

**Supplemental Table 1.** NAD and known small molecule PARP-1 inhibitors. Column # 1 - formal and popular names for each small molecule; column # 2 - CID number; column # 3 - formulas in SMILES format; column #4 - skeletal formulas of each compound. Row 1 shows NAD; rows 2 - 24 show known PARP-1 inhibitors; row 25 shows Pyrrolocarbazole, derivatives of which have strong similarity to known PARP-1 inhibitors; rows 26 - 27 include minor groove binding molecules that have been shown to inhibit DNA-dependent PARP-1 activation [16].

	Name	CID	SMILES	
1	NAD	5893	<chem>C1=CC(=C[N+](=C1)C2C(C(C(O2)COP(=O)(O)OP(=O)(O)OCC3C(C(C(O3)N4C=NC5=C4N=CN=C5N)O)O)O)C(=O)N</chem>	
2	Nicotinamide	936	<chem>C1=CC(=CN=C1)C(=O)N</chem>	
3	3AB/ PARP inhib. I	1645	<chem>C1=CC(=CC(=C1)N)C(=O)N</chem>	
4	PARP Inhibitor II, INH2BP	72356	<chem>C1=CC(=O)OC2=C1C(=C(C=C2)N)I</chem>	
5	PARP Inhibitor III, DPQ	3164	<chem>C1CCN(CC1)CCCCOC2CNC(=O)C3=CC=CC=C23</chem>	
6	PARP Inhibitor IV, IQD	1340	<chem>C1=CC2=C(C=CNC2=O)C(=C1)O</chem>	
7	4-ANI/ PARP inhib. V	1720	<chem>C1=CC2=C(C=CC3=C2C(=C1)C(=O)NC3=O)N</chem>	
8	PARP Inhibitor VI, NU1025	63306	<chem>CC1=NC(=O)C2=C(N1)C(=CC=C2)O</chem>	
9	6(5H)-Phenanthridinone	1853	<chem>C1=CC=C2C(=C1)C3=C(C=CC=C3NC2=O</chem>	
10	PARP Inhibitor VIII, PJ34	16760621	<chem>CN(C)CC(=O)NC1=CC2=C(C=C1)NC(=O)C3=CC=CC=C32.Cl</chem>	
11	PARP Inhibitor IX, EB-47	16760406	<chem>C1CN(CCN1CC(=O)NC2=CC=CC3=C2CNC3=O)C(=O)C4C(C(C(O4)N5C=NC6=C5N=CN=C6N)O)O.O.Cl.Cl</chem>	
12	PARP inhibitor X, TIQ-A	9899130	<chem>C1=CC=C2C(=C1)C3=C(C=NC2=O)SC=C3</chem>	
13	PARP Inhibitor XI, DR2313	10219702	<chem>CC1=NC(=O)C2=C(N1)C=CSC2</chem>	
14	PARP Inhibitor XII	57347661	<chem>CC1=CC=C(C=C1)C2=N(C3=C(C=CC=C3N=C2)C(=O)N</chem>	
15	PARP Inhibitor XV, UPF-1035	659976	<chem>C1=CC=C(C=C1)C(=O)OC2=CC=CC3=C2C=NC3=O</chem>	
16	Olaparib	23725625	<chem>C1CC1C(=O)N2CCN(CC2)C(=O)C3=C(C=CC(=C3)CC4=NNC(=O)C5=CC=CC=C54)F</chem>	
17	ABT-888 (Veliparib)	11960529	<chem>CC1(CCCN1)C2=NC3=C(C=CC=C3N2)C(=O)N</chem>	

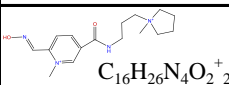
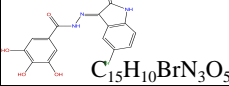
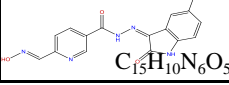
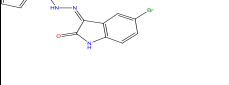
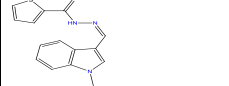
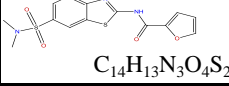
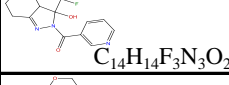
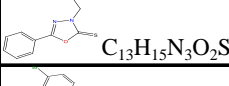
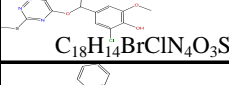
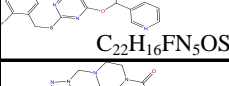
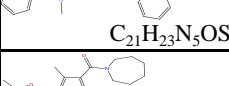
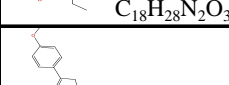
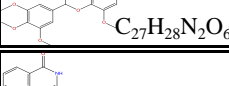
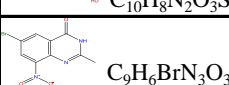
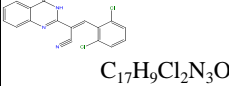
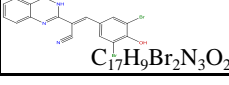

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19	BSI-201 Iniparib	9796068	<chem>C1=CC(=C(C=C1C(=O)N)[N+](=O)[O-])I</chem>	
20	AG14361	9840076	<chem>CN(C)CC1=CC=C(C=C1)C2=NC3=CC=CC4=C3N2CCNC4=O</chem>	
21	A-966492	16665853	<chem>C1CC(NC1)C2=CC(=C(C=C2)C3=NC4=C(C=CC=C4N3)C(=O)N)F</chem>	
22	MK-4827	24958200	<chem>C1CC(NC1)C2=CC(=C(C=C2)N3C=C4C=CC=C(C4=N3)C(=O)N</chem>	
23	BYK49187	15285131	<chem>CC1=C(N=CN1)C2CCN(CC2)C3=NC4=CC=CC5=C4N3CCCC5=O</chem>	
24	BYK20370	25113763	<chem>CC1=C(N2C=C(C=C(C2=N1)O)Cl)C</chem>	
25	Pyrrolocarbazole derivative (only similar to published inh.)	58890072	<chem>C1CC2=C(CCC1=O)C3=C(C4C2NC5=CC=CC=C45)C(=O)NC3=O</chem>	
26	Diminazene	2354	<chem>C1=CC(=CC=C1C(=N)N)NN=NC2=CC=C(C=C2)C(=N)N</chem>	
27	Hoechst 33342	1464	<chem>CCOC1=CC=C(C=C1)C2=NC3=C(N2)C=C(C=C3)C4=NC5=C(N4)C=C(C=C5)N6CCN(CC6)C</chem>	

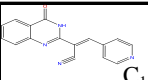
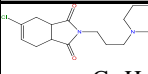
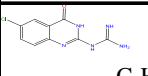
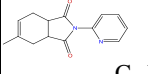
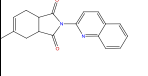
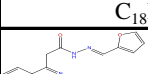
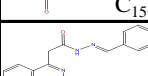
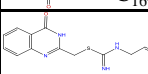
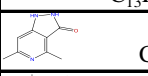
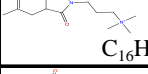
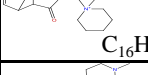
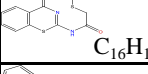
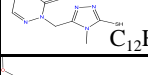
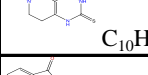
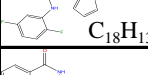
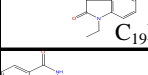
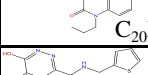
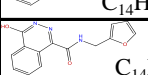
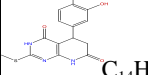

**Supplemental Table 2.** The results of pilot screen of ICCB known bioactivities. Column # 1 shows the values of PARP-1 inhibition; column # 2 – the plate number and the position on the plate; column # 3 – name of each small molecule; column # 4 – known biological activity.

<b>Value</b>	<b>Position</b>	<b>NAME</b>	
1.22	2-H9	A-23187	Calcium ionophore
2.34	3-C2	Loperamide	Calcium channels
2.01	3-D6	PCO-400	Potassium channels
2.07	4-A4	b-Lapachone	topoisomerase 1 inhibitor
2.06	4-A5	Parthenolide	IkappaB kinase inhibitor
1.89	4-A9	Cycloheximide-N-ethylethanoate	FKBP12 inhibitor
0.05	4-B2	Ebselen	glutathione peroxidase mimetic
1.28	4-C7	AG213 (Tyrphostin 47)	EGF-R tyrosine kinase inhibitor
0.05	4-D6	Amino-1,8-naphthalimide [4-Amino-1,8-naphthalimide]	PARP inhibitor
2.03	4-H11	Cytochalasin B	F actin capper
2.00	5-A6	Decoyinine	lowers GTP levels
2.01	5-A9	Dexamethasone	corticosteroid
0.50	5-B3	6,7-ADTN HBr	Dopamine agonist
0.20	5-B5	Diphenyleneiodonium Cl	flavoprotein inhibitor
0.05	5-D6	H9	kinase inhibitor
0.94	5-E8	IBMX	PDE inhibitor (broad spec), adenosineR agonist
0.69	6-A9	PD 98059	MEK inhibitor
0.05	6-B2	Phenanthridinone [6(5H)-Phenanthridinone]	PARP inhibitor
0.18	6-B10	Propidium iodide	DNA intercalator
0.18	6-C5	Quercetin	kinase inhibitor (plus other)
1.25	6-D6	Indirubin	GSK-3beta inhibitor
1.43	6-D11	Piceatannol	Syk inhibitor
1.90	6-H11	Wiskostatin	N-WASP inhibitor
0.18	4-D7	3AB	PARP inhibitor

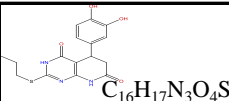
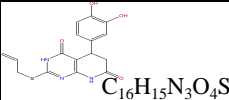
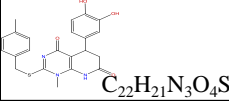
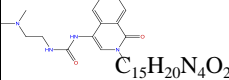
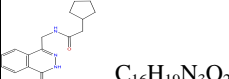
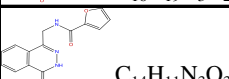
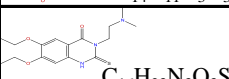

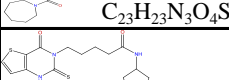
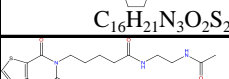
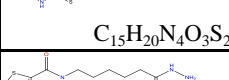
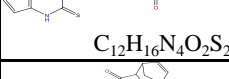
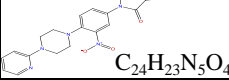
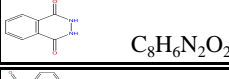
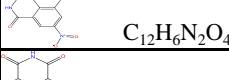
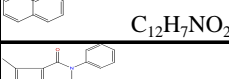
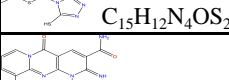
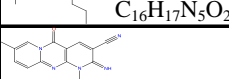
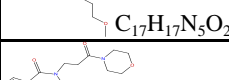
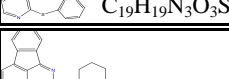
**Supplemental Table 3-1 -- 3-11.** Structural classification of 639 compounds identified as PARP-1 inhibitors by the H4-based screen. Small molecules were classified based on the presence of specific structural cores: **S3-1** – Nicotinamide/Benzamide; **S3-2** - PARP Inhibitor II; **S3-3** - Adenine/Caffeine; **S3-4** - Benzimidazole; **S3-5** - Benzothiazole; **S3-6** - Indole; **S3-7** - Benzofurazan; **S3-8** - 5-imino-5,6-dihydro-7H-[1,3,4]thiadiazolo[3,2-a]pyrimidin-7-one; **S3-9** - Quinoline; **S3-10** - Naphtalene; **S3-11** contains 345 new PARP-1 inhibitors without obvious structural core similarities to other groups. Column # 1 lists the ID number of each small molecule according to the ChemDiv company catalogue; column # 2 – the number of plate in the collection; column # 3 – the position on the plate; column # 4 – skeletal structure of the molecule; column # 5 and 6 – similarity to known PARP-1 inhibitor.

