Supporting Information-1

Rapid Synthesis of Abelson Tyrosine Kinase Inhibitors using Click Chemistry

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High Resolution Mass Spectrometry (HRMS) results of the selected click-inhibitors:

W1-SA9 [$C_{27}H_{24}FN_9O_3S$], $(m/z)_{calculated}$ = 596.1599 [$C_{27}H_{24}FN_9O_3SNa$] $(m/z)_{observed}$ = 596.1586 (ESI-HRMS)

W1-SA10 [$C_{27}H_{24}FN_9O_3S$], $(m/z)_{calculated}$ = 596.1599 [$C_{27}H_{24}FN_9O_3SNa$] $(m/z)_{observed}$ = 596.1590 (ESI-HRMS)

W1-SA17 [$C_{31}H_{27}N_9O_3S$], $(m/z)_{calculated}$ = 606.2036 [$C_{31}H_{28}N_9O_3S$] $(m/z)_{observed}$ = 606.2023 (ESI-HRMS)

W1-SA20 [$C_{28}H_{27}N_9O_3S$], $(m/z)_{calculated}$ = 570.2036 [$C_{28}H_{28}N_9O_3S$] $(m/z)_{observed}$ = 570.2031 (ESI-HRMS)

W1-SA22 [$C_{25}H_{23}N_9O_3S_2$], $(m/z)_{calculated}$ = 584.1258 [$C_{25}H_{23}N_9O_3S_2Na$] $(m/z)_{observed}$ = 584.1251 (ESI-HRMS)

W2-SA3 [$C_{28}H_{26}ClN_9O_3S$], $(m/z)_{calculated}$ = 626.1460 [$C_{28}H_{26}ClN_9O_3SNa$] $(m/z)_{observed}$ = 626.1441 (ESI-HRMS)

W2-SA4 [$C_{26}H_{24}ClN_9O_3S_2$], $(m/z)_{calculated}$ = 632.1024 [$C_{26}H_{24}ClN_9O_3S_2Na$] $(m/z)_{observed}$ = 632.0999 (ESI-HRMS)

W2-SA7 [$C_{28}H_{25}F_2N_9O_3S$], $(m/z)_{calculated}$ = 628.1661 [$C_{28}H_{25}F_2N_9O_3SNa$] $(m/z)_{observed}$ = 628.1692 (ESI-HRMS)

W2-SA13 [$C_{29}H_{28}FN_9O_3S$], $(m/z)_{calculated}$ = 624.1912 [$C_{29}H_{28}FN_9O_3SNa$] $(m/z)_{observed}$ = 624.1939 (ESI-HRMS)

W2-SA17 [$C_{32}H_{29}N_9O_3S$], $(m/z)_{calculated}$ = 642.2006 [$C_{32}H_{29}N_9O_3SNa$] $(m/z)_{observed}$ = 642.2013 (ESI-HRMS)

W2-SA18 [$C_{32}H_{29}N_9O_3S$], $(m/z)_{calculated}$ = 642.2006 [$C_{32}H_{29}N_9O_3SNa$] $(m/z)_{observed}$ = 642.2004 (ESI-HRMS)

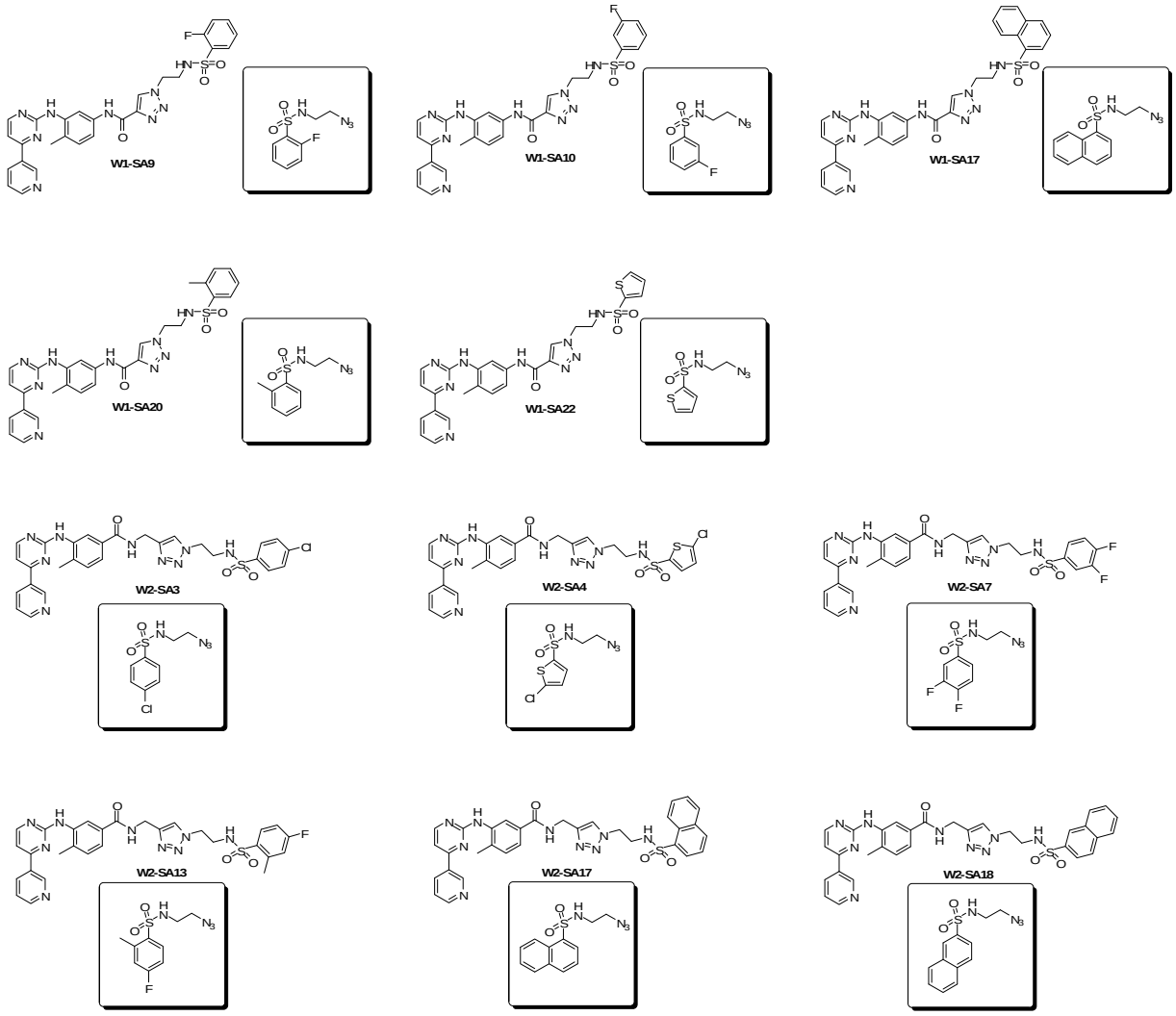
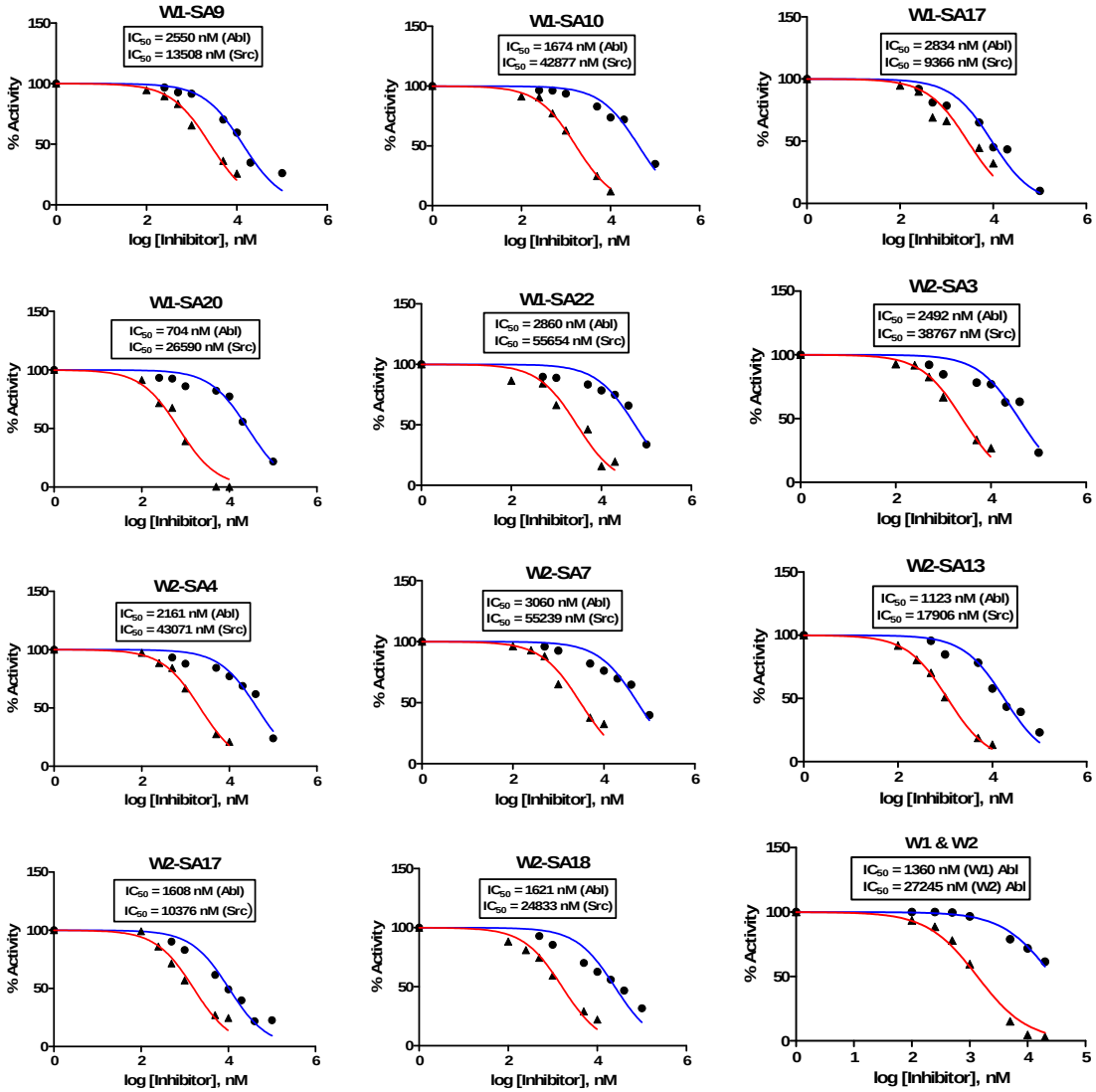


Figure S1. Chemical structures of the potent inhibitors of Abl kinase identified from the screening (Insets shows the structures of the corresponding azides)

IC_{50} evaluation of the click-inhibitors against Abl/Src kinases

Concentration-dependent experiments were performed to confirm the potency of the identified initial hits (structures shown above in Figure S1). All the 11 hits were purified by Semi-Prep reverse-phase HPLC using water with 0.1% TFA and acetonitrile with 0.1% TFA as eluents on a Luna 5 µ C-18 (2) 100A column (50 × 30 mm, 5 micron) at a flow rate of 10 ml/min before subjecting to the detailed inhibition measurements. The dose-dependent inhibition assays were performed by varying the concentration of the inhibitors under fixed enzyme concentration of 50 nM as mentioned before. The IC_{50} values for each inhibitor were calculated from the percentage activity vs. log [concentration of inhibitor] curves generated using the GraphPad Prism software.



Cell culture and Proliferation Assay

Human leukemic cell lines K-562 (p-210 Bcr-Abl expressing chronic myelogenous leukemia) were maintained in RPMI-1640 medium supplemented with L-glutamine and 10% FBS. The cells (0.2-0.4 × 10^6 per mL) were plated in duplicate in 96-well plates containing two different concentrations (50 and 10 µM) of the 11 inhibitor hits identified against recombinant Abl from the in-vitro assay. After incubation at 37 ^oC in 5% CO_2 for 48 h, the effect of the compounds on the cell proliferation was determined by the XTT (sodium 3' – [1-(phenylaminocarbonyl)-3, 4-tetrazolium]-bis (4-methoxy-6-nitro) benzene sulfonic acid hydrate) colorimetric dye reduction method. Briefly, the procedure for the assay was as follows. The XTT was dissolved in hot RPMI media (37 ^oC) at a concentration of 1 mg/mL. Immediately before use, the electron coupling reagent PMS (N-methyl dibenzopyrazine methyl sulfate) was added to the XTT solution giving a PMS concentration of 125 µM (The PMS was stored as 100 mM stock solution in saline at 4 ^oC). 25 µL of this XTT/PMS solution was added to each well in the 96-well plate containing ~ 100 µL per well culture giving a final concentration of 0.2 mg/mL XTT and 25 µM PMS. After incubation at 37 ^oC in 5% CO_2 for 2-6 h the absorbance of each well was measured at a wavelength of 450 nm using Tecan microplate reader and effect of the compounds on the cell proliferation was determined by comparing with the DMSO (no inhibitor) controls. The compounds, unfortunately, did not show significant effect on the cell viability. Even the best inhibitor identified in the cell-based assay (**W2-SA17,** IC_{50} = 1608 nM in in-vitro assay) shows only 60% inhibition of the cell proliferation at 50 µM concentration (All other compounds including the best inhibitor **W1-SA20** from the in-vitro assay were found to be less potent with less than 50% inhibition of cell proliferation at 50 µM concentration. The exact reason for the lack of cellular potency of the compounds is not clear at the moment although we speculate that it could most likely be due either to the poor solubility of the compounds in the assay medium or the cell-impermeability of the compounds. We are currently working on these aspects.

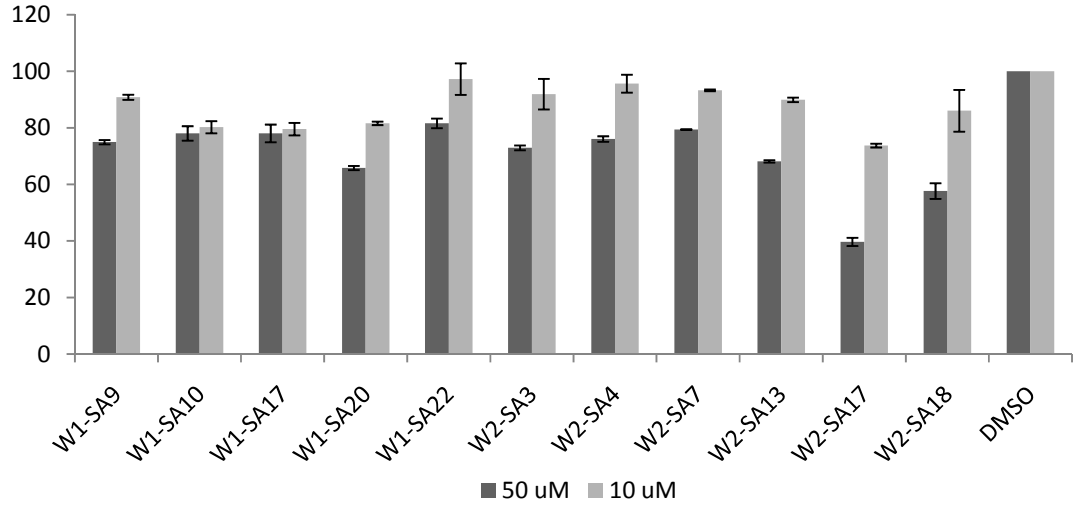


Figure S2. Antiproliferation assay of K-562 cells in the presence of the 11 click-inhibitors at two different concentrations (50 µM and 10 µM). The Y axis represents the cell proliferation

normalized with respect to the no inhibitor control (DMSO alone). Shorter column heights indicate stronger antiproliferative property.

Azide library used for the synthesis of the Imatinib analogue click-library

The azides were synthesized via a highly efficient traceless solid-phase method we recently developed.[1] The synthetic details and characterizations are reported therein.

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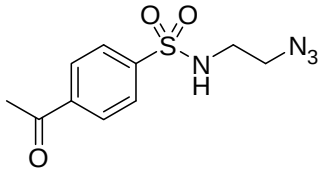
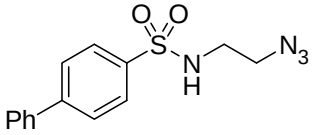
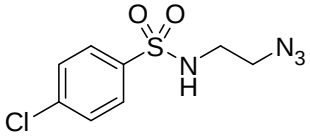
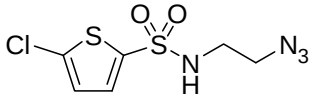
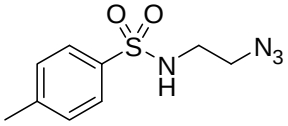
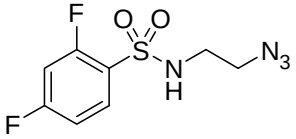
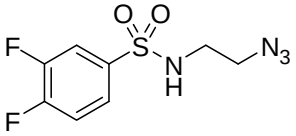
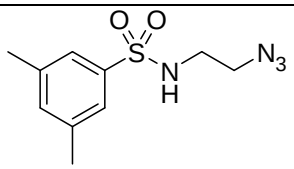
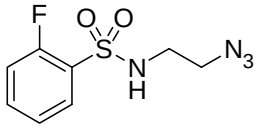
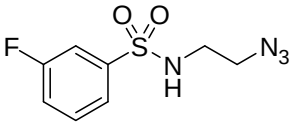
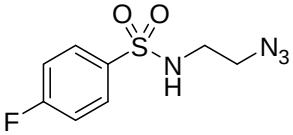
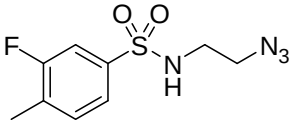
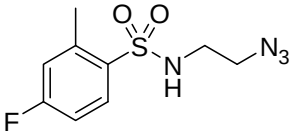
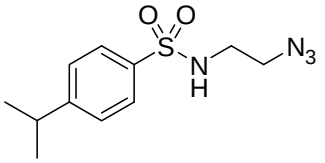
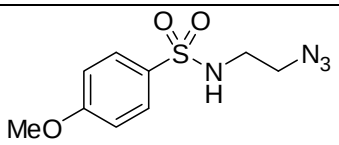
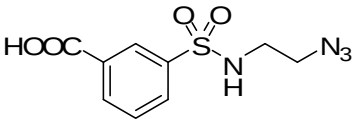
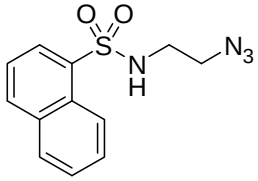
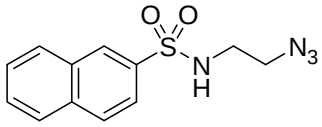
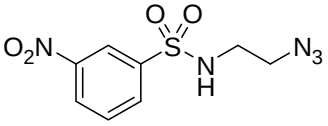
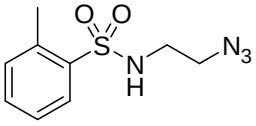
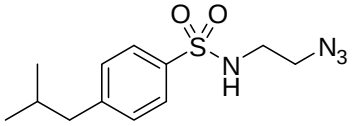
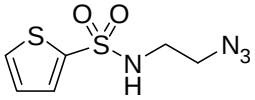
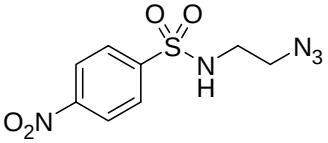
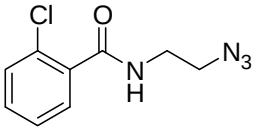
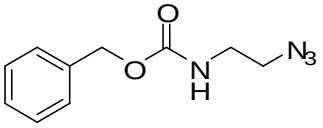
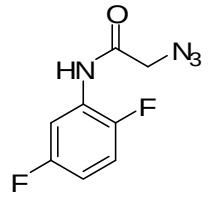
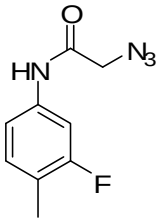
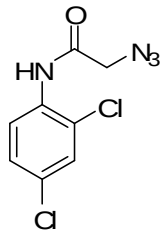
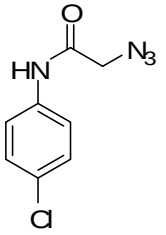
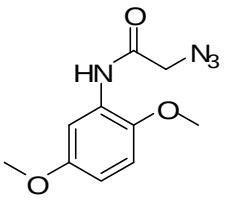
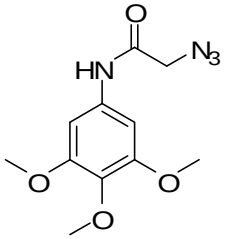
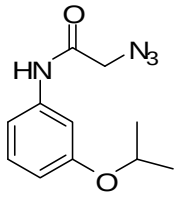
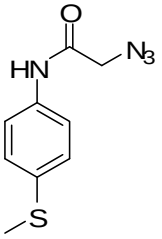
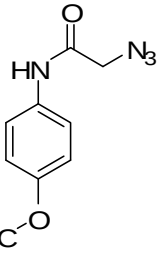
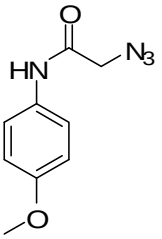
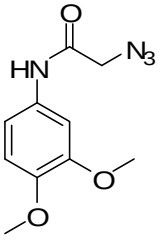
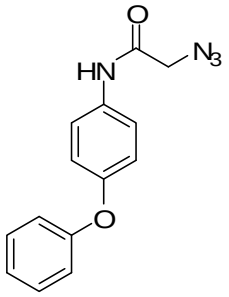
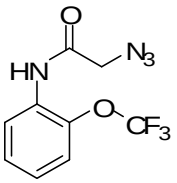
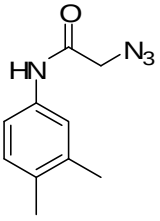
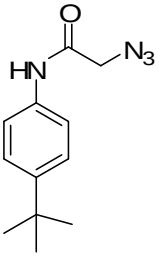
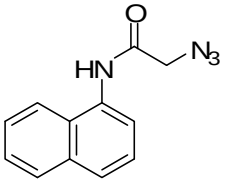
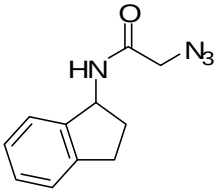
1	 Exact Mass: 268.06	**SA-1**
2	 Exact Mass: 302.08	**SA-2**
3	 Exact Mass: 260.01	**SA-3**
4	 Exact Mass: 265.97	**SA-4**
5	 Exact Mass: 240.07	**SA-5**
6	 Exact Mass: 262.03	**SA-6**
7	 Exact Mass: 262.03	**SA-7**

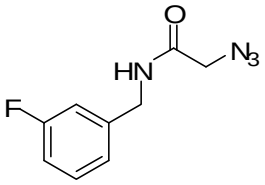
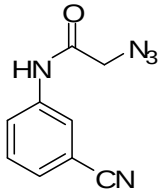
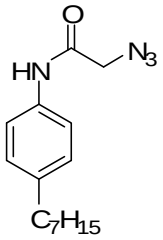
8	 Exact Mass: 254.08	**SA-8**
9	 Exact Mass: 244.04	**SA-9**
10	 Exact Mass: 244.04	**SA-10**
11	 Exact Mass: 244.04	**SA-11**
12	 Exact Mass: 258.06	**SA-12**
13	 Exact Mass: 258.06	**SA-13**
14	 Exact Mass: 268.10	**SA-14**
15	 Exact Mass: 256.06	**SA-15**
16	 Exact mass: 270.04	**SA-16**

17	 Exact Mass: 276.07	**SA-17**
18	 Exact Mass: 276.07	**SA-18**
19	 Exact Mass: 271.04	**SA-19**
20	 Exact Mass: 240.07	**SA-20**
21	 Exact Mass: 282.12	**SA-21**
22	 Exact Mass: 232.01	**SA22**
23	 Exact Mass: 271.04	**SA-23**
24	 Exact Mass: 224.05	**SA-24**
25	 Exact mass: 220.09	**A-25**

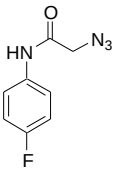
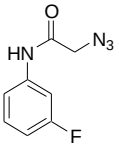
26	 Exact mass: 212.05	**A-26**
27	 Exact mass: 208.07	**A-27**
28	 Exact mass: 243.99	**A-28**
29	 Exact mass: 210.03	**A-29**
30	 Exact mass: 236.09	**A-30**
31	 Exact mass: 266.10	**A-31**

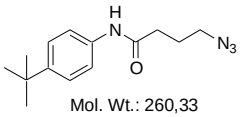
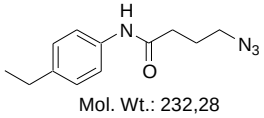
32	 Exact mass: 234.11	**A-32**
33	 Exact mass: 222.05	**A-33**
34	 Exact mass: 260.05	**A-34**
35	 Exact mass: 206.08	**A-35**
36	 Exact mass: 236.09	**A-36**

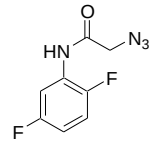
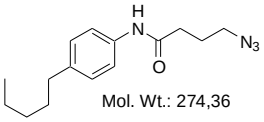
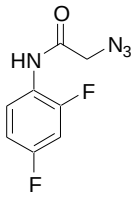
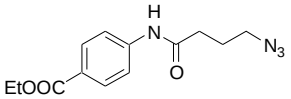
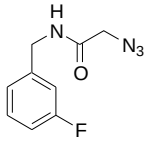
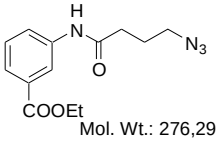
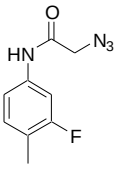
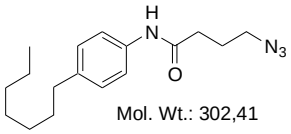
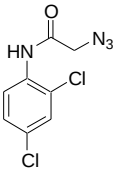
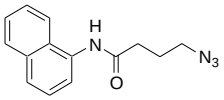
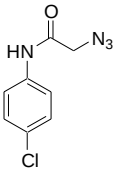
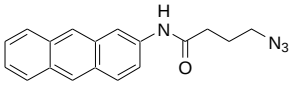
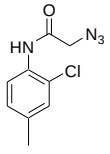
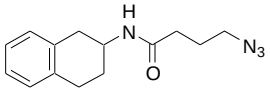
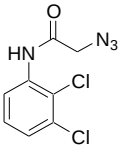
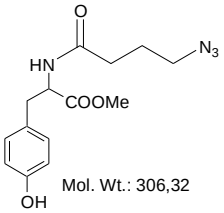
37	 Exact mass: 268.09	**A-37**
38	 Exact mass: 260.05	**A-38**
39	 Exact mass: 204.10	**A-39**
40	 Exact mass: 232.13	**A-40**
41	 Exact mass: 226.08	**A-41**
42	 Exact mass: 216.10	**A-42**

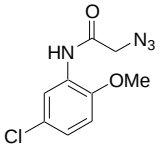
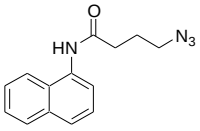
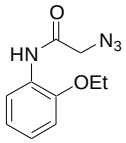
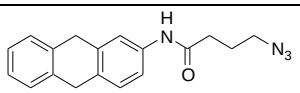
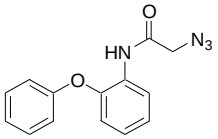
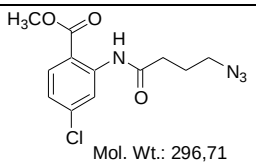
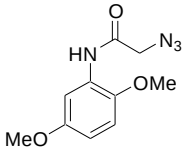
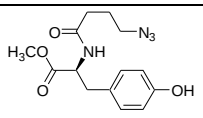
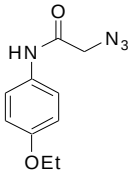
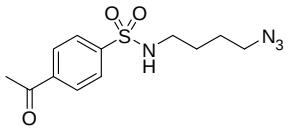
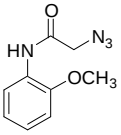
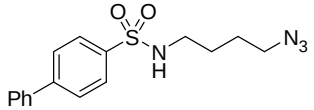
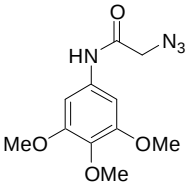
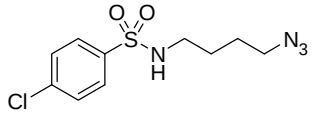
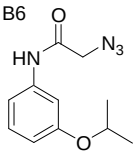
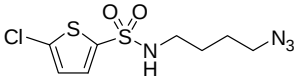
43	 Exact mass: 208.07	**A-43**
44	 Exact mass: 201.06	**A-44**
45	 Exact mass: 274.17	**A-45**

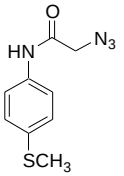
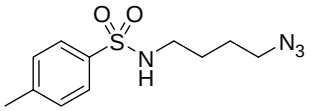
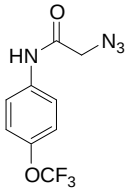
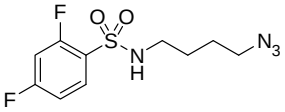
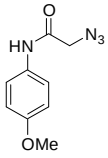
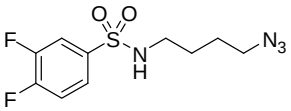
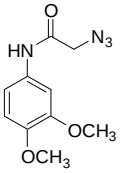
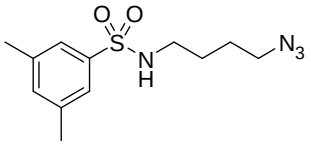
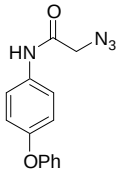
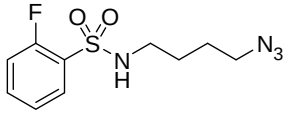
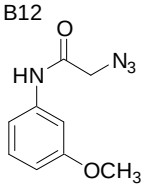
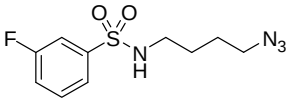
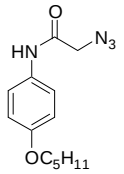
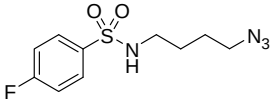
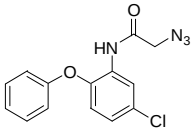
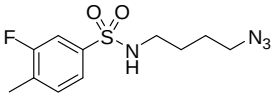
Azide library used for the ADP-alkyne click library

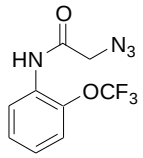
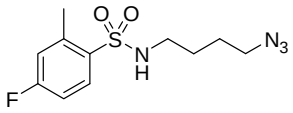
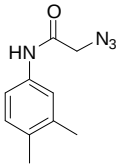
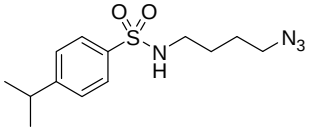
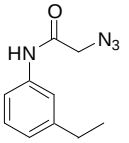
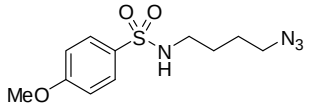
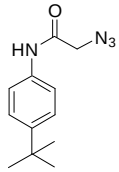
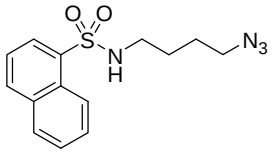
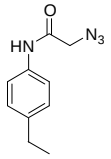
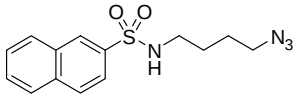
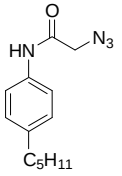
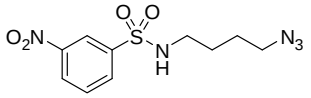
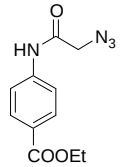
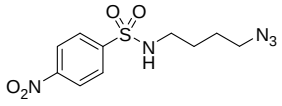
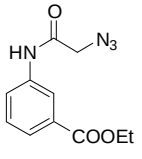
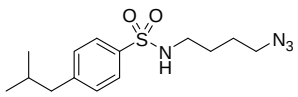
Azide Position in heat-map	Unique ID	Structure
1	A1-2C	 Mol. Wt.: 194,17
2	A2-2C	 Mol. Wt.: 194,17

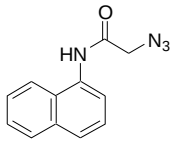
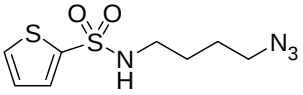
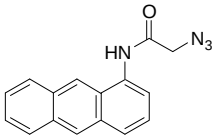
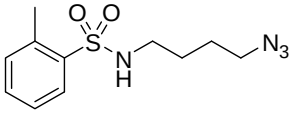
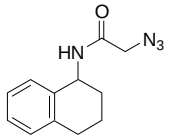
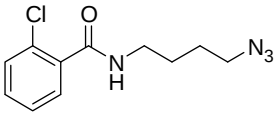
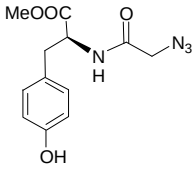
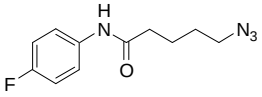
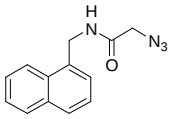
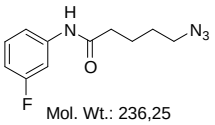
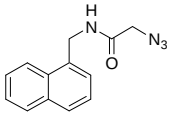
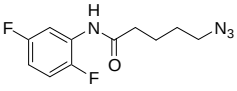
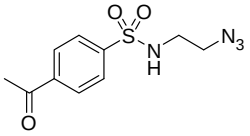
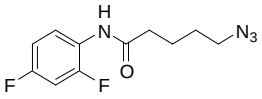
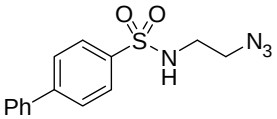
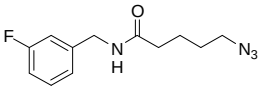
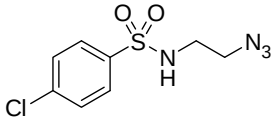
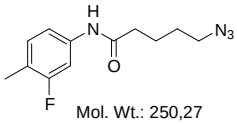
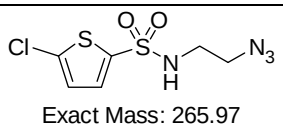
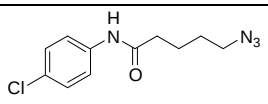
Azide Position in heat-map	Unique ID	Structure
173	G6-4C	 Mol. Wt.: 260,33
174	G7-4C	 Mol. Wt.: 232,28

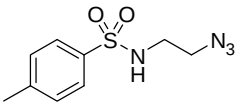
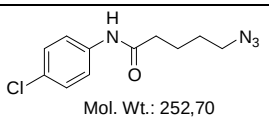
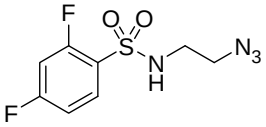
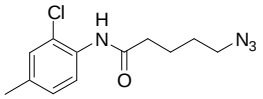
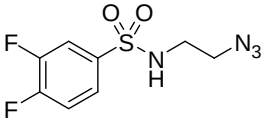
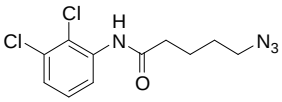
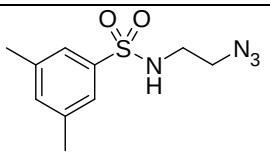
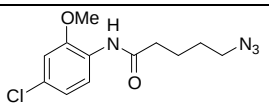
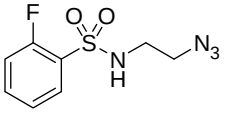
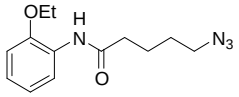
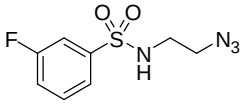
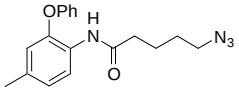
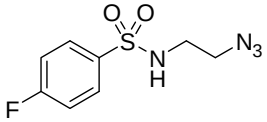
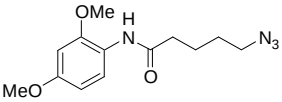
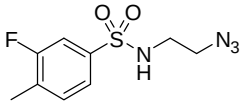
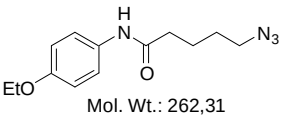
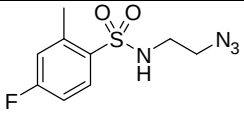
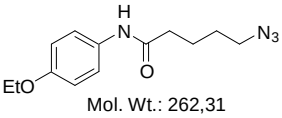
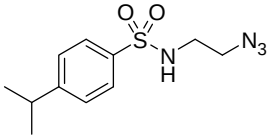
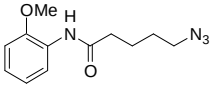
3	A3-2C	 Mol. Wt.: 212,16		175	G8-4C	 Mol. Wt.: 274,36
4	A4-2C	 Mol. Wt.: 212,16		176	G9-4C	 Mol. Wt.: 276,29
5	A5-2C	 Mol. Wt.: 208,19		177	G10-4C	 Mol. Wt.: 276,29
6	A6-2C	 Mol. Wt.: 208,19		178	G11-4C	 Mol. Wt.: 302,41
7	A7-2C	 Mol. Wt.: 245,07		179	G12-4C	 Mol. Wt.: 254,29
8	A8-2C	 Mol. Wt.: 210,62		180	H1-4C	 Mol. Wt.: 304,35
9	A9-2C	 Mol. Wt.: 224,65		181	H2-4C	 Mol. Wt.: 258,32
10	A10-2C	 Mol. Wt.: 245,07		182	H3-4C	 Mol. Wt.: 306,32

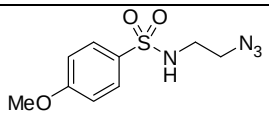
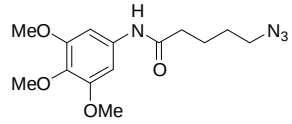
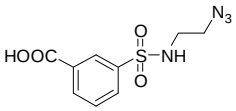
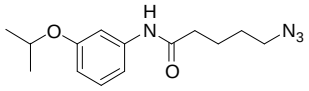
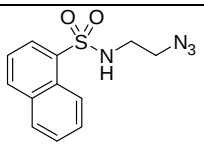
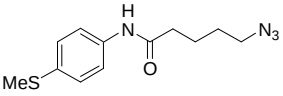
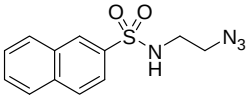
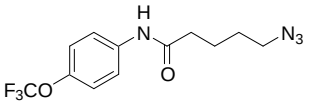
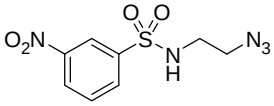
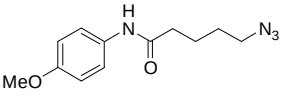
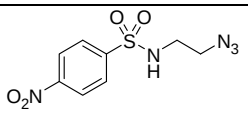
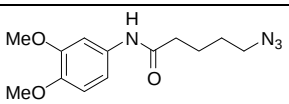
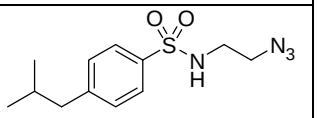
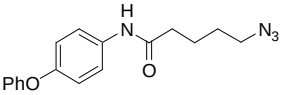
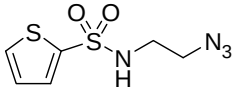
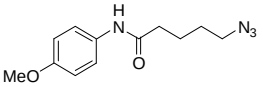
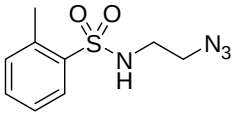
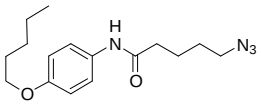
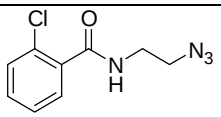
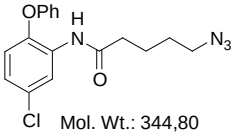
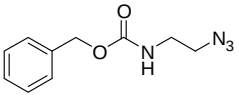
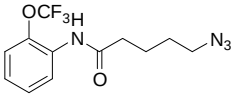
11	A11-2C	 Mol. Wt.: 240,65		183	H4-4C	 Mol. Wt.: 254,29
12	A12-2C	 Mol. Wt.: 220,23		184	H5-4C	 Mol. Wt.: 306,36
13	B1-2C	 Mol. Wt.: 268,27		185	H7-4C	 Mol. Wt.: 296,71
14	B2-2C	 Mol. Wt.: 236,23		186	H8-4C	 Mol. Wt.: 306,32
15	B3-2C	 Mol. Wt.: 220,23		187	E1-4S	 Exact Mass: 296.09
16	B4-2C	 Mol. Wt.: 206,20		188	E2-4S	 Exact Mass: 330.12
17	B5-2C	 Mol. Wt.: 266,25		189	E3-4S	 Exact Mass: 288.04
18	B6-2C	 Mol. Wt.: 234,25		190	E4-4S	 Exact Mass: 294.00

