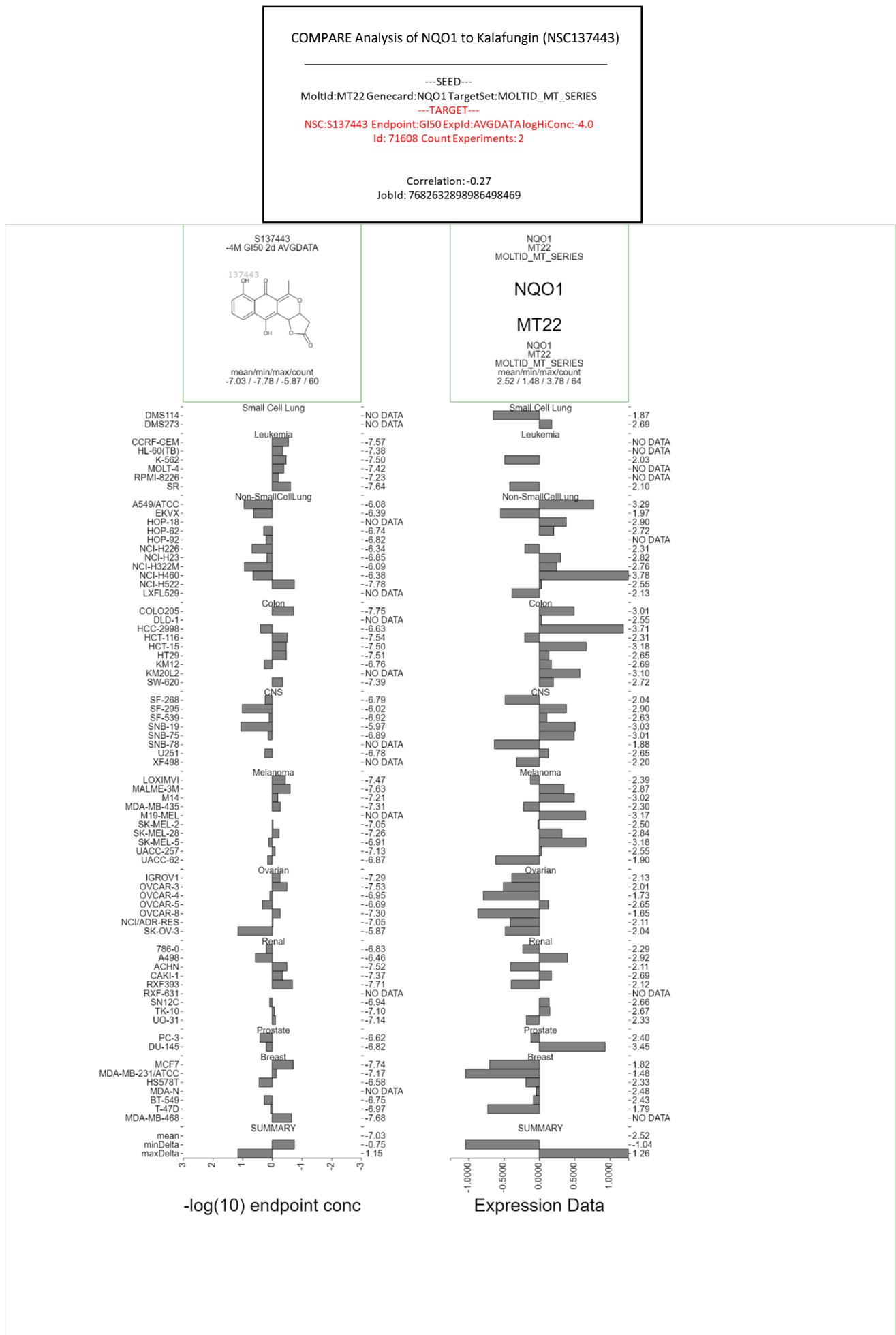


Figure S71

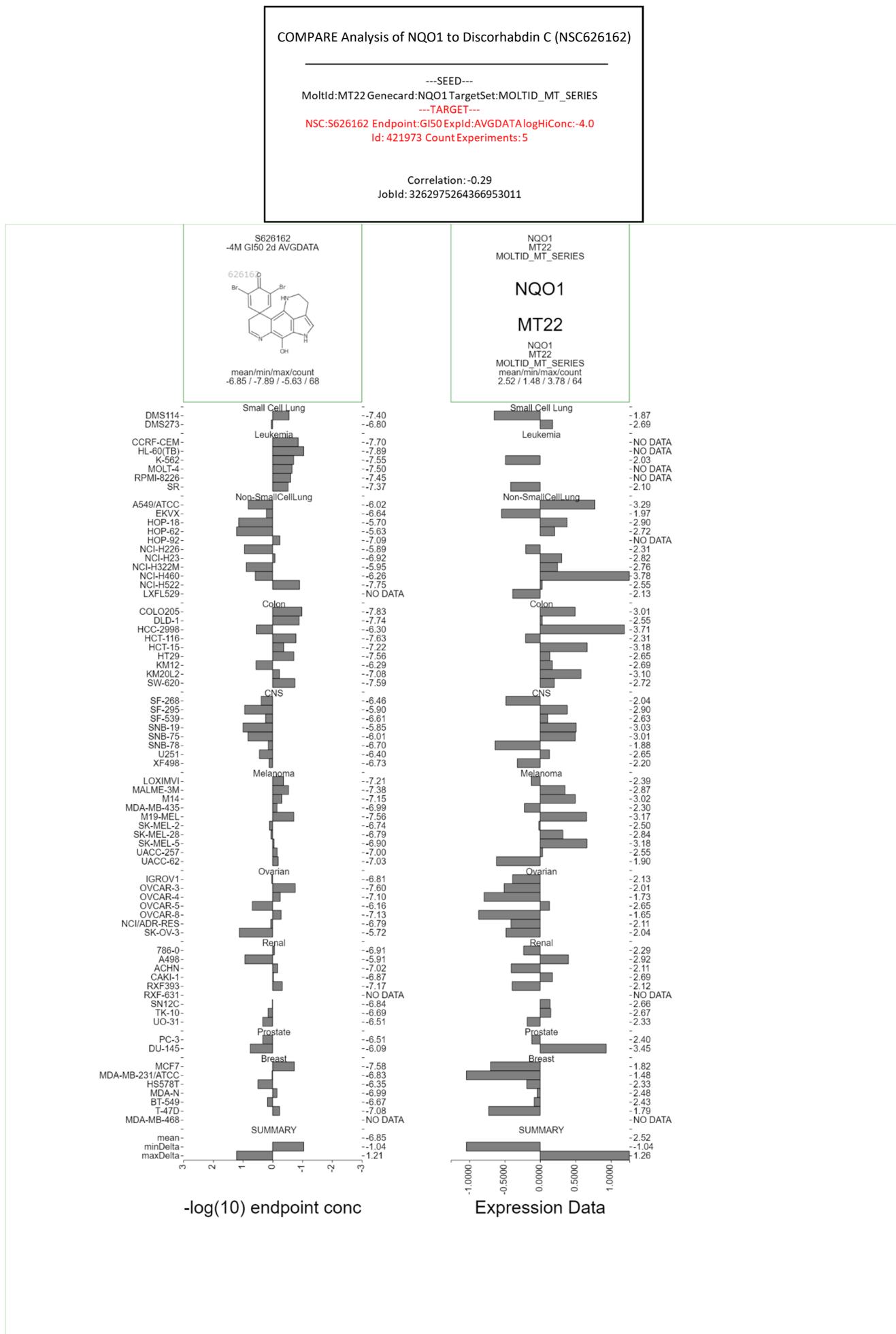