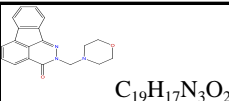
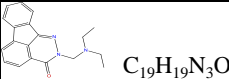
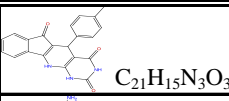


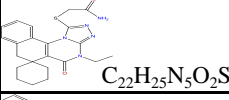
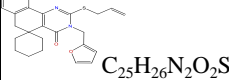
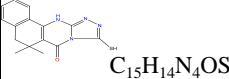
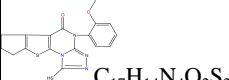
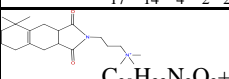
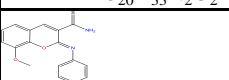
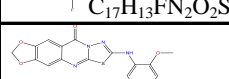
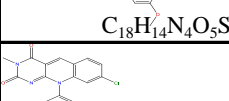
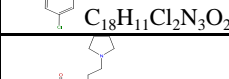
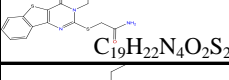
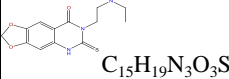
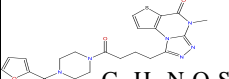
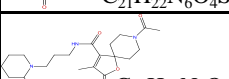
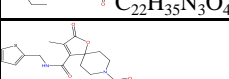
## S3-1 – Nicotinamide/Benzamide

	1	2	3	4	5	6
1	1546-0014	001	C07	 <chem>C16H26N4O2+</chem>	Nicotinamide	
2	2451-0081	002	C02	 <chem>C15H10BrN3O5</chem>	Benzamide/ Indole/ MGB	
3	5556-0387	003	F09	 <chem>C15H10N6O5</chem>	Nicotinamide	
4	1719-1296	001	G08	 <chem>C13H8BrN3O2S</chem>	Substituted Amino- benzamide/ Indole/ MGB	
5	1719-1336	001	H08	 <chem>C15H13N3OS</chem>	Substituted Aminobenzami de/ Indole/ MGB	
6	G786-1566	008	D06	 <chem>C14H13N3O4S2</chem>	Substituted Benzamide?/ Benzothiazole	
7	4607-0208	002	H09	 <chem>C14H14F3N3O2</chem>	Nicotinamide	
8	4719-0299	002	H10	 <chem>C13H15N3O2S</chem>	Benzamide like	
9	4896-3465	003	G02	 <chem>C18H14BrClN4O3S</chem>	Benzamide?	
10	4896-4210	003	A03	 <chem>C22H16FN5OS</chem>	Nicotinamide?	
11	6220-0542	004	H10	 <chem>C21H23N5OS</chem>	Benzamide	
12	C722-0493	007	D08	 <chem>C18H28N2O3</chem>	Substituted Benzamide?	
13	K805-0558	008	F10	 <chem>C27H28N2O6</chem>	Benzamide?	
14	1203-0064	001	E04	 <chem>C10H8N2O3S</chem>	Benzamide	493800 <i>PARP</i> <i>Inhibitor</i> VI, NU1025
15	3606-0037	002	C04	 <chem>C9H6BrN3O3</chem>	Benzamide	493800 <i>PARP</i> <i>Inhibitor</i> VI, NU1025
16	3643-1604	002	H04	 <chem>C17H9Cl2N3O</chem>	Benzamide	493800 <i>PARP</i> <i>Inhibitor</i> VI, NU1025
17	3643-1638	002	A05	 <chem>C17H9Br2N3O2</chem>	Benzamide	493800 <i>PARP</i> <i>Inhibitor</i> VI, NU1025

18	3643-1655	002	B05	 C <sub>16</sub> H <sub>10</sub> N <sub>4</sub> O	Benzamide	493800 <i>PARP Inhibitor VI</i> , NU1025
19	4142-0922	002	G07	 C <sub>16</sub> H <sub>23</sub> ClN <sub>2</sub> O <sub>2</sub>	Substituted Amino- benzamide	<i>PARP Inhibitor IX</i> , EB47
20	4243-0150	002	G08	 C <sub>9</sub> H <sub>8</sub> ClN <sub>5</sub> O	Benzamide	493800 <i>PARP Inhibitor VI</i> , NU1025
21	4493-0928	002	C09	 C <sub>14</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>	Substituted Aminobenzami ne/ Pyridine	<i>PARP Inhibitor IX</i> , EB47
22	4493-0929	002	D09	 C <sub>18</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	Substituted Amino- benzamide/ Quinoxaline	<i>PARP Inhibitor IX</i> , EB47
23	4994-0433	003	H03	 C <sub>15</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub>	Benzamide	Olaparib (AZD2281)
24	4994-0542	003	A04	 C <sub>16</sub> H <sub>13</sub> N <sub>5</sub> O <sub>2</sub>	Benzamide	Olaparib (AZD2281)
25	5742-0594	004	D02	 C <sub>13</sub> H <sub>14</sub> N <sub>4</sub> OS	Benzamide	493800 <i>PARP Inhibitor VI</i> , NU1025
26	5947-0056	004	B05	 C <sub>8</sub> H <sub>9</sub> N <sub>3</sub> O	Nicotinamide	<i>PARP Inhibitor IX</i> , EB47
27	6228-0215	004	B11	 C <sub>16</sub> H <sub>27</sub> N <sub>2</sub> O <sub>2</sub> +	Benzamide?	<i>PARP Inhibitor IX</i> , EB47
28	6228-0595	005	E02	 C <sub>16</sub> H <sub>23</sub> N <sub>2</sub> O <sub>2</sub> +	Substituted Benzamide?	<i>PARP Inhibitor IX</i> , EB47
29	6359-0109	005	H06	 C <sub>16</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub> S <sub>3</sub>	Benzamide	493800 <i>PARP Inhibitor VI</i> , NU1025
30	7832-0165	006	A06	 C <sub>12</sub> H <sub>11</sub> N <sub>5</sub> OS	Benzamide	Olaparib (AZD2281)
31	C200-2670	006	F08	 C <sub>10</sub> H <sub>15</sub> N <sub>3</sub> O <sub>2</sub> S	Substituted Benzamide?	493800 <i>PARP Inhibitor VI</i> , NU1025
32	C612-0960	007	G06	 C <sub>18</sub> H <sub>13</sub> F <sub>2</sub> N <sub>3</sub> OS	Nicotinamide	<i>PARP Inhibitor IX</i> , EB47
33	D163-0928	007	B10	 C <sub>19</sub> H <sub>17</sub> N <sub>3</sub> O <sub>2</sub>	Benzamide	493800 <i>PARP Inhibitor VI</i> , NU1025
34	D163-0929	007	C10	 C <sub>20</sub> H <sub>19</sub> N <sub>3</sub> O <sub>2</sub>	Benzamide	493800 <i>PARP Inhibitor VI</i> , NU1026
35	D216-0576	007	E10	 C <sub>14</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub> S	Benzamide?	Olaparib (AZD2281)
36	D216-0577	007	F10	 C <sub>14</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub>	Benzamide?	Olaparib (AZD2281)
37	D271-0001	007	H10	 C <sub>14</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub> S	Nicotin-amide?	493800 <i>PARP Inhibitor VI</i> , NU1026

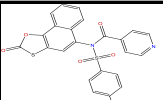


38	D271-0003	007	A11	 C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> O <sub>4</sub> S	Nicotin-amide?	493800 <i>PARP Inhibitor VI</i> , NU1026
39	D271-0004	007	B11	 C <sub>16</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub> S	Nicotin-amide?	493800 <i>PARP Inhibitor VI</i> , NU1026
40	D271-0394	007	C11	 C <sub>22</sub> H <sub>21</sub> N <sub>3</sub> O <sub>4</sub> S	Nicotin-amide?	493800 <i>PARP Inhibitor VI</i> , NU1026
41	E679-0352	008	E03	 C <sub>15</sub> H <sub>20</sub> N <sub>4</sub> O <sub>2</sub>	Benzamide	300270 <i>PARP Inhibitor III</i> , DPQ
42	G786-2274	008	E06	 C <sub>16</sub> H <sub>19</sub> N <sub>3</sub> O <sub>2</sub>	Benzamide	Olaparib (AZD2281)
43	G786-2313	008	F06	 C <sub>14</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub>	Benzamide	Olaparib (AZD2281)
44	K284-7470	008	F08	 C <sub>16</sub> H <sub>23</sub> N <sub>3</sub> O <sub>3</sub> S	Benzamide	493800 <i>PARP Inhibitor VI</i> , NU1025
45	K288-0565	008	G08	 C <sub>23</sub> H <sub>23</sub> N <sub>3</sub> O <sub>4</sub> S	Benzamide	493800 <i>PARP Inhibitor VI</i> , NU1025
46	K292-1481	008	H08	 C <sub>16</sub> H <sub>21</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>	Substituted Benzamide?	528819 <i>PARP Inhibitor XI</i> , DR2313
47	K292-1552	008	A09	 C <sub>15</sub> H <sub>20</sub> N <sub>4</sub> O <sub>3</sub> S <sub>2</sub>	Substituted Benzamide?	528819 <i>PARP Inhibitor XI</i> , DR2313
48	K292-1560	008	B09	 C <sub>12</sub> H <sub>16</sub> N <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	Substituted Benzamide?	528819 <i>PARP Inhibitor XI</i> , DR2313
49	K807-1169	008	G10	 C <sub>24</sub> H <sub>23</sub> N <sub>5</sub> O <sub>4</sub>	Substituted Benzamide?	<i>PARP Inhibitor IX</i> , EB47
50	P38803_AL DRICH	008	F11	 C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	Benzamide	Olaparib (AZD2281)
51	2248-4802	001	E11	 C <sub>12</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>	Benzamide	4ANI, <i>PARP inhib. V</i>
52	N1658_AL DRICH	001	D11	 C <sub>12</sub> H <sub>7</sub> NO <sub>2</sub>	Benzamide	4ANI, <i>PARP inhib. V</i>
53	4159-0181	002	B08	 C <sub>15</sub> H <sub>12</sub> N <sub>4</sub> OS <sub>2</sub>	Substituted Amino-	Phenanthridinone
54	5282-0578	003	H06	 C <sub>16</sub> H <sub>17</sub> N <sub>5</sub> O <sub>2</sub>	Nicotinamide	
55	5282-0891	003	A07	 C <sub>17</sub> H <sub>17</sub> N <sub>5</sub> O <sub>2</sub>	Nicotinamide	
56	G290-1019	008	C06	 C <sub>19</sub> H <sub>19</sub> N <sub>3</sub> O <sub>3</sub> S	Benzamide	Phenanthridinone
57	4711-0020	002	D10	 C <sub>20</sub> H <sub>19</sub> N <sub>3</sub> O	Benzamide	Olaparib (AZD2281)
















58	4711-0033	002	E10	 C <sub>19</sub> H <sub>17</sub> N <sub>3</sub> O <sub>2</sub>	Benzamide	Olaparib (AZD2281)
59	5966-0051	004	E05	 C <sub>19</sub> H <sub>19</sub> N <sub>3</sub> O	Benzamide	Olaparib (AZD2281)
60	4934-0319	003	F03	 C <sub>21</sub> H <sub>15</sub> N <sub>3</sub> O <sub>3</sub>	Nicotinamide	528824 PARP Inhibitor XIV
61	5107-0060	003	H04	 C <sub>12</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>	Nicotinamide	PARP Inhibitor IX, EB47
62	5107-0060	003	H04	 C <sub>12</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>	Nicotinamide	PARP Inhibitor IX, EB47
63	5140-0200	003	A05	 C <sub>22</sub> H <sub>25</sub> N <sub>5</sub> O <sub>2</sub> S	Substituted Benzamide?	493800 PARP Inhibitor VI, NU1025
64	5218-3270	003	F05	 C <sub>25</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub> S	Benzamide?	493800 PARP Inhibitor VI, NU1025
65	5585-0391	003	H09	 C <sub>15</sub> H <sub>14</sub> N <sub>4</sub> OS	Substituted Benzamide?	493800 PARP Inhibitor VI, NU1025
66	5586-2133	003	A10	 C <sub>17</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	Substituted Benzamide?	528819 PARP Inhibitor XI, DR2313
67	6228-0480	005	A02	 C <sub>20</sub> H <sub>33</sub> N <sub>2</sub> O <sub>2</sub> +	Substituted Benzamide?	PARP Inhibitor IX, EB47
68	C200-3022	006	G08	 C <sub>17</sub> H <sub>13</sub> FN <sub>2</sub> O <sub>2</sub> S	Substituted Benzamide?	
69	C200-3045	006	H08	 C <sub>18</sub> H <sub>14</sub> N <sub>4</sub> O <sub>5</sub> S	Benzamide	493800 PARP Inhibitor VI, NU1025
70	C362-0173	007	C03	 C <sub>18</sub> H <sub>11</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>	Nicotinamide	493800 PARP Inhibitor VI, NU1025
71	K263-0536	008	D08	 C <sub>19</sub> H <sub>22</sub> N <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	Substituted Benzamide?	528819 PARP Inhibitor XI, DR2313
72	K284-5080	008	E08	 C <sub>15</sub> H <sub>19</sub> N <sub>3</sub> O <sub>3</sub> S	Benzamide	493800 PARP Inhibitor VI, NU1025
73	E596-0112	008	G02	 C <sub>21</sub> H <sub>22</sub> N <sub>6</sub> O <sub>4</sub> S	Substituted Benzamide?	Phenanthridinone
74	E616-0843	008	H02	 C <sub>22</sub> H <sub>35</sub> N <sub>3</sub> O <sub>4</sub>	Substituted Benzamide?	
75	E616-1041	008	A03	 C <sub>18</sub> H <sub>22</sub> N <sub>2</sub> O <sub>5</sub> S	Substituted Benzamide?	
76	E616-1156	008	B03	 C <sub>23</sub> H <sub>37</sub> N <sub>3</sub> O <sub>5</sub>	Substituted Benzamide?	