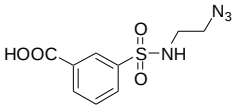
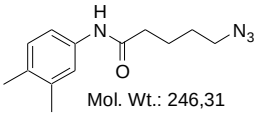
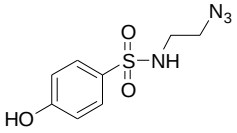
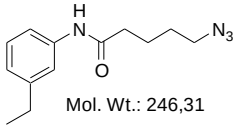
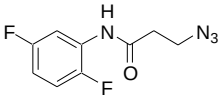
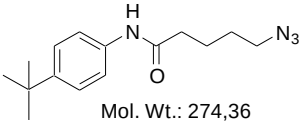
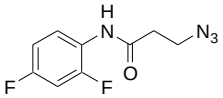
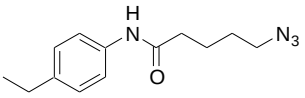
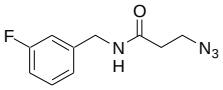
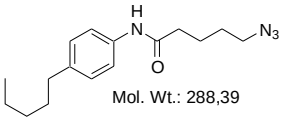
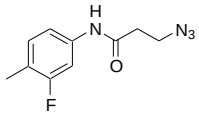
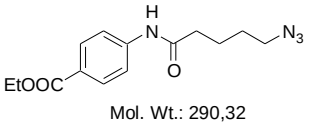
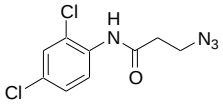
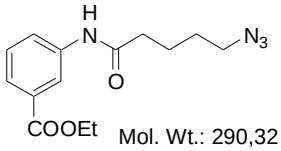
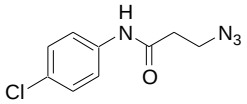
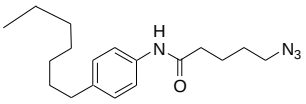
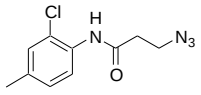
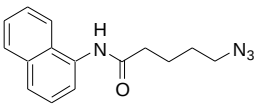
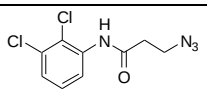
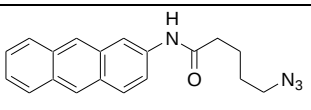
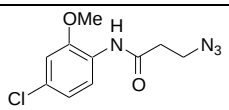
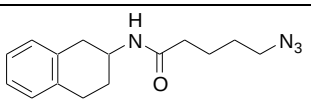
19	B7-2C	 Mol. Wt.: 222,27		191	E5-4S	 Exact Mass: 268.10
20	B8-2C	 Mol. Wt.: 260,17		192	E6-4S	 Exact Mass: 290.06
21	B9-2C	 Mol. Wt.: 206,20		193	E7-4S	 Exact Mass: 290.06
22	B10-2C	 Mol. Wt.: 236,23		194	E8-4S	 Exact Mass: 282.12
23	B11-2C	 Mol. Wt.: 268,27		195	E9-4S	 Exact Mass: 272.07
24	B12-2C	B12  Mol. Wt.: 206,20		196	E10-4S	 Exact Mass: 272.07
25	C1-2C	 Mol. Wt.: 262,31		197	E11-4S	 Exact Mass: 272.07
26	C2-2C	 Mol. Wt.: 302,72		198	E12-4S	 Exact Mass: 286.09

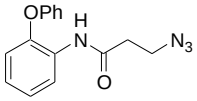
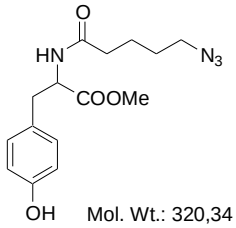
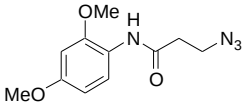
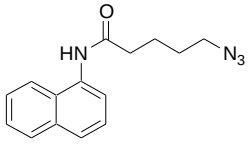
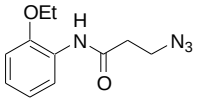
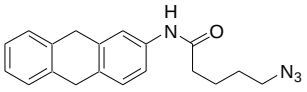
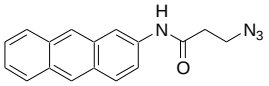
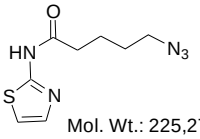
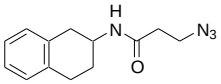
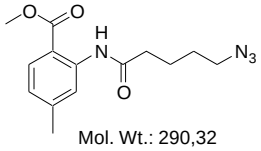
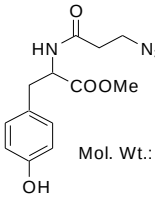
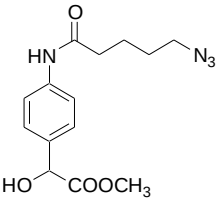
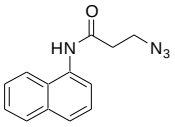
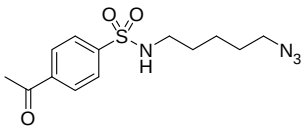
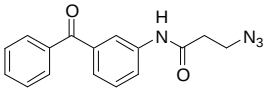
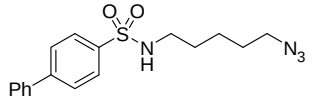
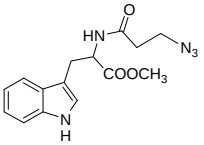
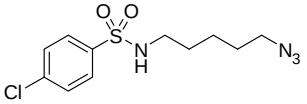
27	C3-2C	 Mol. Wt.: 260,17		199	F1-4S	 Exact Mass: 286.09
28	C4-2C	 Mol. Wt.: 204,23		200	F2-4S	 Exact Mass: 296.13
29	C5-2C	 Mol. Wt.: 204,23		201	F3-4S	 Exact Mass: 284.09
30	C6-2C	 Mol. Wt.: 232,28		202	F5-4S	 Exact Mass: 304.10
31	C7-2C	 Mol. Wt.: 204,23		203	F6-4S	 Exact Mass: 304.10
32	C8-2C	 Mol. Wt.: 246,31		204	F7-4S	 Exact Mass: 299.07
33	C9-2C	 Mol. Wt.: 248,24		205	F8-4S	 Exact Mass: 299.07
34	C10-2C	 Mol. Wt.: 248,24		206	F9-4S	 Exact Mass: 310.15

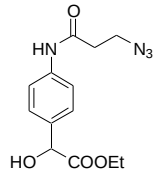
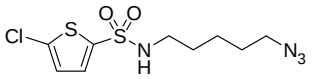
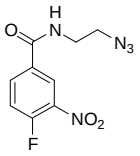
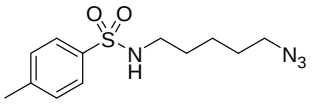
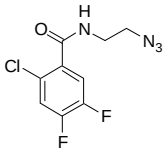
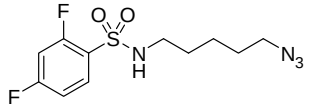
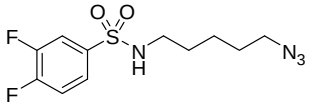
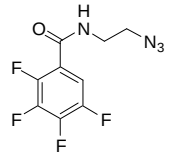
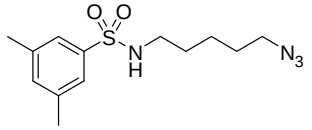
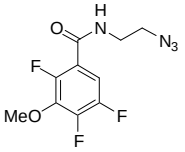
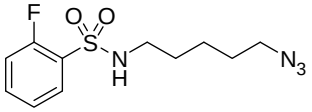
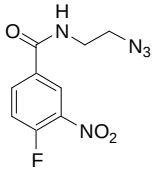
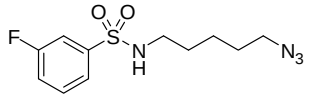
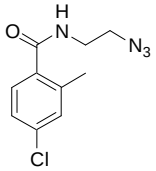
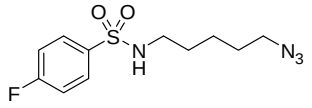
35	C11-2C	 Mol. Wt.: 226,23	207	F10-4S	 Exact Mass: 260.04
36	C12-2C	 Mol. Wt.: 276,29	208	F11-4S	 Exact Mass: 268.10
37	D1-2C	 Mol. Wt.: 230,27	209	F12-4S	 Exact Mass: 252.08
38	D2-2C	 Mol. Wt.: 278,26	210	A1-5C	 Mol. Wt.: 236,25
39	D3-2C	 Mol. Wt.: 240,26	211	A2-5C	 Mol. Wt.: 236,25
40	D4-2C	 Mol. Wt.: 240,26	212	A3-5C	 Mol. Wt.: 254,24
41	A1-2S	 Exact Mass: 268.06	213	A4-5C	 Mol. Wt.: 254,24
42	A2-2S	 Exact Mass: 302.08	214	A5-5C	 Mol. Wt.: 250,27
43	A3-2S	 Exact Mass: 260.01	215	A6-5C	 Mol. Wt.: 250,27
44	A4-2S	 Exact Mass: 265.97	216	A7-5C	 Mol. Wt.: 252,70

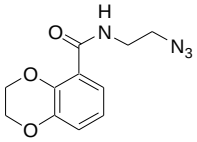
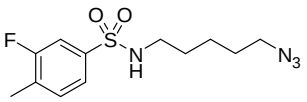
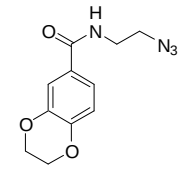
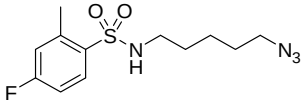
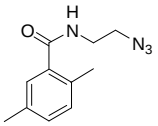
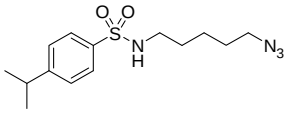
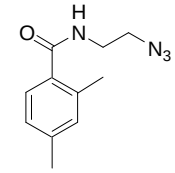
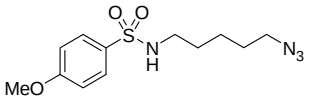
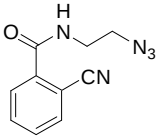
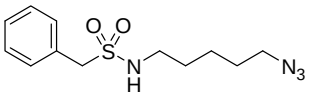
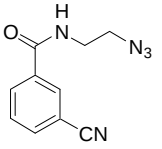
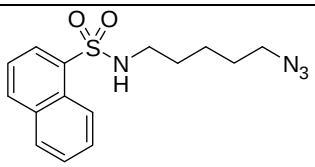
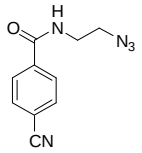
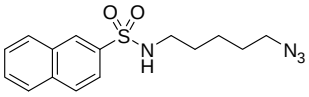
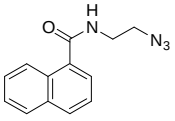
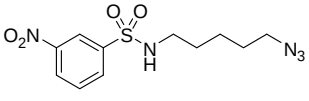
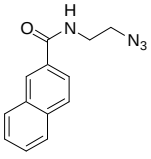
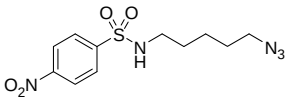
45	A5-2S	 Exact Mass: 240.07	217	A8-5C	 Mol. Wt.: 252,70
46	A6-2S	 Exact Mass: 262.03	218	A9-5C	 Mol. Wt.: 266,73
47	A7-2S	 Exact Mass: 262.03	219	A10-5C	 Mol. Wt.: 287,14
48	A8-2S	 Exact Mass: 254.08	220	A11-5C	 Mol. Wt.: 282,73
49	A9-2S	 Exact Mass: 244.04	221	A12-5C	 Mol. Wt.: 262,31
50	A10-2S	 Exact Mass: 244.04	222	B1-5C	 Mol. Wt.: 324,38
51	A11-2S	 Exact Mass: 244.04	223	B2-5C	 Mol. Wt.: 278,31
52	A12-2S	 Exact Mass: 258.06	224	B3-5C	 Mol. Wt.: 262,31
53	B1-2S	 Exact Mass: 258.06	225	B3-5C	 Mol. Wt.: 262,31
54	B2-2S	 Exact Mass: 268.10	226	B4-5C	 Mol. Wt.: 248,28

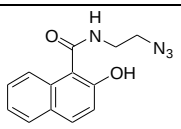
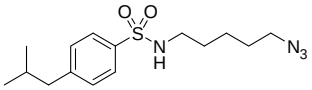
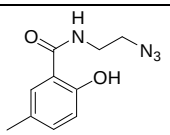
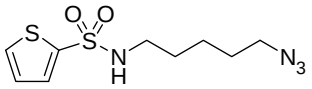
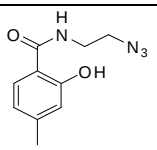
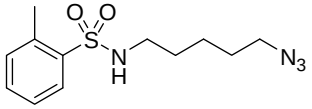
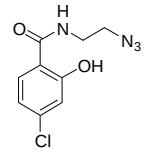
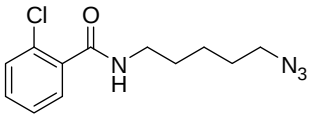
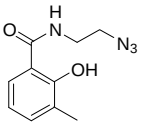
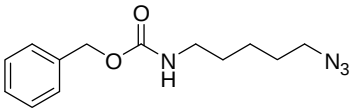
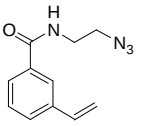
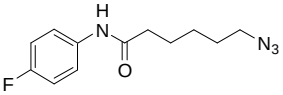
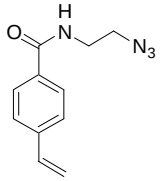
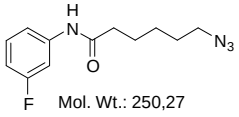
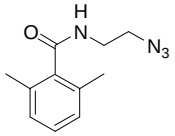
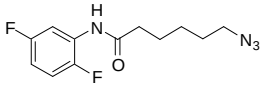
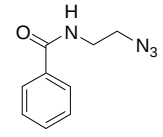
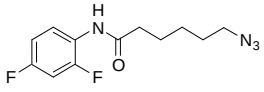
55	B3-2S	 Exact Mass: 256.06		227	B5-5C	 Mol. Wt.: 308,33
56	C2-2S	 Mol. Wt.: 270,27		228	B6-5C	 Mol. Wt.: 276,33
57	B5-2S	 Exact Mass: 276.07		229	B7-5C	 Mol. Wt.: 264,35
58	B6-2S	 Exact Mass: 276.07		230	B8-5C	 Mol. Wt.: 302,25
59	B7-2S	 Exact Mass: 271.04		231	B9-5C	 Mol. Wt.: 248,28
60	B8-2S	 Exact Mass: 271.04		232	B10-5C	 Mol. Wt.: 278,31
61	B9-2S	 Exact Mass: 282.12		233	B11-5C	 Mol. Wt.: 310,35
62	B10-2S	 Exact Mass: 232.01		234	B12-5C	 Mol. Wt.: 248,28
63	B11-2S	 Exact Mass: 240.07		235	C1-5C	 Mol. Wt.: 304,39
64	B12-2S	 Exact Mass: 224.05		236	C2-5C	 Mol. Wt.: 344,80
65	C1-2S	 Exact Mass: 220.10		237	C3-5C	 Mol. Wt.: 302,25

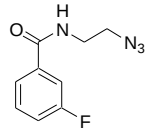
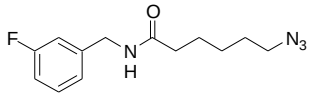
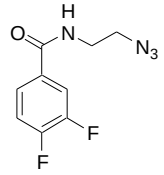
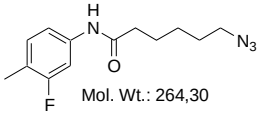
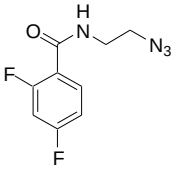
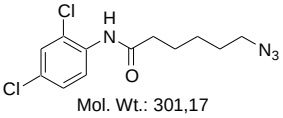
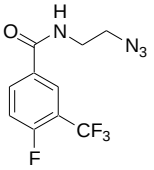
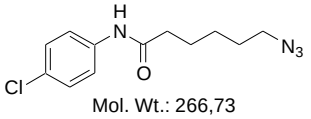
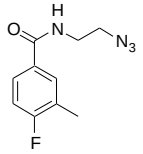
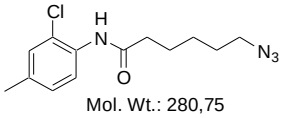
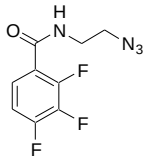
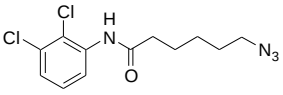
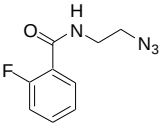
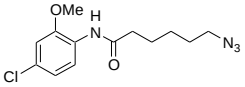
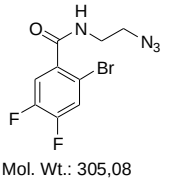
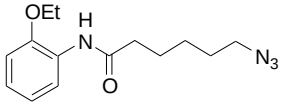
66	C2-2S	 Mol. Wt.: 270,27		238	C4-5C	 Mol. Wt.: 246,31
67	C3-2S	 Mol. Wt.: 242,26		239	C5-5C	 Mol. Wt.: 246,31
68	A3-3C(am)	 Mol. Wt.: 226,18		240	C6-5C	 Mol. Wt.: 274,36
69	A4-3C(am)	 Mol. Wt.: 226,18		241	C7-5C	 Mol. Wt.: 246,31
70	A5-3C(am)	 Mol. Wt.: 222,22		242	C8-5C	 Mol. Wt.: 288,39
71	A6-3C(am)	 Mol. Wt.: 222,22		243	C9-5C	 Mol. Wt.: 290,32
72	A7-3C(am)	 Mol. Wt.: 259,09		244	C10-5C	 Mol. Wt.: 290,32
73	A8-3C(am)	 Mol. Wt.: 224,65		245	C11-5C	 Mol. Wt.: 316,44
74	A9-3C(am)	 Mol. Wt.: 238,67		246	C12-5C	 Mol. Wt.: 268,31
75	A10-3C(am)	 Mol. Wt.: 259,09		247	D1-5C	 Mol. Wt.: 318,37
76	A11-3C(am)	 Mol. Wt.: 254,67		248	D2-5C	 Mol. Wt.: 272,35

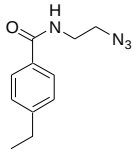
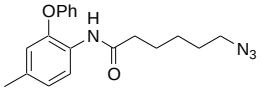
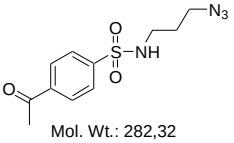
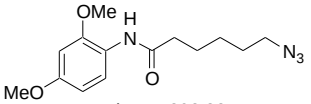
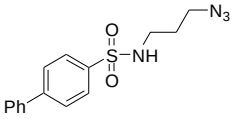
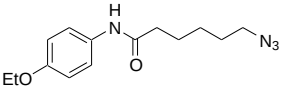
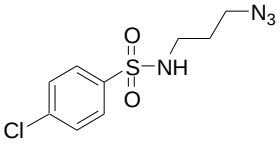
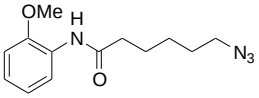
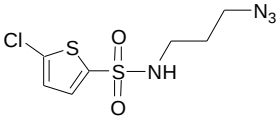
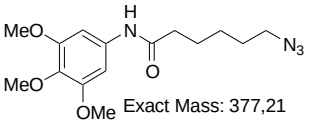
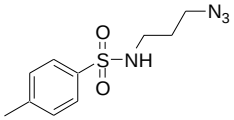
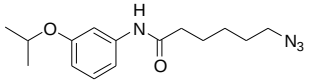
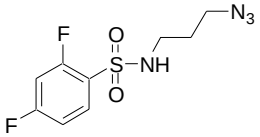
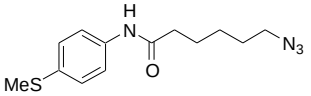
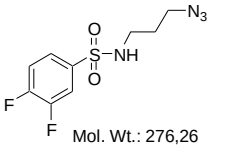
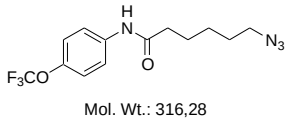
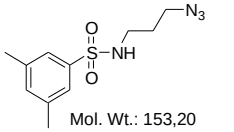
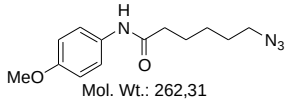
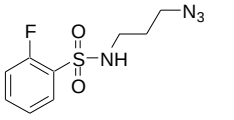
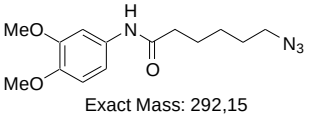
77	B1-3C(am)	 Mol. Wt.: 282,30		249	D3-5C	 Mol. Wt.: 320,34
78	B2-3C(am)	 Mol. Wt.: 250,25		250	D4-5C	 Mol. Wt.: 268,31
79	A12-3C(am)	 Mol. Wt.: 234,25		251	D5-5C	 Mol. Wt.: 320,39
80	D1-3C(am)	 Mol. Wt.: 290,32		252	D6-5C	 Mol. Wt.: 225,27
81	D2-3C(am)	 Mol. Wt.: 244,29		253	D7-5C	 Mol. Wt.: 290,32
82	D3-3C(am)	 Mol. Wt.: 292,29		254	D8-5C	 Mol. Wt.: 306,32
83	D4-3C(am)	 Mol. Wt.: 240,26		255	A1-5S	 Exact Mass: 310.11
84	D5-3C(am)	 Mol. Wt.: 294,31		256	A2-5S	 Exact Mass: 344.13
85	D6-3C(am)	 Mol. Wt.: 315,33		257	A3-5S	 Exact Mass: 302.06

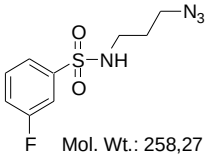
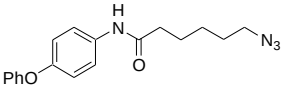
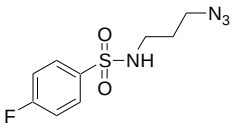
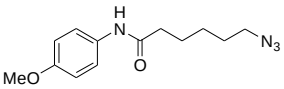
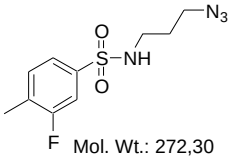
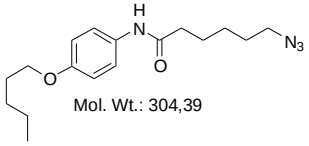
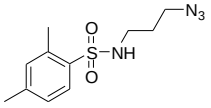
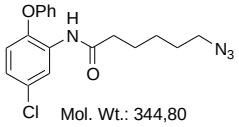
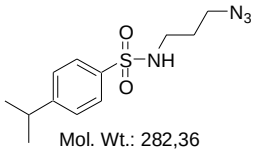
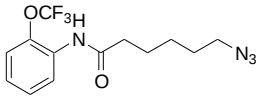
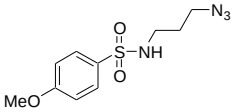
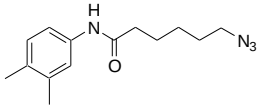
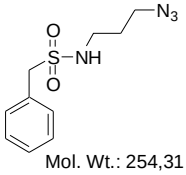
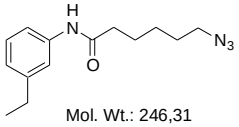
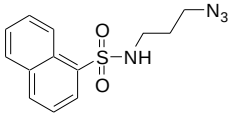
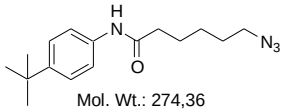
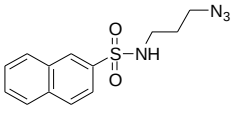
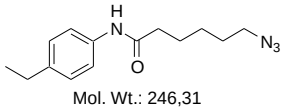
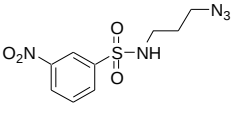
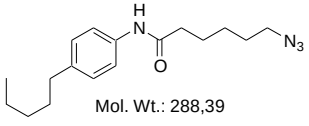
86	D7-3C(am)	 Mol. Wt.: 292,29		258	A4-5S	 Exact Mass: 308.02
87	E1-3C	 Mol. Wt.: 253,19		259	A5-5S	 Exact Mass: 282.12
88	E2-3C	 Mol. Wt.: 260,63		260	A6-5S	 Exact Mass: 304.08
89	E3-3C	 Mol. Wt.: 244,17		261	A7-5S	 Exact Mass: 304.08
90	E4-3C	 Mol. Wt.: 262,16		262	A8-5S	 Exact Mass: 296.13
91	E5-3C	 Mol. Wt.: 274,20		263	A9-5S	 Exact Mass: 286.09
92	E6-3C	 Mol. Wt.: 253,19		264	A10-5S	 Exact Mass: 286.09
93	E7-3C	 Mol. Wt.: 238,67		265	A11-5S	 Exact Mass: 286.09

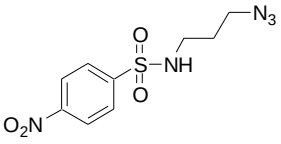
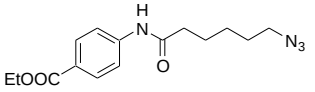
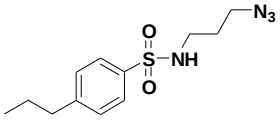
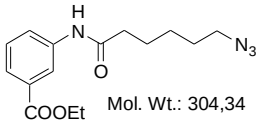
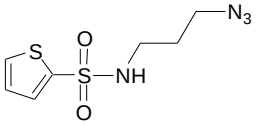
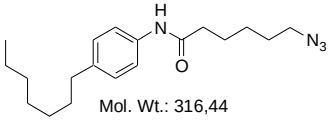
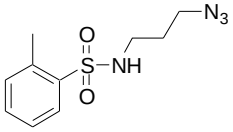
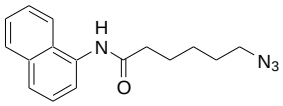
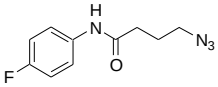
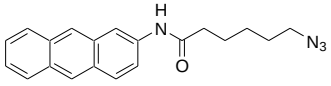
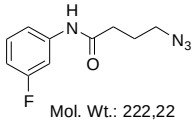
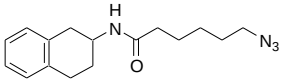
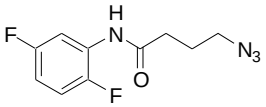
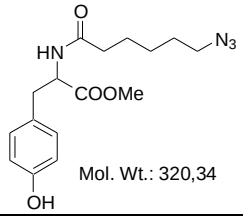
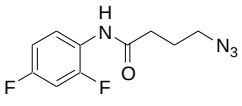
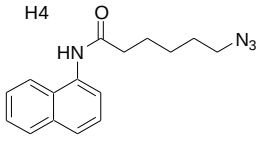
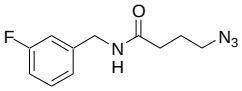
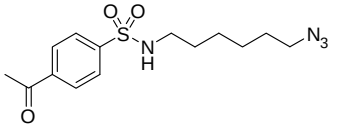
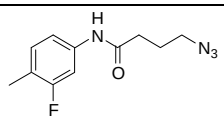
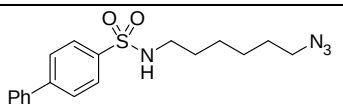
94	E8-3C	 Mol. Wt.: 248,24		266	A12-5S	 Exact Mass: 300.11
95	E9-3C	 Mol. Wt.: 248,24		267	B1-5S	 Exact Mass: 300.11
96	E10-3C	 Mol. Wt.: 218,26		268	B2-5S	 Exact Mass: 310.15
97	E11-3C	 Mol. Wt.: 218,26		269	B3-5S	 Exact Mass: 298.11
98	E12-3C	 Mol. Wt.: 215,21		270	B4-5S	 Exact Mass: 282.12
99	F1-3C	 Mol. Wt.: 215,21		271	B5-5S	 Exact Mass: 318.12
100	F2-3C	 Mol. Wt.: 215,21		272	B6-5S	 Exact Mass: 318.12
101	F3-3C	 Mol. Wt.: 240,26		273	B7-5S	 Exact Mass: 313.08
102	F4-3C	 Mol. Wt.: 240,26		274	B8-5S	 Exact Mass: 313.08

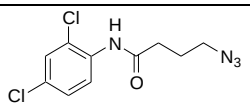
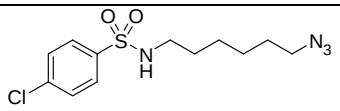
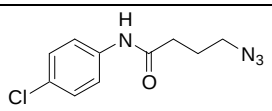
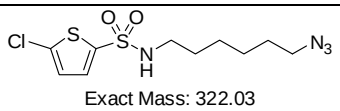
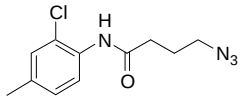
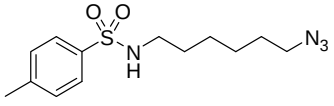
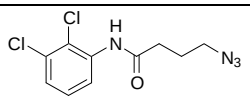
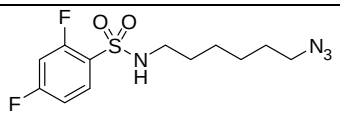
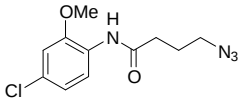
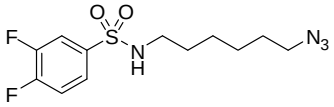
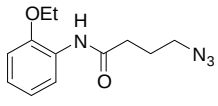
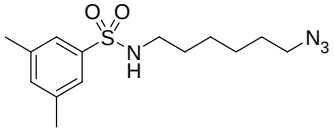
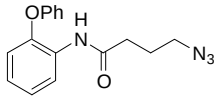
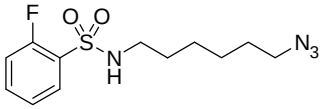
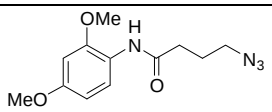
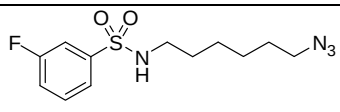
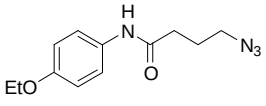
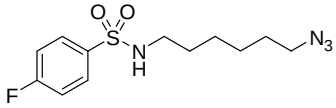
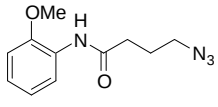
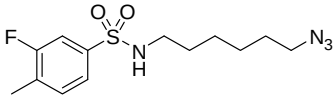
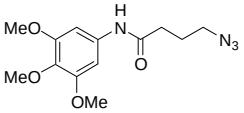
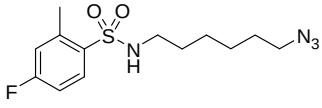
103	F5-3C	 Mol. Wt.: 256,26		275	B9-5S	 Exact Mass: 324.16
104	F6-3C	 Mol. Wt.: 220,23		276	B10-5S	 Exact Mass: 274.06
105	F7-3C	 Mol. Wt.: 220,23		277	B11-5S	 Exact Mass: 282.12
106	F8-3C	 Mol. Wt.: 240,65		278	B12-5S	 Exact Mass: 266.09
107	F9-3C	 Mol. Wt.: 220,23		279	C1-5S	 Exact Mass: 262.14
108	F10-3C	 Mol. Wt.: 216,24		280	E1-6C	 Exact Mass: 250,12
109	F11-3C	 Mol. Wt.: 216,24		281	E2-6C	 Mol. Wt.: 250,27
110	F12-3C	 Mol. Wt.: 218,26		282	E3-6C	 Mol. Wt.: 268,26
111	G1-3C	 Mol. Wt.: 190,20		283	E4-6C	 Mol. Wt.: 268,26

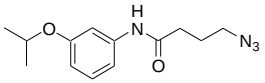
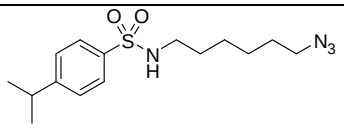
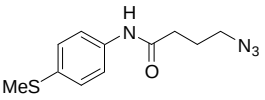
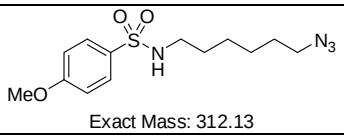
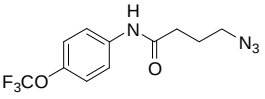
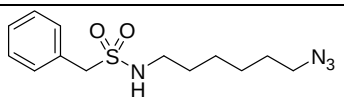
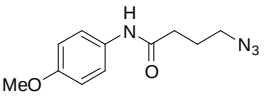
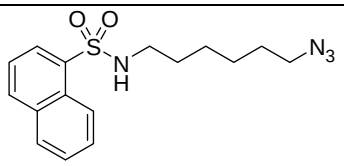
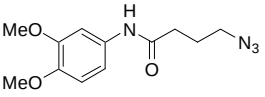
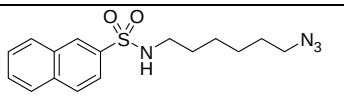
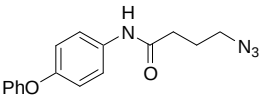
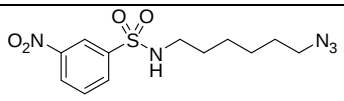
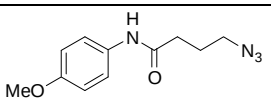
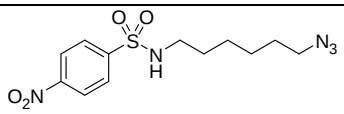
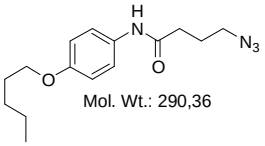
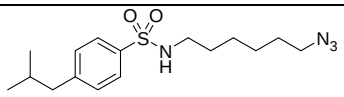
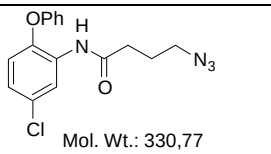
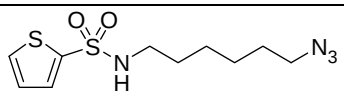
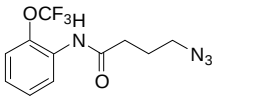
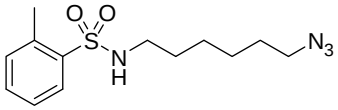
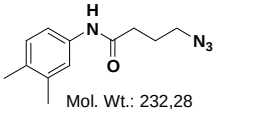
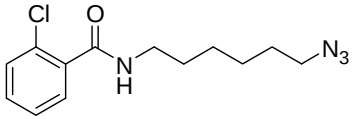
112	G2-3C	 Mol. Wt.: 208,19		284	E5-6C	 Mol. Wt.: 264,30
113	G3-3C	 Mol. Wt.: 226,18		285	E6-6C	 Mol. Wt.: 264,30
114	G4-3C	 Mol. Wt.: 226,18		286	E7-6C	 Mol. Wt.: 301,17
115	G5-3C	 Mol. Wt.: 276,19		287	E8-6C	 Mol. Wt.: 266,73
116	G6-3C	 Mol. Wt.: 222,22		288	E9-6C	 Mol. Wt.: 280,75
117	G7-3C	 Mol. Wt.: 244,17		289	E10-6C	 Mol. Wt.: 301,17
118	G8-3C	 Mol. Wt.: 208,19		290	E11-6C	 Exact Mass: 296,10
119	G9-3C	 Mol. Wt.: 305,08		291	E12-6C	 Exact Mass: 276,16

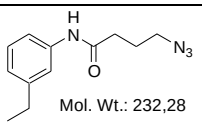
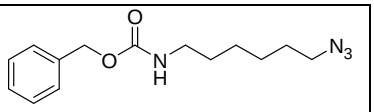
120	G10-3C	 Mol. Wt.: 218,26		292	F1-6C	 Mol. Wt.: 338,40
121	G1-3S	 Mol. Wt.: 282,32		293	F2-6C	 Mol. Wt.: 292,33
122	G2-3S	 Mol. Wt.: 316,38		294	F3-6C	 Exact Mass: 309,19
123	G3-3S	 Mol. Wt.: 274,73		295	F4-6C	 Exact Mass: 306,18
124	G4-3S	 Exact Mass: 279,99		296	F5-6C	 Exact Mass: 377,21
125	G5-3S	 Mol. Wt.: 254,31		297	F6-6C	 Mol. Wt.: 290,36
126	G6-3S	 Mol. Wt.: 276,26		298	F7-6C	 Mol. Wt.: 278,37
127	G7-3S	 Mol. Wt.: 276,26		299	F8-6C	 Mol. Wt.: 316,28
128	G8-3S	 Mol. Wt.: 153,20		300	F9-6C	 Mol. Wt.: 262,31
129	G9-3S	 Mol. Wt.: 258,27		301	F10-6C	 Exact Mass: 292,15

130	G10-3S	 Mol. Wt.: 258,27		302	F11-6C	 Exact Mass: 324,16
131	G11-3S	 Mol. Wt.: 258,27		303	F12-6C	 Mol. Wt.: 262,31
132	G12-3S	 Mol. Wt.: 272,30		304	G1-6C	 Mol. Wt.: 304,39
133	H1-3S	 Mol. Wt.: 268,34		305	G2-6C	 Mol. Wt.: 344,80
134	H2-3S	 Mol. Wt.: 282,36		306	G3-6C	 Mol. Wt.: 302,25
135	H3-3S	 Mol. Wt.: 270,31		307	G4-6C	 Mol. Wt.: 246,31
136	H4-3S	 Mol. Wt.: 254,31		308	G5-6C	 Mol. Wt.: 246,31
137	H5-3S	 Mol. Wt.: 290,34		309	G6-6C	 Mol. Wt.: 274,36
138	H6-3S	 Mol. Wt.: 290,34		310	G7-6C	 Mol. Wt.: 246,31
139	H7-3S	 Mol. Wt.: 285,28		311	G8-6C	 Mol. Wt.: 288,39

140	H8-3S	 Mol. Wt.: 285,28		312	G9-6C	 Mol. Wt.: 290,32
141	H9-3S	 Mol. Wt.: 282,36		313	G10-6C	 Mol. Wt.: 304,34
142	H10-3S	 Mol. Wt.: 246,31		314	G11-6C	 Mol. Wt.: 316,44
143	H11-3S	 Mol. Wt.: 254,31		315	G12-6C	 Mol. Wt.: 268,31
144	E1-4C	 Mol. Wt.: 222,22		316	H1-6C	 Mol. Wt.: 318,37
145	E2-4C	 Mol. Wt.: 222,22		317	H2-6C	 Mol. Wt.: 272,35
146	E3-4C	 Mol. Wt.: 240,21		318	H3-6C	 Mol. Wt.: 320,34
147	E4-4C	 Mol. Wt.: 240,21		319	H4-6C	 Mol. Wt.: 268,31
148	E5-4C	 Mol. Wt.: 236,25		320	E1-6S	 Exact Mass: 324.13
149	E6-4C	 Mol. Wt.: 236,25		321	E2-6S	 Exact Mass: 358.15

150	E7-4C	 Mol. Wt.: 273,12		322	E3-6S	 Exact Mass: 316.08
151	E8-4C	 Mol. Wt.: 238,67		323	E4-6S	 Exact Mass: 322.03
152	E9-4C	 Mol. Wt.: 252,70		324	E5-6S	 Exact Mass: 296.13
153	E10-4C	 Mol. Wt.: 273,12		325	E6-6S	 Exact Mass: 318.10
154	E11-4C	 Mol. Wt.: 268,70		326	E7-6S	 Exact Mass: 318.10
155	E12-4C	 Mol. Wt.: 248,28		327	E8-6S	 Exact Mass: 310.15
156	F1-4C	 Mol. Wt.: 296,32		328	E9-6S	 Exact Mass: 300.11
157	F2-4C	 Mol. Wt.: 264,28		329	E10-6S	 Exact Mass: 300.11
158	F3-4C	 Mol. Wt.: 248,28		330	E11-6S	 Exact Mass: 300.11
159	F4-4C	 Mol. Wt.: 234,25		331	E12-6S	 Exact Mass: 314.12
160	F5-4C	 Mol. Wt.: 294,31		332	F1-6S	 Exact Mass: 314.12