Figure S72

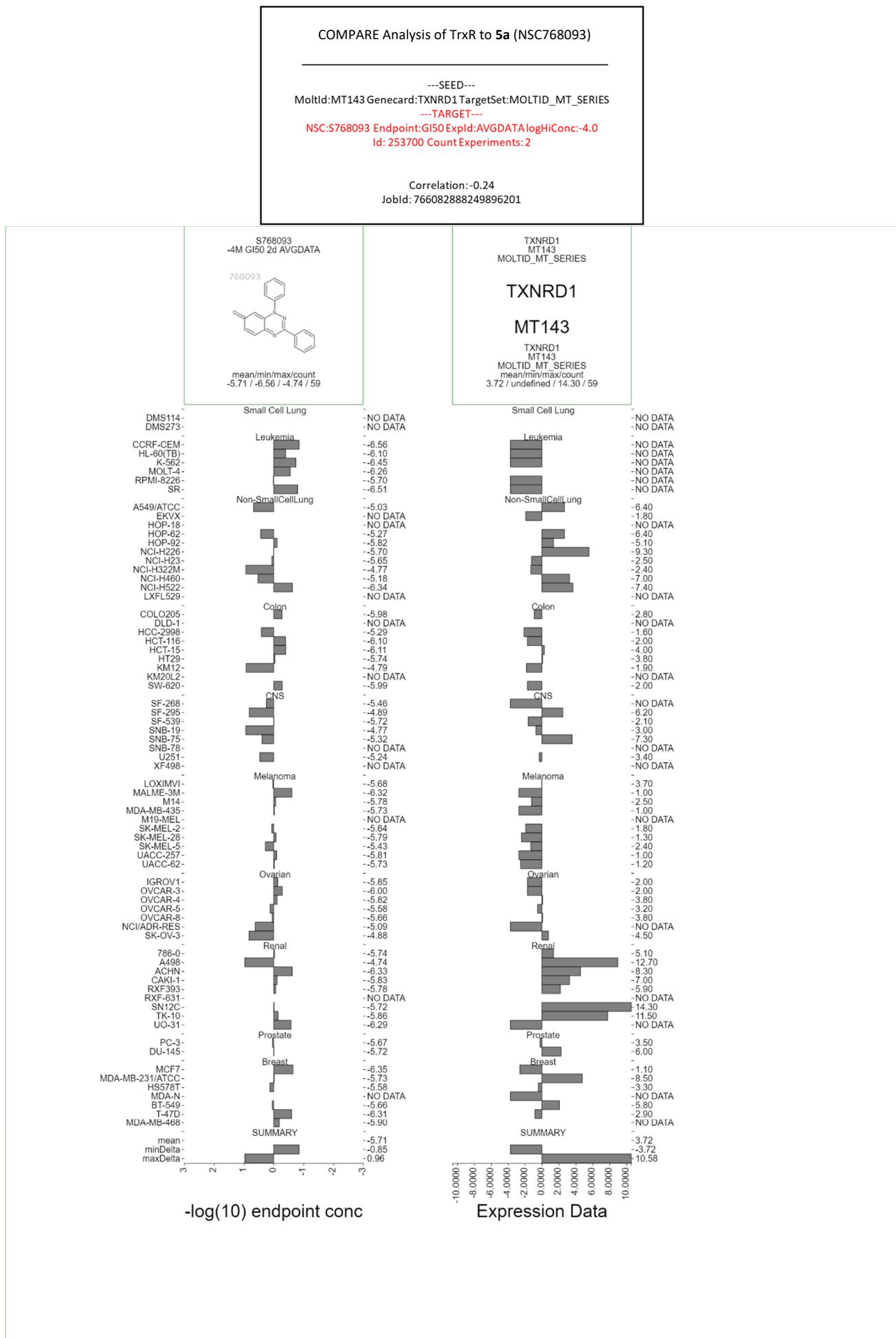


Figure S73