## S3-2 - PARP Inhibitor II



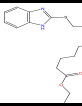



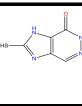


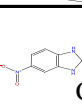
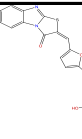
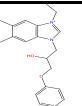
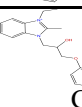
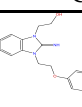

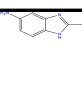



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1	1080-0356	001	E03	 C <sub>23</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> S	407850 <i>PARP Inhibitor II, INH<sub>2</sub>BP</i>
2	1440-2871	001	D06	 C <sub>18</sub> H <sub>11</sub> BrN <sub>2</sub> O <sub>4</sub>	407850 <i>PARP Inhibitor II, INH<sub>2</sub>BP</i>
3	1440-2880	001	E06	 C <sub>18</sub> H <sub>11</sub> N <sub>3</sub> O <sub>6</sub>	407850 <i>PARP Inhibitor II, INH<sub>2</sub>BP</i>
4	1615-0026	001	E07	 C <sub>20</sub> H <sub>12</sub> O <sub>3</sub>	407850 <i>PARP Inhibitor II, INH<sub>2</sub>BP</i>
5	4789-3425	002	C11	 C <sub>23</sub> H <sub>22</sub> O <sub>6</sub>	407850 <i>PARP Inhibitor II, INH<sub>2</sub>BP</i>
6		004	C05	 C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>	407850 <i>PARP Inhibitor II, INH<sub>2</sub>BP</i>
7	6944-0004	005	F08	 C <sub>25</sub> H <sub>24</sub> N <sub>2</sub> O <sub>5</sub>	407850 <i>PARP Inhibitor II, INH<sub>2</sub>BP</i>
8	6944-0066	005	H08	 C <sub>15</sub> H <sub>12</sub> O <sub>5</sub>	407850 <i>PARP Inhibitor II, INH<sub>2</sub>BP</i>
9	6944-0105	005	A09	 C <sub>25</sub> H <sub>22</sub> N <sub>2</sub> O <sub>4</sub>	407850 <i>PARP Inhibitor II, INH<sub>2</sub>BP</i>
10	6944-0110	005	B09	 C <sub>19</sub> H <sub>22</sub> O <sub>3</sub>	407850 <i>PARP Inhibitor II, INH<sub>2</sub>BP</i>
11	6944-0126	005	D09	 C <sub>22</sub> H <sub>24</sub> N <sub>4</sub> O <sub>4</sub>	407850 <i>PARP Inhibitor II, INH<sub>2</sub>BP</i>
12	6944-0140	005	E09	 C <sub>15</sub> H <sub>12</sub> ClNO <sub>4</sub>	407850 <i>PARP Inhibitor II, INH<sub>2</sub>BP</i>
13	C301-4598	007	A02	 C <sub>18</sub> H <sub>14</sub> FN <sub>3</sub> O <sub>4</sub> S	407850 <i>PARP Inhibitor II, INH<sub>2</sub>BP</i>
14	C301-6438	007	C02	 C <sub>11</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S	407850 <i>PARP Inhibitor II, INH<sub>2</sub>BP</i>
15	C566-0094	007	C06	 C <sub>18</sub> H <sub>14</sub> Br <sub>2</sub> O <sub>4</sub> S	407850 <i>PARP Inhibitor II, INH<sub>2</sub>BP</i>
16	C566-0138	007	D06	 C <sub>15</sub> H <sub>7</sub> Br <sub>2</sub> ClO <sub>4</sub> S	407850 <i>PARP Inhibitor II, INH<sub>2</sub>BP</i>
17	5591-1932	003	E10	 C <sub>13</sub> H <sub>8</sub> N <sub>2</sub> O <sub>6</sub> S <sub>2</sub>	407850 <i>PARP Inhibitor II, INH<sub>2</sub>BP</i>

18	6807-0730	005	B08	 <chem>C<sub>23</sub>H<sub>13</sub>N<sub>2</sub>O<sub>5</sub>S<sub>2</sub></chem>	407850 <i>PARP Inhibitor</i> II, INH <sub>2</sub> BP
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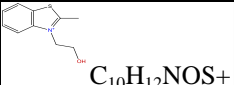
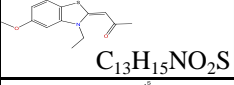
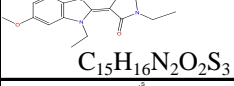
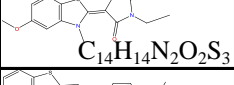
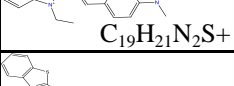
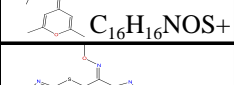
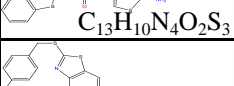
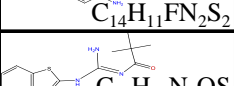
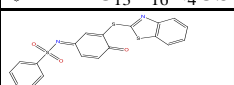
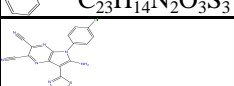
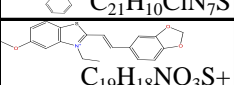
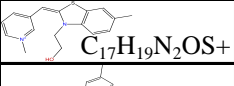
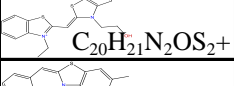
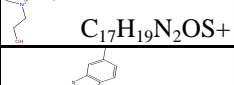
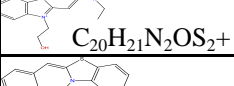
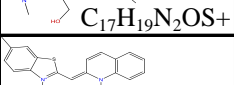
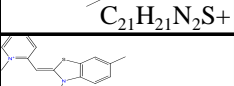
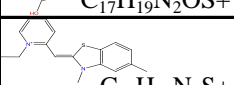
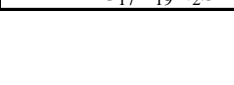

## S3-3 - Adenine/Cafeine

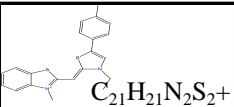
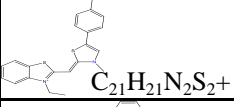
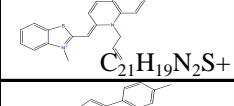
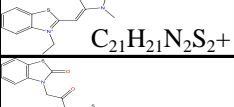
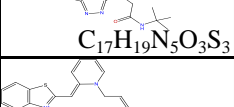
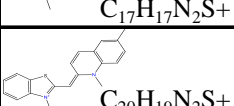
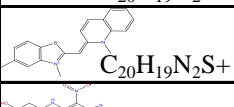
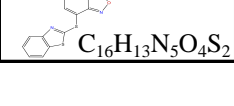

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1	1185-1661	001	B04	 <chem>C13H19N5O3S</chem>	Adenine
2	2280-2944	001	F11	 <chem>C9H12N4O2S</chem>	Adenine
3	3601-0852	002	B04	 <chem>C10H14N4O2S</chem>	Adenine
4	3736-0228	002	G05	 <chem>C10H12N4O2S</chem>	Adenine
5	4236-1085	002	F08	 <chem>C14H15FN6O2</chem>	Adenosine
6	4244-2141	002	H08	 <chem>C15H13ClN4O4S</chem>	Adenosine
7	5228-0325	003	H05	 <chem>C9H13N5O3</chem>	Adenine
8	5241-0492	003	E06	 <chem>C12H11N5S</chem>	Adenosine
9	5254-2680	003	F06	 <chem>C10H14N4O2S</chem>	Adenine
10	5339-0389	003	F07	 <chem>C10H15N5O3</chem>	Adenine
11	5646-0037	003	F11	 <chem>C16H19N5O2S</chem>	Adenosine
12	5692-1348	003	H11	 <chem>C11H16N4O2S</chem>	Adenine
13	5947-0082	004	D05	 <chem>C14H22N4O2S</chem>	Adenine
14	7639-0037	006	D04	 <chem>C19H17N5</chem>	Adenine
15	C470-0539	007	G04	 <chem>C20H32N6O4</chem>	Adenine

## S3-4 - Benzimidazole

	1	2	3	4	5
1	1069-0089	001	D03	 $C_{12}H_{15}N_3S$	Mercapto-benzimidazole
2	2144-0960	001	B11	 $C_9H_{10}N_2S$	Mercapto-benzimidazole
3	2683-0170	002	E02	 $C_{19}H_{22}N_4O_4S$	Mercapto-benzimidazole
4	5055-9162	003	E04	 $C_{16}H_{14}N_2S$	Mercapto-benzimidazole
5	6025-5977	004	H06	 $C_7H_5ClN_2S$	Mercapto-benzimidazole
6	7286-0604	006	E03	 $C_6H_4BrN_3S$	Mercapto-benzimidazole?
7	C301-6439	007	D02	 $C_{11}H_8N_4OS$	Mercapto-benzimidazole? <a href="#">Aminobenzimide?</a>
8	1247-0021	001	A05	 $C_{19}H_{19}N_3^+$	Benzimidazole?/ <a href="#">Quinoline?</a>
9	3945-0101	002	E06	 $C_{16}H_{18}N_3^+$	Benzimidazole
10	4872-0199	002	E11	 $C_{15}H_{10}ClN_5O_5$	Benzimidazole
11	4919-0202	003	E03	 $C_{22}H_{12}N_2O_6S$	Benzimidazole
12	5010-0425	003	D04	 $C_{20}H_{25}N_2O_2^+$	Benzimidazole
13	5103-0523	003	G04	 $C_{19}H_{22}FN_2O_2^+$	Benzimidazole
14	5390-1481	003	C08	 $C_{18}H_{21}N_3O_3$	Benzimidazole
15	6232-0264	005	A04	 $C_{16}H_{13}N_5S$	Benzimidazole
16	6843-3187	005	C08	 $C_{19}H_{15}N_7$	Benzimidazole
17	C456-0034	007	D04	 $C_9H_8N_4S$	Benzimidazole
18	C456-0050	007	E04	 $C_{15}H_{12}N_4S$	Benzimidazole
19	C456-0058	007	F04	 $C_{16}H_{14}N_4OS$	Benzimidazole

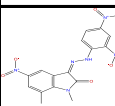
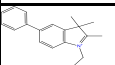
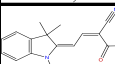
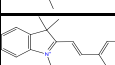
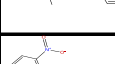
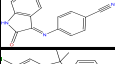
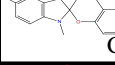
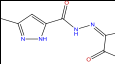
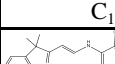
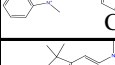
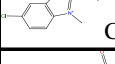
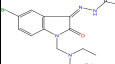
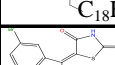
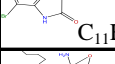
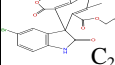
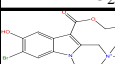
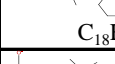
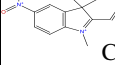
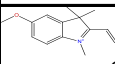
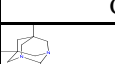
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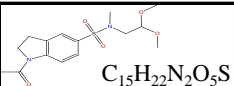
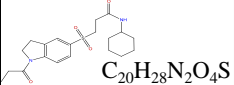
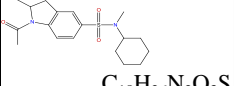
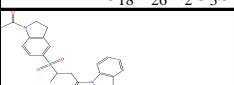
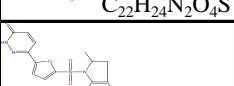
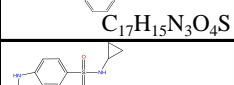
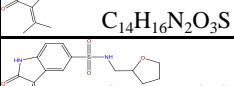
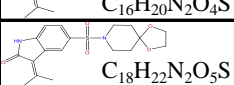
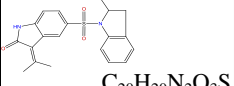
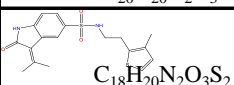

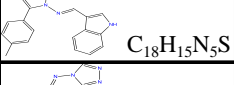
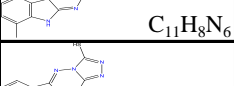
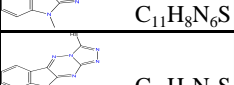
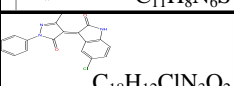
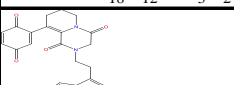
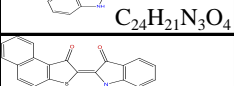
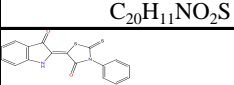
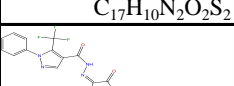
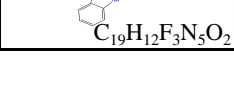
	1	2	3	4	5
1	0118-0082	001	C02	 $C_{10}H_{12}NOS^+$	Benzothiazole
2	1365-0041	001	D05	 $C_{13}H_{15}NO_2S$	Benzothiazole
3	1365-0203	001	G05	 $C_{15}H_{16}N_2O_2S_3$	Benzothiazole/ MGB?
4	1365-0208	001	H05	 $C_{14}H_{14}N_2O_2S_3$	Benzothiazole
5	1495-0025	001	F06	 $C_{19}H_{21}N_2S^+$	Benzothiazole
6	1499-0133	001	G06	 $C_{16}H_{16}NOS^+$	Benzothiazole
7	1822-0349	001	E09	 $C_{13}H_{10}N_4O_2S_3$	Benzothiazole
8	3167-0429	002	B03	 $C_{14}H_{11}FN_2S_2$	Benzothiazole
9	3652-0228	002	D05	 $C_{13}H_{16}N_4OS$	Benzothiazole
10	5591-2869	003	G10	 $C_{23}H_{14}N_2O_3S_3$	Benzothiazole
11	5830-0010	004	E03	 $C_{21}H_{10}ClN_7S$	Benzothiazole
12	5984-0397	004	D06	 $C_{19}H_{18}NO_3S^+$	Benzothiazole
13	6253-0696	005	H05	 $C_{17}H_{19}N_2OS^+$	Benzothiazole/ Pyridine
14	6253-0698	005	A06	 $C_{20}H_{21}N_2OS_2^+$	Benzothiazole
15	6253-0703	005	B06	 $C_{17}H_{19}N_2OS^+$	Benzothiazole
16	6253-0705	005	C06	 $C_{20}H_{21}N_2OS_2^+$	Benzothiazole
17	6253-0720	005	D06	 $C_{17}H_{19}N_2OS^+$	Benzothiazole
18	7165-0066	005	E10	 $C_{21}H_{21}N_2S^+$	Quinoline Benzothiazole
19	7165-0073	005	G10	 $C_{17}H_{19}N_2OS^+$	Benzothiazole
20	7165-0075	005	H10	 $C_{17}H_{19}N_2S^+$	Benzothiazole

