

Supplementary material

Targeting HIV-1 RNase H: *N'*-(2-Hydroxybenzylidene)-3,4,5-Trihydroxybenzoylhydrazone as Selective Inhibitor Active against NNRTIs-Resistant Variants

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Table S1. Percentage of conservation of the amino acid residue in the corresponding position.

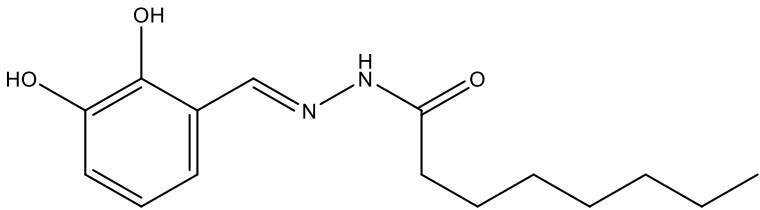
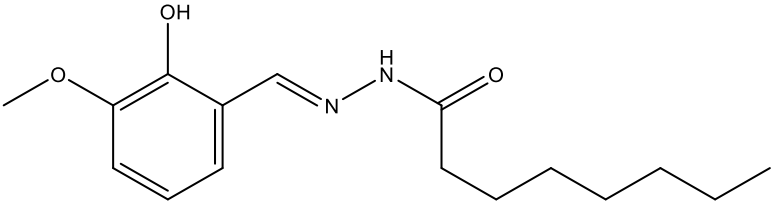
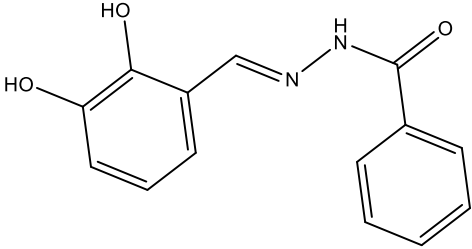
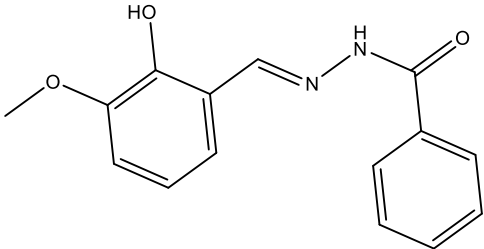
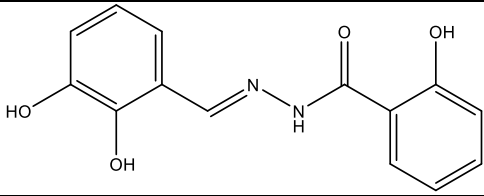
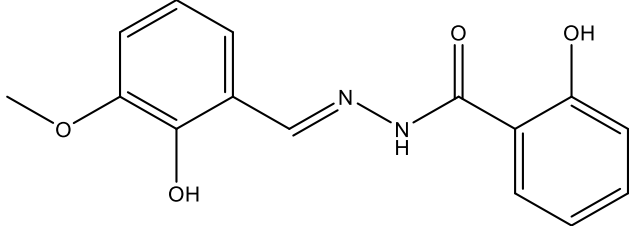
HIV-1 RT position	Amino acid	% of conservation
427	Y	100.00
428	Q	100.00
429	L	99.90
430	E	99.80
431	K	96.20
432	E	77.00
433	P	100.00
434	I	98.20
435	V	35.60
436	G	95.60
437	A	84.00
438	E	99.90
439	T	99.90
440	F	99.30
441	Y	99.90
442	V	100.00
443	D	99.80
444	G	99.90
445	A	100.00
446	A	93.90
447	S	9.00
448	R	96.70
449	E	95.40
450	T	97.70
451	K	98.20
452	L	59.60
453	G	99.80