161	F6-4C	 Mol. Wt.: 262,31	333	F2-6S	 Exact Mass: 324.16
162	F7-4C	 Mol. Wt.: 250,32	334	F3-6S	 Exact Mass: 312.13
163	F8-4C	 Mol. Wt.: 288,23	335	F4-6S	 Exact Mass: 296.13
164	F9-4C	 Mol. Wt.: 234,25	336	F5-6S	 Exact Mass: 332.13
165	F10-4C	 Mol. Wt.: 264,28	337	F6-6S	 Exact Mass: 332.13
166	F11-4C	 Mol. Wt.: 296,32	338	F7-6S	 Exact Mass: 327.10
167	F12-4C	 Mol. Wt.: 234,25	339	F8-6S	 Exact Mass: 327.10
168	G1-4C	 Mol. Wt.: 290,36	340	F9-6S	 Exact Mass: 338.18
169	G2-4C	 Mol. Wt.: 330,77	341	F10-6S	 Exact Mass: 288.07
170	G3-4C	 Mol. Wt.: 288,23	342	F11-6S	 Exact Mass: 296.13
171	G4-4C	 Mol. Wt.: 232,28	343	F12-6S	 Exact Mass: 280.11

172	G5-4C	 Mol. Wt.: 232,28		344	G1-6S	 Exact Mass: 276.16

References

1. Srinivasan, R.; Tan, L. P.; Wu, H.; Yang, P. -Y.; Kalesh, K. A.; Yao, S. Q. *Org. Biol. Chem.* 2009, 7, 1821-1828.

Supporting Information-2

Rapid Synthesis of Abelson Tyrosine Kinase Inhibitors using Click Chemistry

Karunakaran A. Kalesh,[a] Kai Liu[b] and Shao Q. Yao,[a,b,c,*]

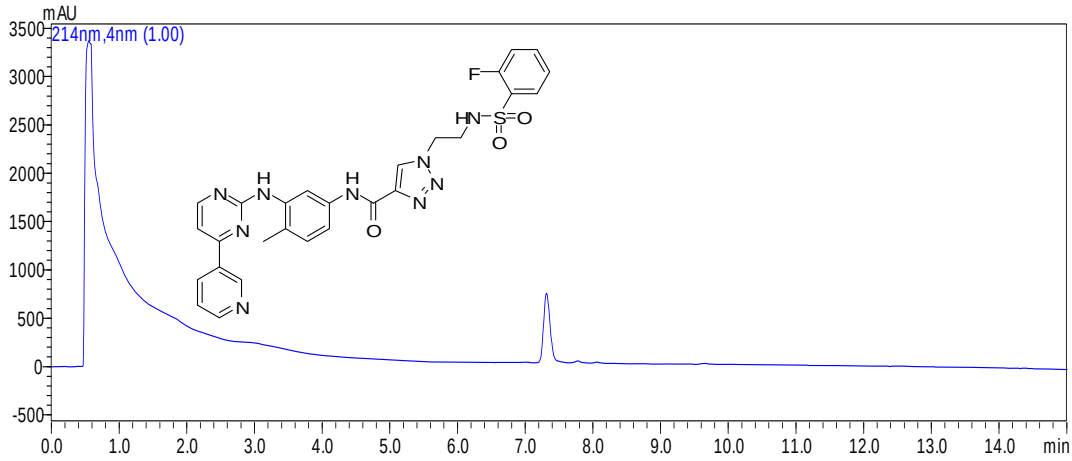
Departments of Chemistry [a] and Biological Sciences,[b] NUS MedChem Program of the Life Sciences Institute,[c] National University of Singapore, Singapore 117543

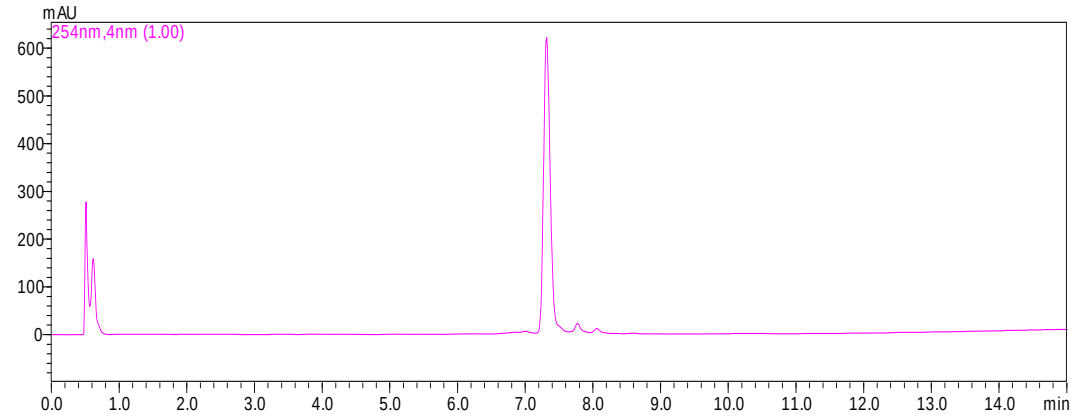
Contents:

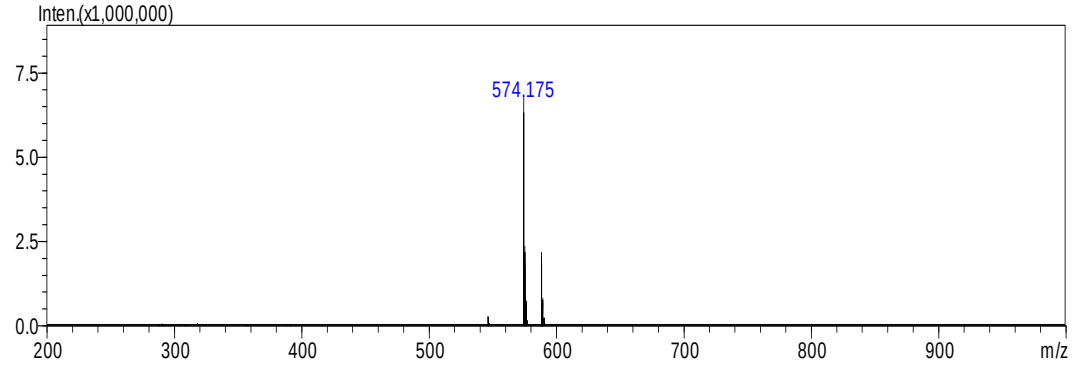
1. 1. LC-MS profiles of the purified click-inhibitors from the Imatinib analogue library

Gradient : 20 to 100% ACN in 10 min, 100 to 100 till 13 min, to 20 in 13.5 min; C-18 column

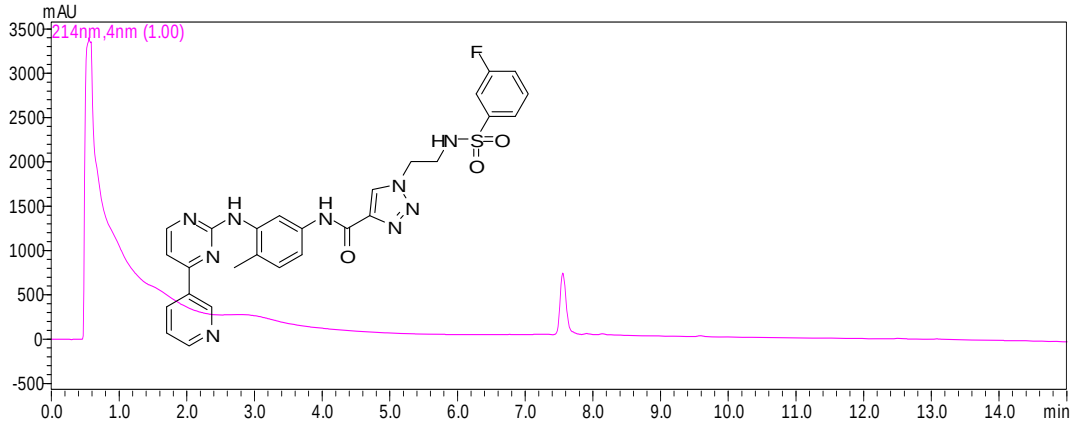
W1-SA9

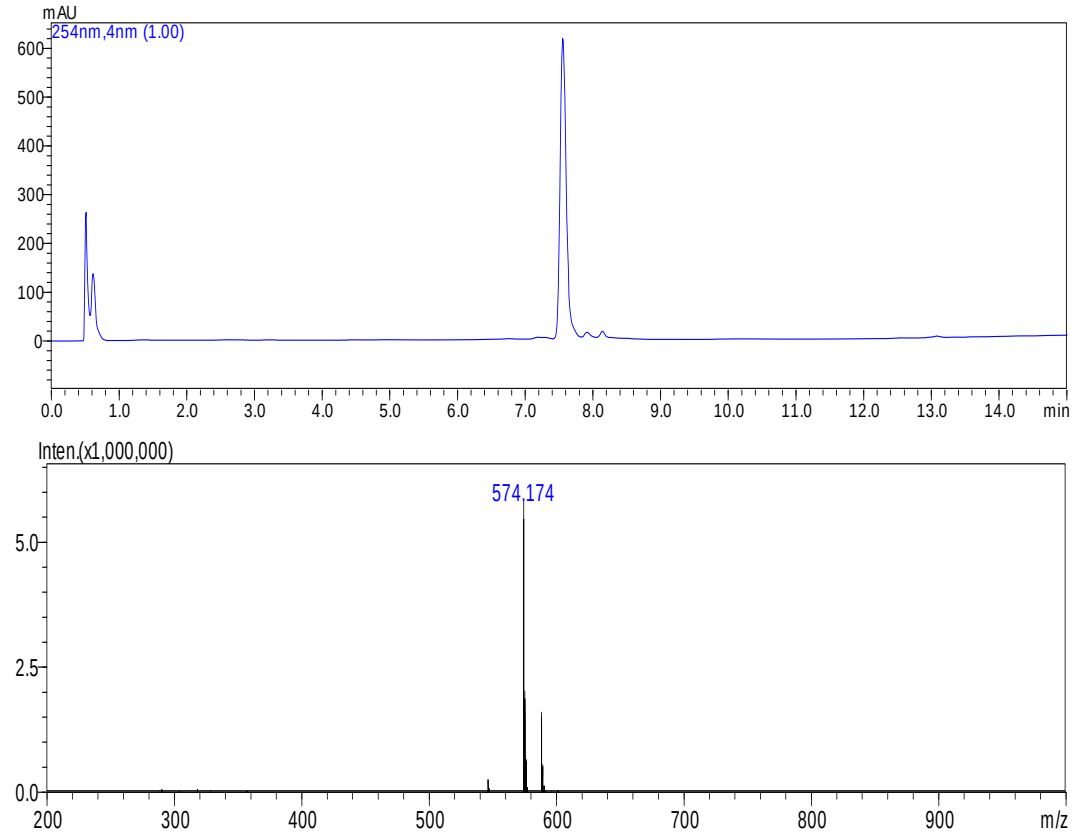



mAU
254nm,4nm (1.00)
600
500
400
300
200
100
0
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
min

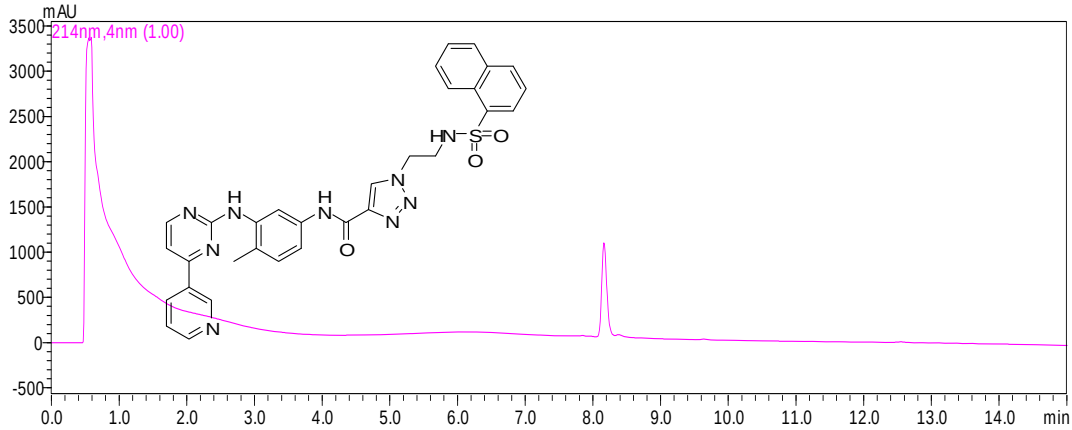

Inten.(x1,000,000)
574.175
7.5
5.0
2.5
0.0
200
300
400
500
600
700
800
900
m/z

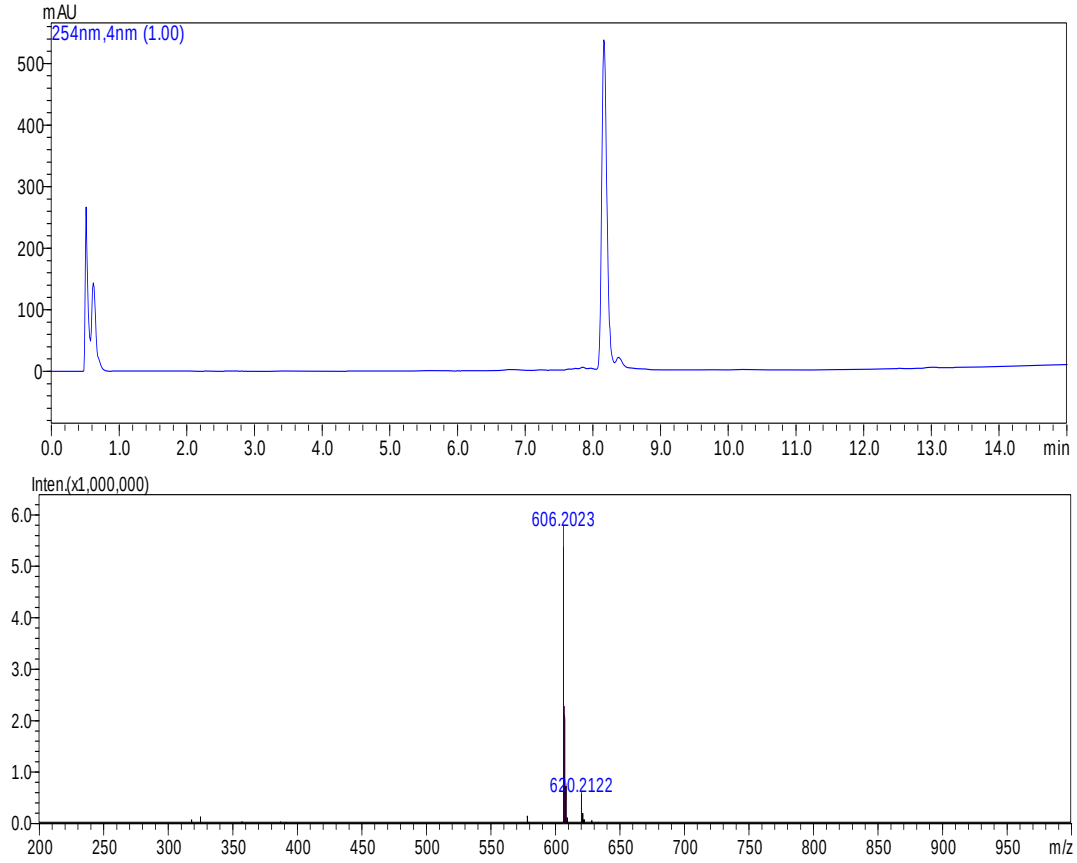
W1-SA10


mAU
214nm,4nm (1.00)
3500
3000
2500
2000
1500
1000
500
0
-500
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
min
F
HN
S
O
O
H
N
N
N
N
H
N
N
N
O
N

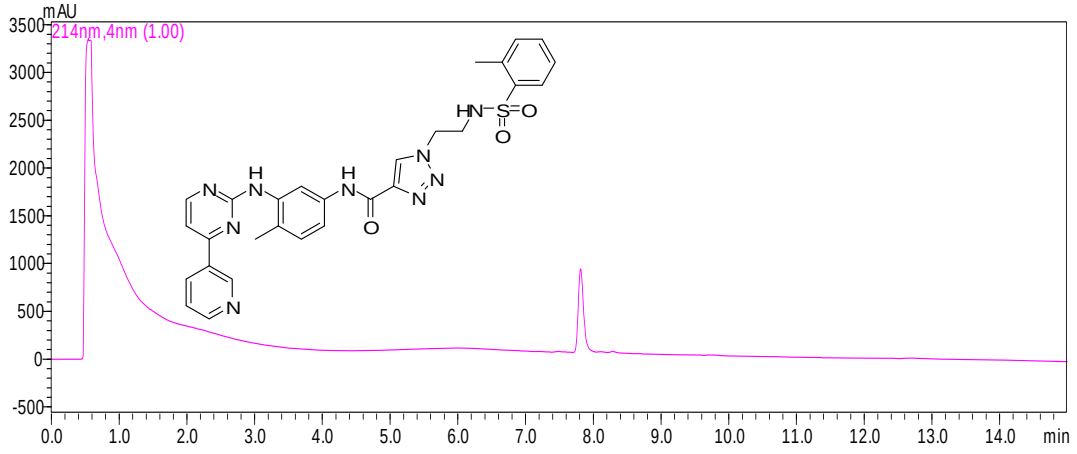

mAU
254nm,4nm (1.00)
600
500
400
300
200
100
0
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 min
Inten.(x1,000,000)
574.174
5.0
2.5
0.0
200 300 400 500 600 700 800 900 m/z

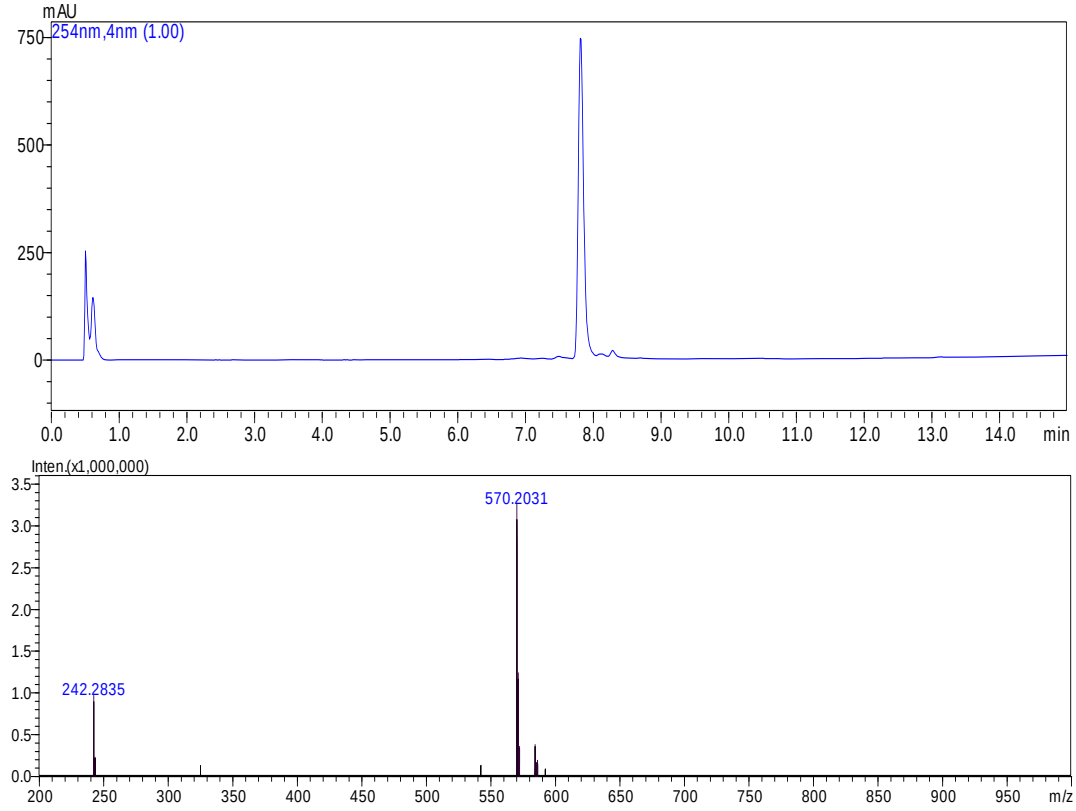
W1-SA17


mAU
214nm,4nm (1.00)
3500
3000
2500
2000
1500
1000
500
0
-500
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 min

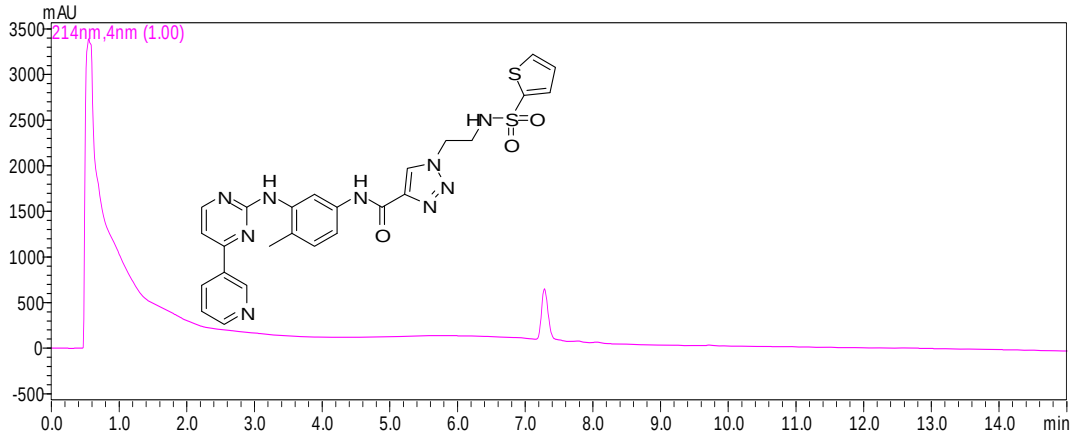

mAU
254nm,4nm (1.00)
min
Inten.(x1,000,000)
606.2023
620.2122
m/z

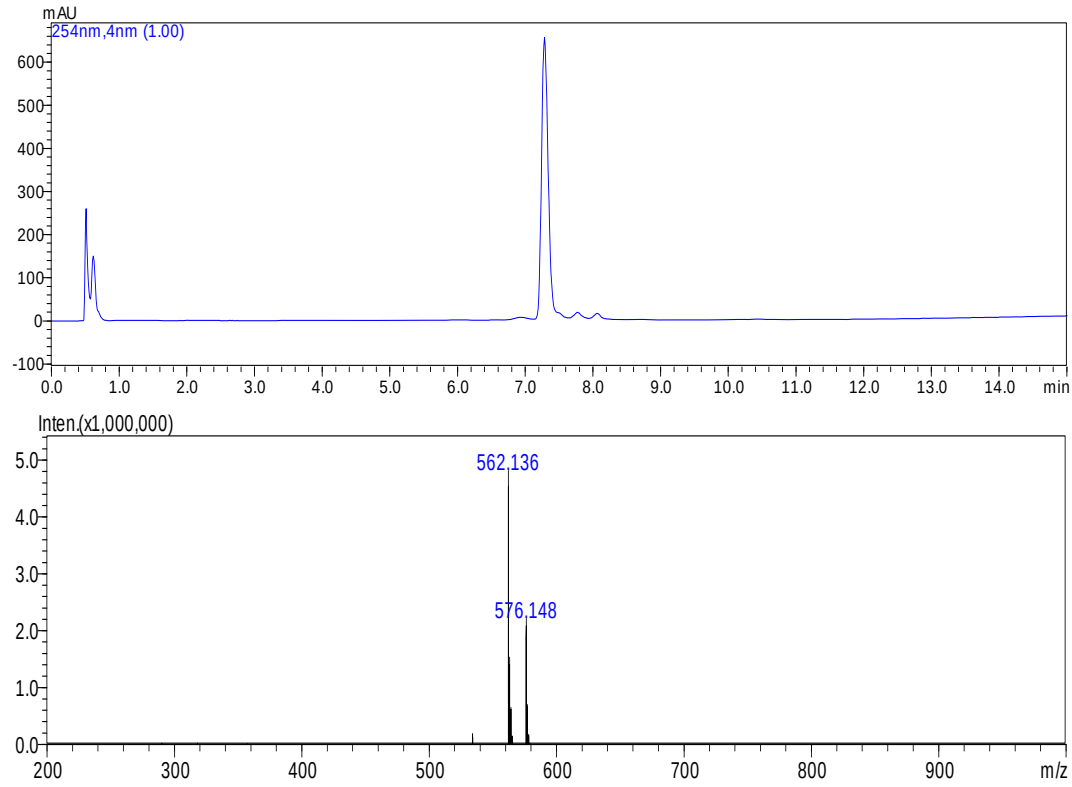
W1-SA20


mAU
214nm,4nm (1.00)
min

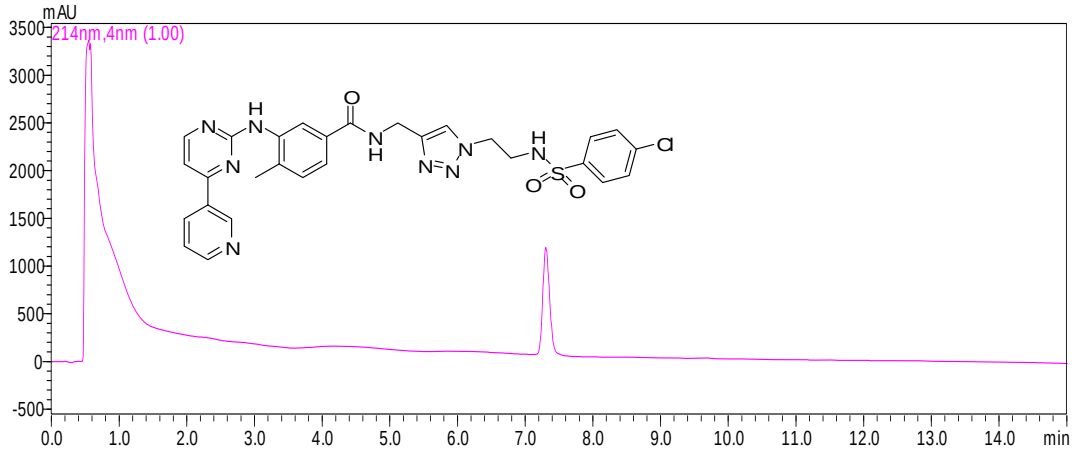

mAU
254nm,4nm (1.00)
750
500
250
0
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 min
Inten.(x1,000,000)
570.2031
242.2835
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 m/z

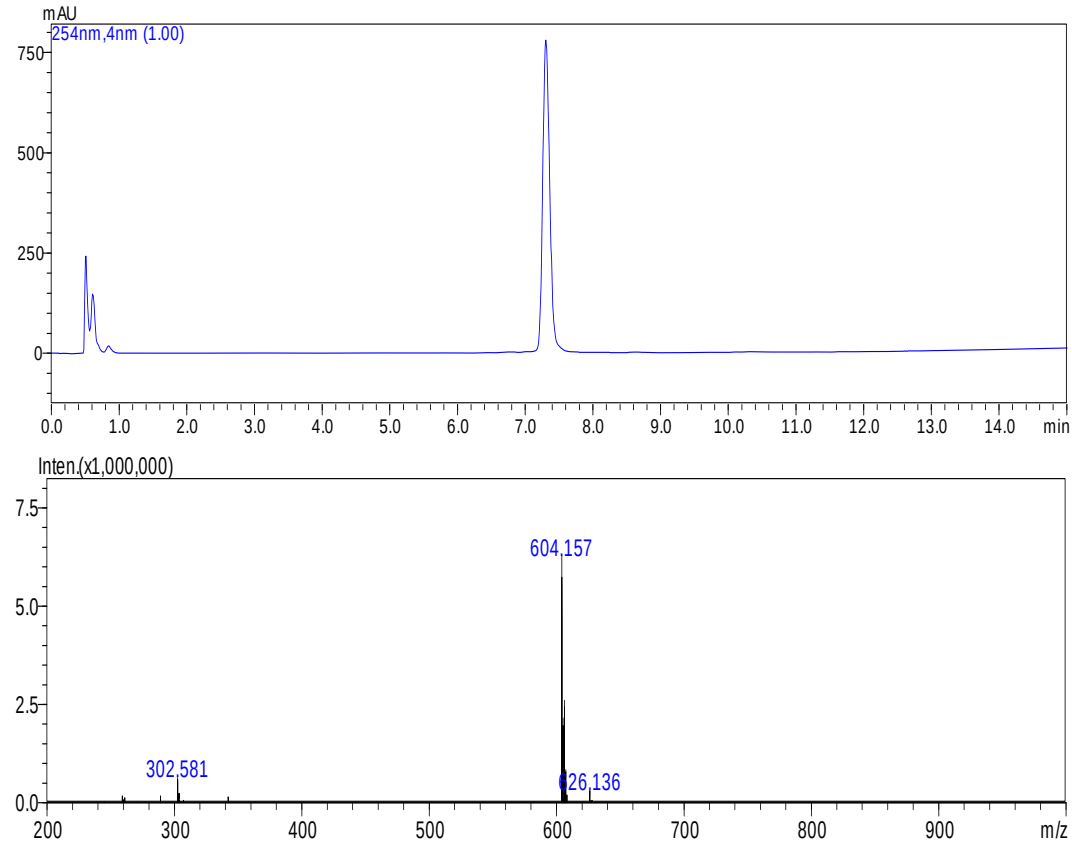
W1-SA22


mAU
214nm,4nm (1.00)
3500
3000
2500
2000
1500
1000
500
0
-500
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 min

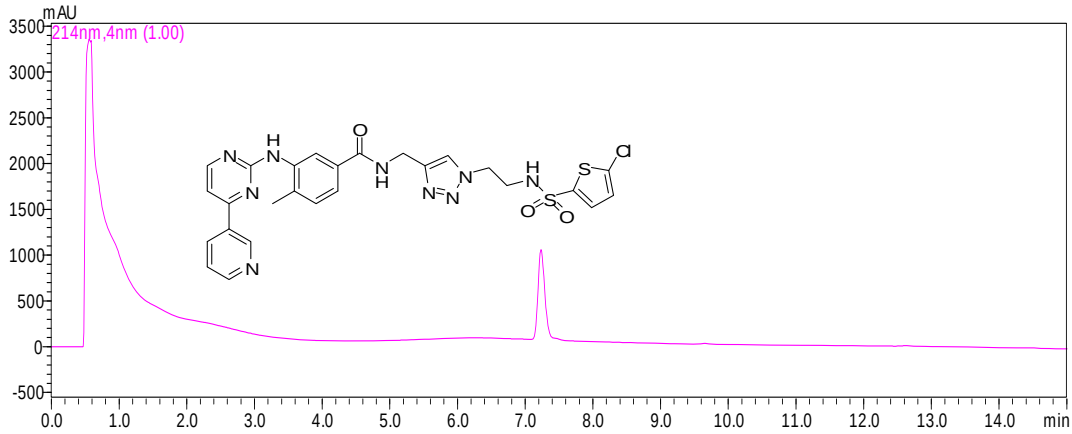

mAU
254nm,4nm (1.00)
600
500
400
300
200
100
0
-100
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 min
Inten.(x1,000,000)
562.136
576.148
5.0
4.0
3.0
2.0
1.0
0.0
200 300 400 500 600 700 800 900 m/z

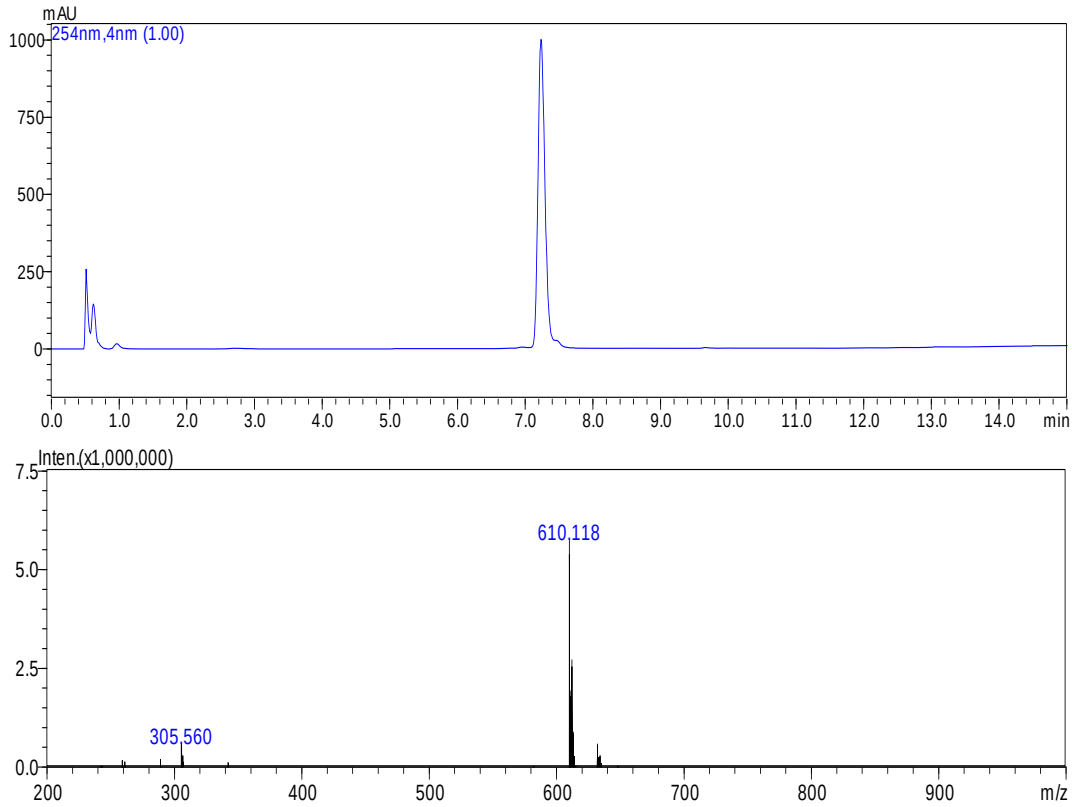
W2-SA3


mAU
214nm,4nm (1.00)
3500
3000
2500
2000
1500
1000
500
0
-500
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 min

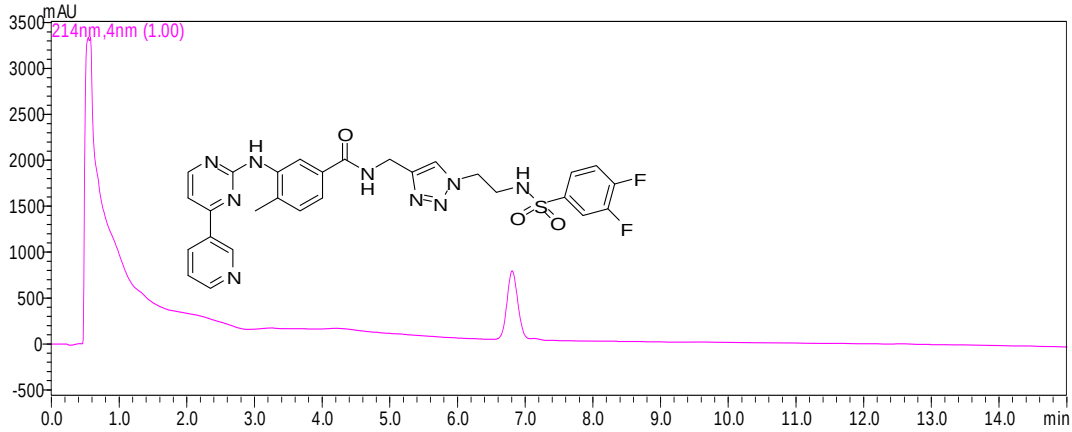

mAU
254nm,4nm (1.00)
750
500
250
0
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 min
Inten.(x1,000,000)
7.5
5.0
2.5
0.0
604.157
302.581
626.136
200 300 400 500 600 700 800 900 m/z

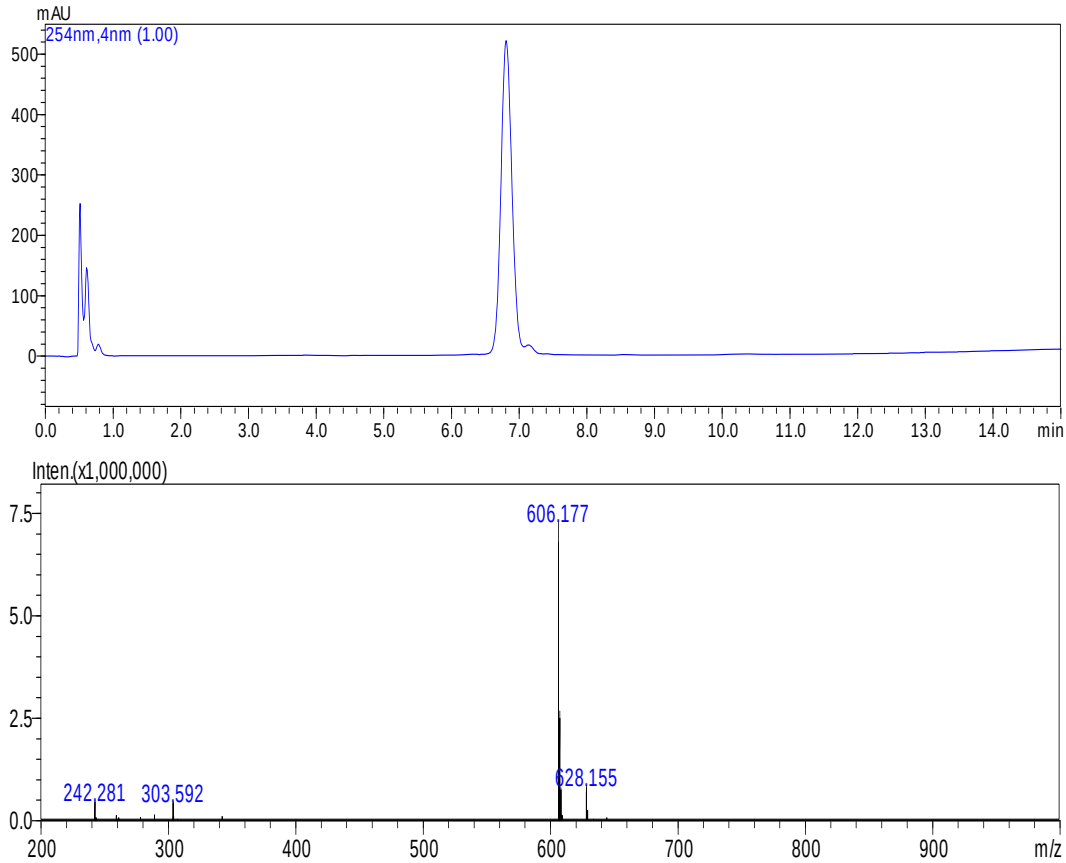
W2-SA4


mAU
214nm,4nm (1.00)
3500
3000
2500
2000
1500
1000
500
0
-500
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 min

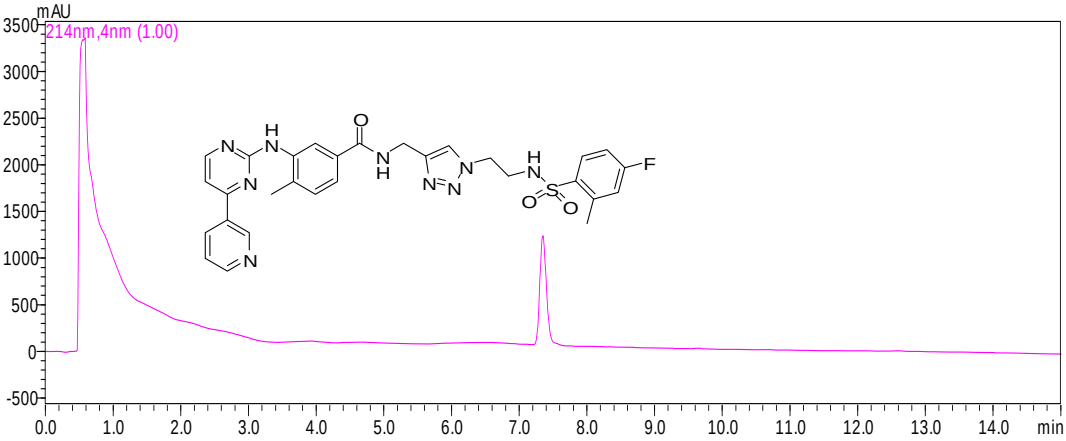

mAU
254nm,4nm (1.00)
1000
750
500
250
0
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 min
Inten.(x1,000,000)
7.5
5.0
2.5
0.0
610.118
305.560
200 300 400 500 600 700 800 900 m/z