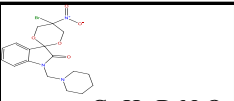
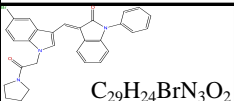
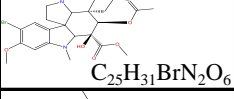
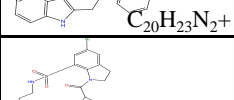
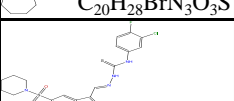
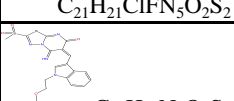
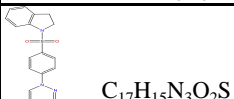

21	7165-0795	006	A02	 <chem>C21H21N2S2+</chem>	Benzothiazole
22	7165-0796	006	B02	 <chem>C21H21N2S2+</chem>	Benzothiazole
23	7165-0807	006	D02	 <chem>C21H19N2S+</chem>	Quinoline Benzothiazole
24	7165-0835	006	E02	 <chem>C21H21N2S2+</chem>	Benzothiazole
25	7255-3860	006	D03	 <chem>C17H19N5O3S3</chem>	Benzothiazole
26	7771-0711	006	C05	 <chem>C17H17N2S+</chem>	Benzothiazole
27	7771-0743	006	E05	 <chem>C20H19N2S+</chem>	Quinoline Benzothiazole
28	7771-0753	006	F05	 <chem>C20H19N2S+</chem>	Quinoline Benzothiazole
29	K784-6214	008	B10	 <chem>C16H13N5O4S2</chem>	Benzothiazole




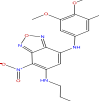
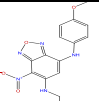
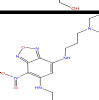
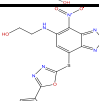
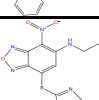
## S3-6 - Indole

	1	2	3	4	5
1	1348-0866	001	B05	 C <sub>16</sub> H <sub>12</sub> N <sub>6</sub> O <sub>7</sub>	Indole
2	1362-0200	001	C05	 C <sub>19</sub> H <sub>22</sub> N <sup>+</sup>	Indole
3	1439-0176	001	C06	 C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> O	Indole
4	1541-0004	001	B07	 C <sub>21</sub> H <sub>25</sub> N <sub>2</sub> <sup>+</sup>	Indole
5	1699-1424	001	E08	 C <sub>15</sub> H <sub>8</sub> N <sub>4</sub> O <sub>3</sub>	Indole
6	1923-0048	001	H09	 C <sub>19</sub> H <sub>17</sub> IN <sub>2</sub> O <sub>3</sub>	Indole
7	1936-2046	001	B10	 C <sub>13</sub> H <sub>10</sub> BrN <sub>5</sub> O <sub>2</sub>	MGB?
8	2421-0052	001	H11	 C <sub>19</sub> H <sub>20</sub> ClN <sub>2</sub> <sup>+</sup>	Indole
9	2421-0298	002	B02	 C <sub>20</sub> H <sub>22</sub> ClN <sub>2</sub> <sup>+</sup>	Indole/ MGB?
10	4072-2913	002	C07	 C <sub>18</sub> H <sub>19</sub> BrN <sub>4</sub> O <sub>2</sub> S	Indole/ MGB?
11	4896-0742	003	A02	 C <sub>11</sub> H <sub>5</sub> Br <sub>2</sub> N <sub>3</sub> O <sub>2</sub> S	Indole/ BA like
12	5587-0183	003	D10	 C <sub>22</sub> H <sub>25</sub> BrN <sub>2</sub> O <sub>7</sub>	Indole
13	5926-0045	004	C04	 C <sub>18</sub> H <sub>24</sub> BrN <sub>2</sub> O <sub>4</sub> <sup>+</sup>	Indole
14	6253-0066	005	A05	 C <sub>19</sub> H <sub>19</sub> N <sub>2</sub> O <sub>2</sub> <sup>+</sup>	Indole
15	6253-0495	005	B05	 C <sub>21</sub> H <sub>24</sub> NO <sub>2</sub> <sup>+</sup>	Indole
16	6583-0310	005	D07	 C <sub>19</sub> H <sub>25</sub> N <sub>3</sub>	Indole
17	7771-0535	006	G04	 C <sub>24</sub> H <sub>28</sub> NO <sub>3</sub> <sup>+</sup>	Indole
18	7771-0670	006	A05	 C <sub>22</sub> H <sub>22</sub> NO <sub>4</sub> <sup>+</sup>	Indole
19	7771-0704	006	B05	 C <sub>22</sub> H <sub>25</sub> N <sub>2</sub> <sup>+</sup>	Indole
20	C066-3077	006	D06	 C <sub>9</sub> H <sub>6</sub> ClNO	Indole

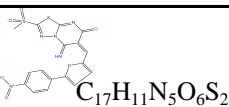
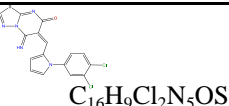
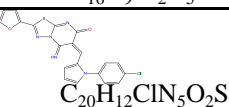
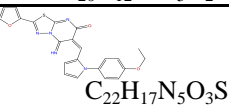
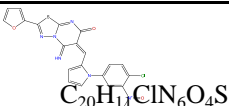
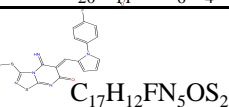
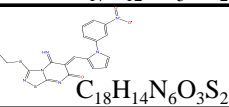
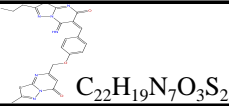
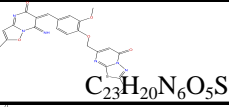
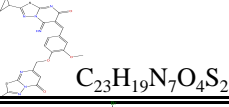
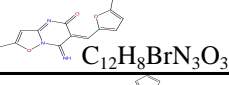
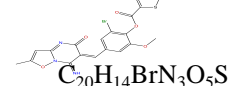
21	C324-2667	007	E02	 <chem>C15H22N2O5S</chem>	Indole?
22	C361-2059	007	B03	 <chem>C20H28N2O4S</chem>	Indole?
23	E667-0090	008	D03	 <chem>C18H26N2O3S</chem>	Indole?
24	E746-0671	008	B04	 <chem>C22H24N2O4S</chem>	Indole?
25	E959-1820	008	F04	 <chem>C17H15N3O4S</chem>	Indole?
26	E966-0516	008	G04	 <chem>C14H16N2O3S</chem>	Indole?
27	E966-0521	008	H04	 <chem>C16H20N2O4S</chem>	Indole?
28	E966-0548	008	A05	 <chem>C18H22N2O5S</chem>	Indole?
29	E966-0571	008	B05	 <chem>C20H20N2O3S</chem>	Indole?
30	E966-0620	008	C05	 <chem>C18H20N2O3S2</chem>	Indole?
31	K780-0136	008	D09	 <chem>C11H11NO</chem>	Indole
32	4896-1409	003	B02	 <chem>C18H15N5S</chem>	Indole
33	4896-2167	003	C02	 <chem>C11H8N6</chem>	Indole
34	4896-2883	003	D02	 <chem>C11H8N6S</chem>	Indole
35	4896-3047	003	E02	 <chem>C11H8N6S</chem>	Indole
36	4896-4941	003	C03	 <chem>C18H12ClN3O2</chem>	Indole
37	5605-0007	003	C11	 <chem>C24H21N3O4</chem>	Indole
38	5984-0157	004	F05	 <chem>C20H11NO2S</chem>	Indole
39	5984-0171	004	H05	 <chem>C17H10N2O2S2</chem>	Indole
40	6196-0080	004	E10	 <chem>C19H12F3N5O2</chem>	Indole

41	6260-2307	005	E06	 $C_{17}H_{20}BrN_3O_5$	Indole
42	6637-1033	005	H07	 $C_{29}H_{24}BrN_3O_2$	Indole
43	6944-0056	005	G08	 $C_{25}H_{31}BrN_2O_6$	Indoline
44	C104-0030	006	E07	 $C_{20}H_{23}N_2^+$	Indole
45	C137-2374	006	F07	 $C_{20}H_{28}BrN_3O_3S$	Indole?
46	C348-0024	007	F02	 $C_{21}H_{21}ClFN_5O_2S_2$	Indole
47	C356-0052	007	G02	 $C_{24}H_{21}N_5O_5S_2$	Indole
48	E746-0060	008	A04	 $C_{17}H_{15}N_3O_2S$	Indoline





















## S3-7 - Benzofurazan

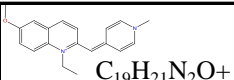
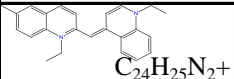
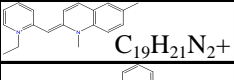
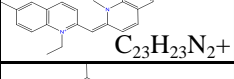
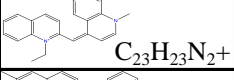
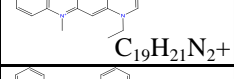
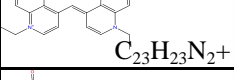
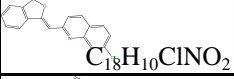
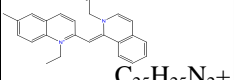
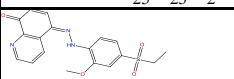
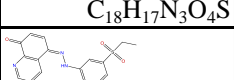
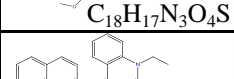
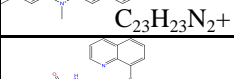
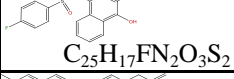
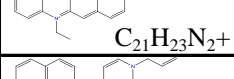
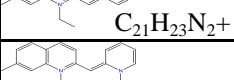
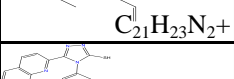
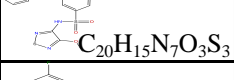
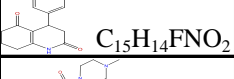
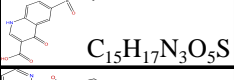
	1	2	3	4	5
1	3660-0336	002	E05	 C <sub>14</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub>	Benzofurazan
2	C091-0115	006	G06	 C <sub>17</sub> H <sub>19</sub> N <sub>5</sub> O <sub>7</sub>	Benzofurazan
3	C091-0248	006	H06	 C <sub>15</sub> H <sub>15</sub> N <sub>5</sub> O <sub>5</sub>	Benzofurazan
4	C091-0304	006	A07	 C <sub>17</sub> H <sub>26</sub> N <sub>6</sub> O <sub>4</sub>	Benzofurazan
5	K784-6198	008	A10	 C <sub>16</sub> H <sub>12</sub> N <sub>6</sub> O <sub>5</sub> S	Benzofurazan
6	K786-2882		C10	 C <sub>15</sub> H <sub>16</sub> N <sub>6</sub> O <sub>5</sub> S	Benzofurazan

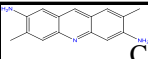
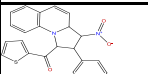
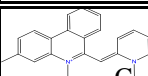
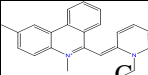
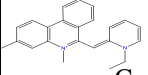
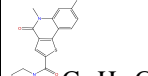
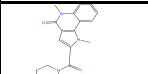
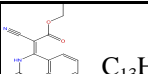
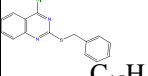
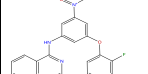
S3-8 - 5-imino-5,6-dihydro-7H-[1,3,4]thiadiazolo[3,2-a]pyrimidin-7-one

	1	2	3	4
1	C356-0074	007	H02	 C <sub>17</sub> H <sub>11</sub> N <sub>5</sub> O <sub>6</sub> S <sub>2</sub>
2	C370-3531	007	E03	 C <sub>16</sub> H <sub>9</sub> Cl <sub>2</sub> N <sub>5</sub> OS
3	C370-4282	007	F03	 C <sub>20</sub> H <sub>12</sub> ClN <sub>5</sub> O <sub>2</sub> S
4	C370-4289	007	G03	 C <sub>22</sub> H <sub>17</sub> N <sub>5</sub> O <sub>3</sub> S
5	C370-4307	007	H03	 C <sub>20</sub> H <sub>11</sub> ClN <sub>6</sub> O <sub>4</sub> S
6	C370-5084	007	A04	 C <sub>17</sub> H <sub>12</sub> FN <sub>5</sub> OS <sub>2</sub>
7	C370-5164	007	B04	 C <sub>18</sub> H <sub>14</sub> N <sub>6</sub> O <sub>3</sub> S <sub>2</sub>
8	C679-0721	007	A08	 C <sub>22</sub> H <sub>19</sub> N <sub>7</sub> O <sub>3</sub> S <sub>2</sub>
9	C679-1685	007	B08	 C <sub>23</sub> H <sub>20</sub> N <sub>6</sub> O <sub>5</sub> S
10	C679-1708	007	C08	 C <sub>23</sub> H <sub>19</sub> N <sub>7</sub> O <sub>4</sub> S <sub>2</sub>
11	C482-0405	007	H04	 C <sub>12</sub> H <sub>8</sub> BrN <sub>3</sub> O <sub>3</sub>
12	C482-0623	007	A05	 C <sub>20</sub> H <sub>14</sub> BrN <sub>3</sub> O <sub>5</sub> S