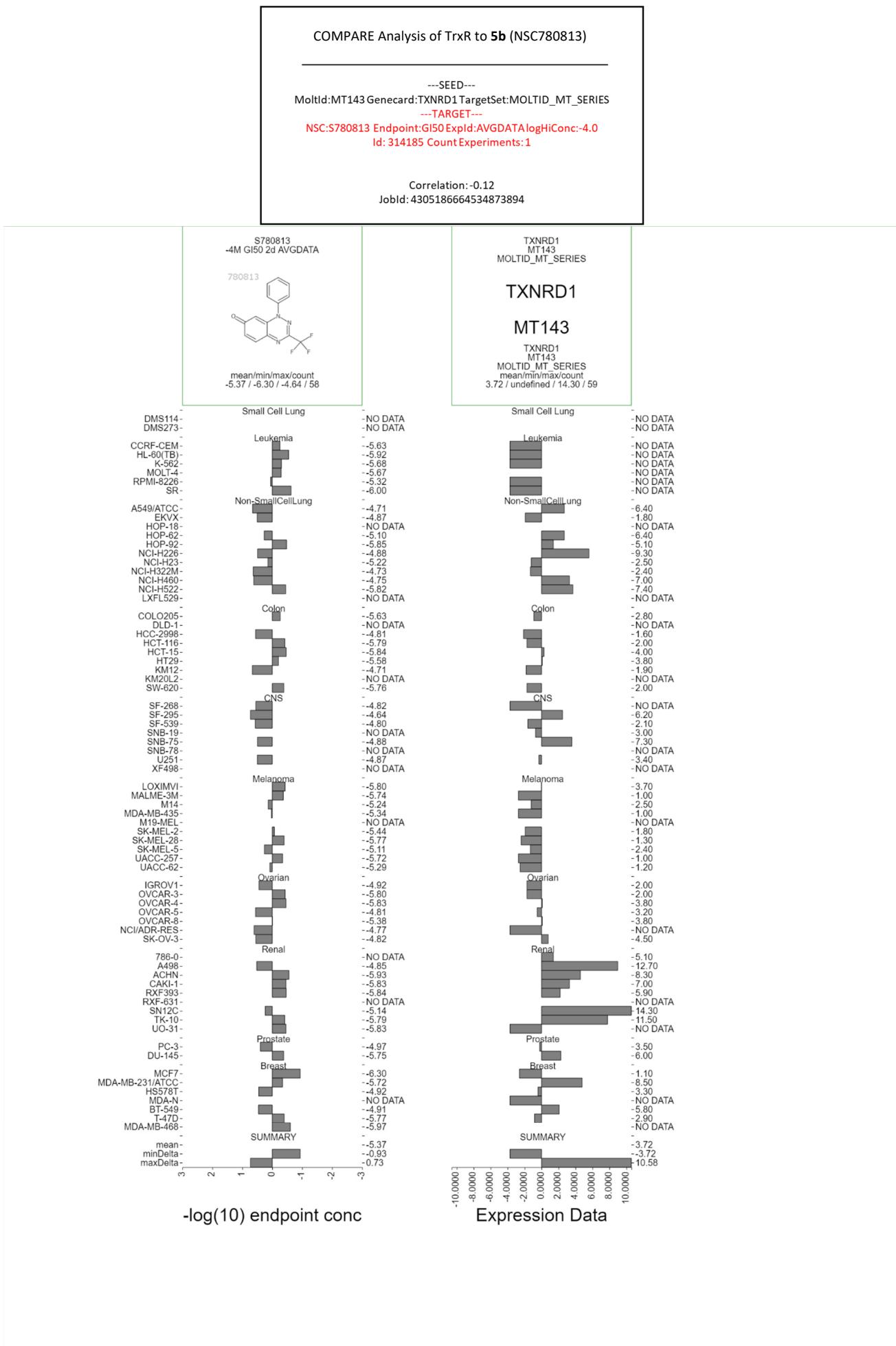


Figure S74

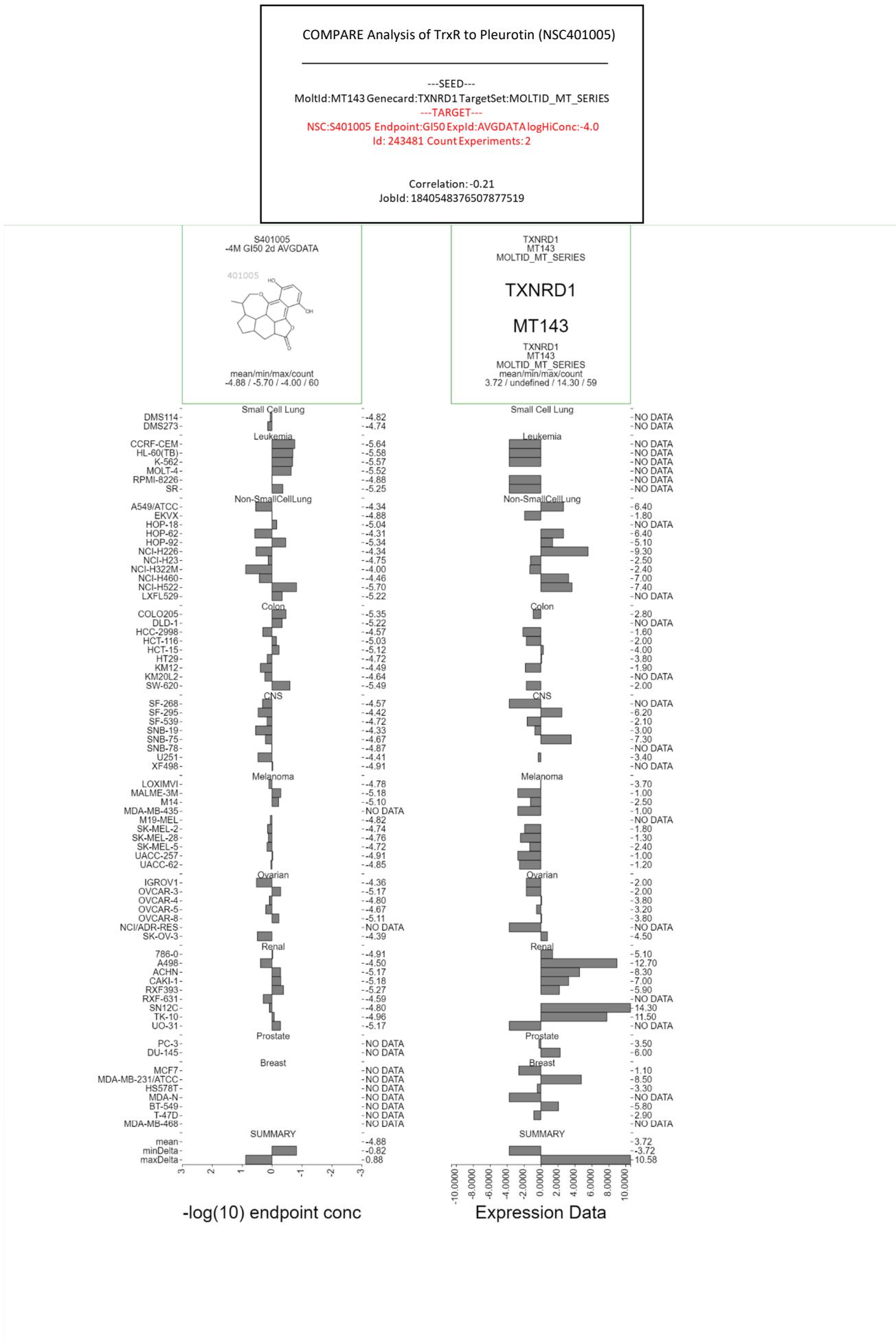