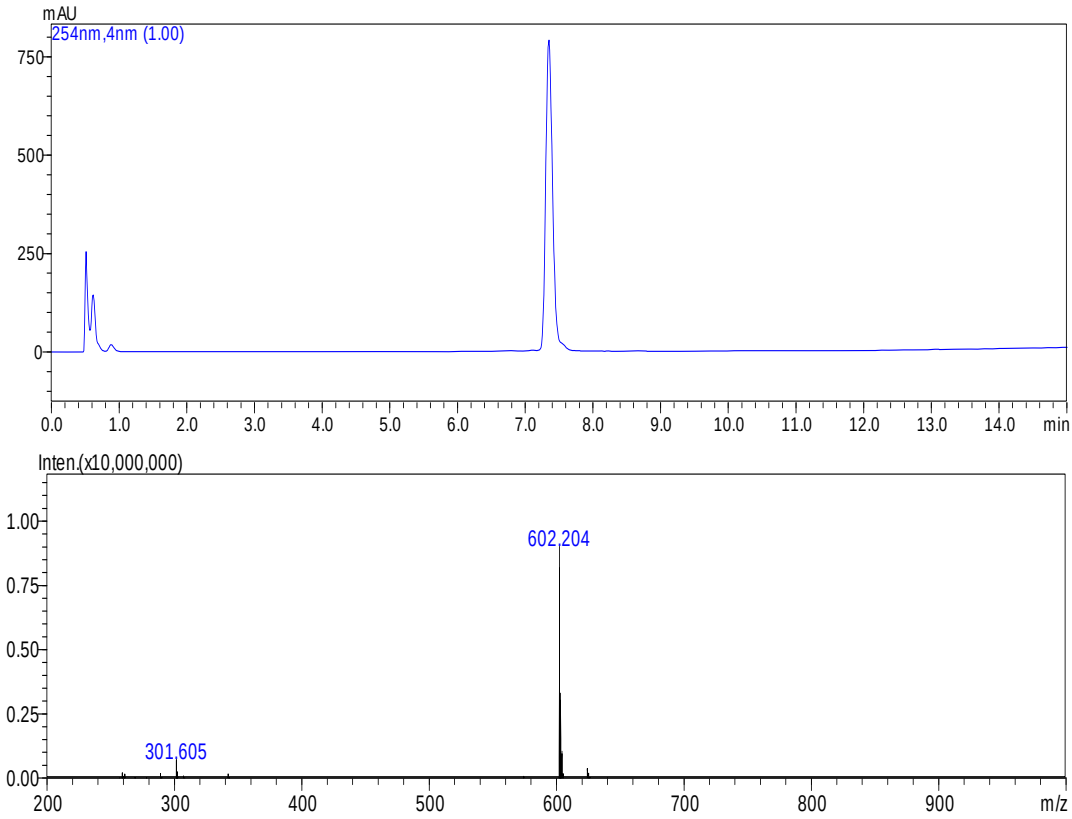
W2-SA7


mAU
214nm,4nm (1.00)
3500
3000
2500
2000
1500
1000
500
0
-500
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 min

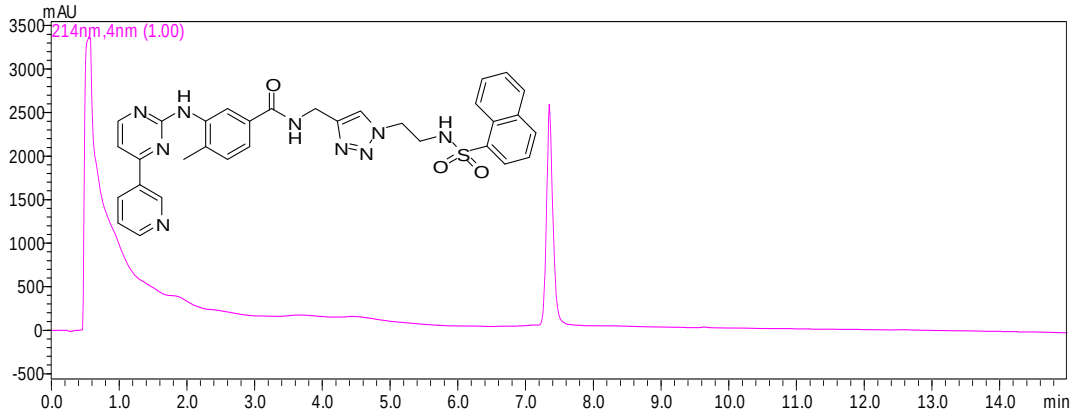

mAU
254nm,4nm (1.00)
500
400
300
200
100
0
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 min
Inten.(x1,000,000)
7.5
5.0
2.5
0.0
606.177
628.155
242.281
303.592
200 300 400 500 600 700 800 900 m/z

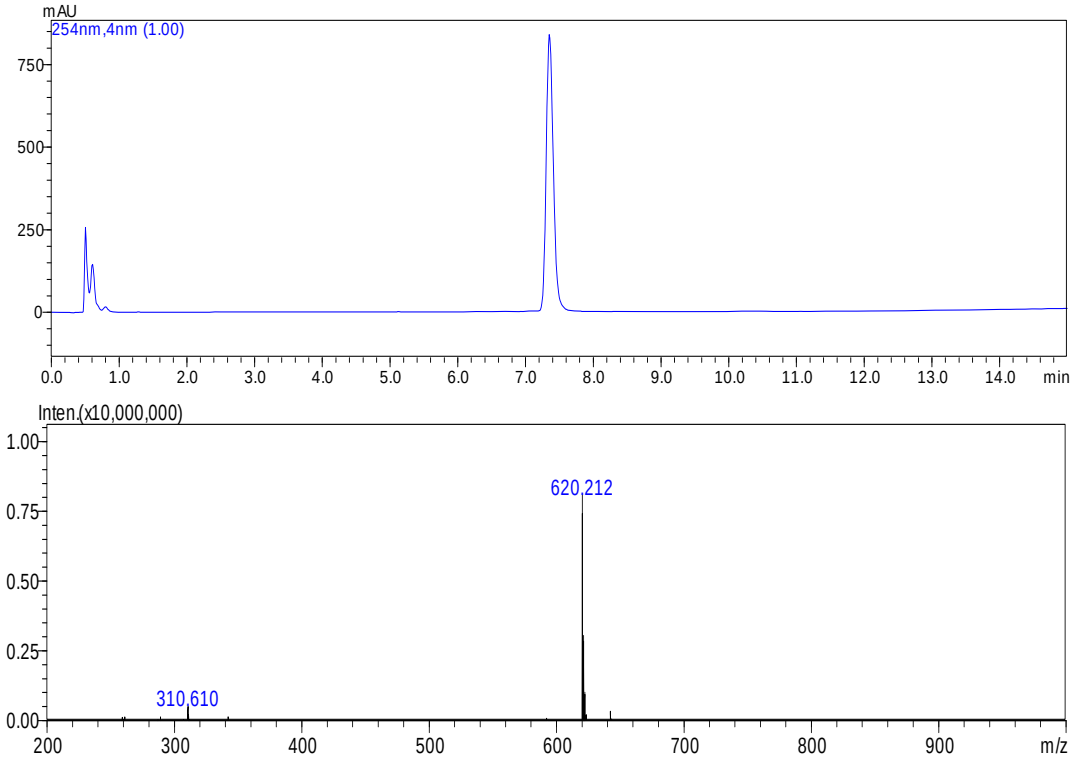
W2-SA13


mAU
214nm,4nm (1.00)
3500
3000
2500
2000
1500
1000
500
0
-500
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 min

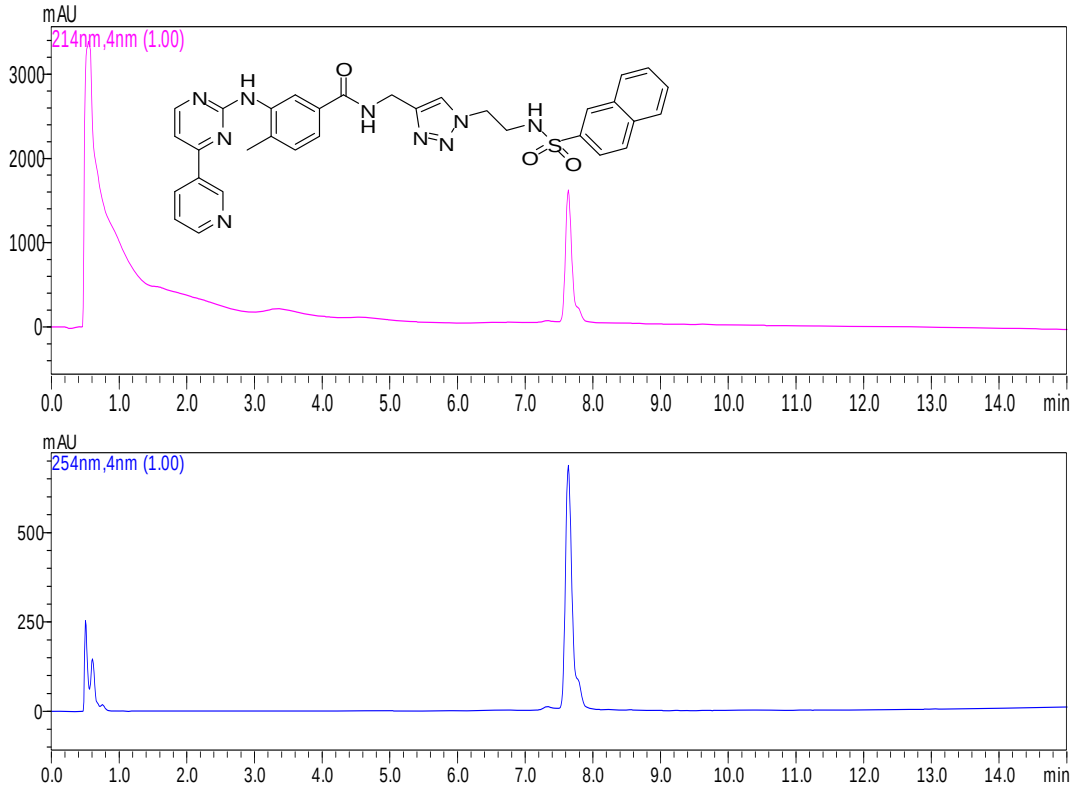

mAU
254nm,4nm (1.00)
750
500
250
0
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 min
Inten.(x10,000,000)
1.00
0.75
0.50
0.25
0.00
602.204
301.605
200 300 400 500 600 700 800 900 m/z

W2-SA17

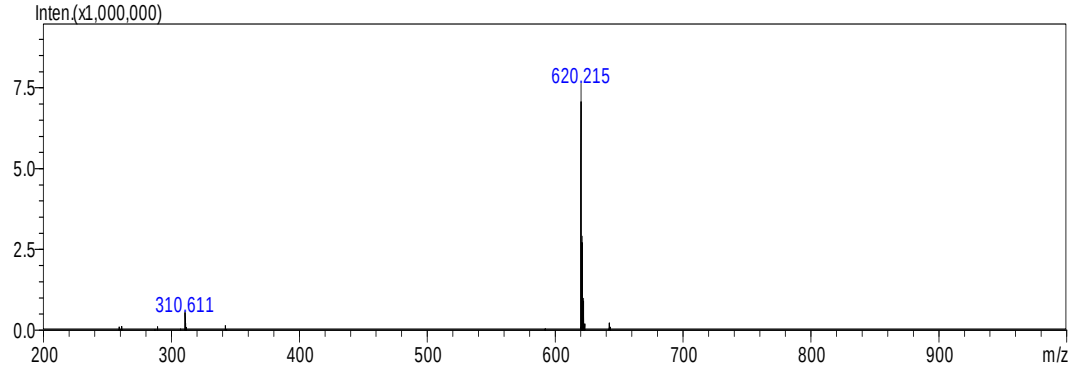

mAU
214nm,4nm (1.00)
3500
3000
2500
2000
1500
1000
500
0
-500
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 min


mAU
254nm,4nm (1.00)
750
500
250
0
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 min
Inten.(x10,000,000)
1.00
0.75
0.50
0.25
0.00
620.212
310.610
200 300 400 500 600 700 800 900 m/z

W2-SA18

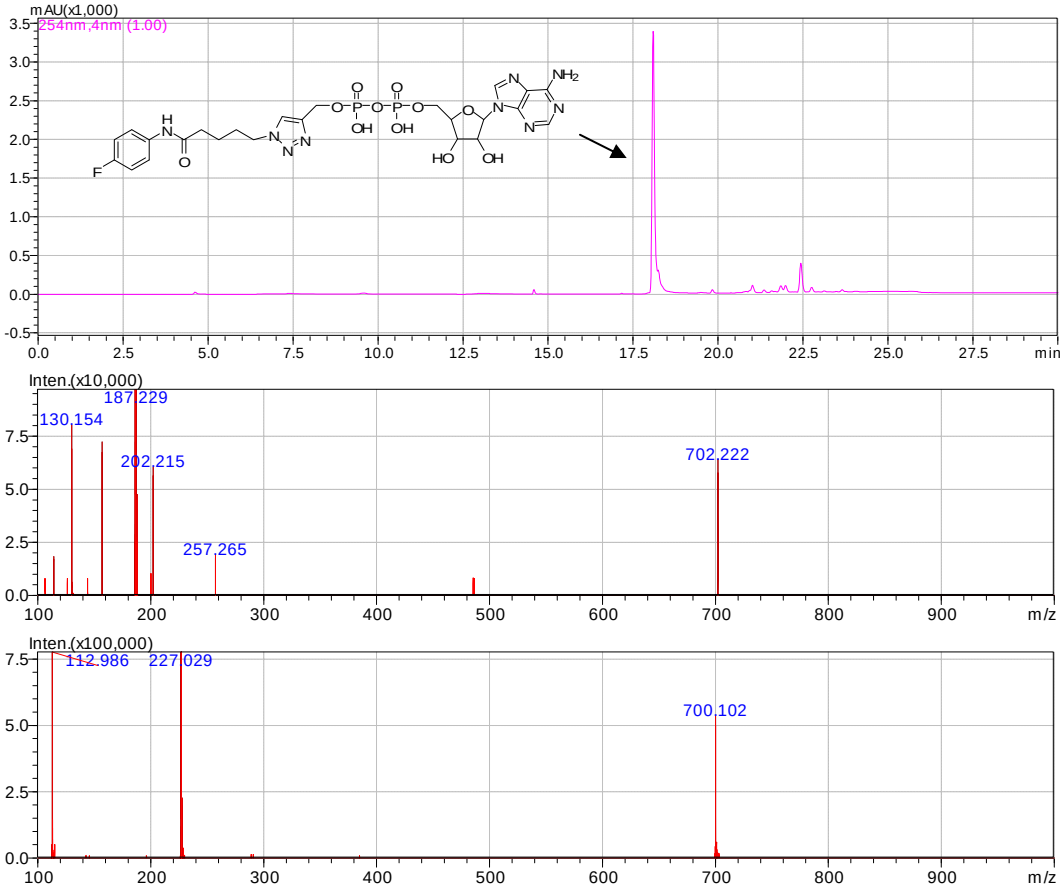

mAU
214nm,4nm (1.00)
3000
2000
1000
0
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 min

mAU
254nm,4nm (1.00)
500
250
0
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 min

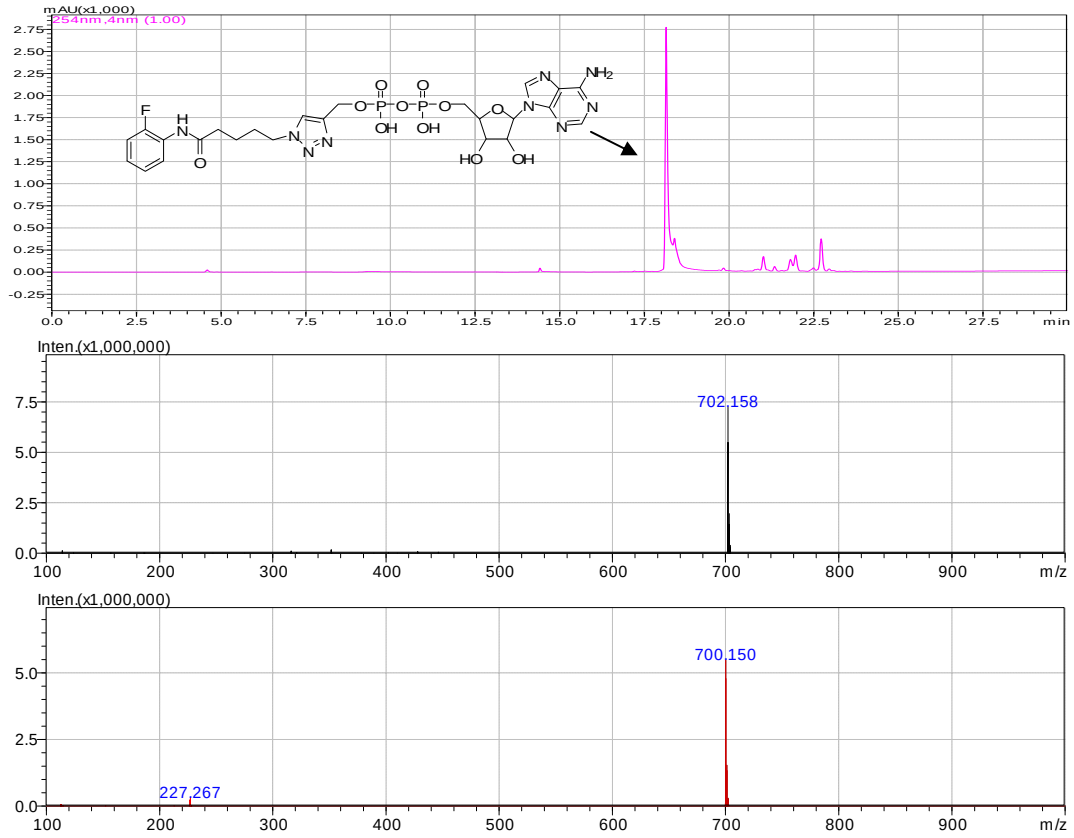


1. 2. LC-MS profiles of the click-library of ADP- alkyne and the traceless azides

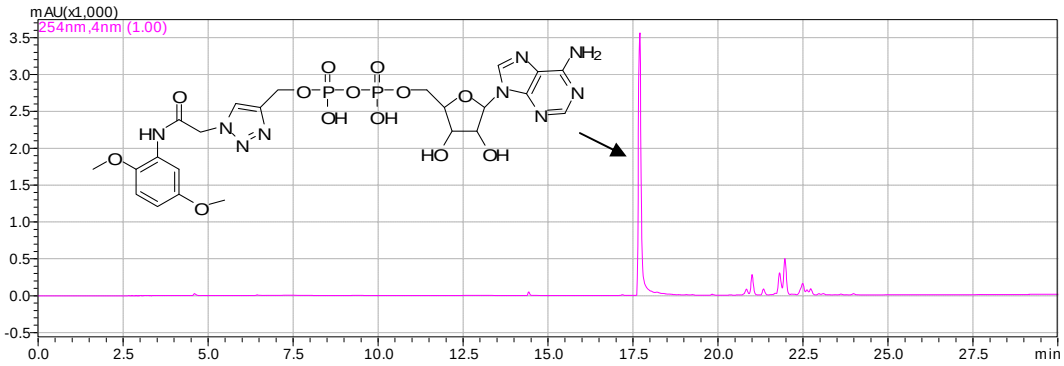
A1-5C

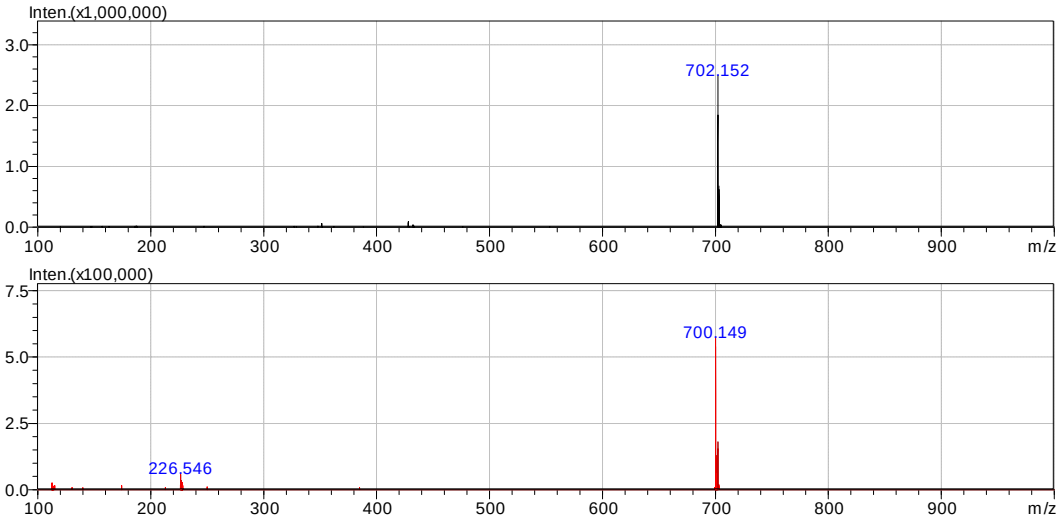


A2-5C

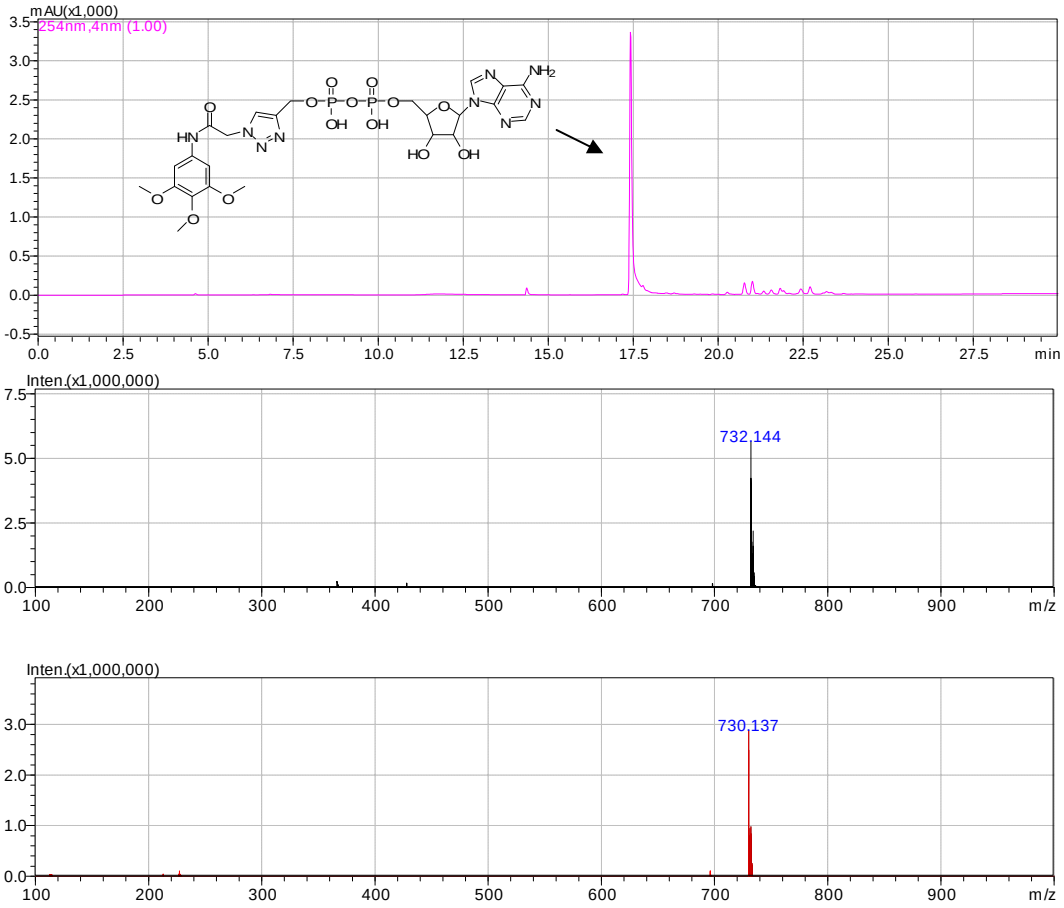

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
702.158
m/z
Inten.(x1,000,000)
700.150
227.267
m/z

B2-2C

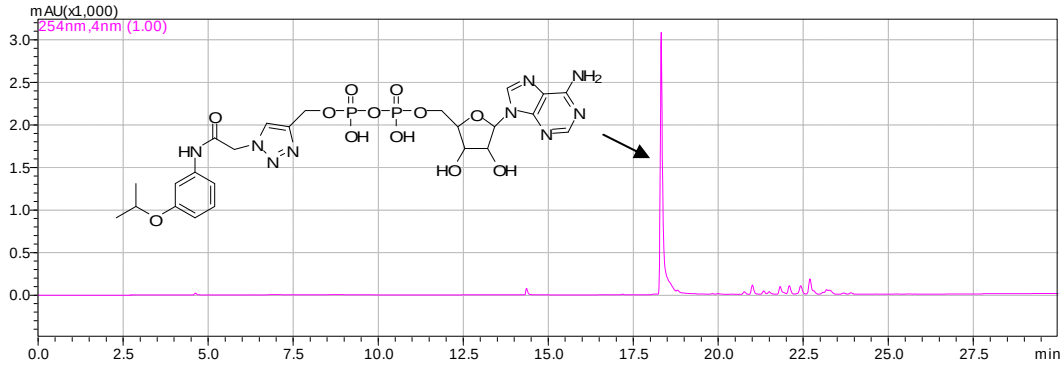

mAU(x1,000)
254nm,4nm (1.00)
min


Inten.(x1,000,000)
702.152
Inten.(x100,000)
700.149
226.546
m/z

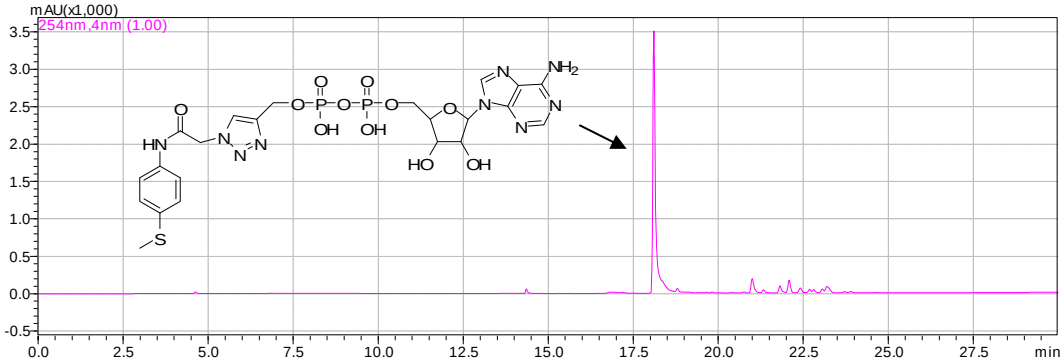
B5-2C


mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
732.144
m/z
Inten.(x1,000,000)
730.137
m/z

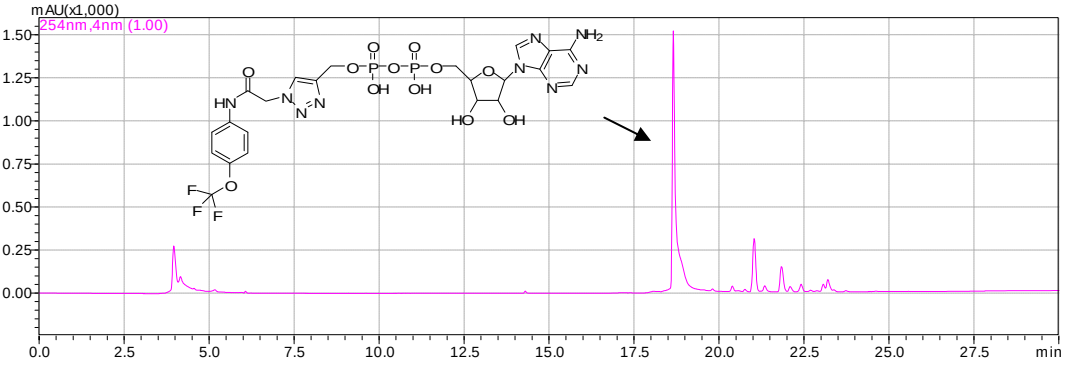
B6-2C



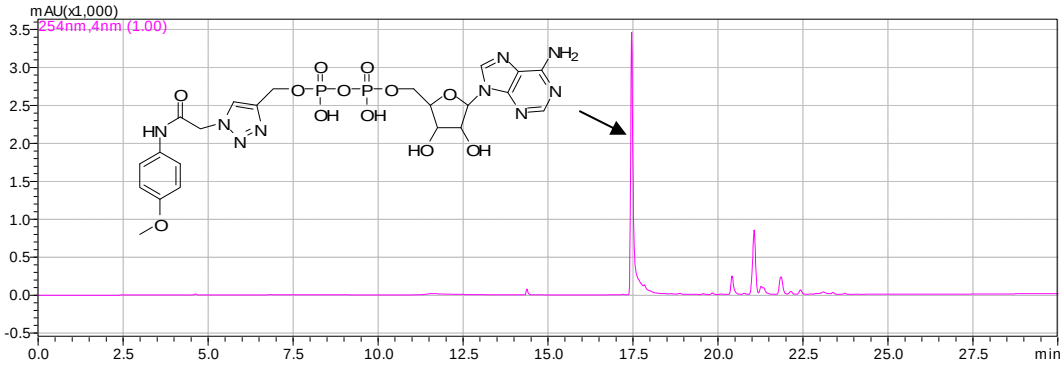
B7-2C



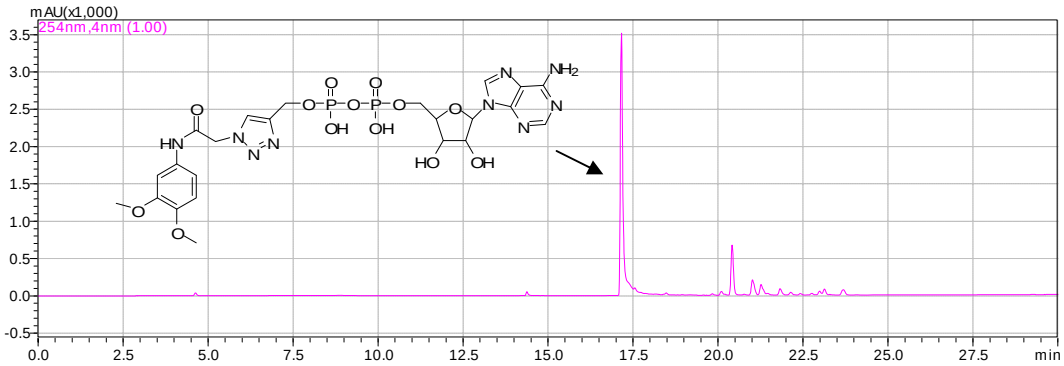
B8-2C



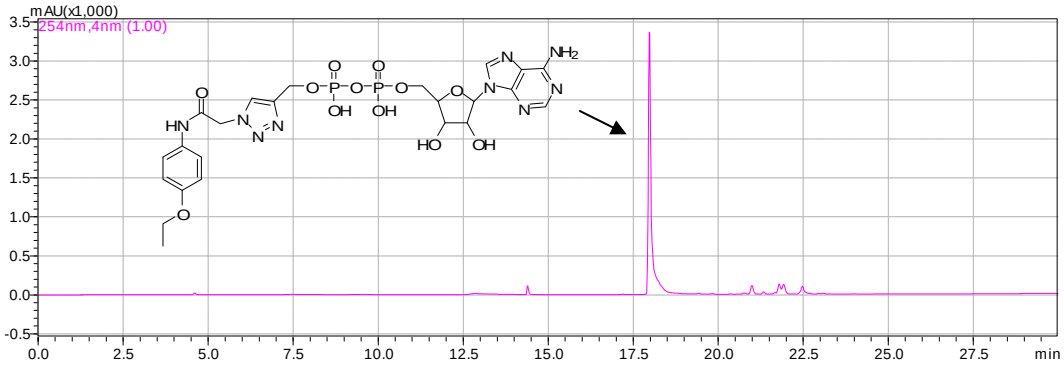
B9-2C



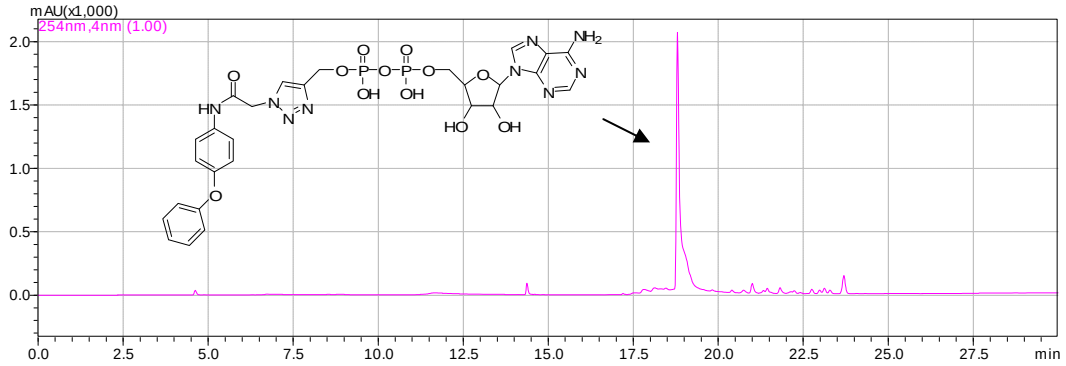
B10-2C



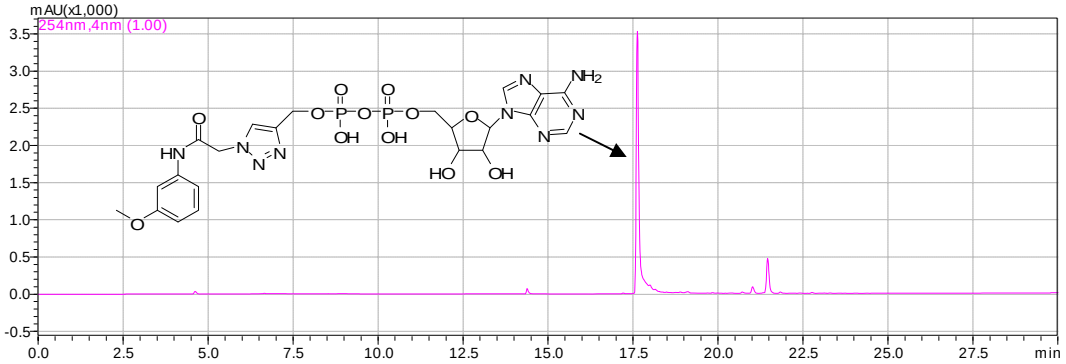
B3-2C



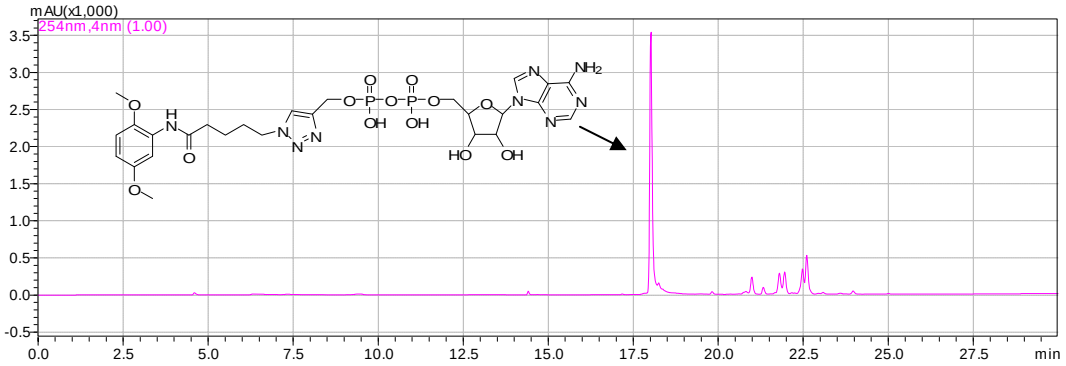
B11-2C

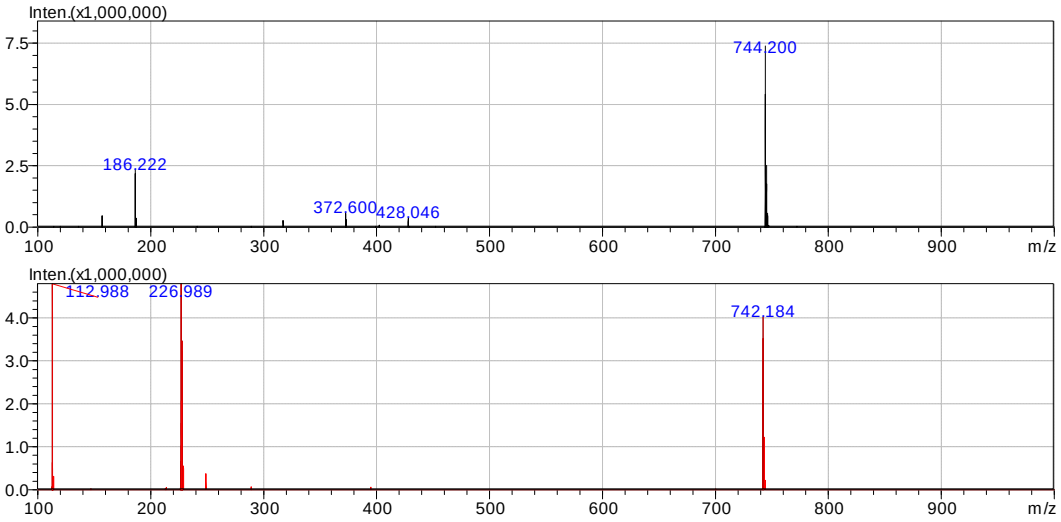


B12-2C

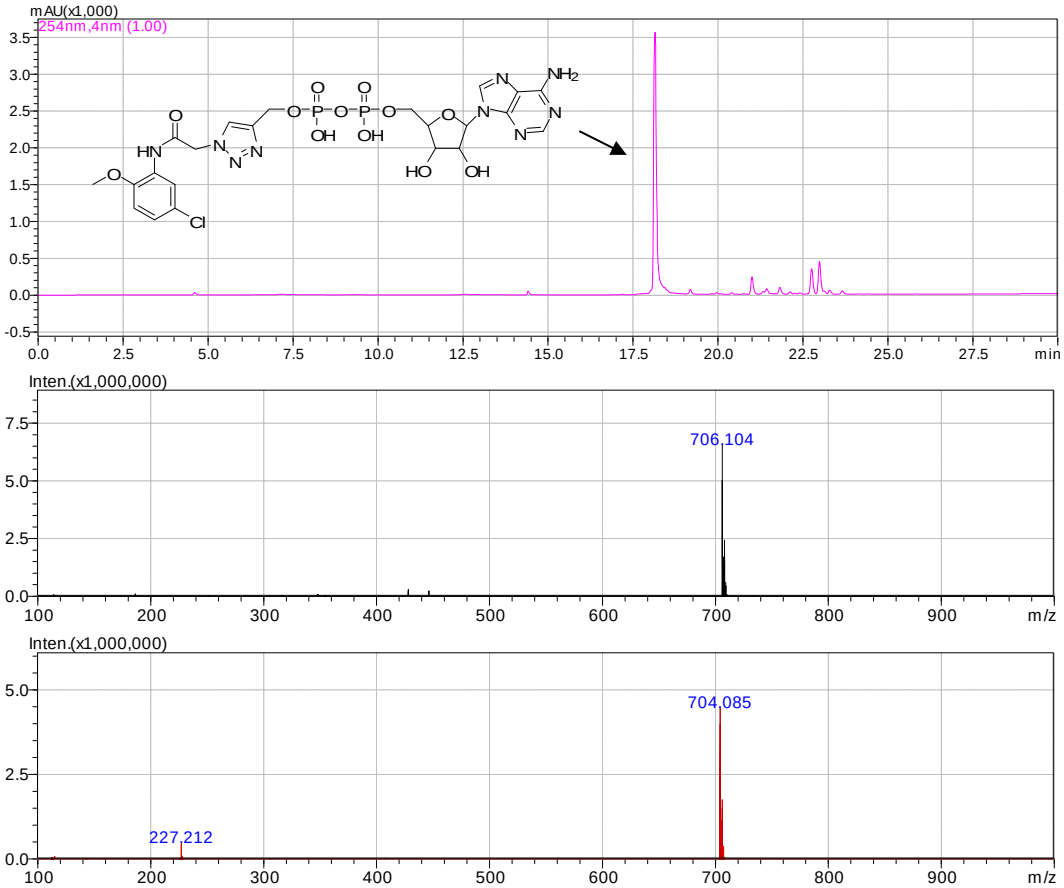


B2-5C

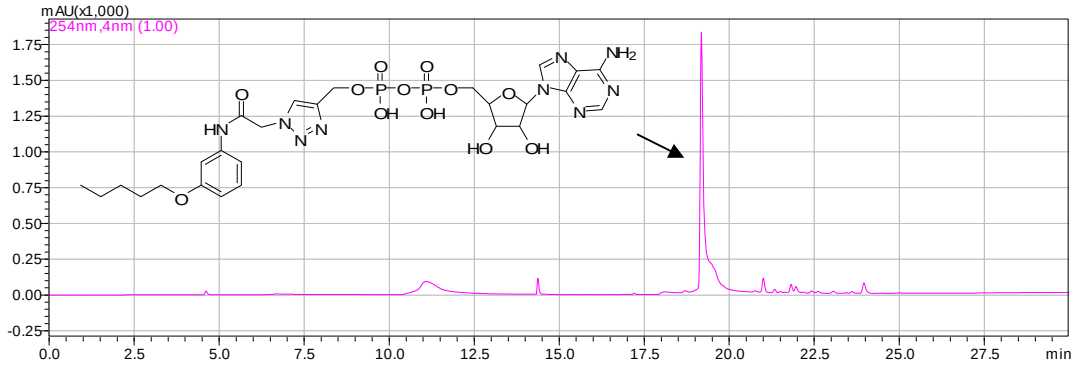



Inten.(x1,000,000)
744.200
186.222
372.600
428.046
m/z
Inten.(x1,000,000)
112.988
226.989
742.184
m/z