## S3-9 - Quinoline

















	1	2	3	4	5
1	0099-0209	001	B02	 $C_{12}H_{14}N^+$	Quinoline
2	0422-0118	001	F02	 $C_{10}H_7Cl_2NO_2$	Quinoline
3	0986-0007	001	B03	 $C_{11}H_{11}N_2O^+$	Quinoline
4	1365-0165	001	E05	 $C_{18}H_{18}N_2O_2S_2$	Quinoline
5	1365-0179	001	F05	 $C_{17}H_{18}N_2O_3S$	Quinoline
6	1607-0150	001	D07	 $C_{11}H_{11}NO_2$	Quinoline
7	2055-0058	001	E10	 $C_{15}H_{15}N_3OS_2$	Quinoline
8	3853-0028	002	B06	 $C_{18}H_{19}N_2^+$	Quinoline
9	3853-0032	002	C06	 $C_{17}H_{17}N_2^+$	Quinoline
10	4971-0044	003	G03	 $C_{23}H_{23}N_2^+$	Quinoline
11	5294-0006	003	C07	 $C_{19}H_{13}NO_3$	Quinoline
12	5509-0001	003	G08	 $C_{19}H_{16}NO_2^+$	Quinoline
13	5509-0002	003	H08	 $C_{16}H_{14}NO^+$	Quinoline
14	5509-0003	003	A09	 $C_{18}H_{15}FN^+$	Quinoline
15	5984-0371	004	B06	 $C_{16}H_{14}N_2O$	Quinoline
16	5984-0373	004	C06	 $C_{20}H_{23}N_3$	Quinoline
17	5984-0401	004	E06	 $C_{19}H_{16}NO_2^+$	Quinoline
18	6253-0534	005	C05	 $C_{21}H_{19}N_2^+$	Quinoline
19	6253-0536	005	D05	 $C_{21}H_{19}N_2^+$	Quinoline
20	6253-0562	005	E05	 $C_{18}H_{19}N_2O^+$	Quinoline

21	6253-0587	005	F05	 $C_{19}H_{21}N_2O^+$	Quinoline
22	7165-0007	005	D10	 $C_{24}H_{25}N_2^+$	Quinoline
23	7165-0069	005	F10	 $C_{19}H_{21}N_2^+$	Quinoline
24	7165-0232	005	A11	 $C_{23}H_{23}N_2^+$	Quinoline
25	7165-0250	005	B11	 $C_{23}H_{23}N_2^+$	Quinoline
26	7165-0265	005	C11	 $C_{19}H_{21}N_2^+$	Quinoline
27	7165-0448	005	D11	 $C_{23}H_{23}N_2^+$	Quinoline
28	7165-0474	005	E11	 $C_{18}H_{10}ClNO_2$	Quinoline/ Coumarine
29	7165-0683	005	F11	 $C_{25}H_{25}N_2^+$	Quinoline
30	7165-0735	005	G11	 $C_{18}H_{17}N_3O_4S$	Quinoline
31	7165-0736	005	H11	 $C_{18}H_{17}N_3O_4S$	Quinoline
32	7165-0800	006	C02	 $C_{23}H_{23}N_2^+$	Quinoline
33	7287-0084	006	G03	 $C_{25}H_{17}FN_2O_3S_2$	Quinoline
34	7771-0718	006	D05	 $C_{21}H_{23}N_2^+$	Quinoline/ Pyridine
35	7771-0797	006	G05	 $C_{21}H_{23}N_2^+$	Quinoline/ Pyridine
36	7771-0816	006	H05	 $C_{21}H_{23}N_2^+$	Quinoline/ Pyridine
37	7832-0186	006	B06	 $C_{20}H_{15}N_7O_3S_3$	Quinoline
38	C276-0761	006	E10	 $C_{15}H_{14}FNO_2$	Quinoline?
39	K511-0001	008	C09	 $C_{15}H_{17}N_3O_5S$	Quinoline
40	K906-2202	008	B11	 $C_{14}H_{13}N_5O_3S_3$	Quinoline

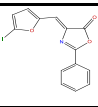
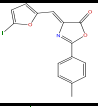
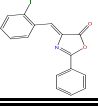
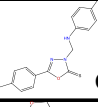
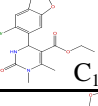
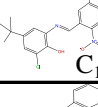
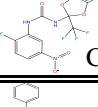
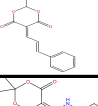
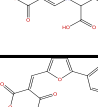
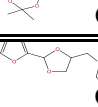
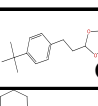
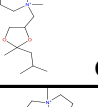
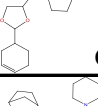
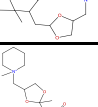
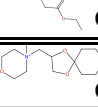
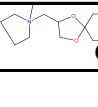


41	6253-0052	005	H04	 C <sub>15</sub> H <sub>15</sub> N <sub>3</sub>	Quinoline/ Intercalator
42	6565-0078	005	C07	 C <sub>23</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub> S	Quinoline
43	7771-0510	006	E04	 C <sub>23</sub> H <sub>23</sub> N <sub>2</sub> <sup>+</sup>	Quinoline/ Pyridine/ Intercalator
44	7771-0519	006	F04	 C <sub>23</sub> H <sub>23</sub> N <sub>2</sub> <sup>+</sup>	Quinoline/ Pyridine/ Intercalator
45	7771-0539	006	H04	 C <sub>23</sub> H <sub>23</sub> N <sub>2</sub> <sup>+</sup>	Quinoline/ Pyridine/ Intercalator
46	C498-0038	007	C05	 C <sub>18</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>2</sub> S	Quinoline/ Substituted Benzamide
47	C593-0426	007	E06	 C <sub>23</sub> H <sub>23</sub> N <sub>5</sub> O <sub>2</sub>	Quinoline/ Substituted Benzamide
48	5586-3582	003	B10	 C <sub>13</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub>	Quinoline?
49	1203-0146	001	F04	 C <sub>15</sub> H <sub>11</sub> ClN <sub>2</sub> S	Quinoline?
50	3651-6382	002	C05	 C <sub>20</sub> H <sub>12</sub> F <sub>2</sub> N <sub>4</sub> O <sub>3</sub>	Quinoline?

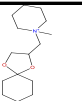







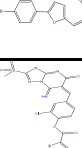













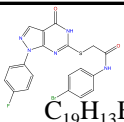
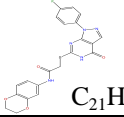
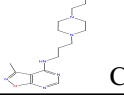
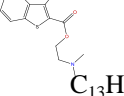
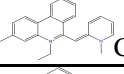
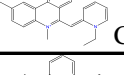
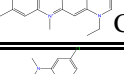
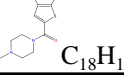
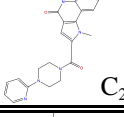
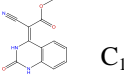
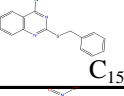
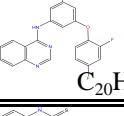
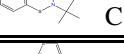
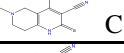
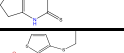
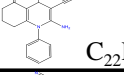
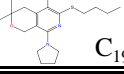
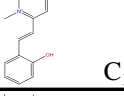
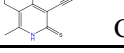
## S3-10 - Naphtalene



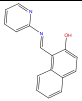







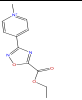
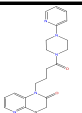



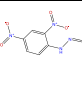


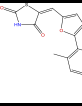


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1	1190-0035	001	D04	 $C_{10}H_3Cl_2NO_4$	Napthoquinone
2	1634-0012	001	G07	 $C_{11}H_7BrO_2$	Naphtalene
3	1697-1661	001	D08	 $C_{14}H_{10}N_4O_3$	Naphtalene
4	4204-0055	002	E08	 $C_{18}H_{11}ClINO_3$	Naphthoquinone
5	5369-0006	003	H07	 $C_{16}H_{16}ClNO_4$	Naphthoquinone
6	5591-3854	003	H10	 $C_{16}H_{13}NO_5S_3$	Naphtalene
7	5591-3872	003	A11	 $C_{19}H_{16}BrNO_3S$	Naphtalene
8	5267-1176	003	G06	 $C_{21}H_{17}N_3O_2$	Naphtalene
9	6232-2814	005	D04	 $C_{14}H_{12}O_3$	Naphthoquinone
10	6623-0252	005	F07	 $C_{15}H_{17}NO$	Naphtalene? (Tetralone)
11	7202-0307	006	F02	 $C_{21}H_{19}NO_5S_2$	Naphtalene
12	7202-1961	006	G02	 $C_{18}H_{11}ClN_4O_3S_2$	Naphthalene/ Triazole
13	7202-2009	006	H02	 $C_{21}H_{18}N_4O_3S_2$	Naphthalene/ Triazole
14	7202-2068	006	A03	 $C_{19}H_{14}N_4O_4S_2$	Naphthalene/ Triazole
15	7202-2236	006	B03	 $C_{20}H_{13}NO_3S_3$	Naphthalene
16	7287-0822	006	H03	 $C_{18}H_{14}N_2O_5S$	Naphthalene

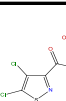


















S3-11 contains 345 new PARP-1 inhibitors without obvious structural core similarities to other groups





















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2	2062-0104	001	G10	 C <sub>15</sub> H <sub>10</sub> INO <sub>3</sub>
3	2062-0626	001	H10	 C <sub>16</sub> H <sub>10</sub> INO <sub>2</sub>
4	2141-0230	001	A11	 C <sub>17</sub> H <sub>17</sub> N <sub>3</sub> OS
5	1670-1776	001	A08	 C <sub>16</sub> H <sub>17</sub> BrN <sub>2</sub> O <sub>5</sub>
6	1688-0128	001	B08	 C <sub>18</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>5</sub>
7	C097-0054	006	B07	 C <sub>15</sub> H <sub>9</sub> F <sub>4</sub> N <sub>3</sub> O <sub>5</sub>
8	3553-1484	002	D03	 C <sub>19</sub> H <sub>14</sub> O <sub>4</sub>
9	5202-0591	003	C05	 C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> O <sub>7</sub>
10	4167-0094	002	C08	 C <sub>17</sub> H <sub>15</sub> NO <sub>7</sub> S
11	6228-0266	004	C11	 C <sub>14</sub> H <sub>22</sub> NO <sub>3</sub> <sup>+</sup>
12	6228-0706	005	A03	 C <sub>21</sub> H <sub>34</sub> NO <sub>3</sub> <sup>+</sup>
13	6228-0778	005	C03	 C <sub>15</sub> H <sub>30</sub> NO <sub>2</sub> <sup>+</sup>
14	6228-0879	005	D03	 C <sub>15</sub> H <sub>26</sub> NO <sub>2</sub> <sup>+</sup>
15	6228-1188	005	G03	 C <sub>19</sub> H <sub>33</sub> NO <sub>2</sub>
16	6228-1189	005	H03	 C <sub>15</sub> H <sub>28</sub> NO <sub>4</sub> <sup>+</sup>
17	5212-2884	003	D05	 C <sub>14</sub> H <sub>26</sub> NO <sub>3</sub> <sup>+</sup>
18	6228-0663	005	G02	 C <sub>14</sub> H <sub>26</sub> NO <sub>2</sub> <sup>+</sup>

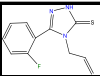
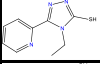
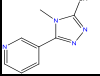
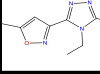
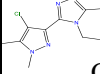
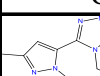
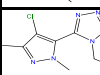
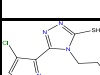
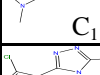
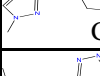
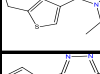
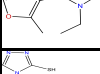
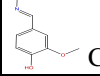
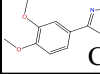
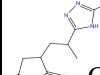
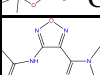
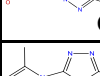
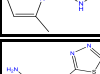
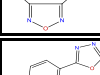
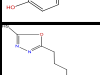
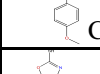
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20	6228-0288	004	D11	 $C_{18}H_{34}NO_2^+$
21	6228-0476	004	H11	 $C_{16}H_{30}NO_3^+$
22	6228-0650	005	F02	 $C_{20}H_{38}NO_2^+$
23	6228-0712	005	B03	 $C_{14}H_{28}NO_2^+$
24	6228-1073	005	E03	 $C_{17}H_{32}N_2O_4^+$
25	6228-1187	005	F03	 $C_{18}H_{34}NO_2^+$
26	6266-1910	005	F06	 $C_{15}H_{10}BrNO_3$
27	C356-0367	007	A03	 $C_{18}H_{11}ClN_4O_5S_3$
28	3570-0705	002	E03	 $C_{19}H_{23}BrO_5$
29	3577-0031	002	F03	 $C_{19}H_{23}BrO_5$
30	3594-0500	002	H03	 $C_{17}H_{13}Br_2NO_4S$
31	4055-0071	002	B07	 $C_{14}H_{25}N_2O_5S^+$
32	4191-1671	002	D08	 $C_9H_{12}N_2O_3$
33	4896-3285	003	F02	 $C_{19}H_{16}N_4O_2S$
34	C151-0185	006	G07	 $C_{16}H_{13}Br_2NO_3$
35	C791-0277	007	G08	 $C_{15}H_{15}N_3O_3S$
36	C200-4587	006	B09	 $C_6H_6N_4OS$
37	E781-0384	008	C04	 $C_{16}H_{17}ClN_6O$
38	E781-0648	008	D04	 $C_{15}H_{17}FN_6$