Figure S75

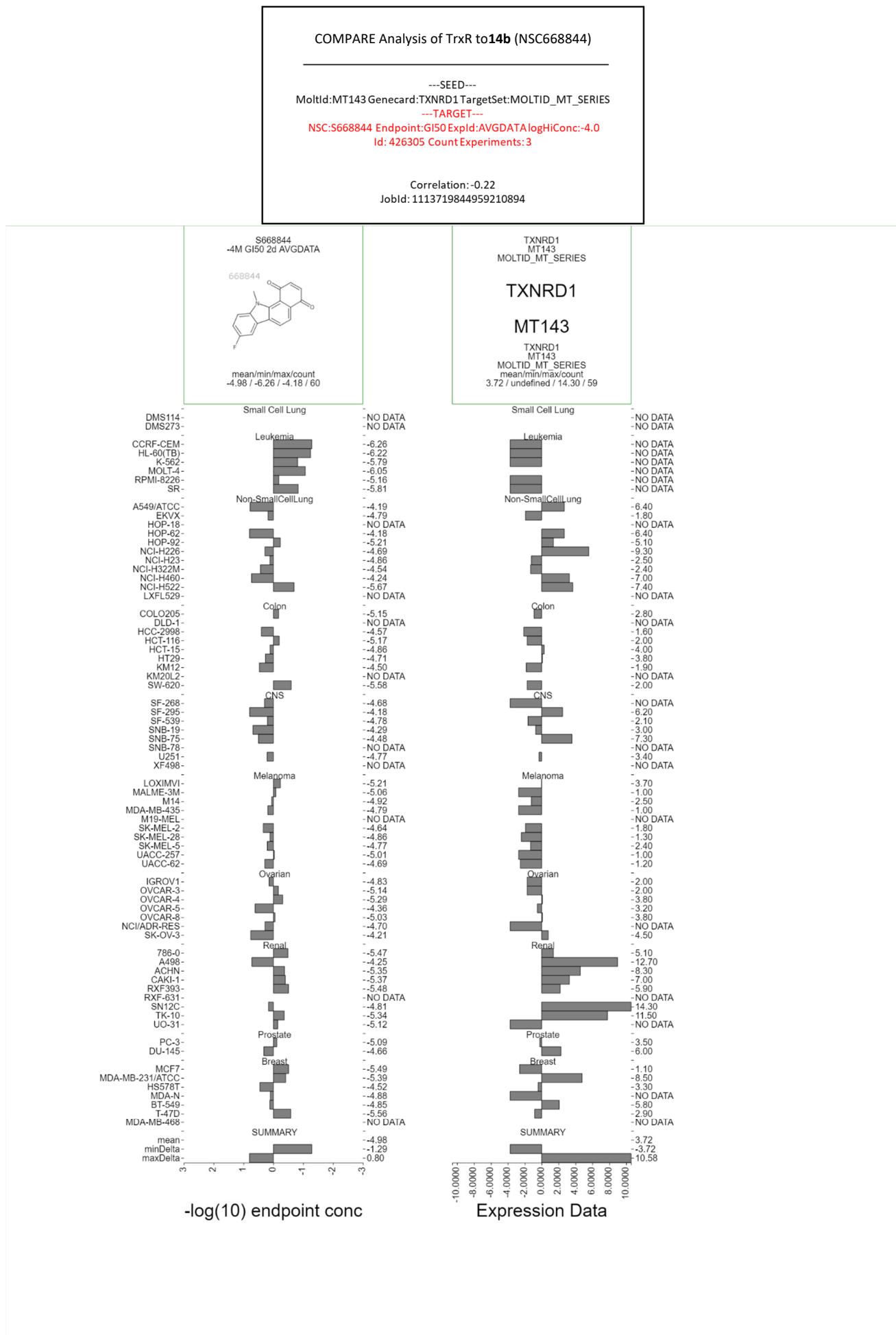


Figure S76