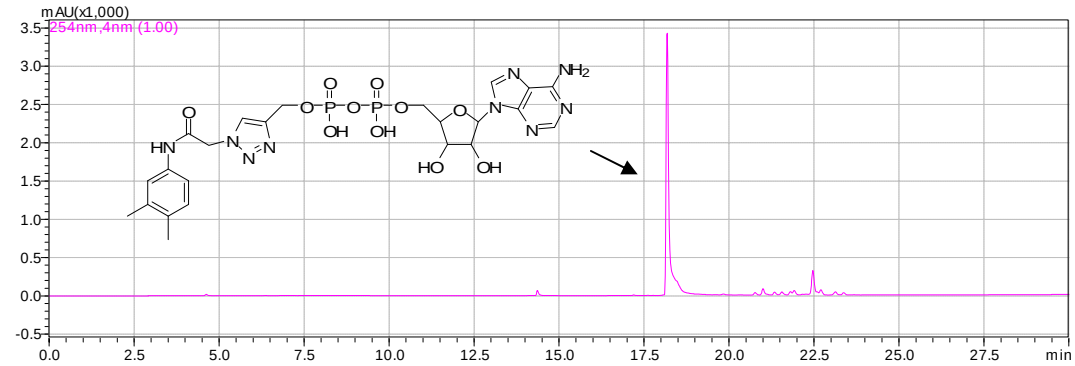
A11-2C


mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
706.104
m/z
Inten.(x1,000,000)
704.085
227.212
m/z

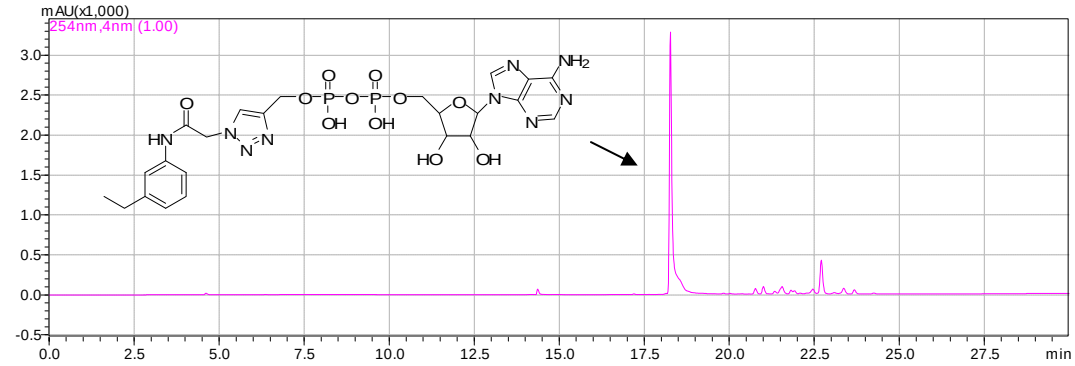
C1-2C



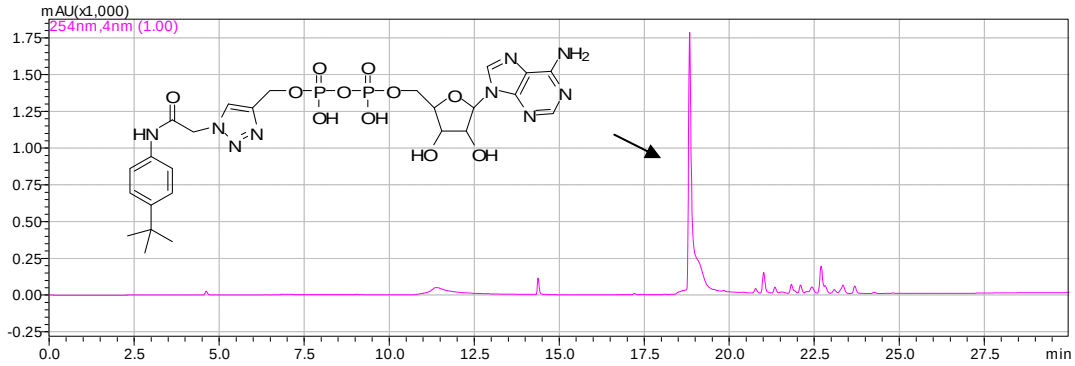
C4-2C



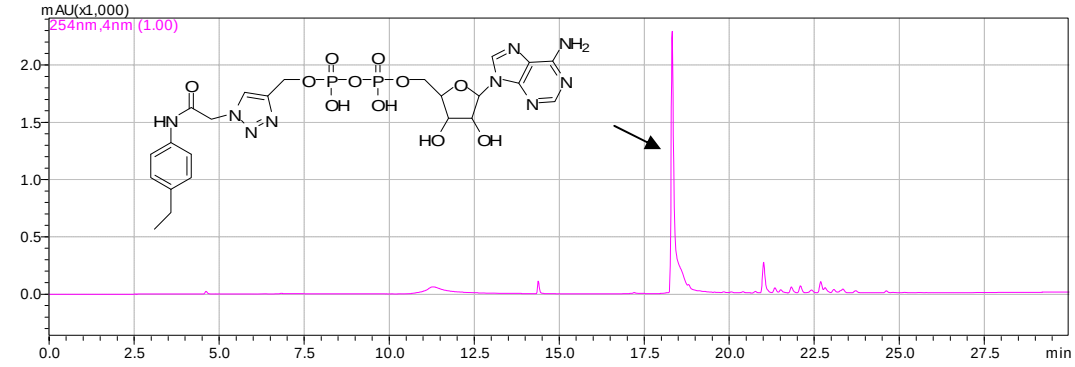
C5-2C



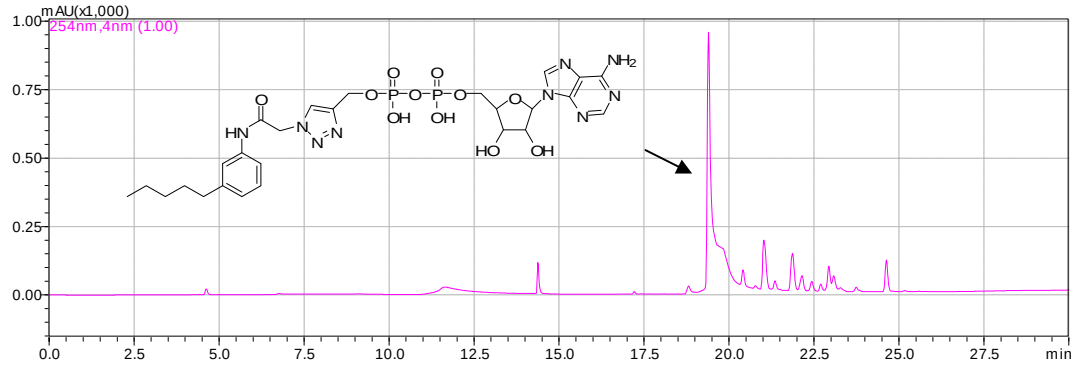
C6-2C



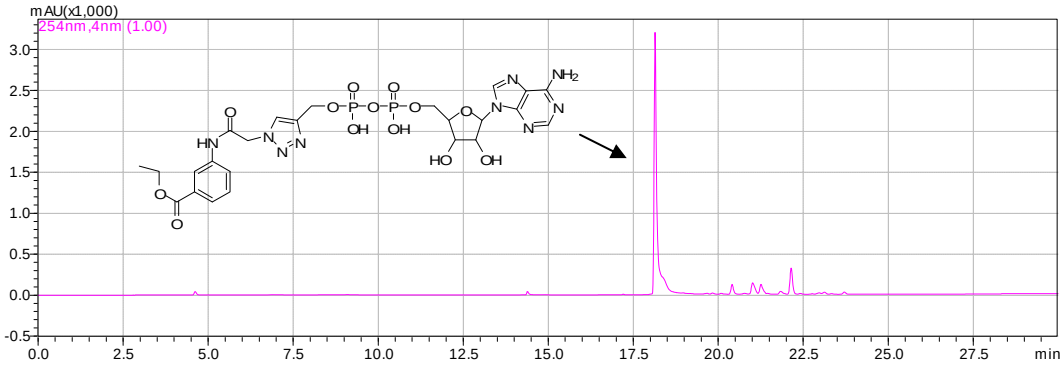
C7-2C



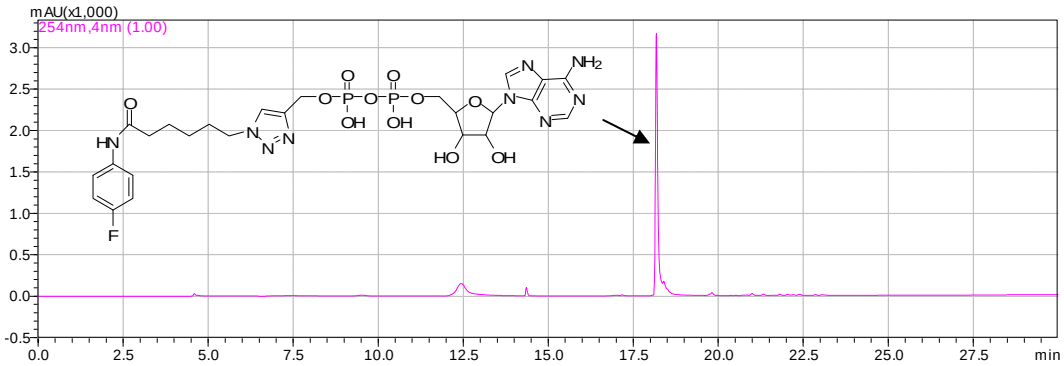
C8-2C

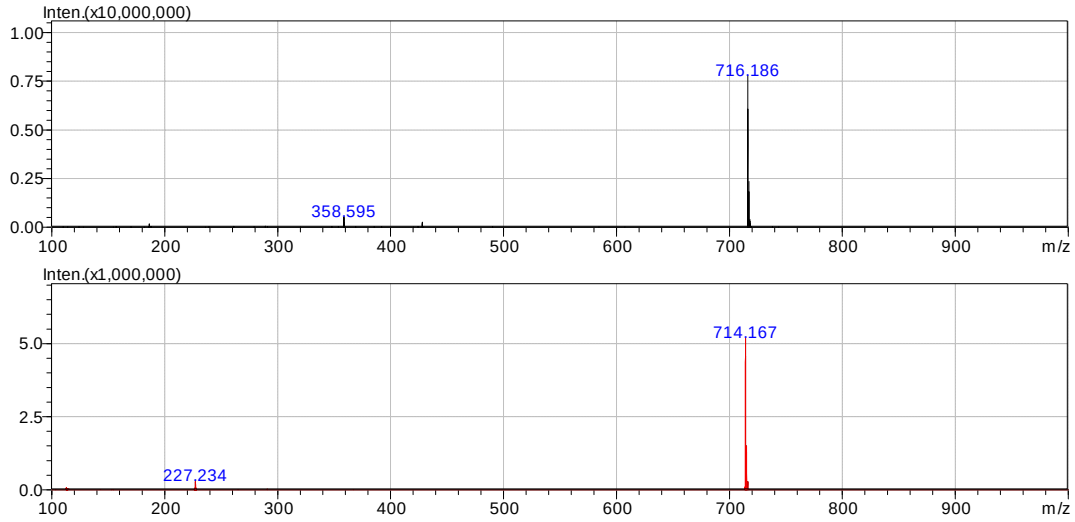


C10-2C

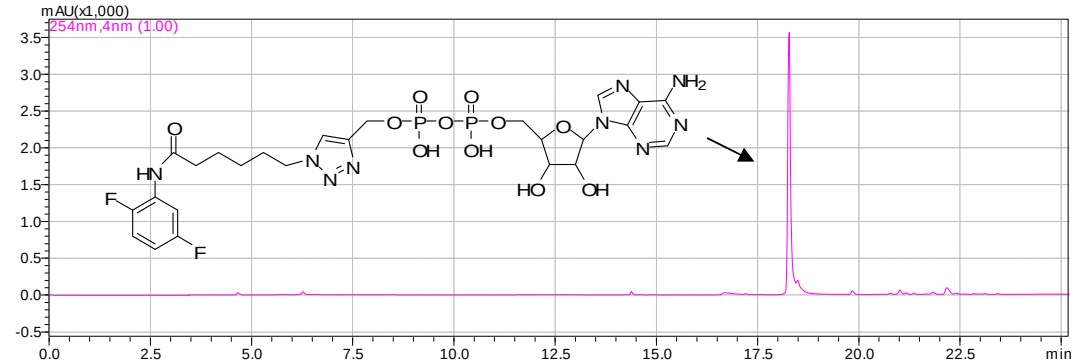

mAU(x1,000)
254nm,4nm (1.00)
min

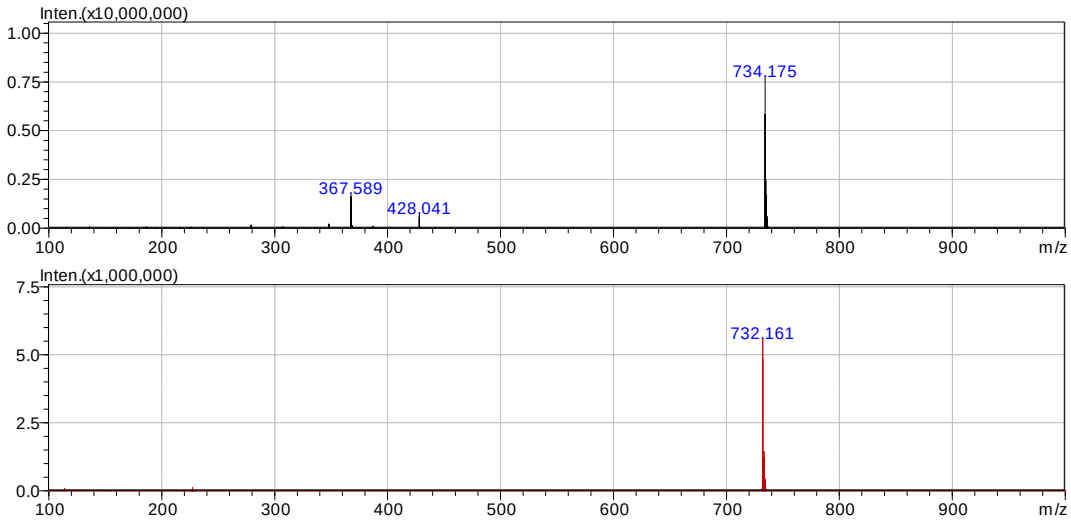
A1-6C


mAU(x1,000)
254nm,4nm (1.00)
min

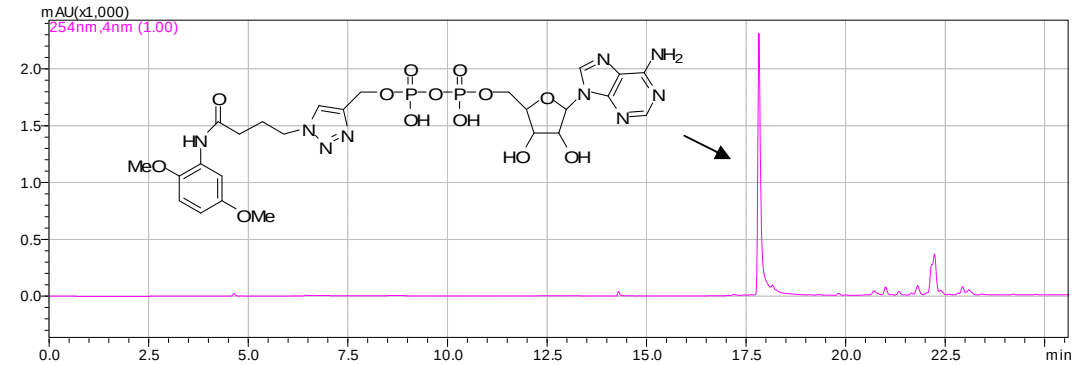

Inten.(x10,000,000)
716.186
358.595
m/z
Inten.(x1,000,000)
714.167
227.234
m/z

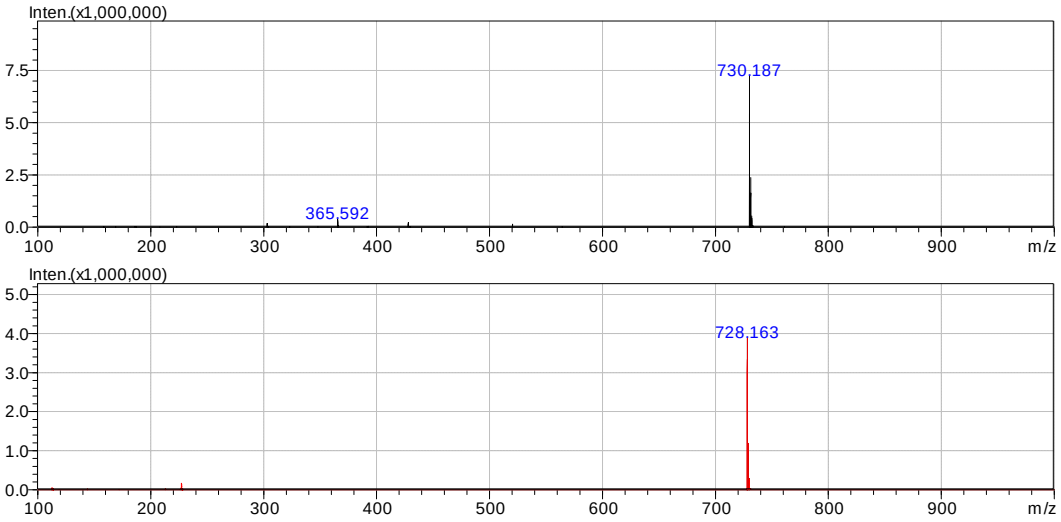
A3-6C


mAU(x1,000)
254nm,4nm (1.00)
min

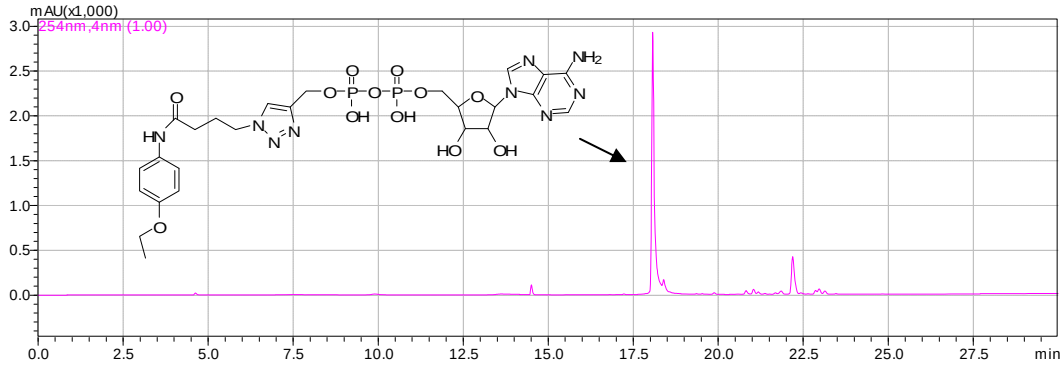

Inten.(x10,000,000)
734.175
367.589
428.041
m/z
Inten.(x1,000,000)
732.161
m/z

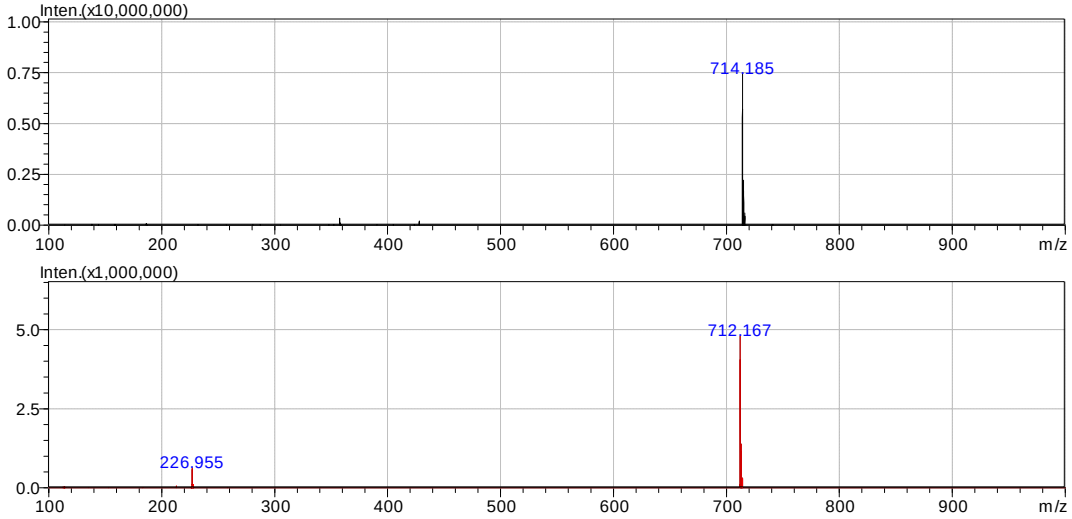
B2-4C


mAU(x1,000)
254nm,4nm (1.00)
min

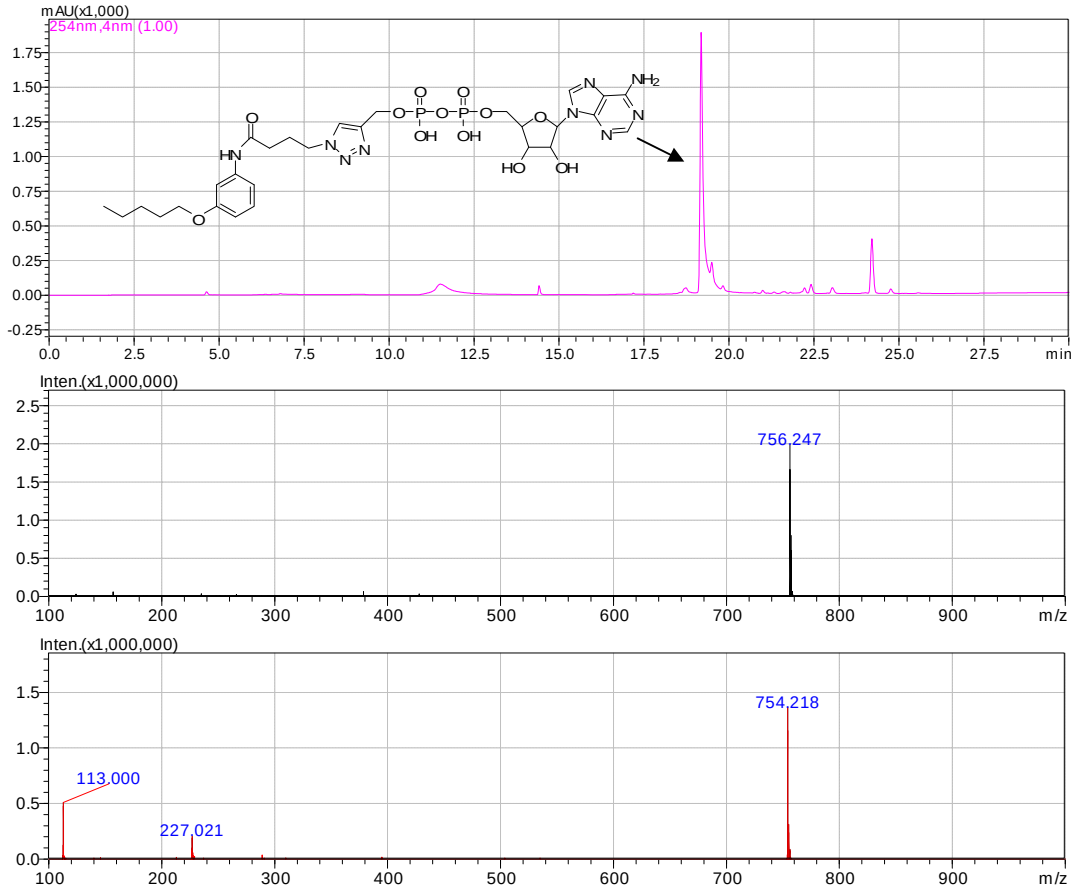

Inten.(x1,000,000)
730.187
365.592
m/z
Inten.(x1,000,000)
728.163
m/z

B3-4C

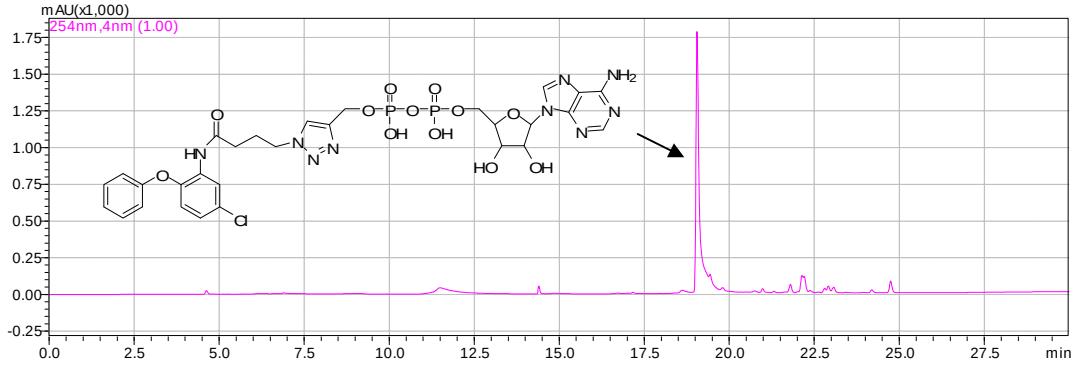

mAU(x1,000)
254nm,4nm (1.00)
min


Inten.(x10,000,000)
714.185
m/z
Inten.(x1,000,000)
712.167
226.955
m/z

C1-4C


mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
756.247
m/z
Inten.(x1,000,000)
754.218
113.000
227.021
m/z

C2-4C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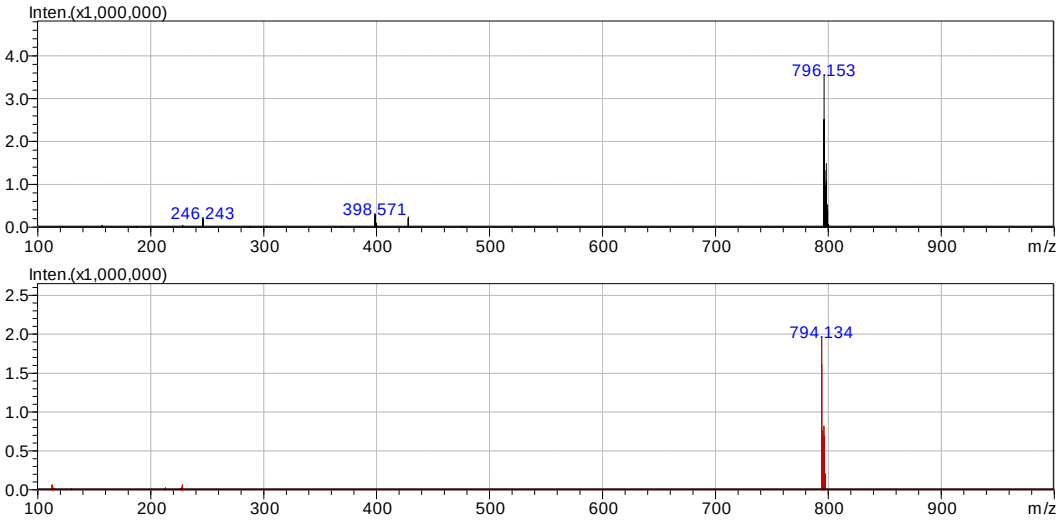
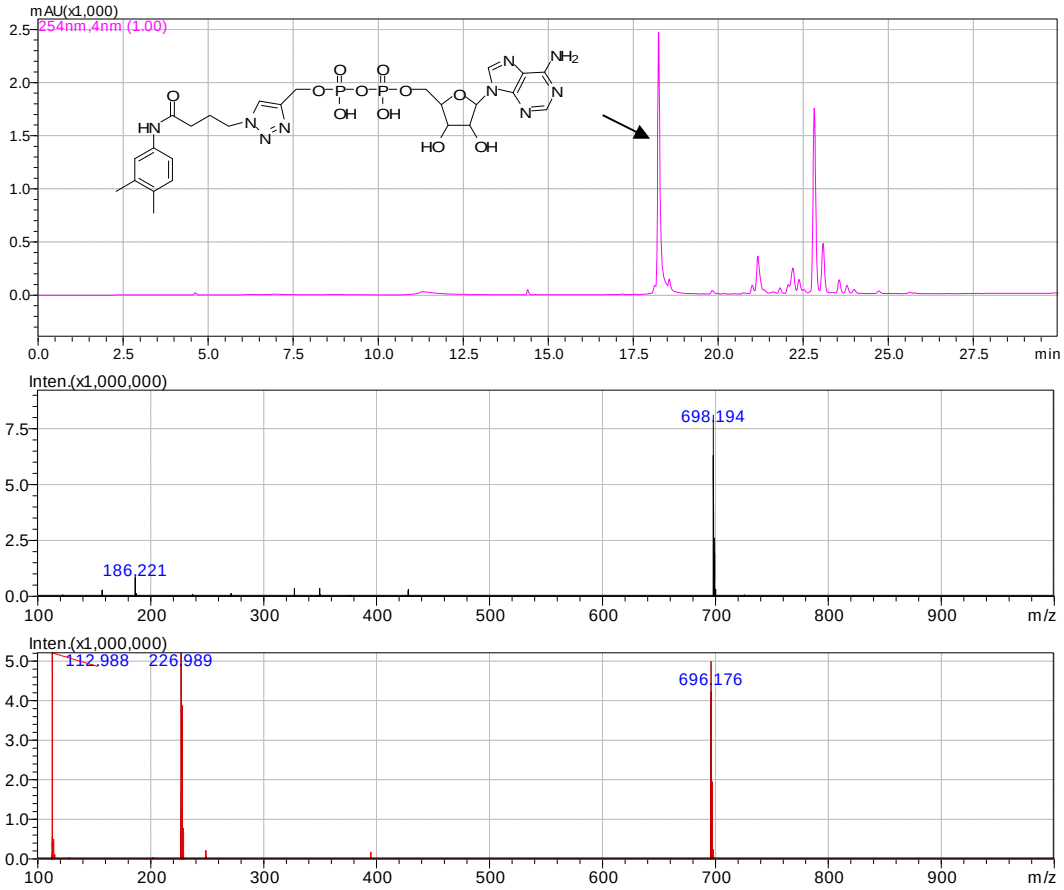
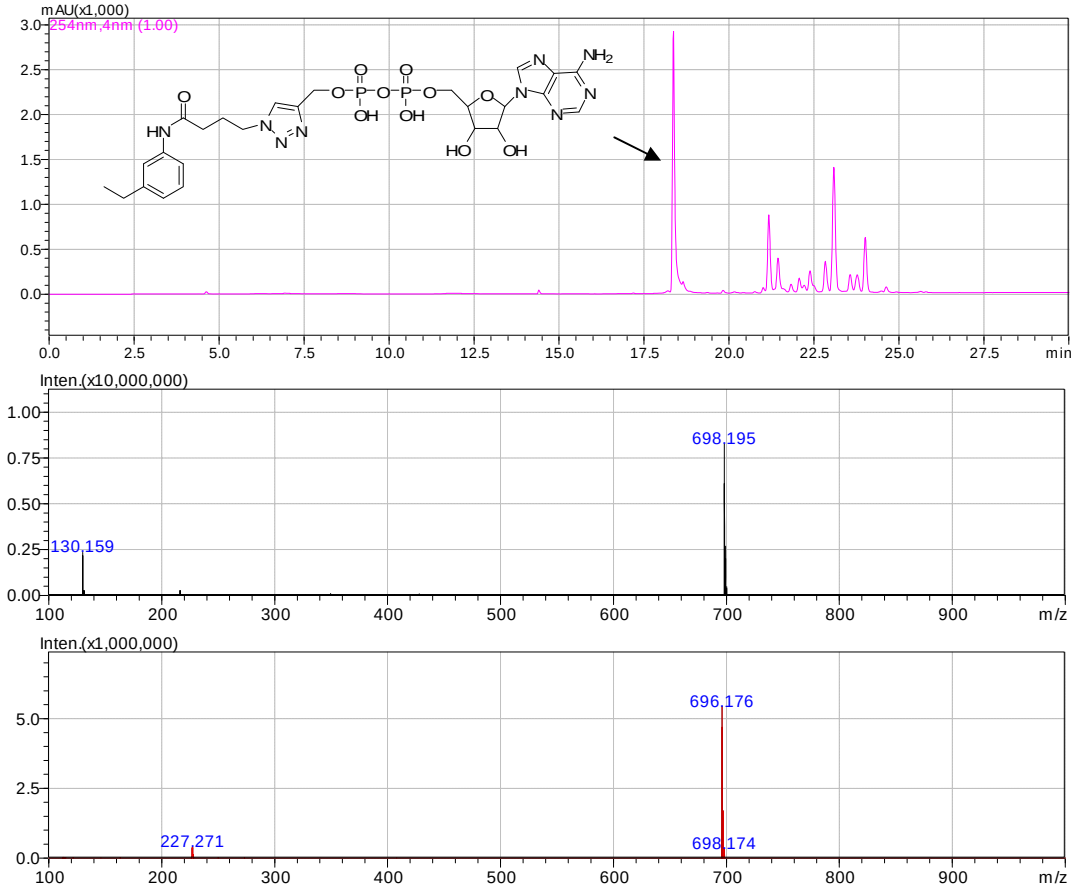
254nm,4nm (1.00)
min


Inten.(x1,000,000)
796.153
246.243
398.571
m/z
Inten.(x1,000,000)
794.134
m/z

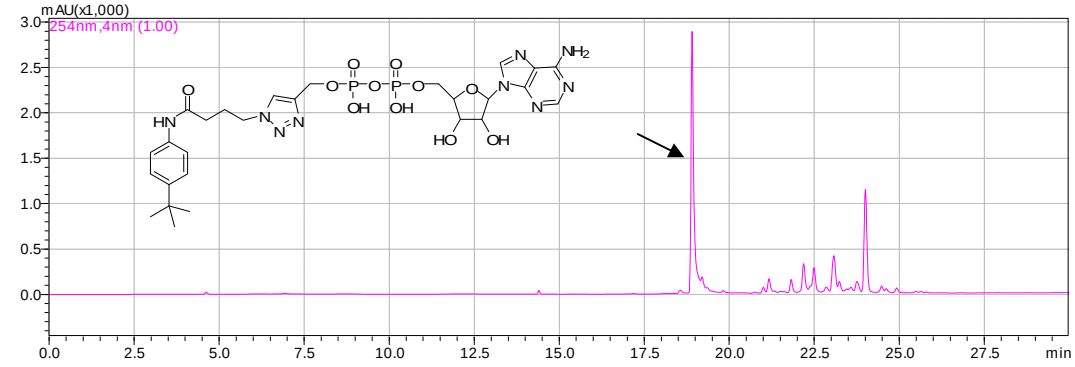
C4-4C

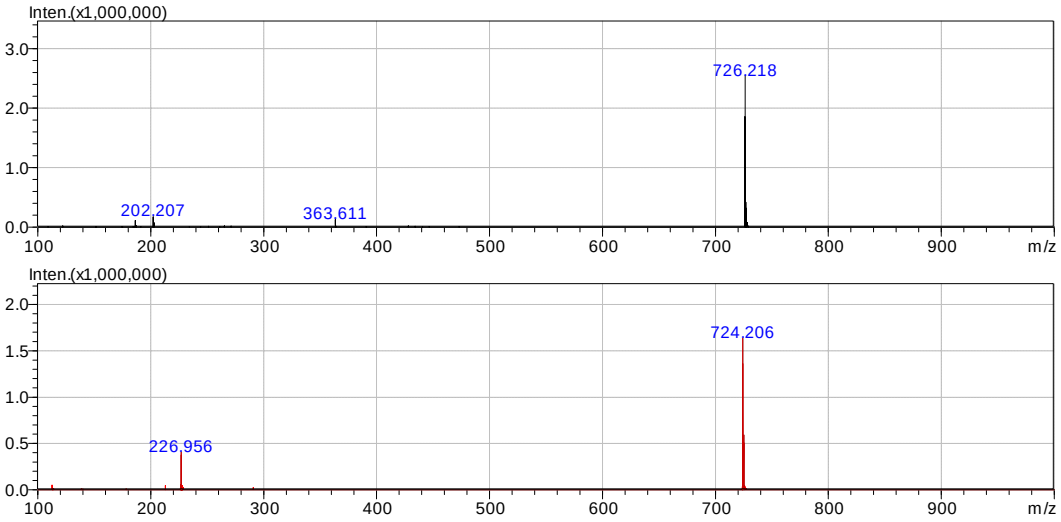

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
698.194
186.221
m/z
Inten.(x1,000,000)
112.988
226.989
696.176
m/z

C5-4C

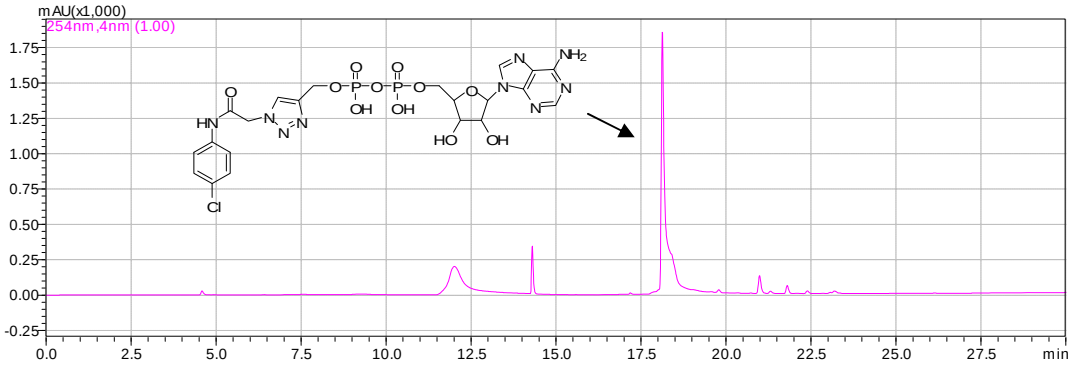

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x10,000,000)
698.195
130.159
m/z
Inten.(x1,000,000)
696.176
227.271
698.174
m/z