39	C099-0343	006	C07	 C <sub>19</sub> H <sub>13</sub> BrFN <sub>5</sub> O <sub>2</sub> S
40	C099-0349	006	D07	 C <sub>21</sub> H <sub>16</sub> FN <sub>5</sub> O <sub>4</sub> S
41	E944-0204	008	E04	 C <sub>16</sub> H <sub>26</sub> N <sub>6</sub> O
42	1710-0003	001	F08	 C <sub>13</sub> H <sub>14</sub> ClNO <sub>2</sub> S
43	7771-0510	006	E04	 C <sub>23</sub> H <sub>23</sub> N <sub>2</sub> <sup>+</sup>
44	7771-0519	006	F04	 C <sub>23</sub> H <sub>23</sub> N <sub>2</sub> <sup>+</sup>
45	7771-0539	006	H04	 C <sub>23</sub> H <sub>23</sub> N <sub>2</sub> <sup>+</sup>
46	C498-0038	007	C05	 C <sub>18</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>2</sub> S
47	C593-0426	007	E06	 C <sub>23</sub> H <sub>23</sub> N <sub>5</sub> O <sub>2</sub>
48	5586-3582	003	B10	 C <sub>13</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub>
49	1203-0146	001	F04	 C <sub>15</sub> H <sub>11</sub> ClN <sub>2</sub> S
50	3651-6382	002	C05	 C <sub>20</sub> H <sub>12</sub> F <sub>2</sub> N <sub>4</sub> O <sub>3</sub>
51	2759-0749	002	G02	 C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> S <sub>2</sub>
52	3132-1829	002	A03	 C <sub>14</sub> H <sub>13</sub> N <sub>3</sub> S <sub>2</sub>
53	4111-1314	002	D07	 C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> S
54	4306-0004	002	A09	 C <sub>22</sub> H <sub>21</sub> N <sub>3</sub> OS <sub>2</sub>
55	6085-0126	004	H09	 C <sub>19</sub> H <sub>27</sub> N <sub>3</sub> OS
56	0126-0222	001	D02	 C <sub>14</sub> H <sub>14</sub> NO <sup>+</sup>
57	0655-0099	001	G02	 C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> S

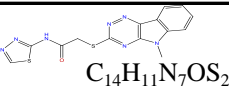
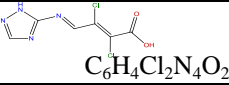
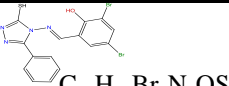
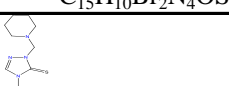
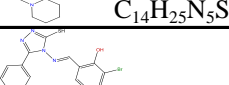
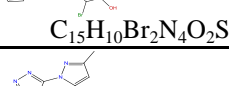
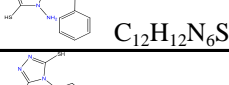
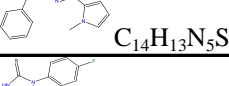
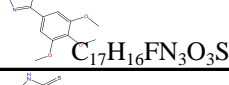
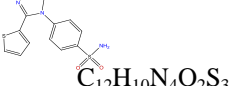
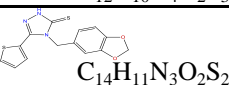
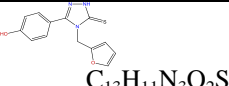
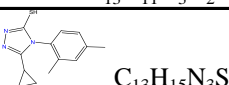
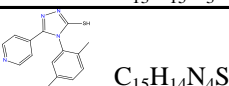
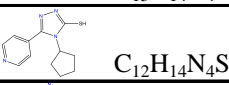
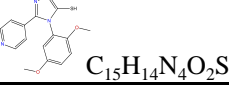
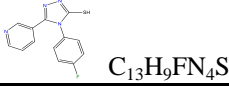
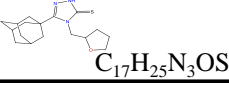
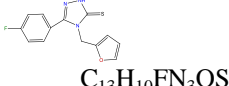
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59	0865-0043	001	A03	 $C_{14}H_{14}N^+$
60	1080-0789	001	F03	 $C_{16}H_{12}N_2O$
61	1142-0034	001	H03	 $C_9H_{10}N_2OS$
62	2421-0135	002	A02	 $C_{17}H_{19}N_2O^+$
63	5984-0304	004	A06	 $C_{16}H_{18}N_2O_4^{2+}$
64	5858-0016	004	H03	 $C_{14}H_{20}NO_4^+$
65	5921-0164	004	B04	 $C_{12}H_{14}N_2O$
66	6228-0295	004	E11	 $C_{18}H_{26}NO_2^+$
67	7404-0007	006	A04	 $C_{13}H_{18}NO_4^+$
68	C066-4192	006	E06	 $C_{11}H_{12}N_3O_3^+$
69	C862-0619	007	A09	 $C_{20}H_{23}N_5O_2S$
70	E534-0249	008	B02	 $C_{17}H_{23}N_3S$
71	K783-6142	008	H09	 $C_8H_8N_2S$
72	cc	001	A02	 $C_{18}H_{18}NS^+$
73	1114-0163	001	G03	 $C_{16}H_{12}N_6O_5S$
74	2368-0687	001	G11	 $C_{18}H_{14}BrN_3O_4S$
75	2513-4331	002	D02	 $C_{16}H_{20}N_4S$
76	5552-0139	003	C09	 $C_{16}H_{11}NO_5S$
77	5777-0232	004	A03	 $C_7H_{11}N_3O_2S$
78	5849-0916	004	G03	 $C_{17}H_{15}BrN_2S$

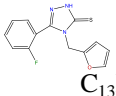
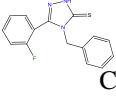
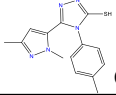
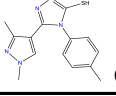
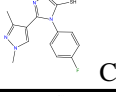
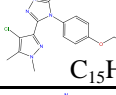
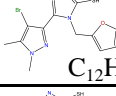
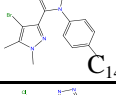
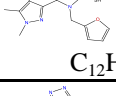
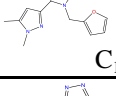
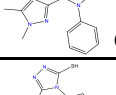
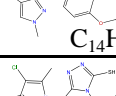
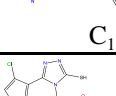
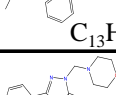
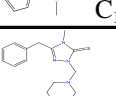
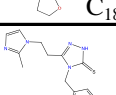
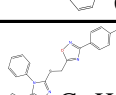
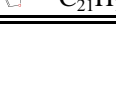
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80	6115-0147	004	A10	 <chem>C7H9N3O3S</chem>
81	6115-0248	004	B10	 <chem>C8H11N3O3S</chem>
82	6250-0004	005	F04	 <chem>C9H8N4OS</chem>
83	G856-5586	008	G06	 <chem>C18H24N2O3S</chem>
84	G856-5601	008	H06	 <chem>C19H19N3O4S</chem>
85	G856-5602	008	A07	 <chem>C15H18N2O3S</chem>
86	G856-5603	008	B07	 <chem>C17H21N3O4S</chem>
87	G856-5604	008	C07	 <chem>C17H22N2O4S</chem>
88	G856-5607	008	D07	 <chem>C18H24N2O3S</chem>
89	G856-5616	008	E07	 <chem>C20H21N3O5S</chem>
90	G856-5620	008	F07	 <chem>C19H26N2O3S</chem>
91	G856-5628	008	G07	 <chem>C15H17N3O3S</chem>
92	G856-5639	008	H07	 <chem>C14H16N2O3S</chem>
93	G856-5646	008	A08	 <chem>C14H18N2O4S</chem>
94	G856-5652	008	B08	 <chem>C18H16N2O5S</chem>
95	6944-0119	005	C09	 <chem>C20H24NO3+</chem>
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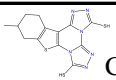
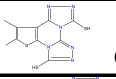
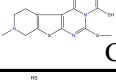
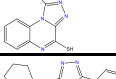
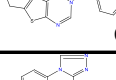
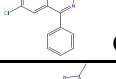
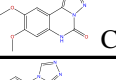
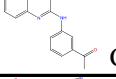
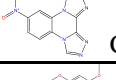
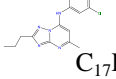
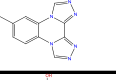
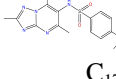
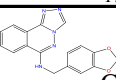
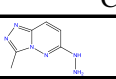
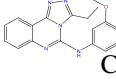
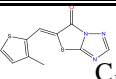
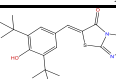
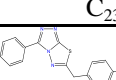
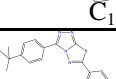
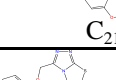
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99	E734-0182	008	G03	 <chem>C18H24N4O4S</chem>
100	6145-0419	004	D10	 <chem>C23H28N2O5S3</chem>
101	C620-0174	007	A07	 <chem>C28H27N5O2</chem>
102	C620-0474	007	B07	 <chem>C29H28N4O4</chem>
103	C620-0475	007	C07	 <chem>C27H29N3O4</chem>
104	5989-2333	004	F06	 <chem>C20H24N2</chem>
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106	0KPI-0079	001	C03	 <chem>C14H20N2S</chem>
107	6220-0414	004	G10	 <chem>C11H12N2S</chem>
108	3733-0015	002	F05	 <chem>C17H14ClN3S</chem>
109	4464-0911	002	B09	 <chem>C16H18N4O2</chem>
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111	D015-0271	007	B09	 <chem>C13H13F3N2O3</chem>
112	4670-0183	002	B10	 <chem>C12H12ClN3OS</chem>
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114	4719-0287	002	G10	 <chem>C13H17N3S</chem>
115	5633-3591	003	E11	 <chem>C13H15N3O2S</chem>
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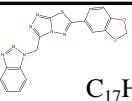
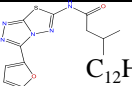
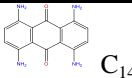
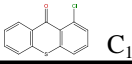
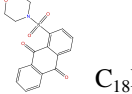
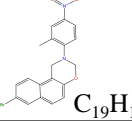
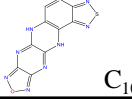
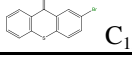
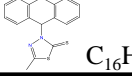
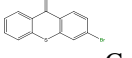
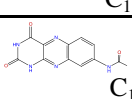
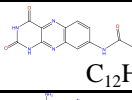
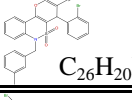
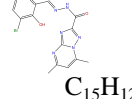
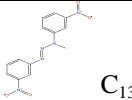
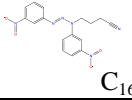
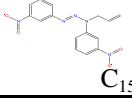
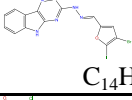
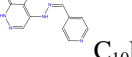
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121	6048-0021	004	A07	 <chem>C8H10N4OS</chem>
122	6049-0226	004	G07	 <chem>C11H16ClN5S</chem>
123	6049-0232	004	H07	 <chem>C9H13N5S</chem>
124	6049-0260	004	A08	 <chem>C9H12ClN5S</chem>
125	6049-0364	004	G08	 <chem>C11H16ClN5OS</chem>
126	6049-0444	004	B09	 <chem>C10H14ClN5S</chem>
127	6049-0461	004	C09	 <chem>C10H13N3S2</chem>
128	6049-0464	004	D09	 <chem>C9H11N3OS</chem>
129		004	C10	 <chem>C10H10N4O2S</chem>
130	6210-0487	004	F10	 <chem>C10H11N3O2S</chem>
131	6521-0200	005	B07	 <chem>C11H17N3O2S</chem>
132	D291-0130	007	D11	 <chem>C8H10N6O2S</chem>
133	K780-1061	008	F09	 <chem>C8H10N4S</chem>
134	7286-2215	006	F03	 <chem>C4H4N6OS</chem>
135	0350-0159	001	E02	 <chem>C8H6N2O2S</chem>
136	4696-1323	002	C10	 <chem>C12H14N2O2S</chem>
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


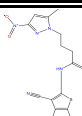
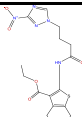
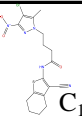