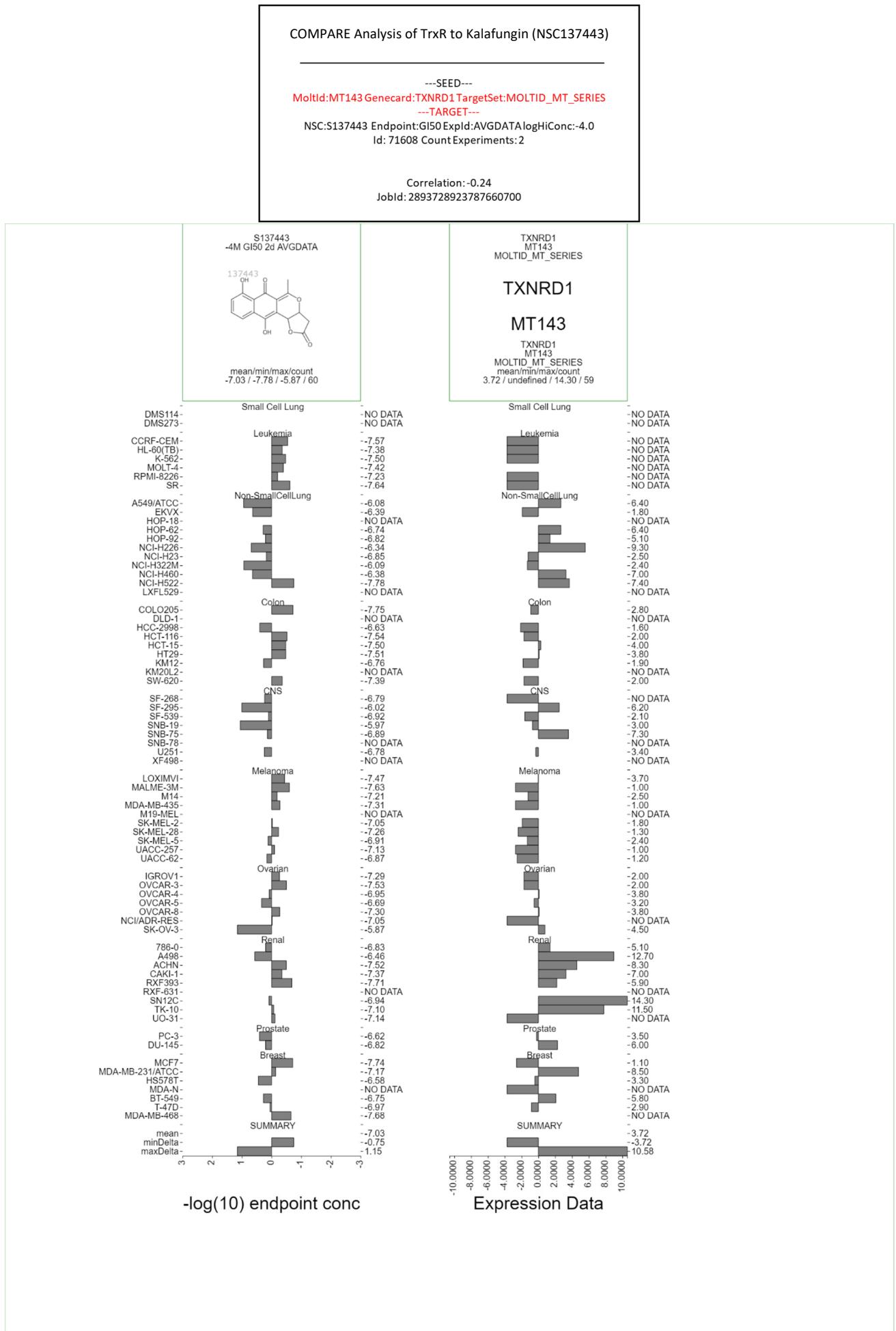


Figure S77

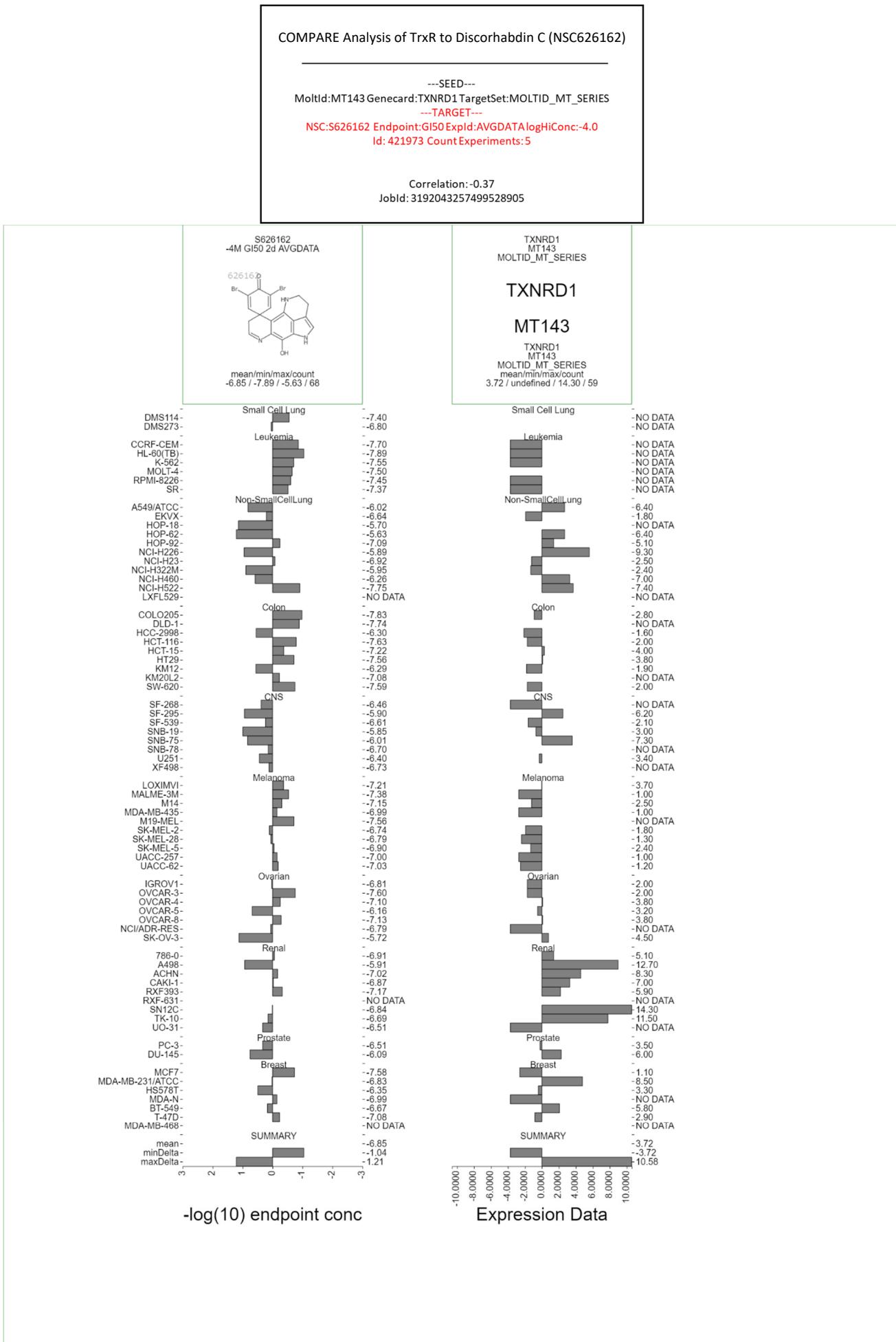