C6-4C

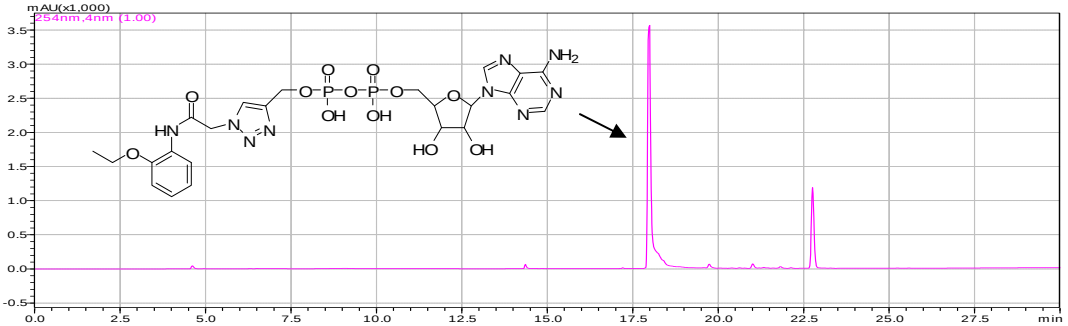

mAU(x1,000)
254nm,4nm (1.00)
min


Inten.(x1,000,000)
726.218
202.207
363.611
m/z
Inten.(x1,000,000)
724.206
226.956
m/z

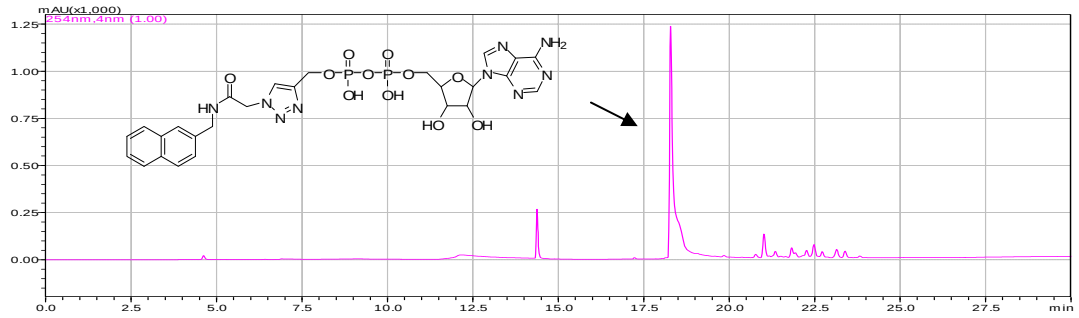
A8-2C


mAU(x1,000)
254nm,4nm (1.00)
min

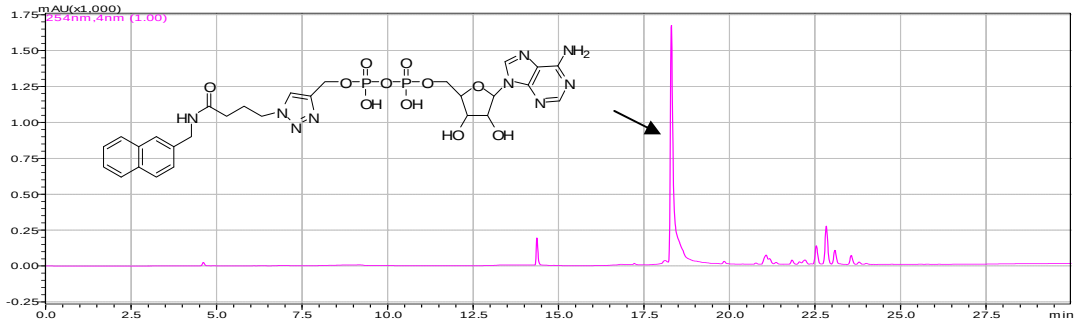
A12-2C


mAU(x1,000)
254nm,4nm (1.00)
min

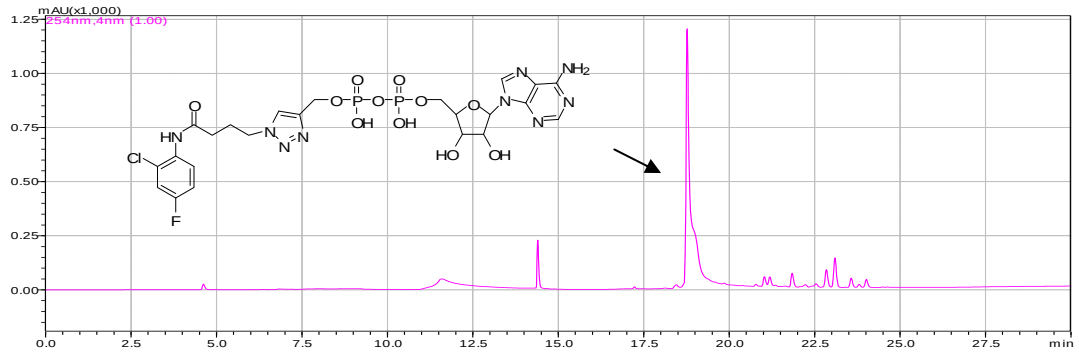
D4-2C



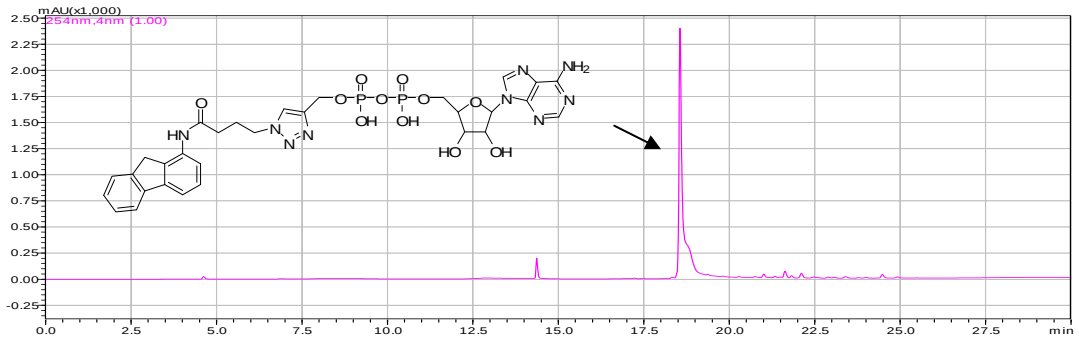
D4-4C



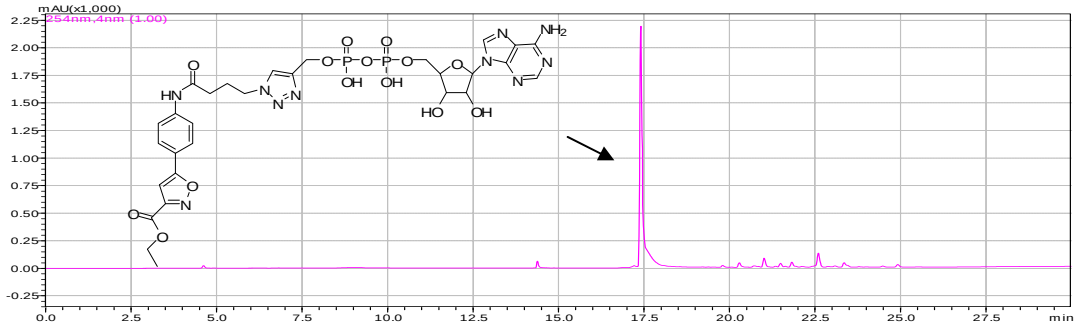
D5-4C



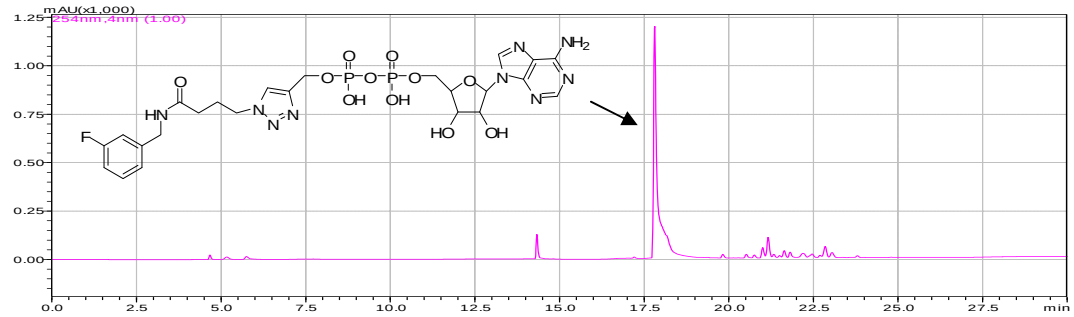
D7-4C



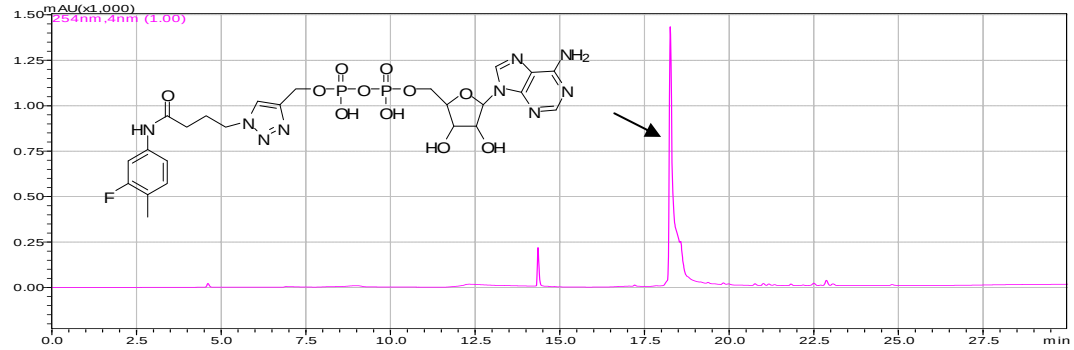
D8-4C



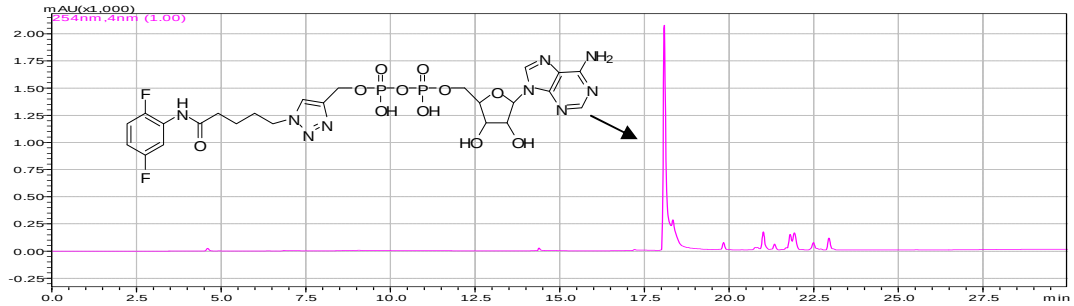
A5-4C

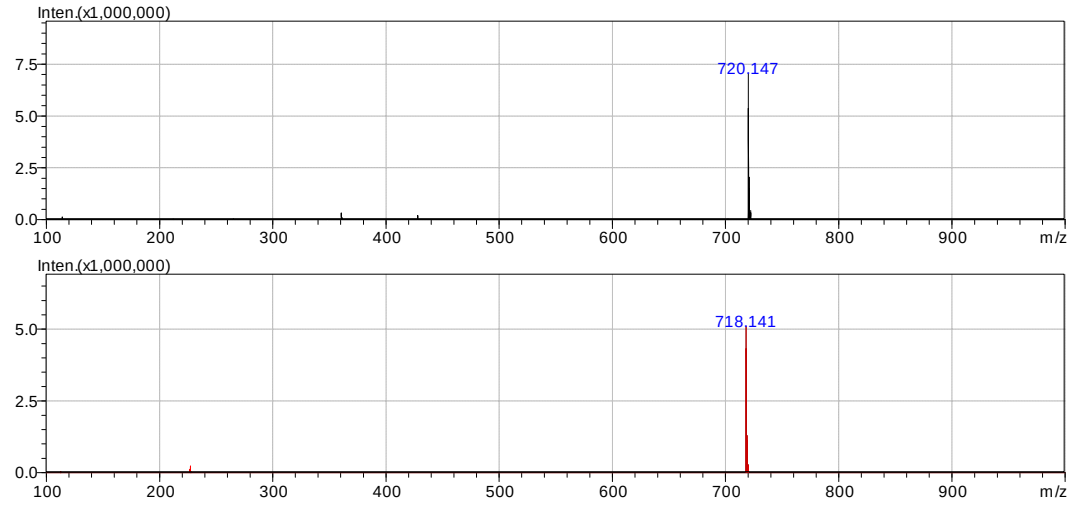


A6-4C

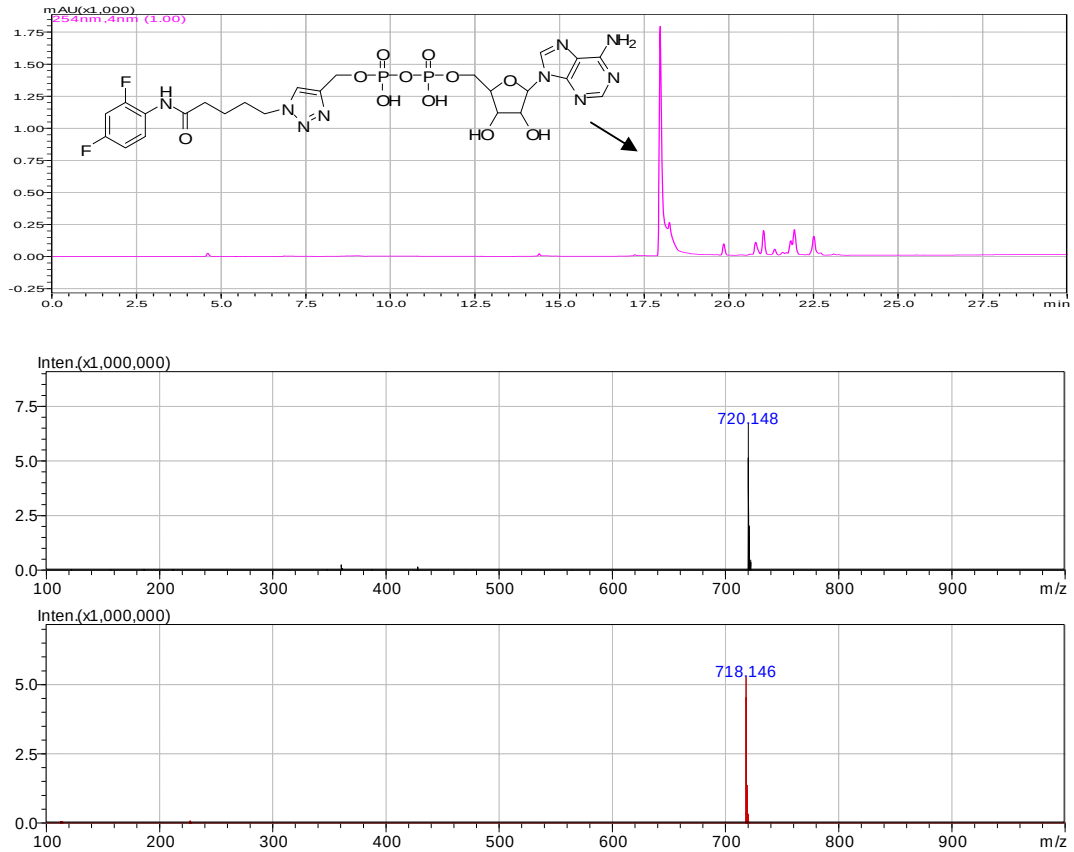

mAU(x1,000)
254nm,4nm (1.00)
min

A3-5C

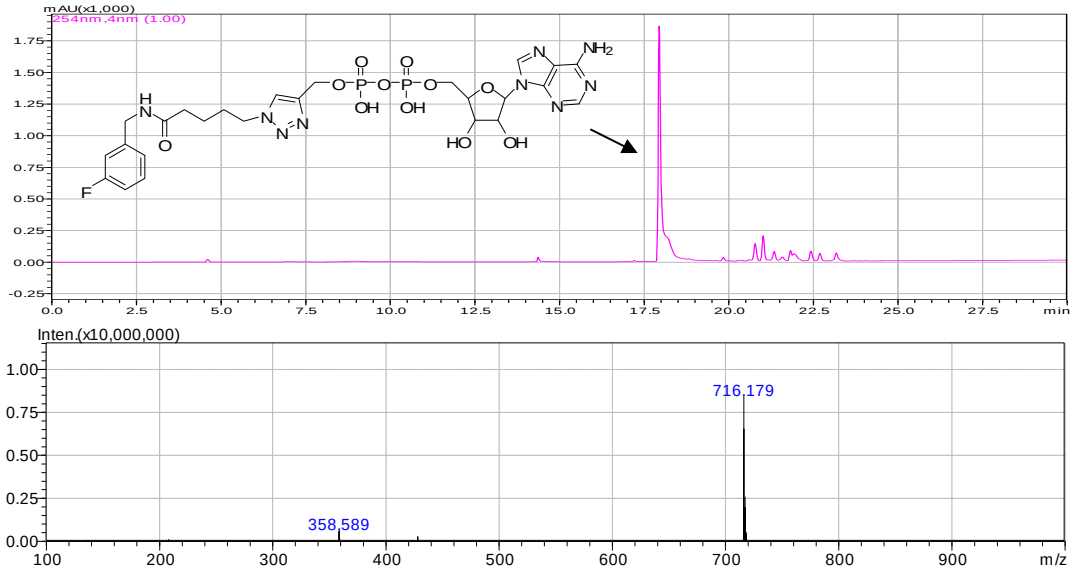

mAU(x1,000)
254nm,4nm (1.00)
min

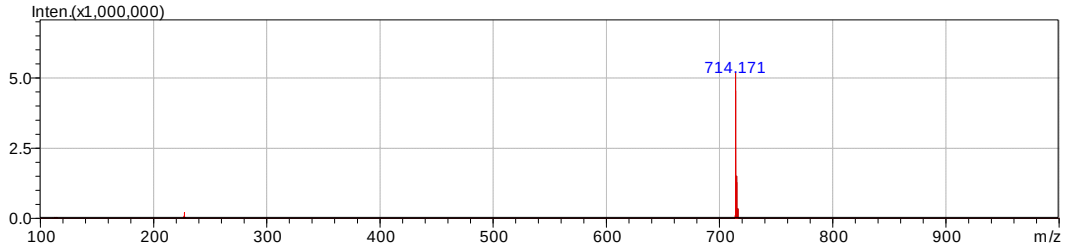

Inten.(x1,000,000)
720.147
m/z
Inten.(x1,000,000)
718.141
m/z

A4-5C

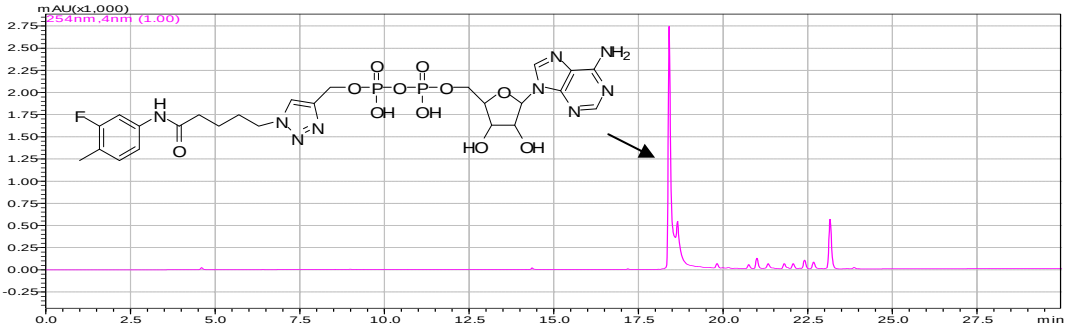

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
720.148
m/z
Inten.(x1,000,000)
718.146
m/z

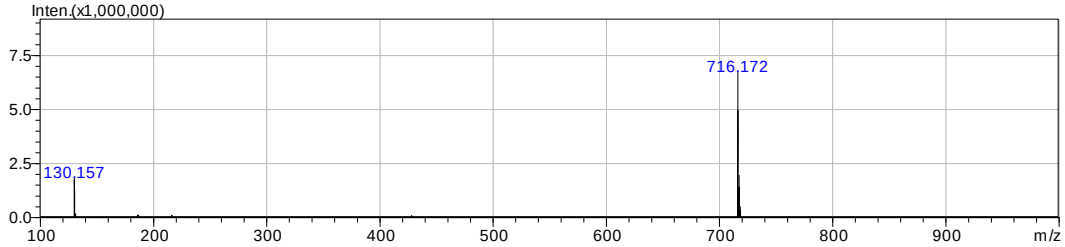
A5-5C

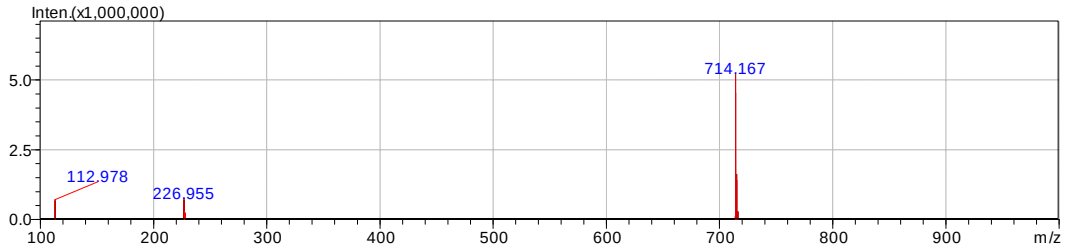

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x10,000,000)
716.179
358.589
m/z


Inten.(x1,000,000)
714.171
m/z

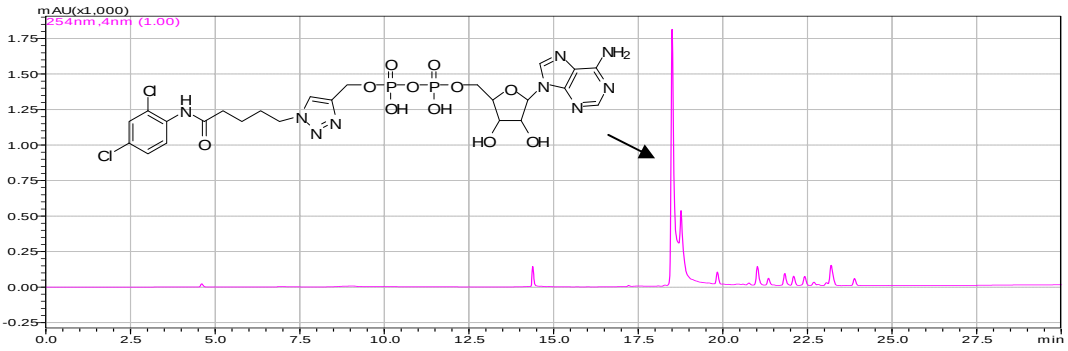
A6-5C

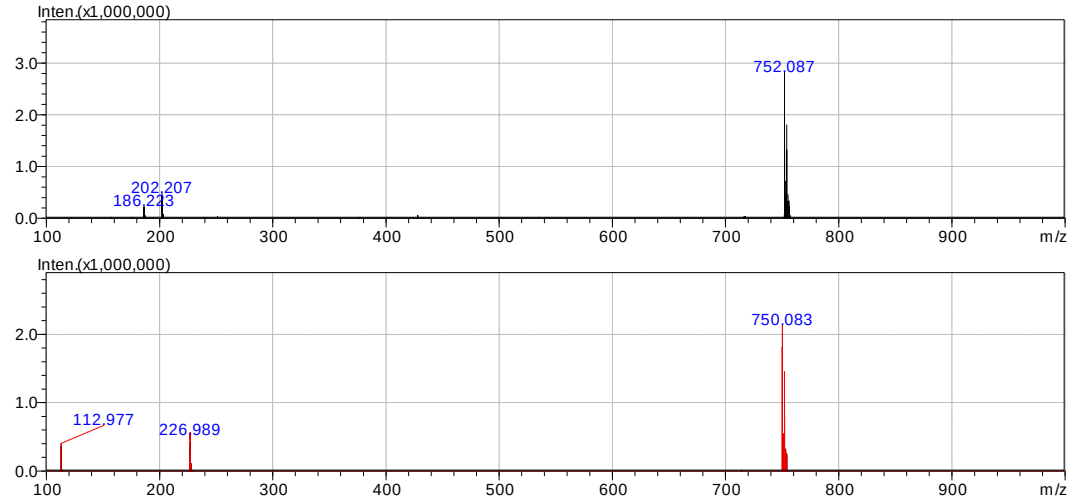

mAU(x1,000)
254nm,4nm (1.00)
min


Inten.(x1,000,000)
716.172
130.157
m/z

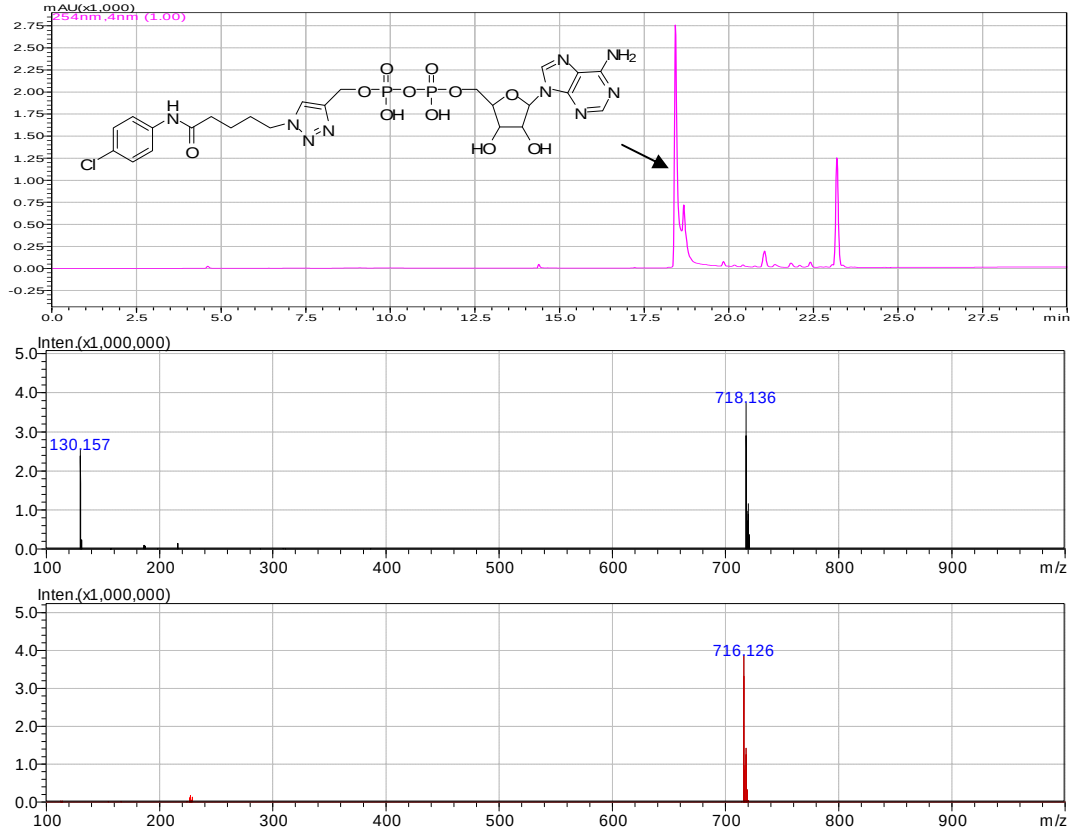

Inten.(x1,000,000)
714.167
112.978
226.955
m/z

A7-5C

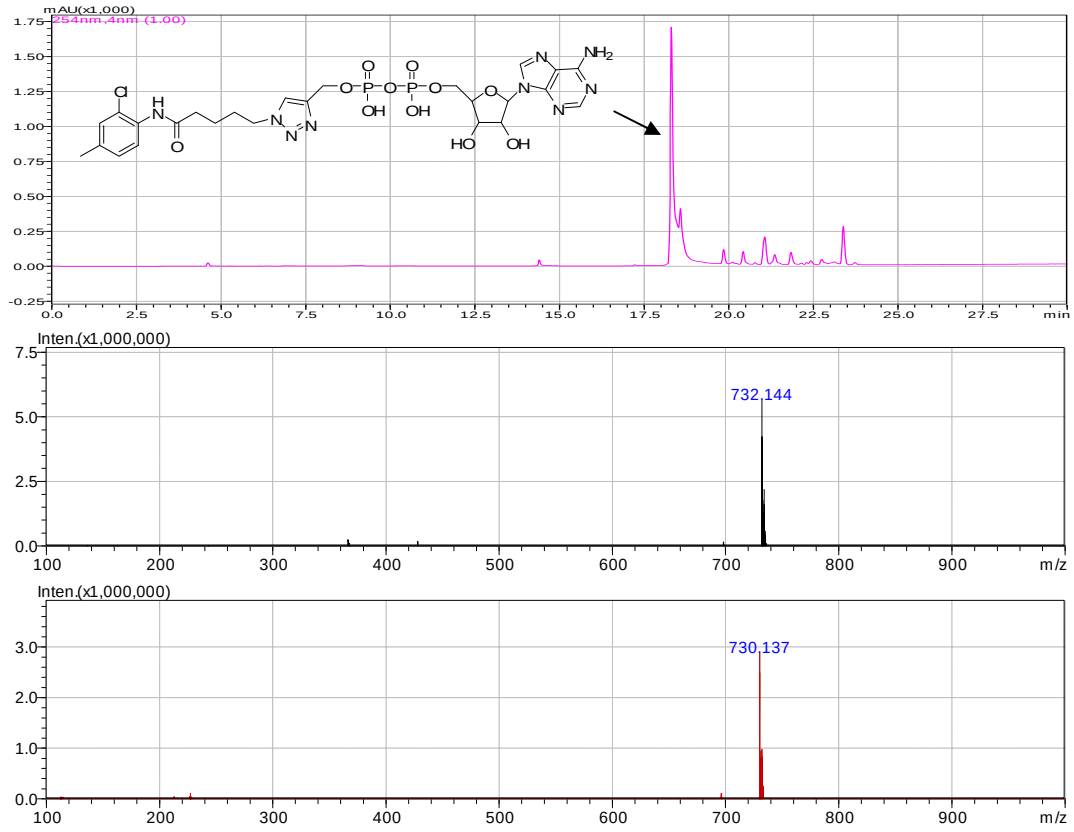

mAU(x1,000)
254nm,4nm (1.00)
min


Inten.(x1,000,000)
752.087
202.207
186.213
m/z
Inten.(x1,000,000)
750.083
112.977
226.989
m/z

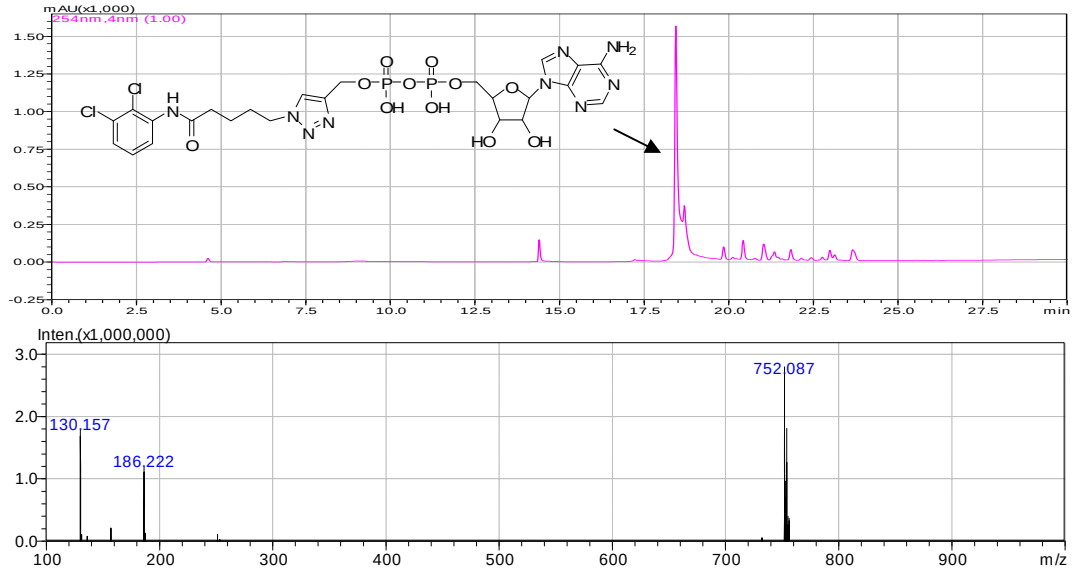
A8-5C

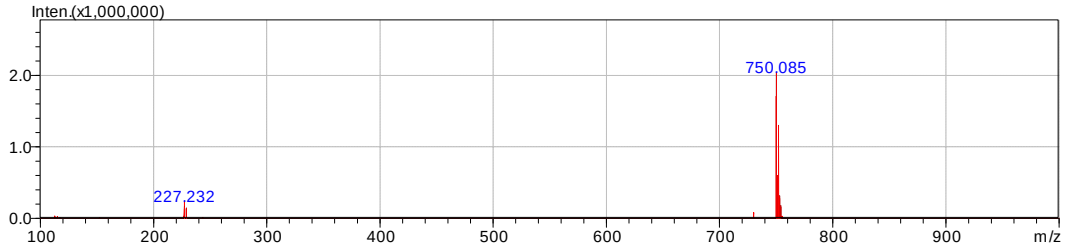

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
718.136
130.157
m/z
Inten.(x1,000,000)
716.126
m/z

A9-5C

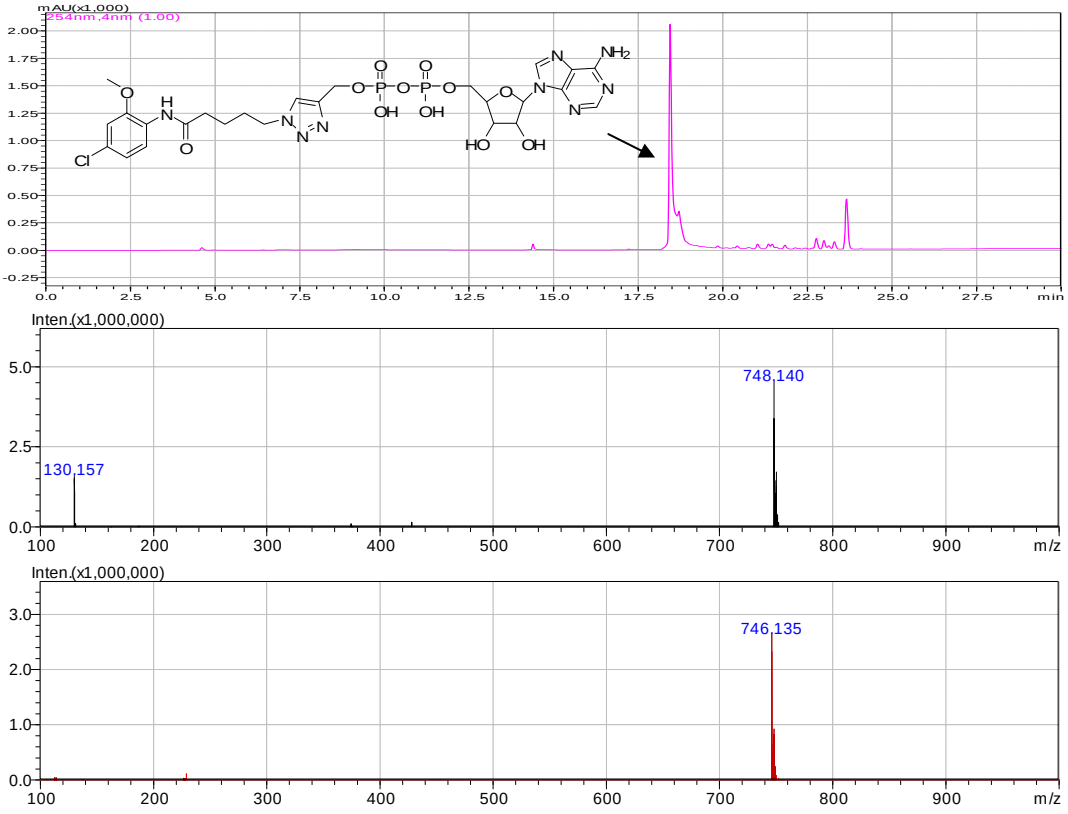

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
732.144
m/z
Inten.(x1,000,000)
730.137
m/z

A10-5C

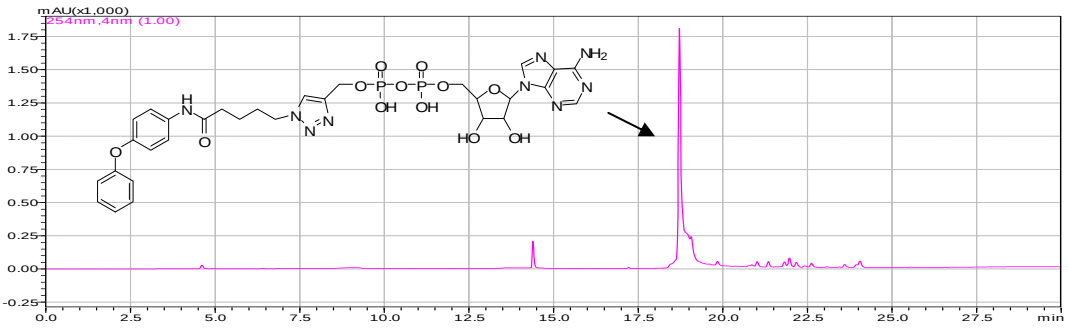

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
752.087
130.157
186.222
m/z