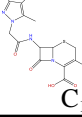










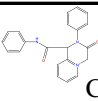


















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140	C301-3836	006	E11	 C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>2</sub>
141	1927-7417	001	A10	 C <sub>15</sub> H <sub>10</sub> Br <sub>2</sub> N <sub>4</sub> OS
142	4030-0007	002	A07	 C <sub>14</sub> H <sub>25</sub> N <sub>5</sub> S
143	4896-0340	002	H11	 C <sub>15</sub> H <sub>10</sub> Br <sub>2</sub> N <sub>4</sub> O <sub>2</sub> S
144	4896-4195	003	H02	 C <sub>12</sub> H <sub>12</sub> N <sub>6</sub> S
145	4896-4273	003	B03	 C <sub>14</sub> H <sub>13</sub> N <sub>5</sub> S
146	5236-0076	003	B06	 C <sub>17</sub> H <sub>16</sub> FN <sub>3</sub> O <sub>3</sub> S
147	5236-0120	003	C06	 C <sub>12</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> S <sub>3</sub>
148	5236-0123	003	D06	 C <sub>14</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>
149	5366-2750	003	G07	 C <sub>13</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub> S
150	5742-0465	004	C02	 C <sub>13</sub> H <sub>15</sub> N <sub>3</sub> S
151	5742-1007	004	E02	 C <sub>15</sub> H <sub>14</sub> N <sub>4</sub> S
152	5742-1010	004	F02	 C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> S
153	5742-1015	004	G02	 C <sub>15</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> S
154	5742-1018	004	H02	 C <sub>13</sub> H <sub>9</sub> FN <sub>4</sub> S
155	5933-0676	004	D04	 C <sub>17</sub> H <sub>25</sub> N <sub>3</sub> OS
156	5933-0687	004	E04	 C <sub>13</sub> H <sub>10</sub> FN <sub>3</sub> OS
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


















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159	5933-0736	004	A05	 C <sub>15</sub> H <sub>12</sub> FN <sub>3</sub> S
160	6049-0116	004	B07	 C <sub>14</sub> H <sub>15</sub> N <sub>5</sub> S
161	6049-0121	004	C07	 C <sub>14</sub> H <sub>15</sub> N <sub>5</sub> S
162	6049-0149	004	D07	 C <sub>13</sub> H <sub>12</sub> FN <sub>5</sub> S
163	6049-0155	004	E07	 C <sub>15</sub> H <sub>16</sub> ClN <sub>5</sub> OS
164	6049-0225	004	F07	 C <sub>12</sub> H <sub>12</sub> BrN <sub>5</sub> OS
165	6049-0275	004	B08	 C <sub>14</sub> H <sub>14</sub> BrN <sub>5</sub> S
166	6049-0277	004	C08	 C <sub>12</sub> H <sub>12</sub> ClN <sub>5</sub> OS
167	6049-0292	004	D08	 C <sub>12</sub> H <sub>13</sub> N <sub>5</sub> OS
168	6049-0293	004	E08	 C <sub>13</sub> H <sub>13</sub> N <sub>5</sub> S
169	6049-0295	004	F08	 C <sub>14</sub> H <sub>14</sub> ClN <sub>5</sub> OS
170	6049-0372	004	H08	 C <sub>15</sub> H <sub>16</sub> ClN <sub>5</sub> S
171	6049-0398	004	A09	 C <sub>13</sub> H <sub>12</sub> ClN <sub>5</sub> OS
172	6220-1294	004	A11	 C <sub>14</sub> H <sub>18</sub> N <sub>4</sub> OS
173	6232-1273	005	B04	 C <sub>18</sub> H <sub>24</sub> N <sub>4</sub> O <sub>2</sub> S
174	6516-0027	005	A07	 C <sub>15</sub> H <sub>17</sub> N <sub>5</sub> S
175	7012-0549	005	A10	 C <sub>21</sub> H <sub>14</sub> BrN <sub>5</sub> O <sub>2</sub> S






















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178	6280-0685	005	G06	 $C_{12}H_{13}N_5S_3$
179	C301-3719	006	D11	 $C_9H_6N_4S_2$
180	4789-3748	002	D11	 $C_{18}H_{16}N_4S$
181	6618-0003	005	E07	 $C_{15}H_9ClN_4$
182	C200-3973	006	A09	 $C_{12}H_{12}N_4O_3$
183	C301-1229	006	H10	 $C_{17}H_{13}N_5O$
184	C301-1537	006	A11	 $C_{10}H_5N_7O_2$
185	C301-2480	006	C11	 $C_{17}H_{20}ClN_5O_2$
186	C301-3918	006	F11	 $C_{11}H_8N_6$
187	C301-4549	006	H11	 $C_{17}H_{21}N_5O_3S$
188	C301-5920	007	B02	 $C_{17}H_{13}N_5O_2$
189	C430-0847	007	C04	 $C_6H_8N_6$
190	E973-0287	008	D05	 $C_{20}H_{21}N_5O_3$
191	5629-0533	003	D11	 $C_{10}H_7N_3OS_2$
192	6672-0306	005	A08	 $C_{23}H_{25}N_3O_3S$
193	7009-0121	005	F09	 $C_{16}H_{11}ClN_4S$
194	7009-0292	005	G09	 $C_{21}H_{20}N_4O_2S$
195	7009-0641	005	H09	 $C_{17}H_{13}ClN_4O_2S$

196	D221-0305	007	G10	 <chem>C17H11N7O2S</chem>
197	E157-4299	007	F11	 <chem>C12H13N5O2S</chem>
198	1221-0128	001	G04	 <chem>C14H12N4O2</chem>
199	1439-0154	001	B06	 <chem>C13H7ClOS</chem>
200	3594-0962	002	A04	 <chem>C18H15NO5S</chem>
201	3976-0239	002	F06	 <chem>C19H15BrN2O3</chem>
202	5386-0664	003	B08	 <chem>C10H4N8OS</chem>
203	5984-0169	004	G05	 <chem>C13H7BrOS</chem>
204	6232-1901	005	C04	 <chem>C16H12N2OS2</chem>
205	6253-0671	005	G05	 <chem>C13H7BrOS</chem>
206	C248-0004	006	A10	 <chem>C12H9N5O3</chem>
207	C248-0013	006	B10	 <chem>C12H6F3N5O3</chem>
208	E738-0349	008	H03	 <chem>C26H20BrN3O3S</chem>
209	1761-1901	001	D09	 <chem>C15H12Br2N6O2</chem>
210	1184-2227	001	A04	 <chem>C13H11N5O4</chem>
211	1896-0163	001	F09	 <chem>C16H14N6O4</chem>
212	1896-0218	001	G09	 <chem>C15H13N5O4</chem>
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



















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217	4151-0396	002	H07	 C <sub>19</sub> H <sub>31</sub> N <sub>5</sub>
218	C163-0165	006	B08	 C <sub>16</sub> H <sub>17</sub> N <sub>5</sub> O <sub>3</sub> S
219	C163-0512	006	C08	 C <sub>17</sub> H <sub>21</sub> N <sub>5</sub> O <sub>5</sub> S
220	C226-4309	006	H09	 C <sub>17</sub> H <sub>18</sub> BrN <sub>5</sub> O <sub>3</sub> S
221	C163-0149	006	A08	 C <sub>12</sub> H <sub>15</sub> N <sub>5</sub> O <sub>4</sub>
222	C614-6004	007	H06	 C <sub>25</sub> H <sub>31</sub> N <sub>5</sub> O <sub>2</sub>
223	D052-0023	007	H09	 C <sub>17</sub> H <sub>19</sub> ClN <sub>4</sub> O <sub>6</sub> S
224	G262-0986	008	B06	 C <sub>12</sub> H <sub>17</sub> N <sub>5</sub> OS <sub>2</sub>
225	K788-7062	008	E10	 C <sub>9</sub> H <sub>9</sub> NO <sub>3</sub> S
226	5785-1359	004	B03	 C <sub>18</sub> H <sub>18</sub> FN <sub>3</sub> O <sub>2</sub>
227	D047-0137	007	F09	 C <sub>17</sub> H <sub>23</sub> F <sub>2</sub> N <sub>3</sub> O
228	C226-2735	006	E09	 C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> O <sub>3</sub> S
229	C226-2884	006	F09	 C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
230	C226-3516	006	G09	 C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O <sub>6</sub> S
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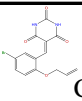
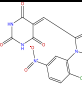




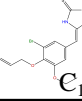




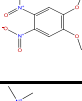



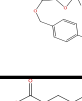






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234	G008-2661	008	E05	 C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O <sub>4</sub> S
235	G008-2935	008	F05	 C <sub>18</sub> H <sub>15</sub> F <sub>3</sub> N <sub>4</sub> O <sub>5</sub> S <sub>2</sub>
236	G008-2980	008	G05	 C <sub>14</sub> H <sub>18</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub> S <sub>2</sub>
237	G008-3184	008	H05	 C <sub>15</sub> H <sub>13</sub> F <sub>3</sub> N <sub>2</sub> O <sub>3</sub> S <sub>3</sub>
238	E692-1229	008	F03	 C <sub>19</sub> H <sub>25</sub> BrFN <sub>3</sub> O <sub>5</sub> S
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243	7202-3000	006	C03	 C <sub>13</sub> H <sub>9</sub> NO <sub>5</sub> S
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











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254	6937-0081	005	E08	 <chem>C19H29N3O4S</chem>
255	E565-0447	008	D02	 <chem>C20H21N5O3S2</chem>
256	E596-0108	008	F02	 <chem>C22H30N6O2S</chem>
257	C785-0977	007	F08	 <chem>C20H26N4O2S</chem>
258	1636-0309	001	H07	 <chem>C14H11BrN2S</chem>
259	1726-0132	001	A09	 <chem>C15H17NOS2</chem>
260	1726-0133	001	B09	 <chem>C12H11NOS2</chem>
261	4782-0199	002	B11	 <chem>C21H28N2O2</chem>
262	5599-0684	003	B11	 <chem>C21H26NO+</chem>
263	5324-0025	003	E07	 <chem>C19H24NOS+</chem>
264	5008-0192	003	B04	 <chem>C18H15OS+</chem>
265	7954-5044	006	C06	 <chem>C19H18N2O7</chem>
266	E002-1461	007	E11	 <chem>C24H31N3OS</chem>
267	E635-0288	008	C03	 <chem>C27H34N4O3S</chem>
268		001	D11	 <chem>C20H12N2O4S</chem>
269	3643-1400	002	G04	 <chem>C10H5Cl2NO2</chem>

270	3584-0059	002	G03	 <chem>C11H7Cl2NO2S2</chem>
271	3977-1344	002	G06	 <chem>C17H16N2O6S</chem>
272	C151-0296	006	H07	 <chem>C18H20N2O</chem>
273	5218-3347	003	G05	 <chem>C10H13N3O2S</chem>
274	5371-4617	003	A08	 <chem>C14H13N5O2S</chem>
275	E547-0133	008	C02	 <chem>C14H13N5OS3</chem>
276	6850-0232	005	D08	 <chem>C21H19N5OS3</chem>
277	5144-0082	003	B05	 <chem>C15H19N3O2S</chem>
278	5510-0886	003	B09	 <chem>C15H17N3O2S</chem>
279	1689-0147	001	C08	 <chem>C10H20N3O2+</chem>
280	2158-0062	001	C11	 <chem>C15H20NO+</chem>
281	3788-1509	002	H05	 <chem>C15H21N3OS</chem>
282	3843-0342	002	A06	 <chem>C11H22N3O3+</chem>
283	5320-4478	003	D07	 <chem>C13H22N+</chem>
284	5504-0086	003	E08	 <chem>C12H20N+</chem>
285	5830-1466	004	F03	 <chem>C13H26N+</chem>
286	6228-0352	004	F11	 <chem>C18H36NO2+</chem>
287	6228-0489	005	B02	 <chem>C13H20NO3+</chem>
288		004	G11	 <chem>C24H34NO2+</chem>
289	7150-0154	005	B10	 <chem>C13H22NO+</chem>
290	7150-0157	005	C10	 <chem>C14H26NO2+</chem>

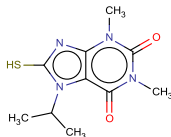
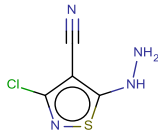
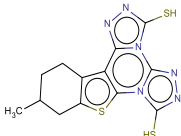
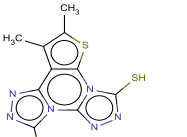
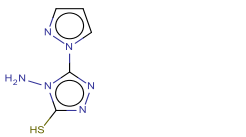
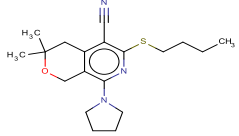
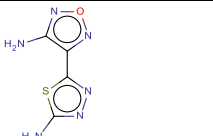
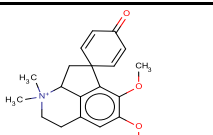
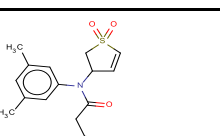
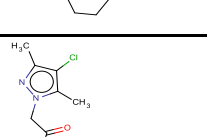


291	7405-3436	006	B04	 $C_{12}H_{24}NO^+$
292	3130-0766	002	H02	 $C_8H_{10}ClN_3O$
293	5554-0068	003	D09	 $C_{17}H_{32}NO^+$
294	6228-0529	005	C02	 $C_{13}H_{24}NO^+$
295	3886-1222	002	D06	 $C_9H_{18}NO^+$
296	6080-0058	004	F09	 $C_{13}H_{20}N^+$
297	6080-0081	004	G09	 $C_{17}H_{20}NO^+$
298	D019-1004	007	C09	 $C_{18}H_{18}N_4S$
299	D019-1188	007	D09	 $C_{19}H_{22}N_4O_4S$
300	C087-1385	006	F06	 $C_{19}H_{24}ClN_3S_2$
301	K788-6323	008	D10	 $C_{18}H_{26}ClN_3OS$
302	C499-0070	007	D05	 $C_{21}H_{25}N_3OS$
303	C499-0691	007	E05	 $C_{20}H_{22}N_4O_3S$
304	C499-0753	007	F05	 $C_{18}H_{21}N_3O_4S$
305	C499-1005	007	G05	 $C_{22}H_{19}N_3O_3S$
306	C499-1006	007	H05	 $C_{24}H_{25}N_3OS$
307	C202-0324	006	D09	 $C_{22}H_{28}BrN_5O_2$
308	K832-4321	008	H10	 $C_{15}H_{10}BrF_2N_5OS$
309	C301-2064	006	B11	 $C_{17}H_{16}N_6$
310	C850-0735	007	H08	 $C_{13}H_{16}N_6O$