Figure S78

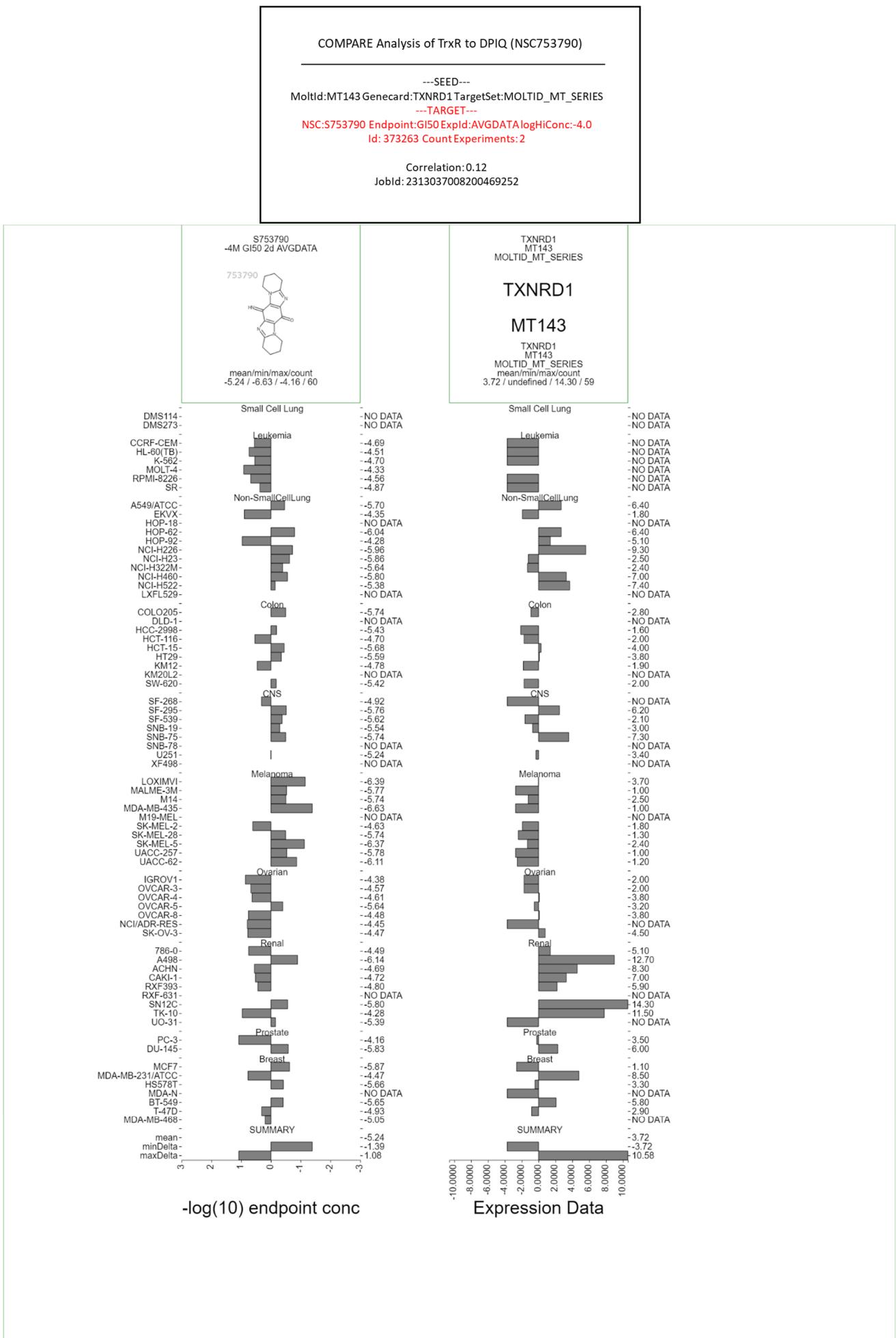


Figure S79