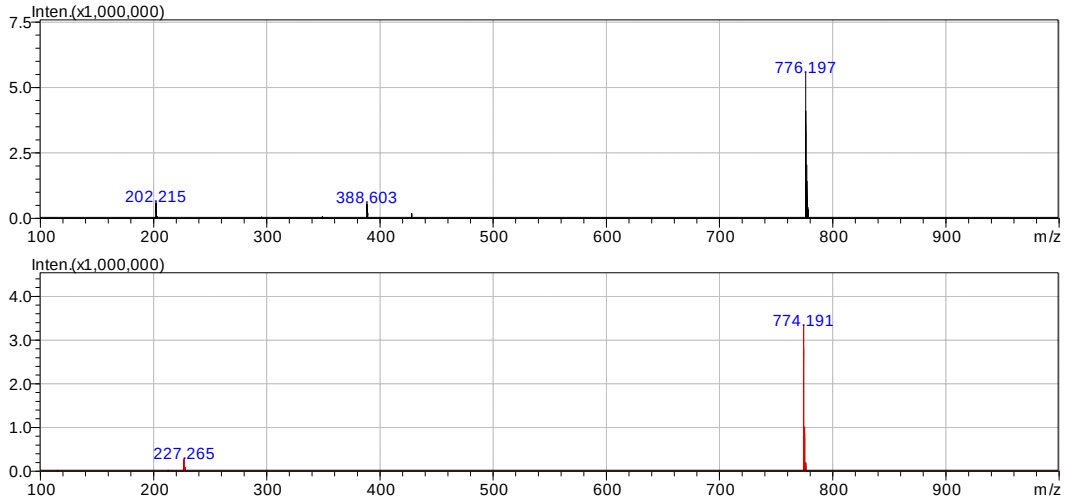

Inten.(x1,000,000)
750.085
227.232
m/z

A11-5C

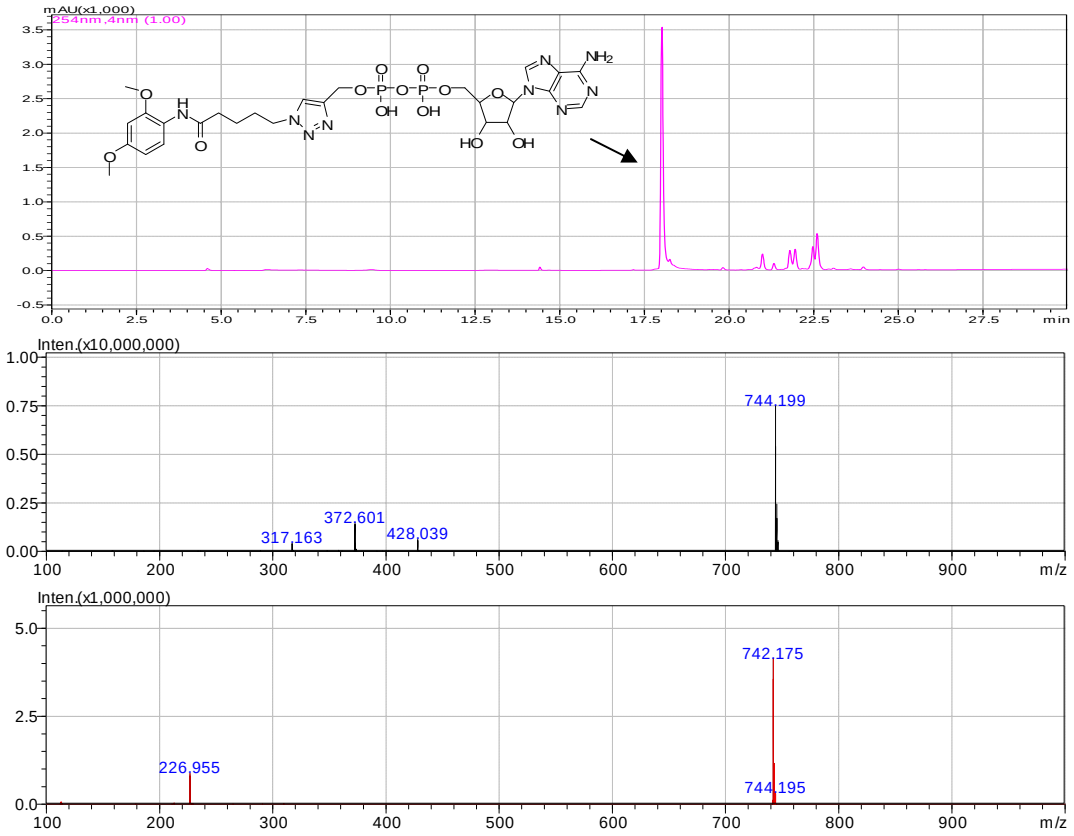

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
748.140
130.157
m/z
Inten.(x1,000,000)
746.135
m/z

B1-5C

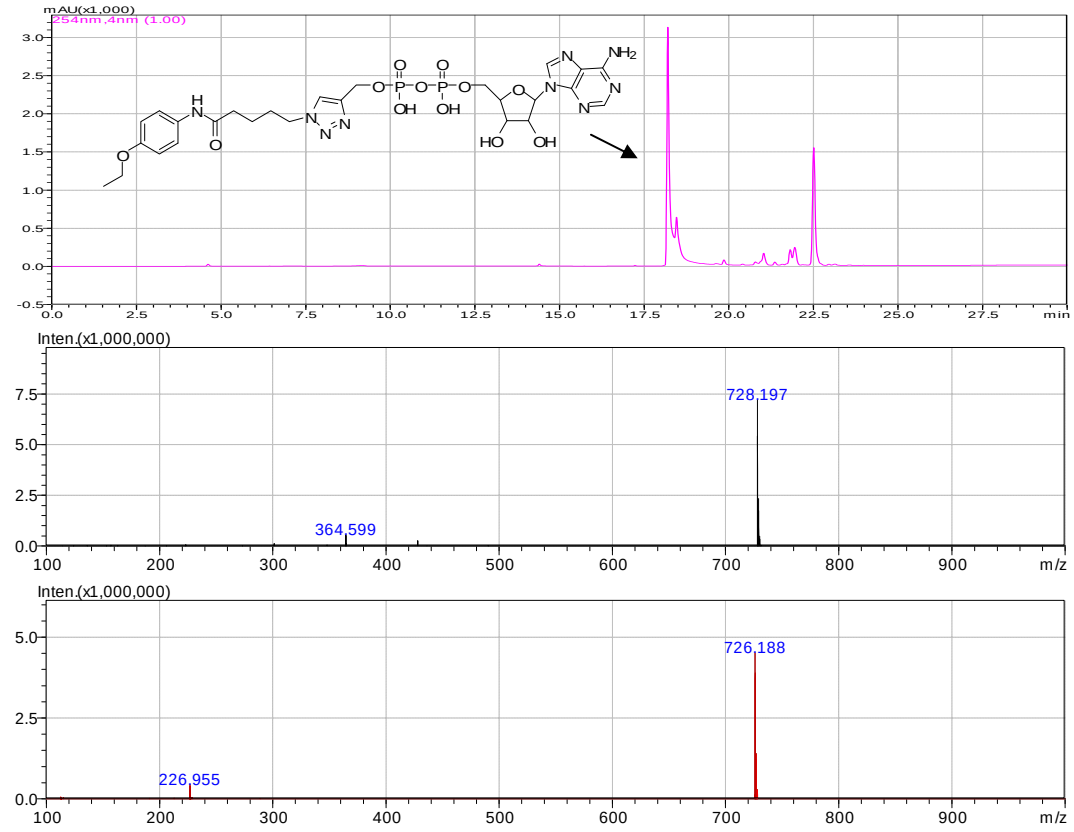

mAU(x1,000)
254nm,4nm (1.00)
min


Inten.(x1,000,000)
776.197
202.215
388.603
m/z
Inten.(x1,000,000)
774.191
227.265
m/z

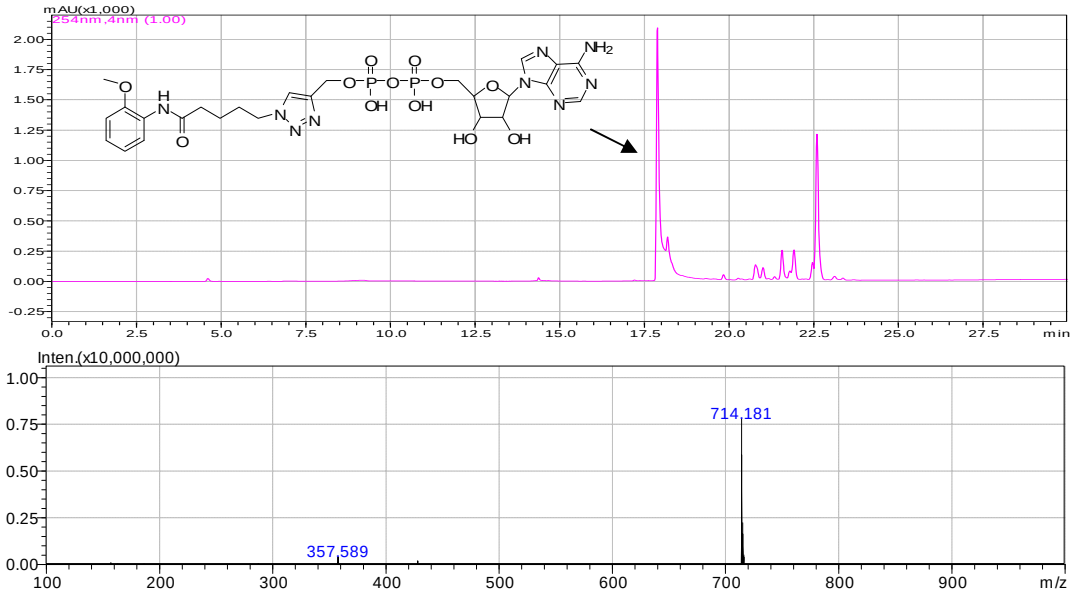
B2-5C

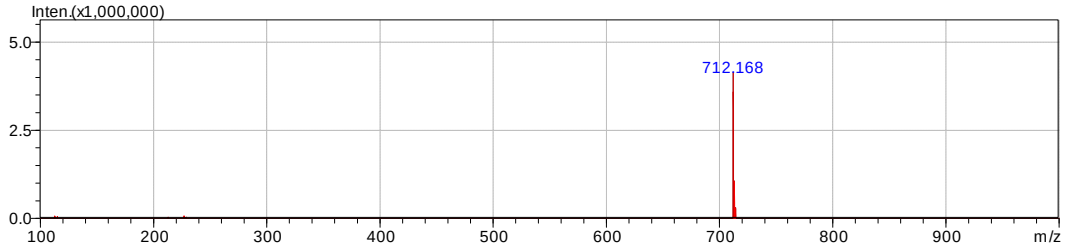

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x10,000,000)
744.199
372.601
317.163
428.039
m/z
Inten.(x1,000,000)
742.175
226.955
744.195
m/z

B3-5C

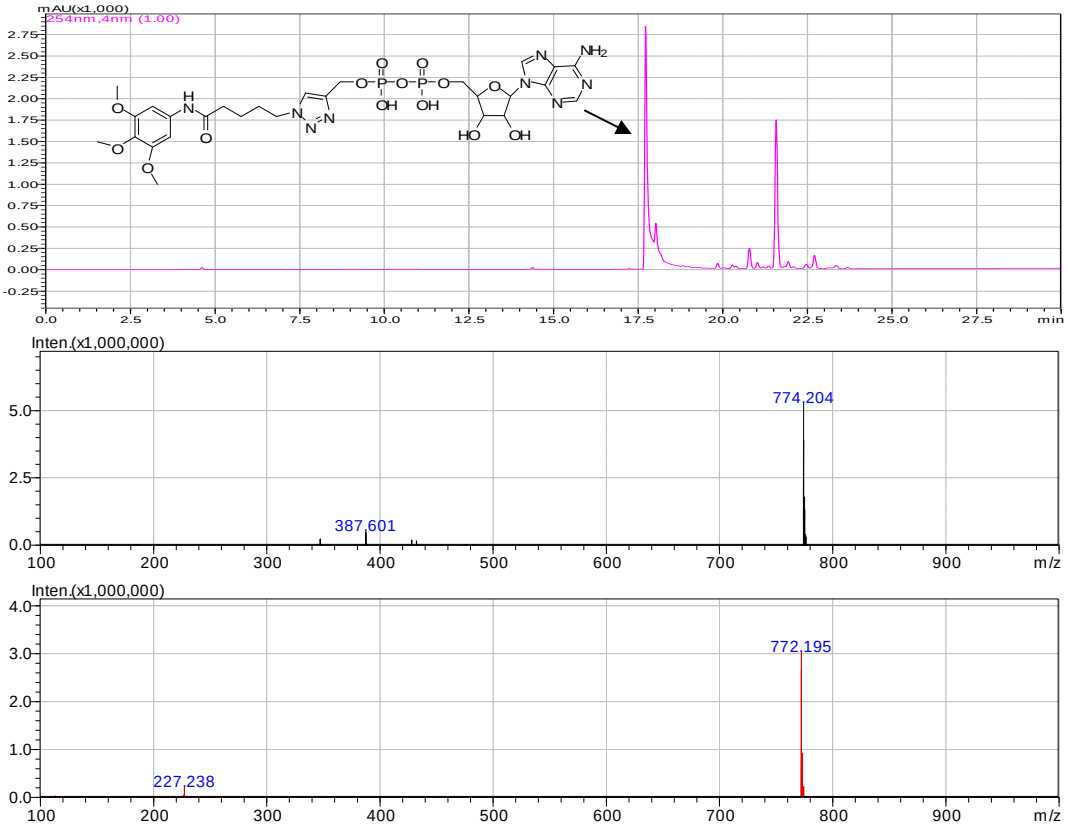

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
728.197
364.599
m/z
Inten.(x1,000,000)
726.188
226.955
m/z

B4-5C

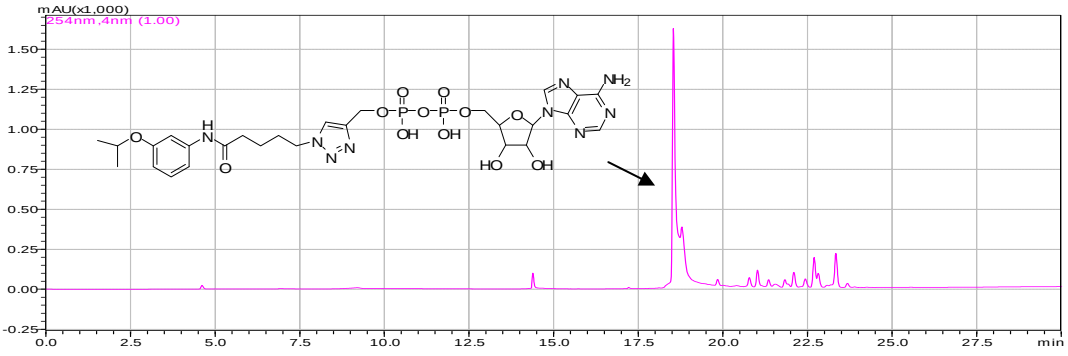

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x10,000,000)
714.181
357.589
m/z

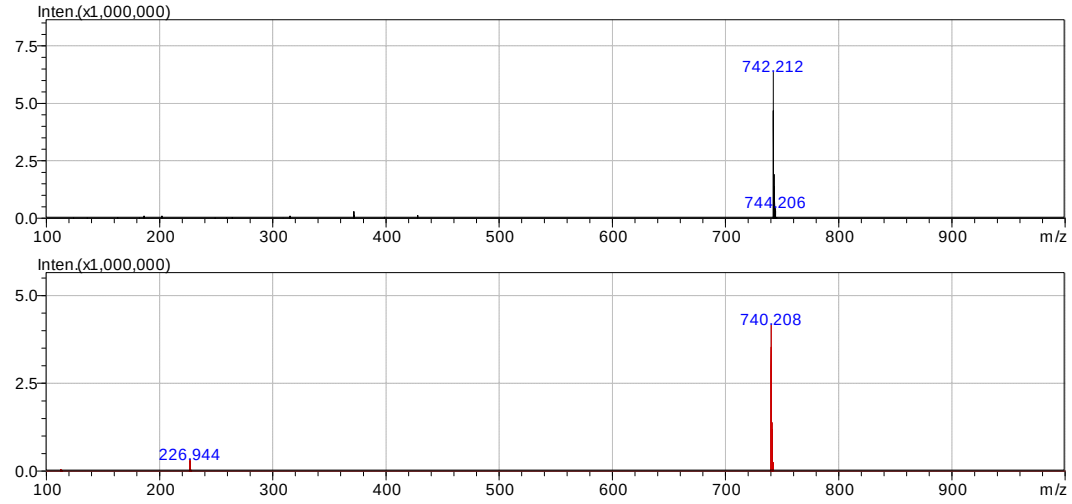

Inten.(x1,000,000)
712.168
m/z

B5-5C

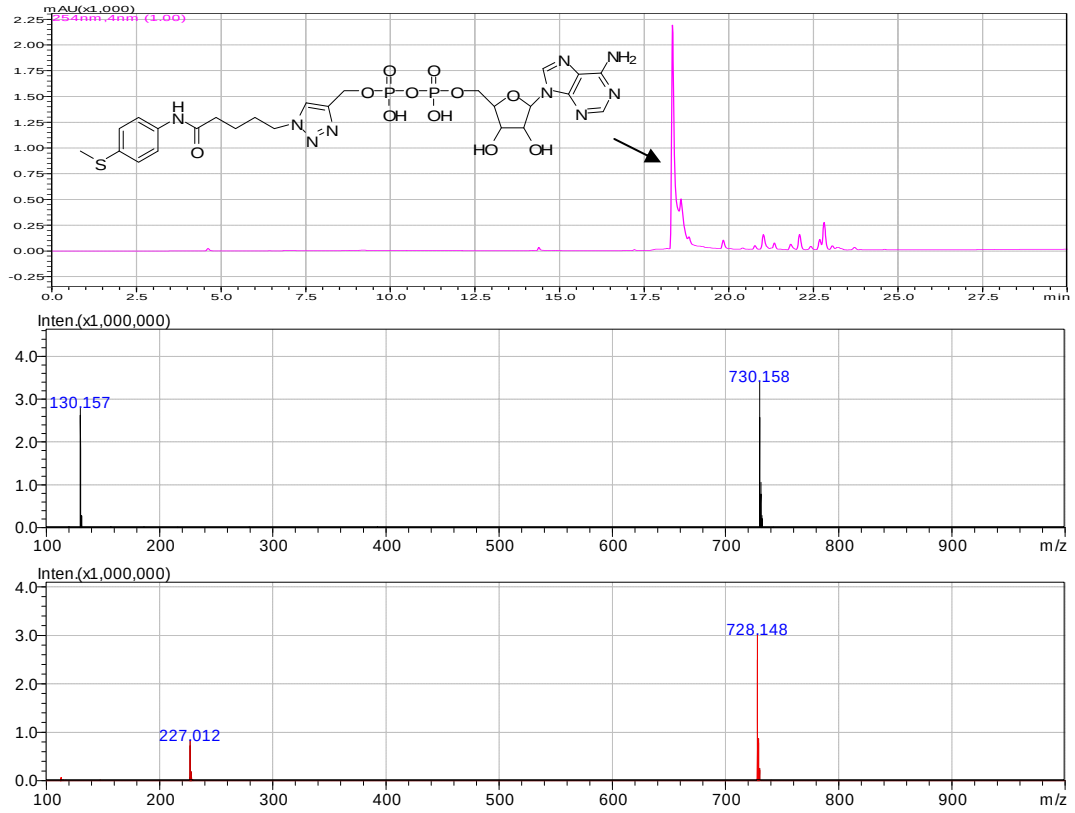

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
774.204
387.601
m/z
Inten.(x1,000,000)
772.195
227.238
m/z

B6-5C

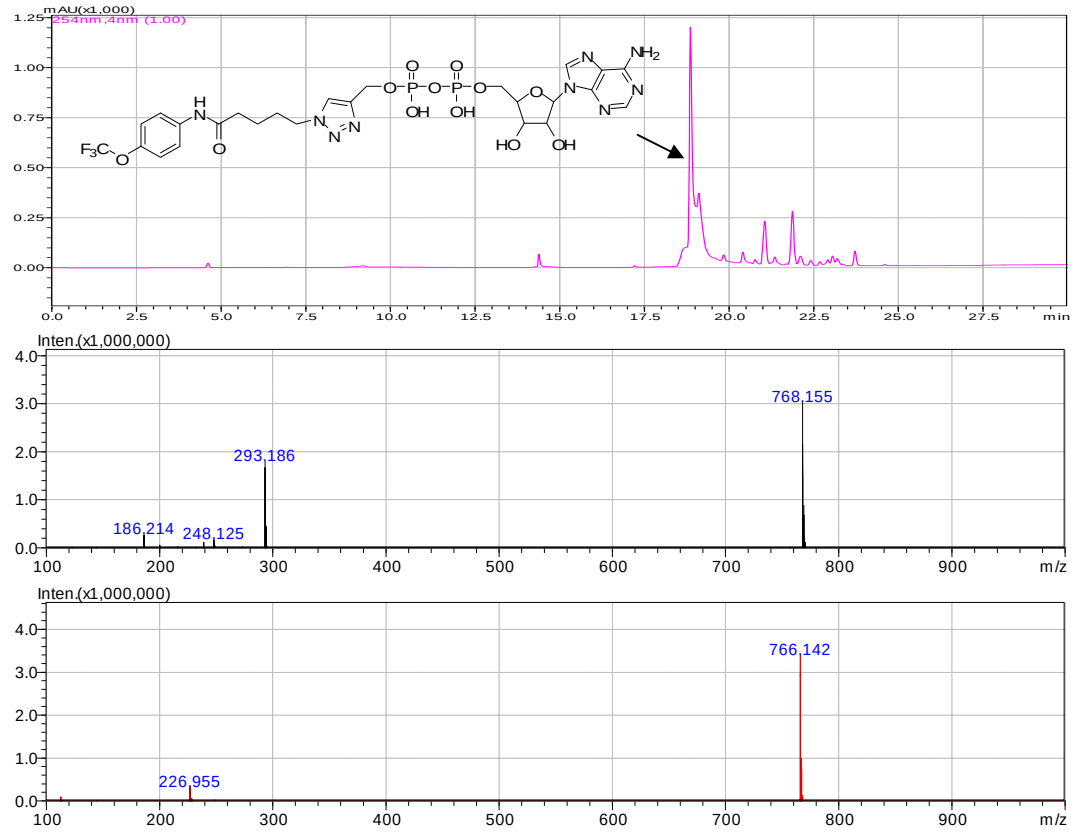

mAU(x1,000)
254nm,4nm (1.00)
min


Inten.(x1,000,000)
742.212
744.206
m/z
Inten.(x1,000,000)
740.208
226.944
m/z

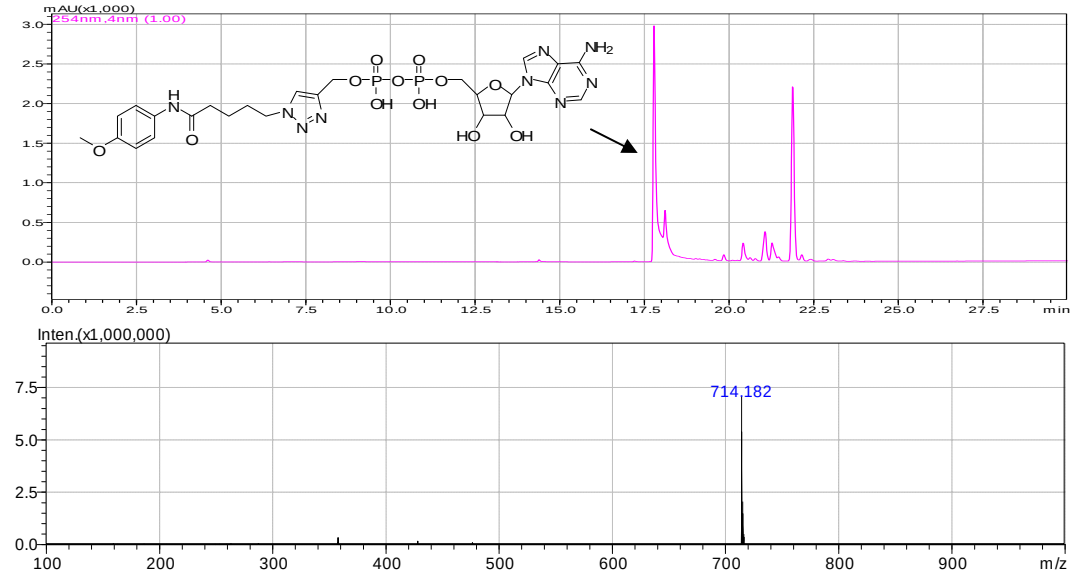
B7-5C

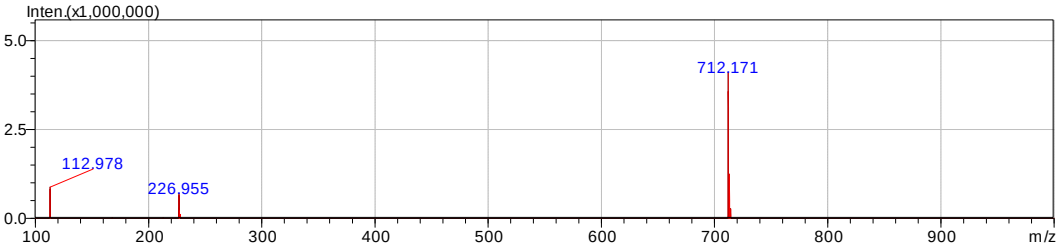

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
730.158
130.157
m/z
Inten.(x1,000,000)
728.148
227.012
m/z

B8-5C

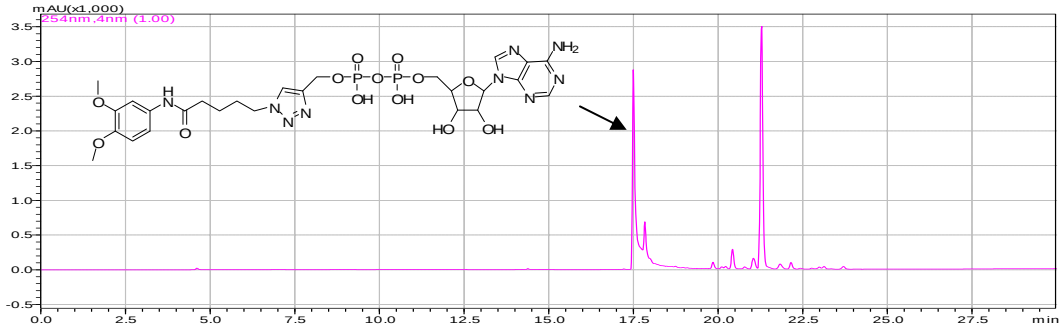

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
768.155
293.186
186.214
248.125
m/z
Inten.(x1,000,000)
766.142
226.955
m/z

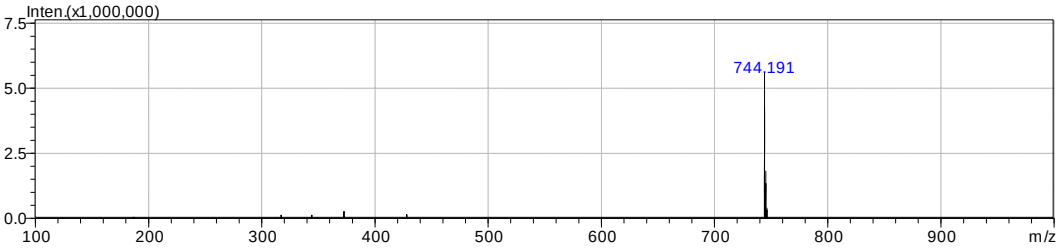
B9-5C

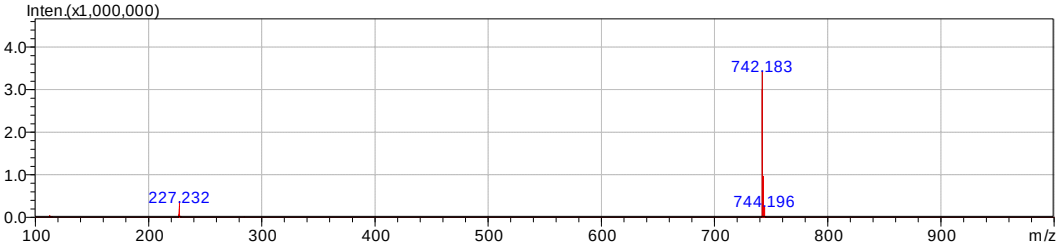

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
714.182
m/z


Inten.(x1,000,000)
712.171
112.978
226.955
m/z

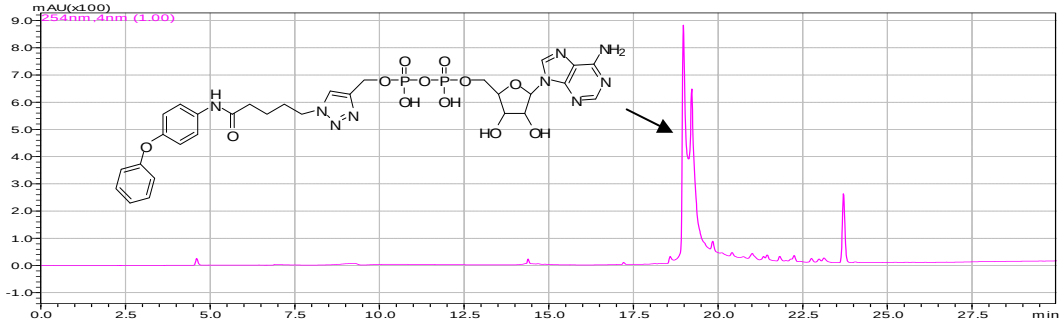
B10-5C

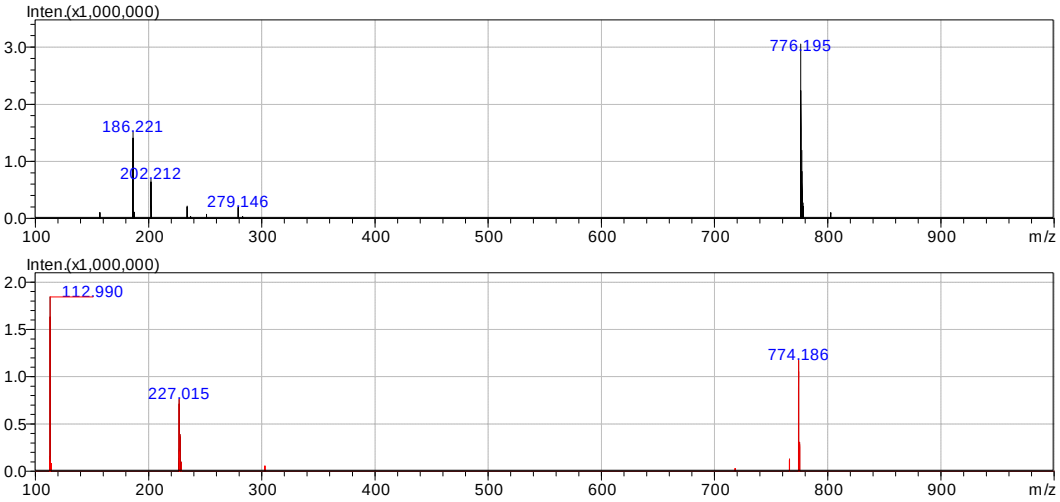

mAU(x1,000)
254nm,4nm (1.00)
min


Inten.(x1,000,000)
744.191
m/z

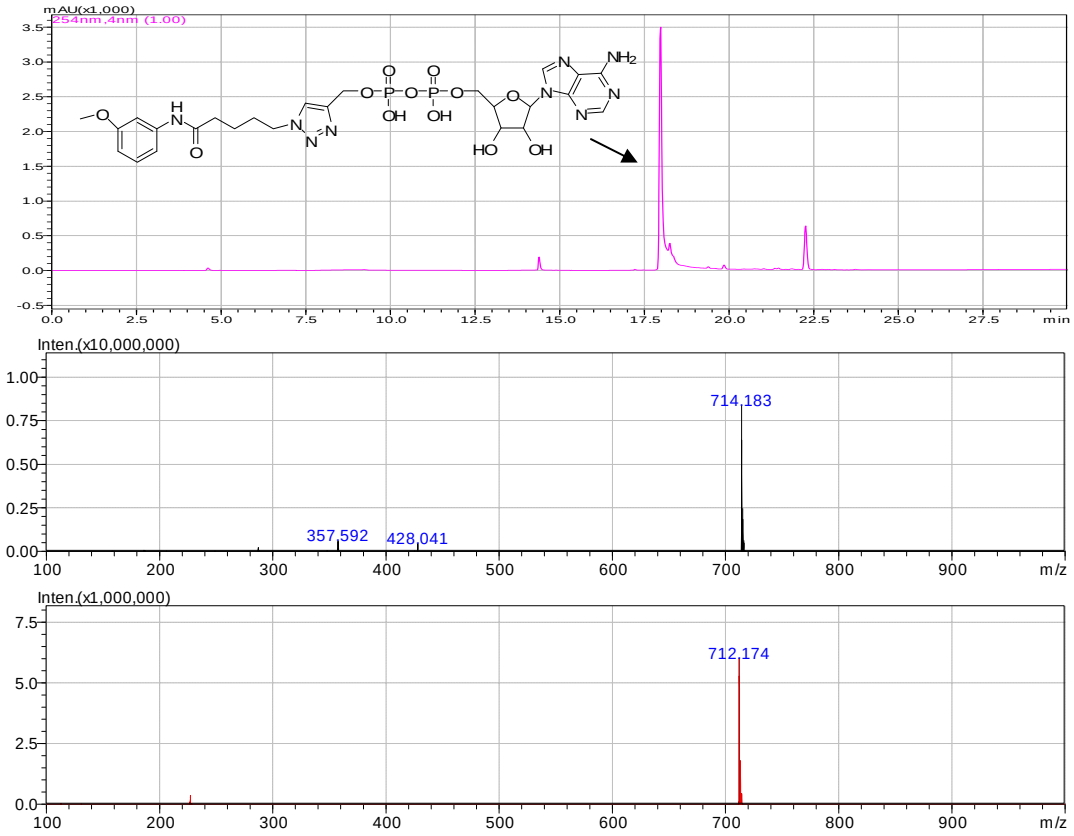

Inten.(x1,000,000)
742.183
227.232
744.196
m/z

B11-5C

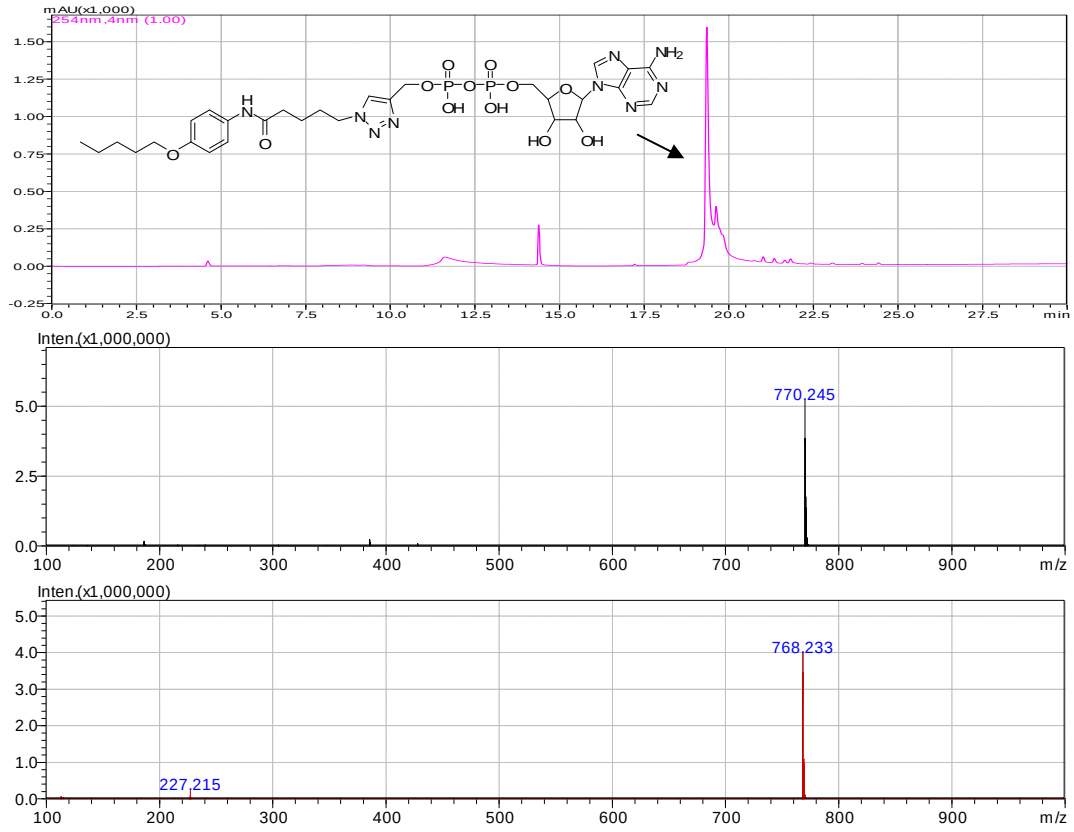

mAU(x100)
254nm,4nm (1.00)
min


Inten.(x1,000,000)
776.195
186.221
202.212
279.146
m/z
Inten.(x1,000,000)
112.990
774.186
227.015
m/z

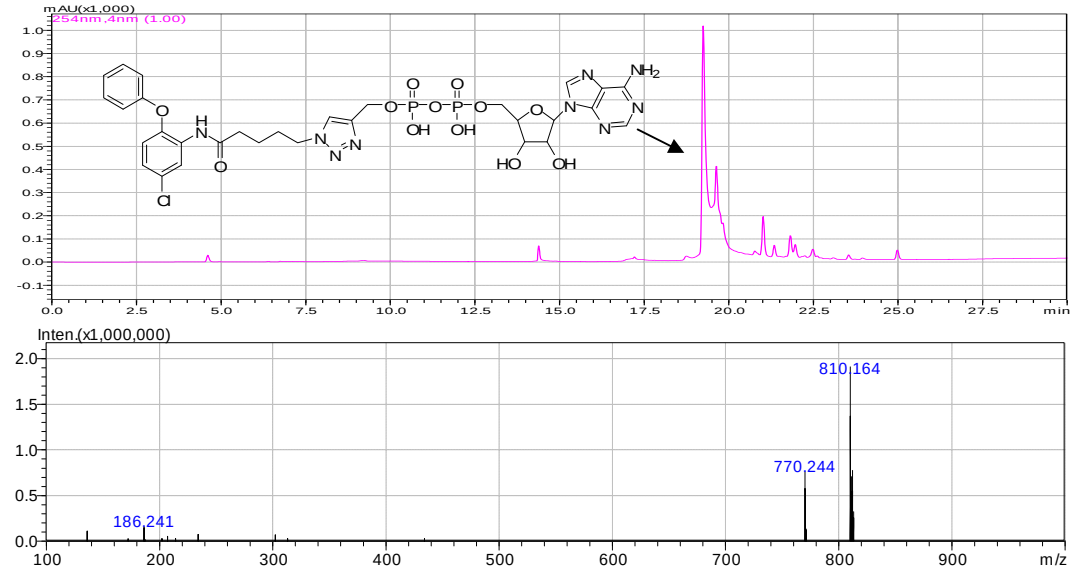
B12-5C

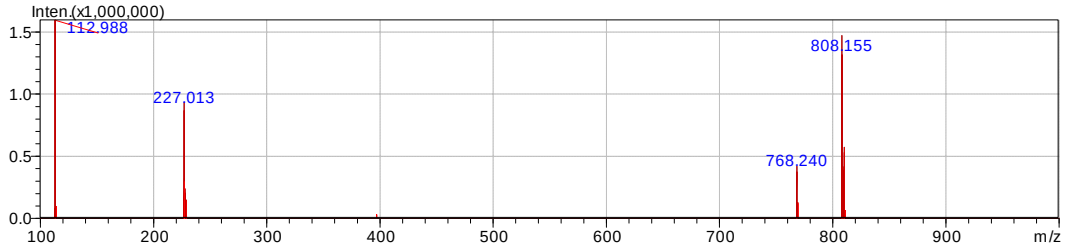

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x10,000,000)
714.183
357.592
428.041
m/z
Inten.(x1,000,000)
712.174
m/z

C1-5C

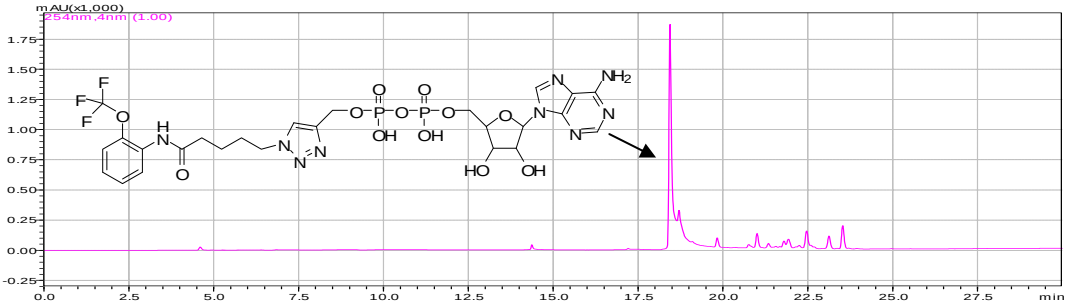

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
770,245
m/z
Inten.(x1,000,000)
768,233
227,215
m/z