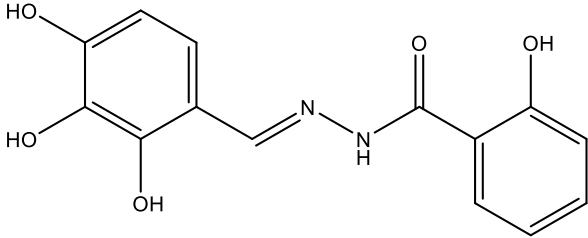
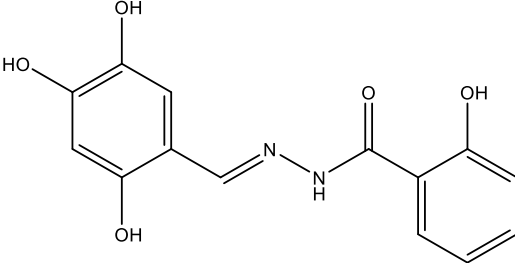
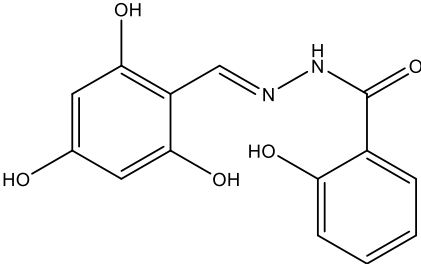
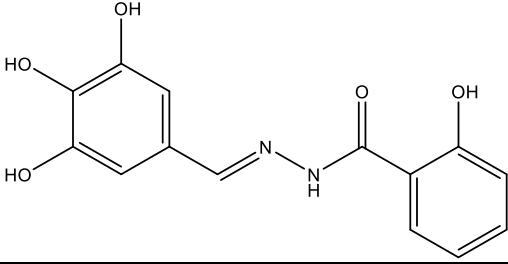
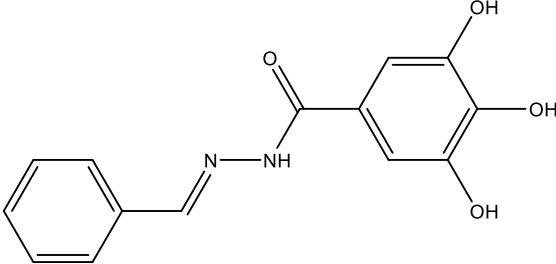
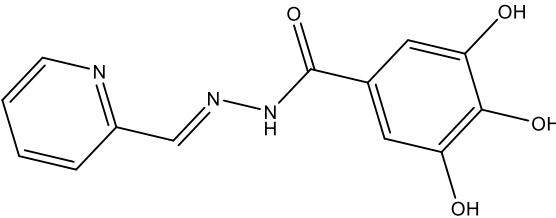
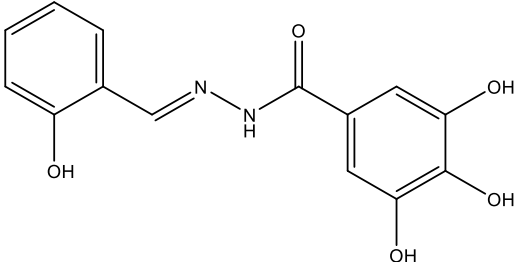
454	K	95.90
455	A	100.00
456	G	99.90
457	Y	100.00
458	V	98.20
459	T	99.90
460	N	11.20
461	R	79.50
462	G	99.90
463	R	97.20
464	Q	99.60
465	K	98.40
466	V	67.10
467	V	75.70
468	T	12.10
469	L	91.00
470	T	87.20
471	D	47.50
472	T	99.90
473	T	100.00
474	N	99.90
475	Q	100.00
476	K	95.70
477	T	76.10
478	E	99.80
479	L	100.00
480	Q	82.90
481	A	100.00
482	I	99.50
483	H	36.30
484	L	98.00
485	A	100.00
486	L	100.00
487	Q	99.80
488	D	99.80
489	S	99.90
490	G	100.00
491	L	37.80
492	E	98.90
493	V	99.60
494	N	100.00
495	I	98.40
496	V	99.40
497	T	100.00
498	D	100.00
499	S	99.90
500	Q	99.90
501	Y	99.90
502	A	97.40
503	L	99.70
504	G	99.90
505	I	99.70

506	I	99.90
507	Q	98.80
508	A	97.60
509	Q	95.60
510	P	100.00
511	D	99.90
512	Q	2.90
513	S	99.90
514	E	96.40
515	S	99.10
516	E	96.70
517	L	88.80
518	V	99.90
519	N	69.10
520	Q	94.80
521	I	99.70
522	I	99.90
523	E	99.80
524	Q	83.20
525	L	99.90
526	I	100.00
527	K	67.70
528	K	99.90
529	E	94.30
530	K	60.80
531	V	69.60
532	Y	99.90
533	L	99.80
534	A	37.10
535	W	99.90
536	V	99.90
537	P	99.90
538	A	99.90
539	H	100.00
540	K	99.90
541	G	99.70
542	I	99.50
543	G	96.40
544	G	99.80
545	N	99.90
546	E	99.30
547	Q	96.60
548	V	94.90
549	D	99.70
550	K	99.70
551	L	99.90
552	V	99.90
553	S	99.90
554	A	100.00
555	G	99.70
556	I	99.10
557	R	99.80

558	K	87.00
559	I	7.40
560	L	100.00

Table S2. Structures and anti-HIV-1 RT RNase H activities of compounds 1–23.

Compound	Structure	HIV-1 RNase H IC ₅₀ (μM)
1		61 ± 11
2		62 ± 2
3		>100
4		>100
5		>100
6		37 ± 5

7		25.26 ± 7.56
8		8.77 ± 3.13
9		9.58 ± 3.43
10		4.12 ± 0.22
11		2.60 ± 0.59
12		3.22 ± 0.54
13		2.32 ± 0.75

14		3.11 ± 0.47
15		0.92 ± 0.02
16		2.15 ± 0.11
17		2.03 ± 0.59
18		1.73 ± 0.07
19		>100

20		0.175 ± 0.002
21		0.62 ± 0.10
22		9.71 ± 1.57
23		0.18 ± 0.03



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