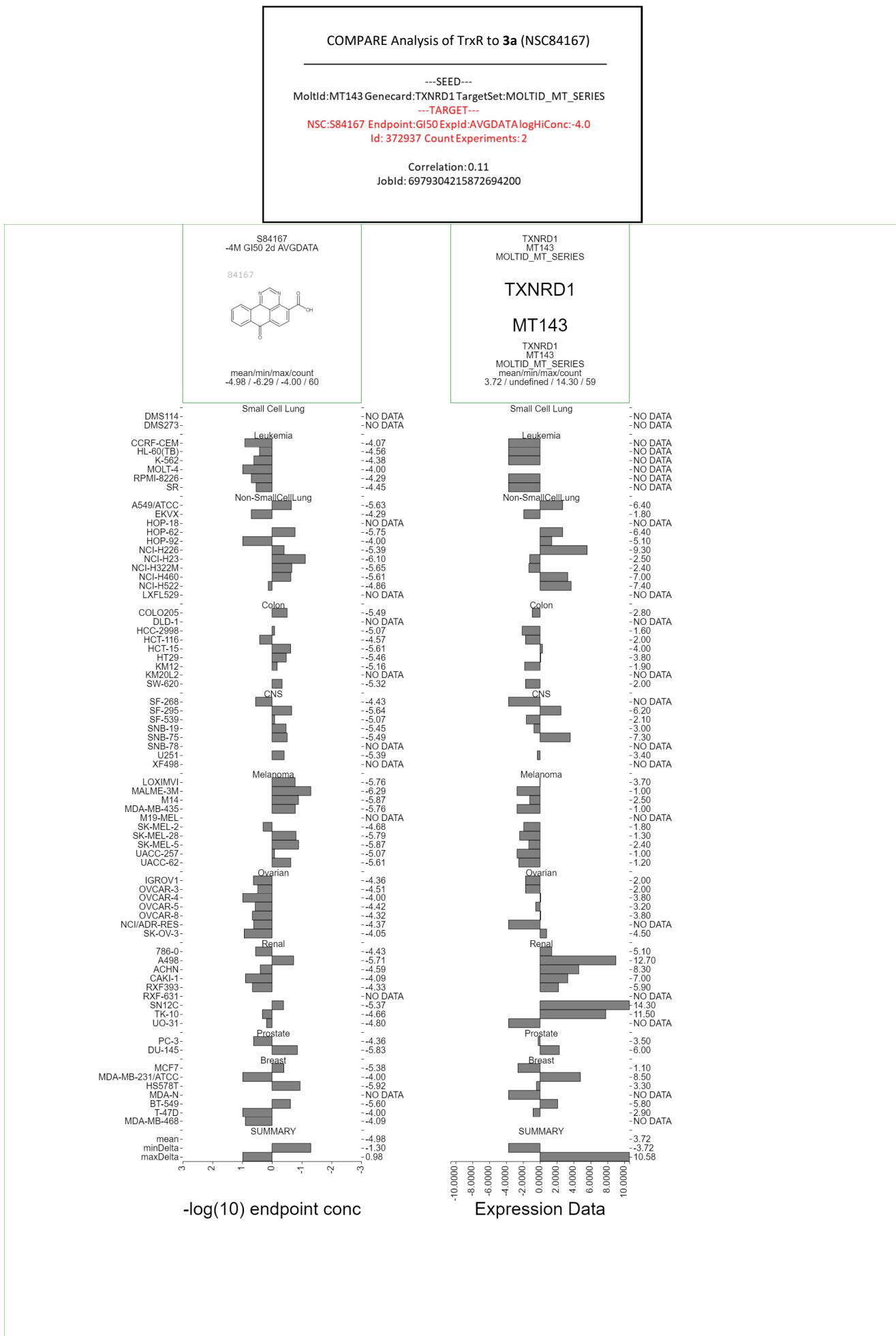


Figure S80

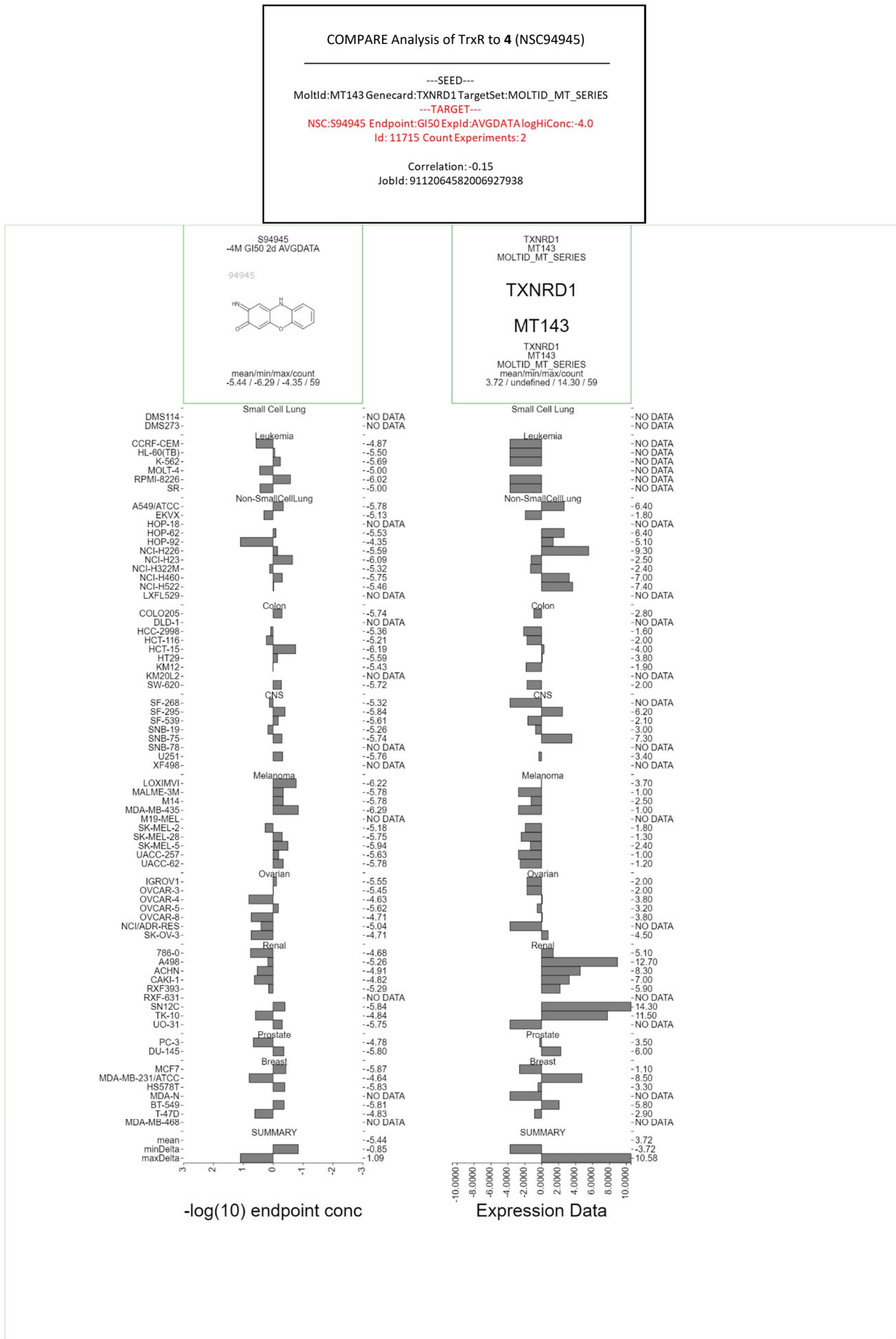