311	3620-0916	002	E04	 C <sub>14</sub> H <sub>11</sub> BrN <sub>2</sub> O <sub>4</sub>
312	C370-0445	007	D03	 C <sub>15</sub> H <sub>9</sub> ClN <sub>4</sub> O <sub>5</sub>
313	1187-0105	001	C04	 C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>4</sub>
314	1530-0255	001	A07	 C <sub>5</sub> H <sub>8</sub> N <sub>4</sub> S
315	C285-0141	006	F10	 C <sub>6</sub> H <sub>7</sub> ClN <sub>4</sub> O <sub>2</sub>
316	1512-0210	001	H06	 C <sub>12</sub> H <sub>13</sub> N <sub>2</sub> O+
317	3620-0875	002	D04	 C <sub>15</sub> H <sub>15</sub> BrN <sub>2</sub> O <sub>3</sub> S
318	5074-0064	003	F04	 C <sub>12</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>2</sub>
319	5556-0108	003	E09	 C <sub>9</sub> H <sub>14</sub> Cl <sub>2</sub> N <sub>3</sub> O+
320	C250-0299	006	C10	 C <sub>16</sub> H <sub>20</sub> N <sub>2</sub> S
321	1238-0035	001	H04	 C <sub>10</sub> H <sub>21</sub> N <sub>2</sub> O <sub>2</sub> +
322	1623-0064	001	F07	 C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>9</sub>
323	1735-0003	001	C09	 C <sub>8</sub> H <sub>16</sub> NO <sub>2</sub> +
324	3331-3468	002	C03	 C <sub>10</sub> H <sub>8</sub> OS
325	4596-0306	002	G09	 C <sub>4</sub> H <sub>3</sub> ClN <sub>4</sub> S
326	3642-0014	002	F04	 C <sub>19</sub> H <sub>28</sub> O <sub>7</sub>
327	4782-0167	002	A11	 C <sub>11</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>
328	5008-0267	003	C04	 C <sub>14</sub> H <sub>20</sub> O <sub>2</sub>
329	5212-3112	003	E05	 C <sub>17</sub> H <sub>32</sub> NO <sub>2</sub> +
330	5556-0461	003	G09	 C <sub>10</sub> H <sub>22</sub> N <sub>3</sub> O <sub>2</sub> +
331	5689-0003	003	G11	 C <sub>15</sub> H <sub>21</sub> NO
332	5701-2415	004	A02	 C <sub>13</sub> H <sub>19</sub> N <sub>3</sub> S

333	5794-0740	004	D03	 <chem>C11H15ClN2O2</chem>
334	6623-0260	005	G07	 <chem>C11H15NO2</chem>
335	7513-0010	006	C04	 <chem>C13H20N2O3</chem>
336	C301-0348	006	G10	 <chem>C19H20ClNO2S</chem>
337	C301-3970	006	G11	 <chem>C8H7ClN4</chem>
338	C761-1499	007	E08	 <chem>C20H27NO3S</chem>
339	D183-0127	007	D10	 <chem>C13H17N7O4</chem>
340	K780-0404	008	E09	 <chem>C11H10ClNO2</chem>
341	K783-3185	008	G09	 <chem>C9H15Cl3N2O3</chem>
342	N089-0202	008	C11	 <chem>C13H21F3NO2+</chem>
343	2,3,5,6-tetrachlorobenzo-1,4-quinone T4271	008	E11	 <chem>C6Cl4O2</chem>
344	1,1-Cyclopentane diacetic acid	008	G11	 <chem>C9H14O4</chem>

**Supplemental Table 4.** 52 small molecules with no similarities to NAD and known PARP-1 inhibitors. This table contains small molecules located in cells I1, I2, J1, and J2 of the 2D matrix shown on **Figure 2BC**. Column # 1 indicates position in 2D matrix, column # 2 lists the ID number of each small molecule according to the ChemDiv company catalogue, column # 3 - the plate number; column # 4 – position on the plate; column # 5 - formulas in SMILES format; column # 6 – skeletal structure.

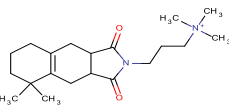
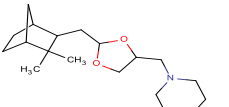
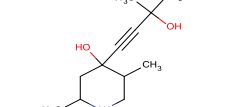
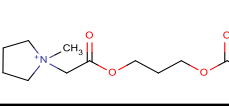
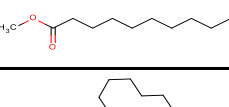
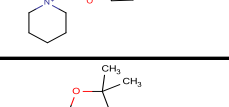
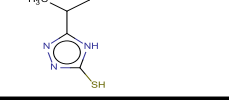
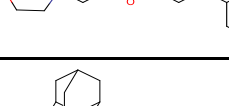
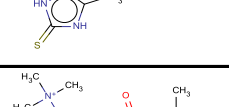
	1	2	3	4	5	6
1	i1	3601-0852	002	B04	<chem>CC(C)n(c(n1)S)c(c12)c(=O)n(C)c(=O)n2C</chem>	
2	i1	4596-0306	002	G09	<chem>N#Cc1c(NN)snc1Cl</chem>	
3	i1	5508-0335	003	F08	<chem>n1nc(S)n2c1c(c3n(c24)c(S)nn4)c5c(s3)CC(C)CC5</chem>	
4	i1	5586-4259	003	C10	<chem>n1nc(S)n(c12)c3c(c(C)c(s3)C)c4n2c(nn4)S</chem>	
5	i1	5720-0252	004	B02	<chem>n1nc(S)n(N)c1-n2nccc2</chem>	
6	i1	6085-0126	004	H09	<chem>C1CCCN1c2nc(SCCCC)c(C#N)c(c23)CC(C)(C)OC3</chem>	
7	i1	7286-2215	006	F03	<chem>n1nc(N)sc1-c2c(N)non2</chem>	
8	i2	6944-0119	005	C09	<chem>COc1c(OC)cc(CC[N+](C)(C)C2C3)c2c1C34C=CC(=O)C=C4</chem>	
9	i2	C761-1499	007	E08	<chem>C1CCCCC1CC(=O)N(C(C2)C=CS2(=O)=O)c(c3)cc(C)cc3C</chem>	
10	i2	D052-0023	007	H09	<chem>Cc1c(Cl)c(C)n(n1)CC(=O)NC2C(=O)N(C23)C(C(=O)O)=C(CS3)COC(=O)C</chem>	

11	i2	4782-0167	002	A11	<chem>CCOC(=O)/C(=N/O)CCC[N+](C)(CC)CC</chem>	
12	i2	6115-0248	004	B10	<chem>O=C(O)CCC(=O)Nc(s1)nnc1CC</chem>	
13	i2	C482-0405	007	H04	<chem>o1c(Br)ccc1/C=C(C(N2)=O)/C(=N/[H])N(C=C23)OC(C)=C3</chem>	
14	i2	C226-4309	006	H09	<chem>C1CCCc(c12)sc(c2C#N)NC(=O)CCCn3nc([N+][O-])=O)c(Br)c3C</chem>	
15	i2	K783-3185	008	G09	<chem>CCOC(=O)NC(C(Cl)(Cl)Cl)N1CCOCC1</chem>	
16	i2	4142-0922	002	G07	<chem>C1CCCCN1CCCN(C2=O)C(=O)C(C23)CC=C(Cl)C3</chem>	
17	j1	5212-3112	003	E05	<chem>CC[N+](C)(CC)CC(=O)OCC(C(C)C1)C(C)C=C1C</chem>	
18	j1	6228-1189	005	H03	<chem>CCOC(=O)CC1(C)OC(CO1)C[N+](2)C)CCCC2</chem>	
19	j1	N089-0202	008	C11	<chem>FC(F)(F)C(=O)OCC(CCC1)C([N+](12C)CCCC2</chem>	
20	j1	6228-0288	004	D11	<chem>CC(C)CC1C(CCCC1)OC(=O)C[N+](2)C)CCCC2</chem>	
21	j1	6228-1187	005	F03	<chem>C1CCCC[N+](1)C)C(=O)OC(CC2)CC2C(C)(C)C</chem>	

22	j1	6944-0056	005	G08	<chem>C1=CCN(CC2)C3C1(CC)[C@@H](OC(=O)C)[C@](O)(C(=O)OC)C4N(C)c(c5C234)cc(c(Br)c5)OC</chem>	
23	j1	5933-0676	004	D04	<chem>O1CCCC1Cn(c(=S)[nH]n2)c2C34CC5C(C3)CC(C4)C5</chem>	
24	j1	1735-0003	001	C09	<chem>C[N+](C)(C)C/C=C1/COC1</chem>	
25	j1	6228-0595	005	E02	<chem>C1CCCC[N+](C)CNC(=O)C(=O)C(C23)C4C=CC3C4</chem>	
26	j1	6228-0879	005	D03	<chem>C1CCC[N+](C)CC2COC(O2)C3CC=CC3</chem>	
27	j1	5504-0086	003	E08	<chem>C=CC#CC[N+](CC)CCCC1</chem>	
28	j1	5008-0267	003	C04	<chem>CC(C)(C)C1=CC(C(C)(C)C)=CC(=O)C1=O</chem>	
29	j1	5320-4478	003	D07	<chem>C=CC[C@H]([N+](C)C)C=CC[C@H]1CC=C</chem>	
30	j1	3886-1222	002	D06	<chem>C1C(O)CC([N+](2)C)C)CCC12</chem>	
31	j1	7405-3436	006	B04	<chem>CCCC[N+](C)C(C)CC12)CC(C2)O</chem>	

32	j1	4030-0007	002	A07	<chem>C1CCCCN1Cn(c2= S)cnn2CN3CCCCC3</chem>	
33	j1	6228-0539	005	D02	<chem>C1CCC[N+]1(C)CC(CO2)OC23CCCC3</chem>	
34	j1	0	005	G02	<chem>C1CCC[N+]1(C)CC(CO2)OC23CCCCC3</chem>	
35	j1	6228-0683	005	H02	<chem>C1CCCC[N+]1(C)C(CO2)OC23CCCCC3</chem>	
36	j1	5212-2884	003	D05	<chem>C1COCC[N+]1(C)C(CO2)OC23CCCCC3</chem>	
37	j1	6228-0778	005	C03	<chem>CC(C)CC1(C)OC(CO1)C[N+]2(C)CCC(C)C2</chem>	
38	j1	6228-0712	005	B03	<chem>C1CCCC[N+]1(C)C(C(O2)OC(C)CC2(C))C</chem>	
39	j1	6228-0529	005	C02	<chem>C1CCC[N+]1(C)C2CCC(C(C23)O)CC3</chem>	
40	j1	5554-0068	003	D09	<chem>C1CCC[N+]1(C)CCOC2CC(CC3)[C@](C)(C)C23C</chem>	
41	j1	7150-0154	005	B10	<chem>C=CC#CC1(O)C(C)C[N+](C)(C)C(C)C1</chem>	
42	j1	5830-1466	004	F03	<chem>C[C@H](C1)[C@H](C)CC12CCCC[N+]2(C)C</chem>	



43	j1	6228-0480	005	A02	<chem>C[N+](C)(C)CCCN(C1=O)C(=O)C(C12)CC3=C(C2)C(C)(C)CCC3</chem>	
44	j1	6228-1188	005	G03	<chem>C1CC(C2)C(C(C)(C)C)C12)CC(O3)OCC3CN4CCCCC4</chem>	
45	j1	7150-0157	005	C10	<chem>CC(C)(O)C#CC1(O)C(C)C[N+](C)(C)C(C)C1</chem>	
46	j2	6228-1073	005	E03	<chem>C1CCC[N+](C)CC(=O)OCCCO(=O)C[N+](C)CC2</chem>	
47	j2	6228-0352	004	F11	<chem>COC(=O)CCCCC(CCCC[N+](C)CCC)CC1</chem>	
48	j2	6228-0650	005	F02	<chem>C1CCCC[N+](C)C(C(=O)OC2CCCC)CCCC2</chem>	
49	j2	6521-0200	005	B07	<chem>[nH]1c(S)nnc1C(C)CC(C(=O)O2)CC2(C)C</chem>	
50	j2	6228-0476	004	H11	<chem>C1COCC[N+](C)C(C(=O)OCC2CC)CCC2</chem>	
51	j2	0KPI-0079	001	C03	<chem>[nH]1c(=S)[nH]c(c1C)C23CC4CC(C2)C(C3)C4</chem>	
52	j2	6228-0215	004	B11	<chem>C[N+](C)(C)CCCN(C1=O)C(=O)C(C12)CC(C)=CC2C</chem>	