Figure S81

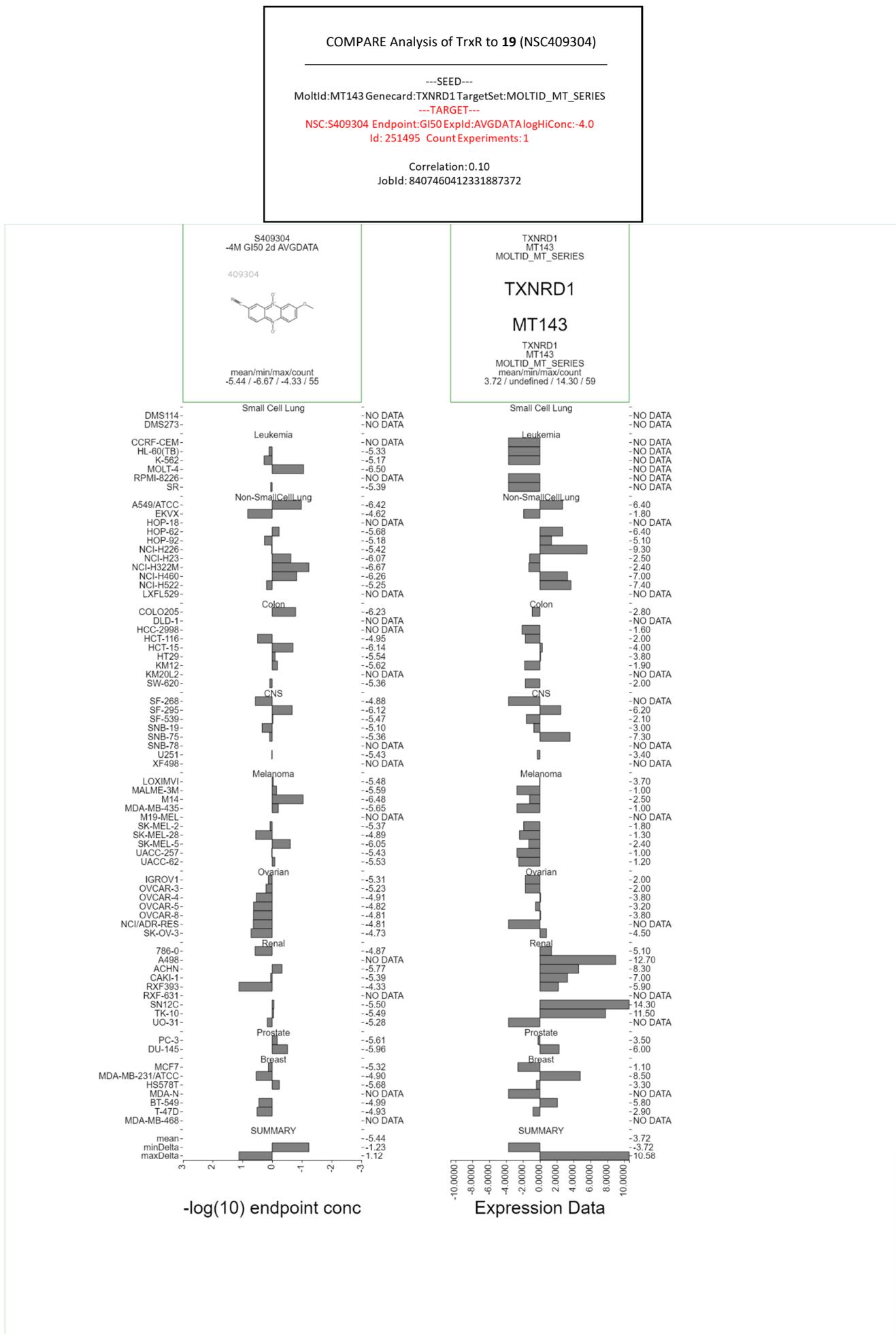


Figure S82