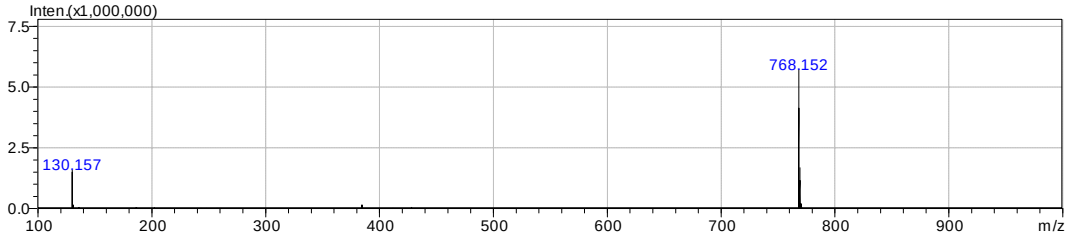
C2-5C

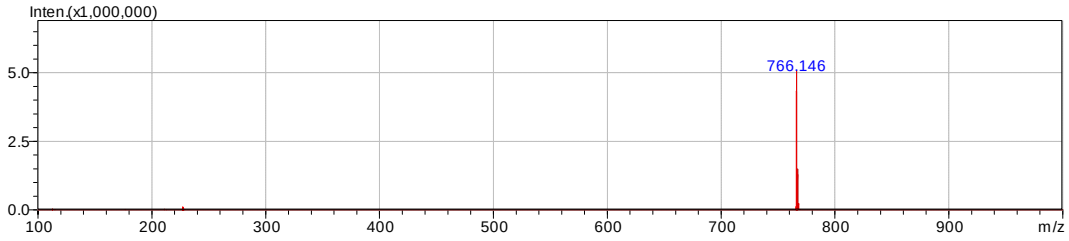

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
810,164
770,244
186,241
m/z


Inten.(x1,000,000)
112.988
227.013
768.240
808.155
m/z

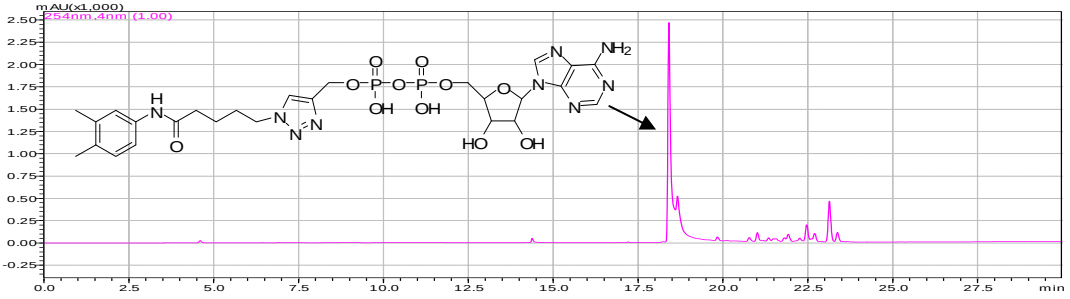
C3-5C

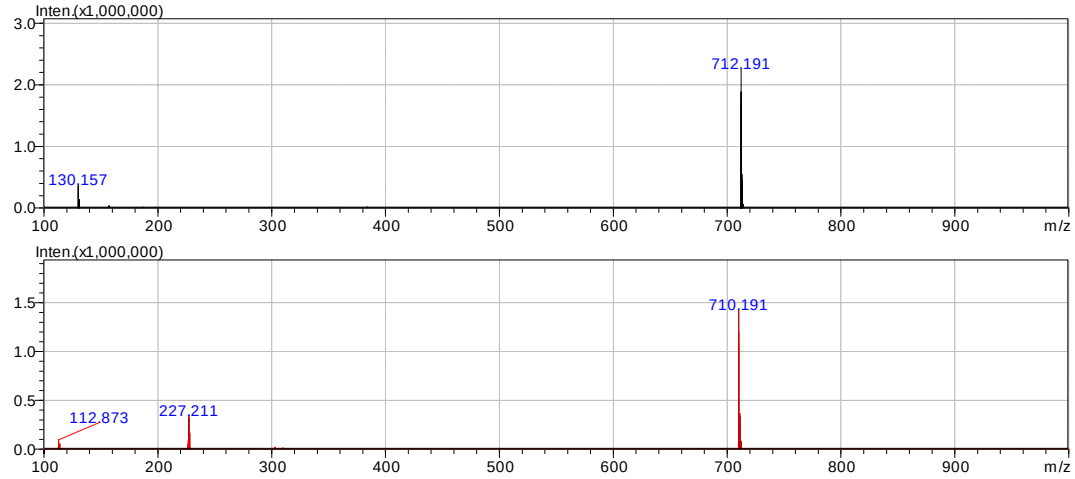

mAU(x1,000)
254nm,4nm (1.00)
min


Inten.(x1,000,000)
768.152
130.157
m/z

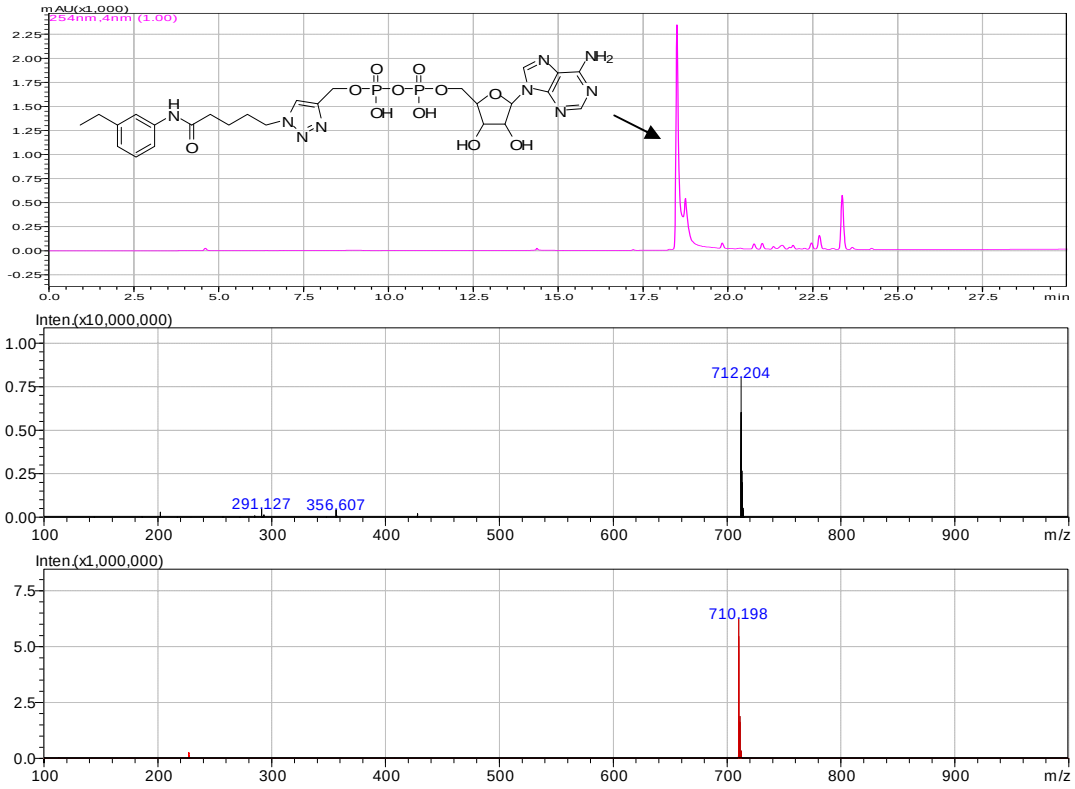

Inten.(x1,000,000)
766.146
m/z

C4-5C

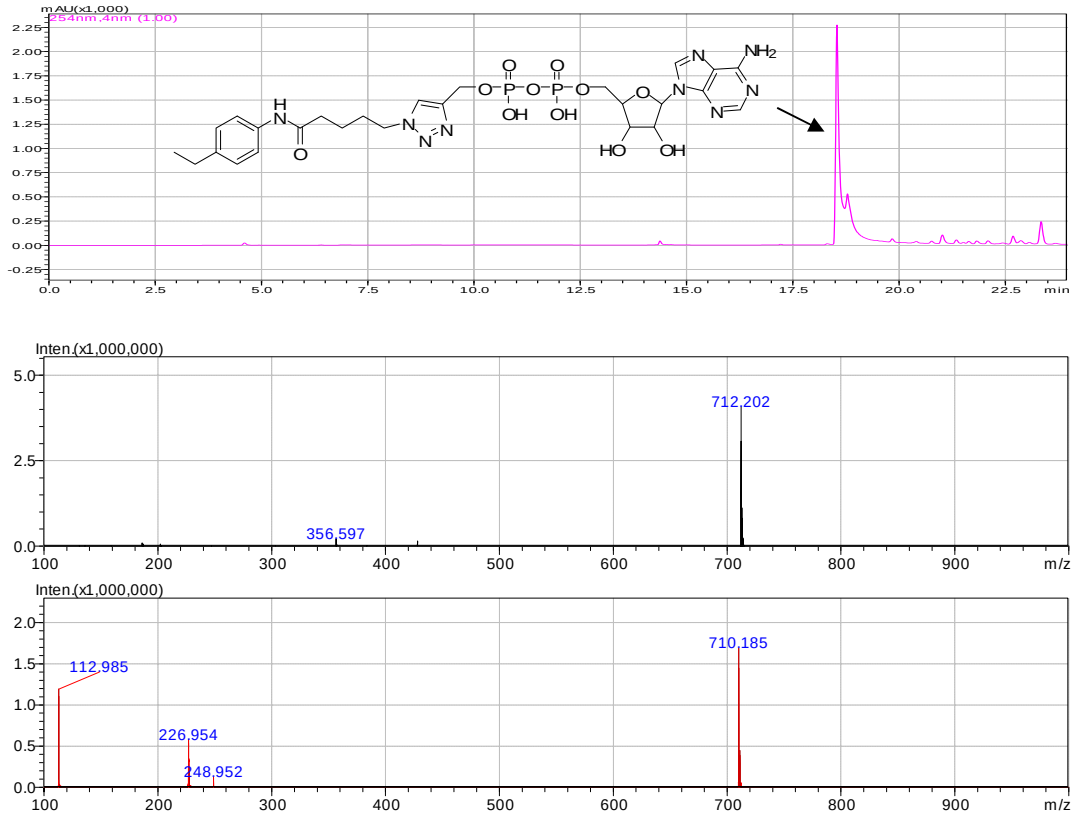

mAU(x1,000)
254nm,4nm (1.00)
min


Inten.(x1,000,000)
712.191
130.157
m/z
Inten.(x1,000,000)
710.191
112.873
227.211
m/z

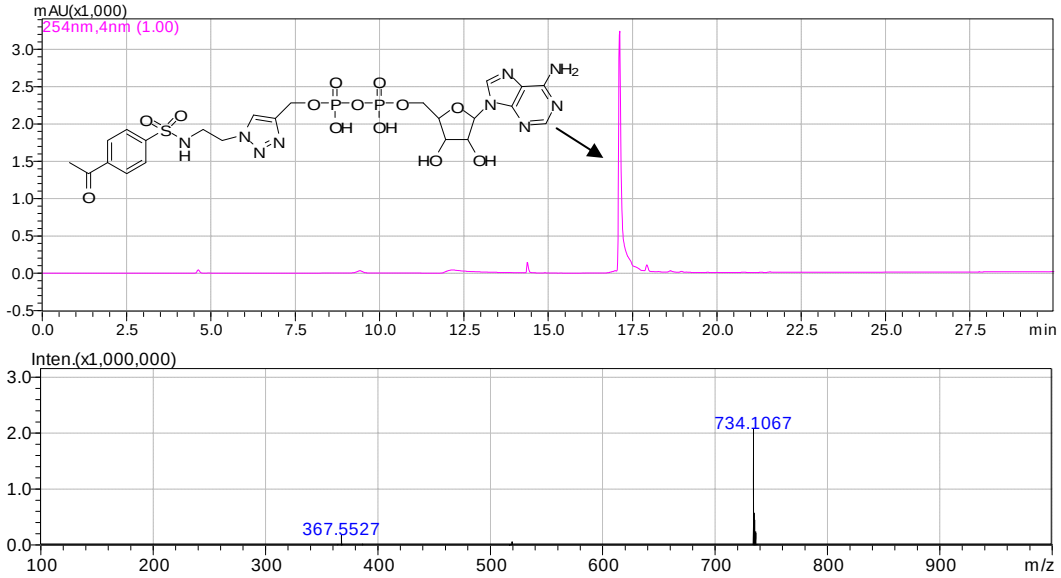
C5-5C

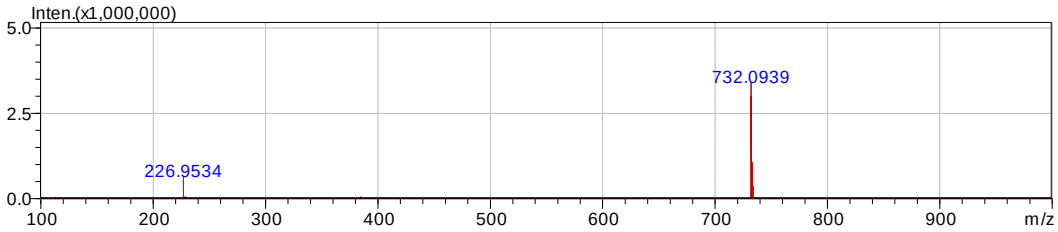

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x10,000,000)
712.204
291.127
356.607
m/z
Inten.(x1,000,000)
710.198
m/z

C7-5C

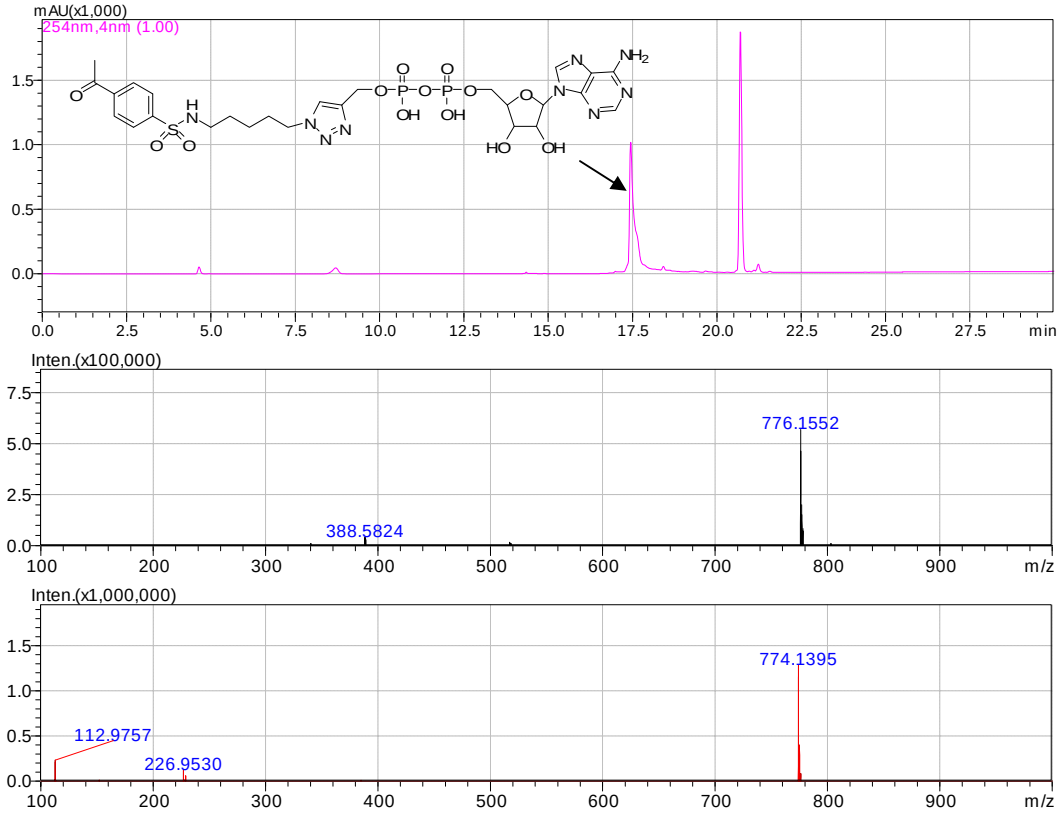

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
712.202
356.597
m/z
Inten.(x1,000,000)
710.185
112.985
226.954
248.952
m/z

SA-A1-2C

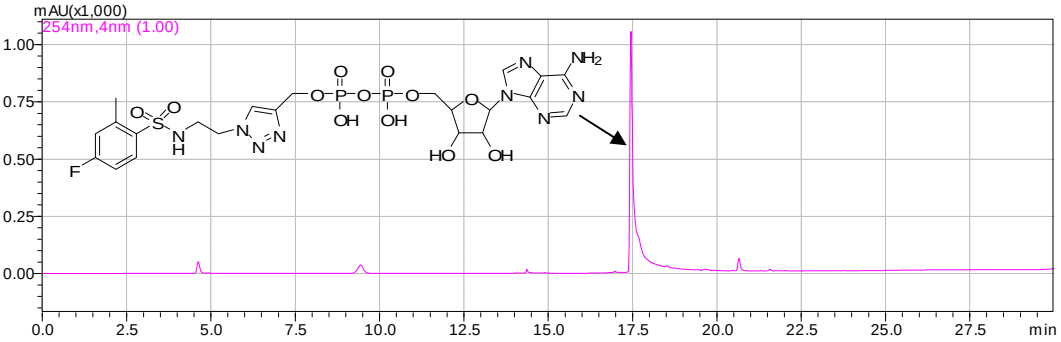

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
734.1067
367.5527
m/z

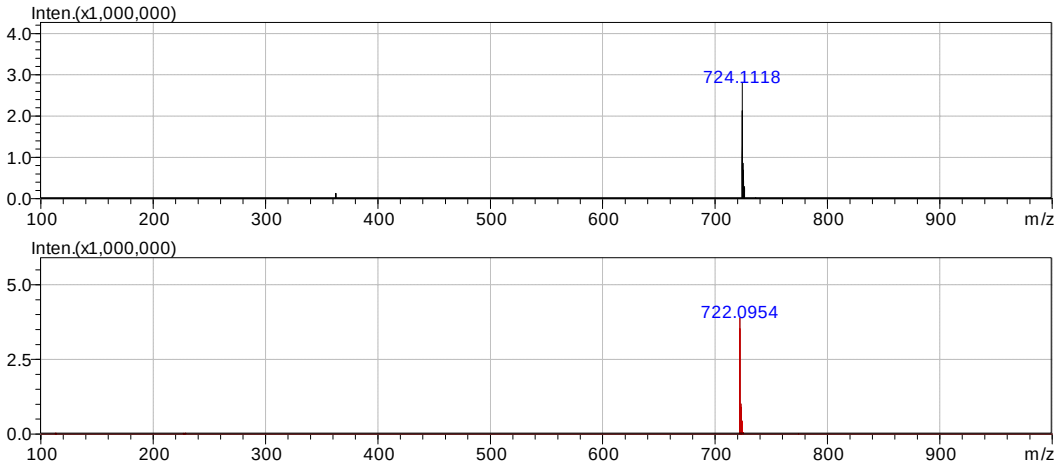


SA-A1-5C

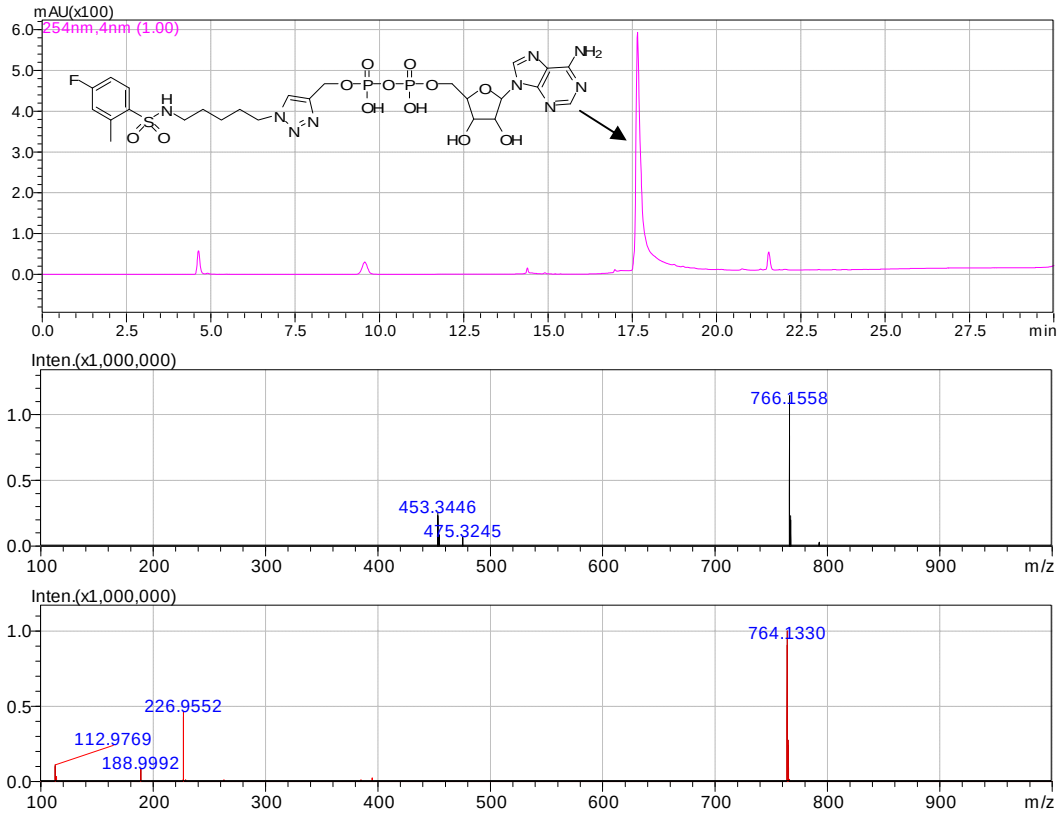


SA-B1-2C

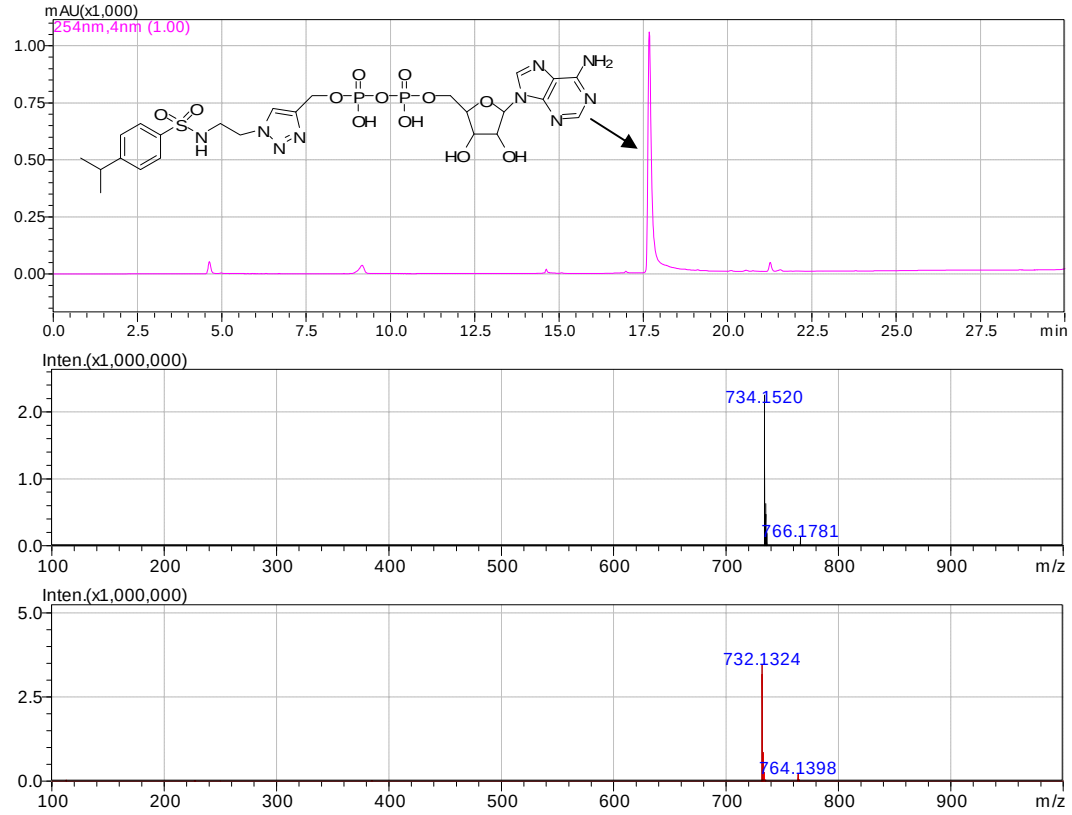



Inten.(x1,000,000)
724.1118
m/z
Inten.(x1,000,000)
722.0954
m/z

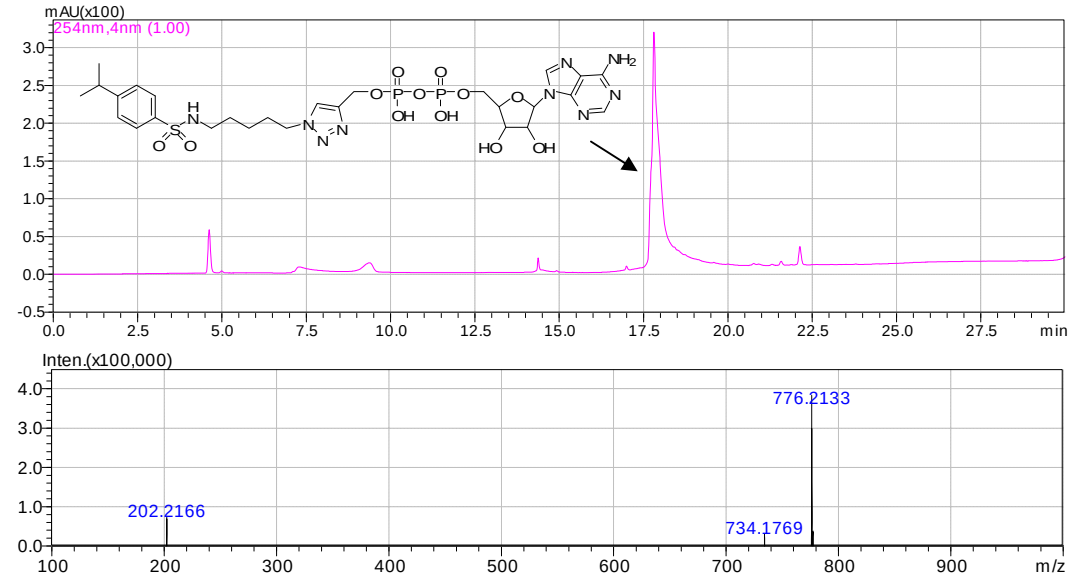
SA-B1-5C

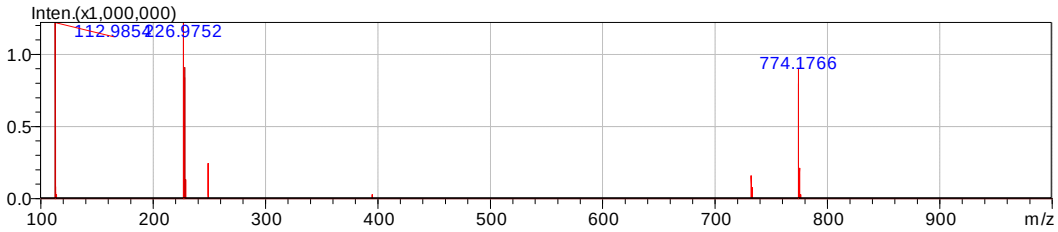

mAU(x100)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
766.1558
453.3446
475.3245
m/z
Inten.(x1,000,000)
764.1330
226.9552
112.9769
188.9992
m/z

SA-B2-2C

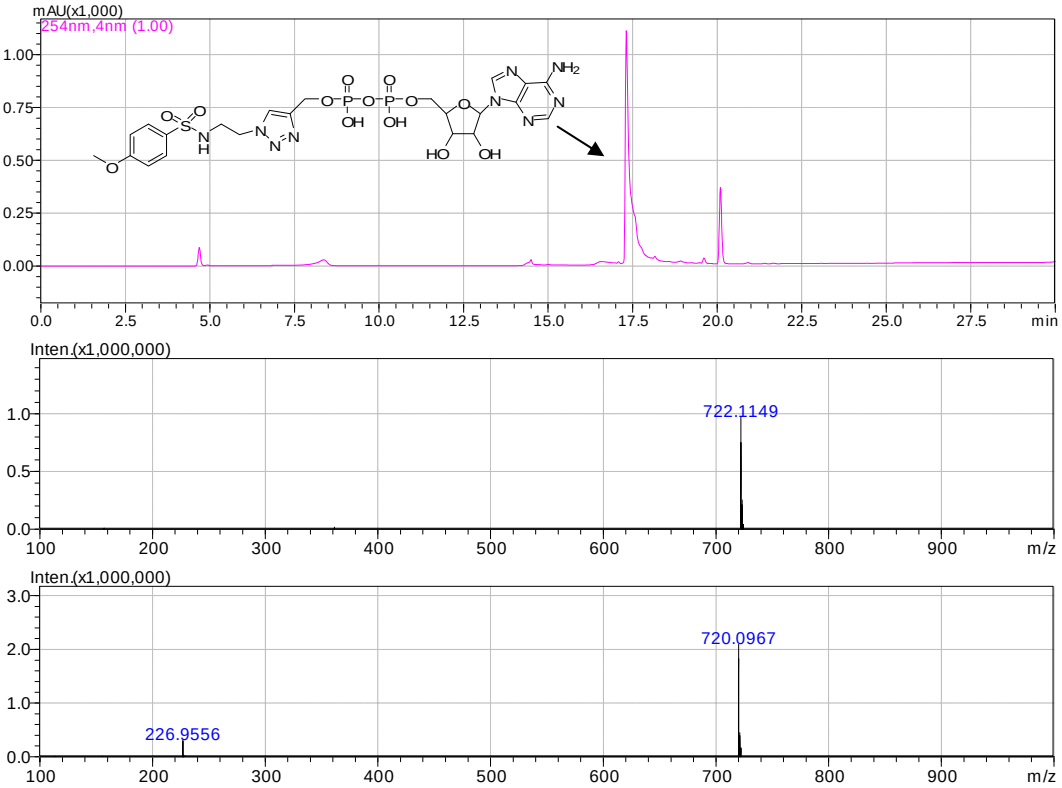


SA-B2-5C

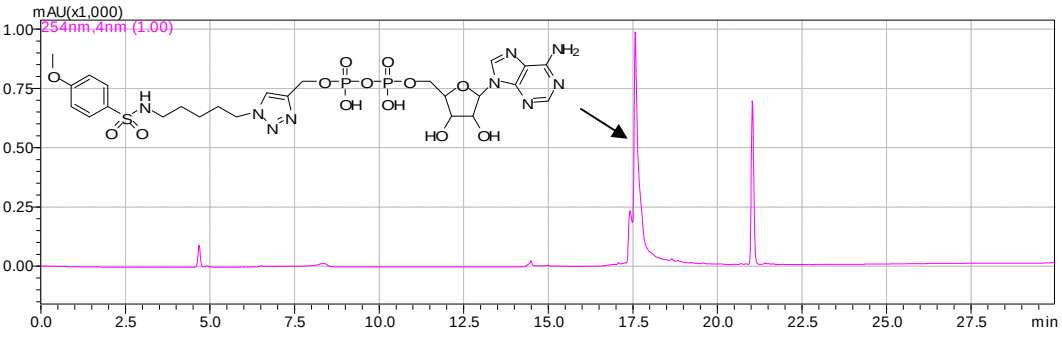


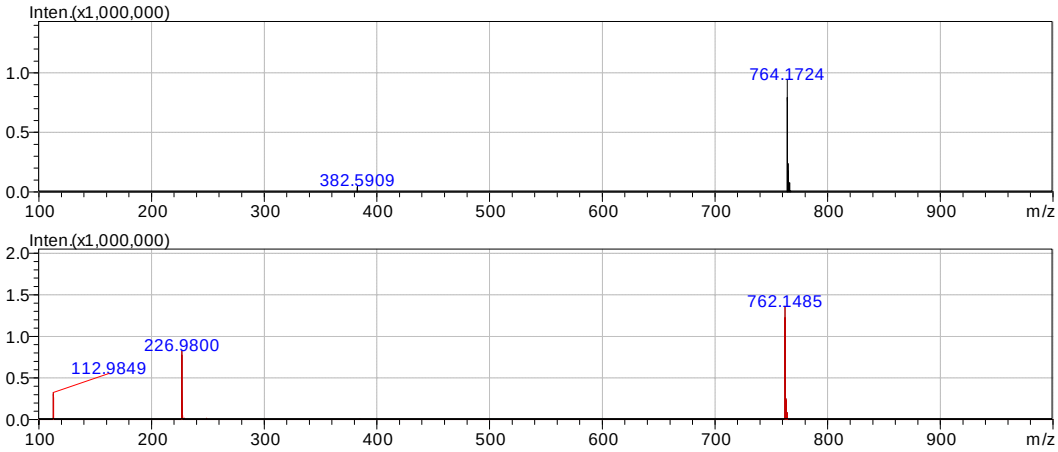


SA-B3-2C

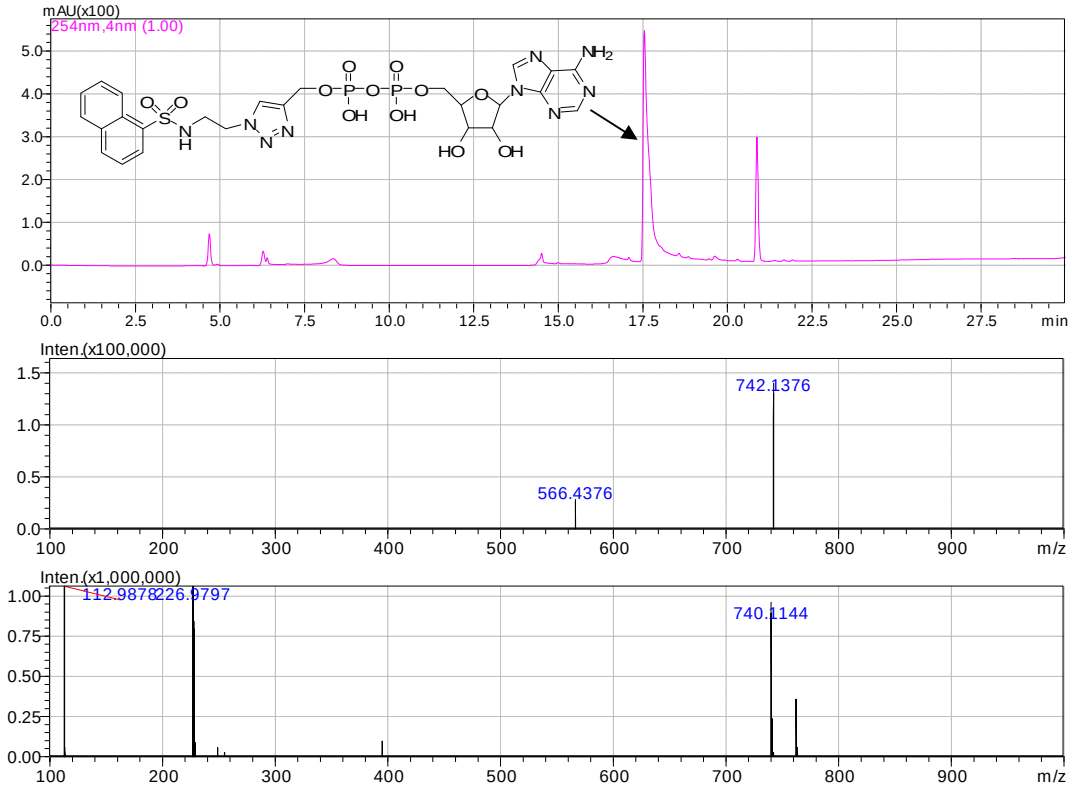


SA-B3-5C

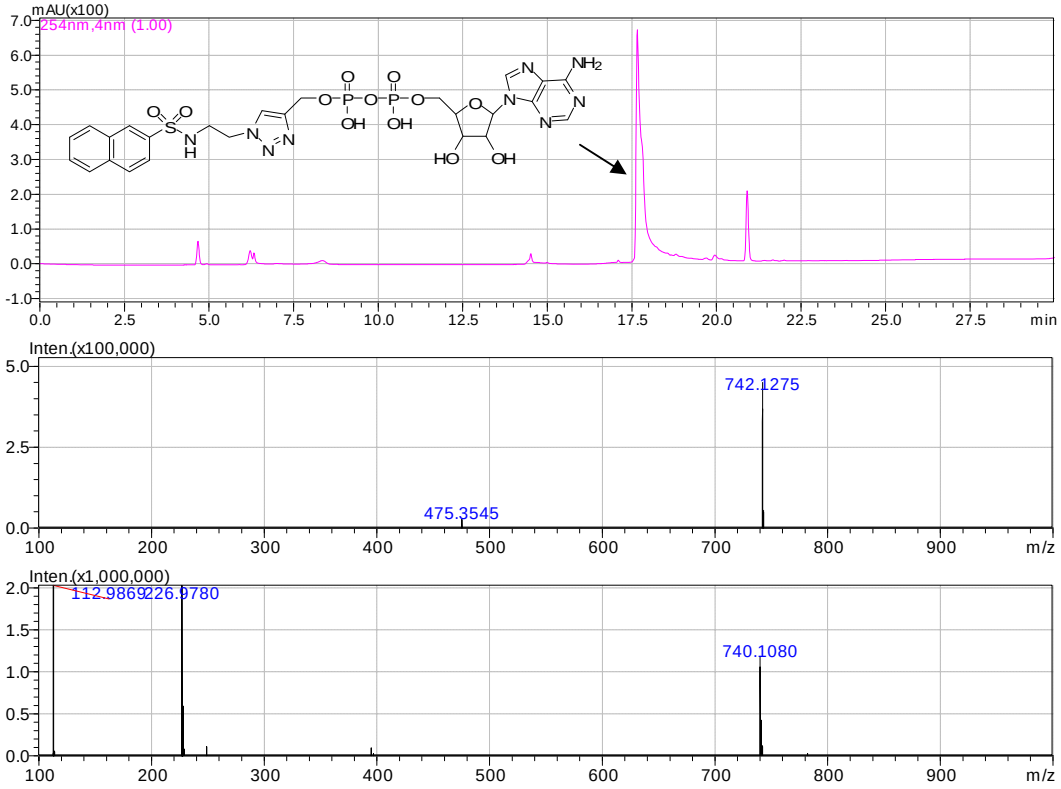



Inten.(x1,000,000)
764.1724
382.5909
m/z
Inten.(x1,000,000)
762.1485
226.9800
112.9849
m/z

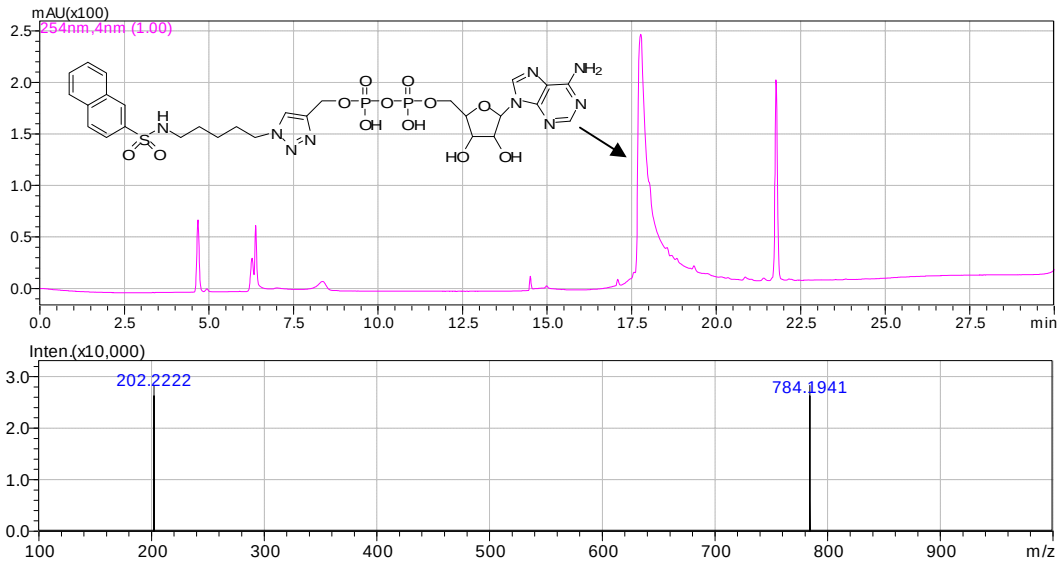
SA-B5-2C


mAU(x100)
254nm,4nm (1.00)
min
Inten.(x100,000)
742.1376
566.4376
m/z
Inten.(x1,000,000)
112.9878
226.9797
740.1144
m/z

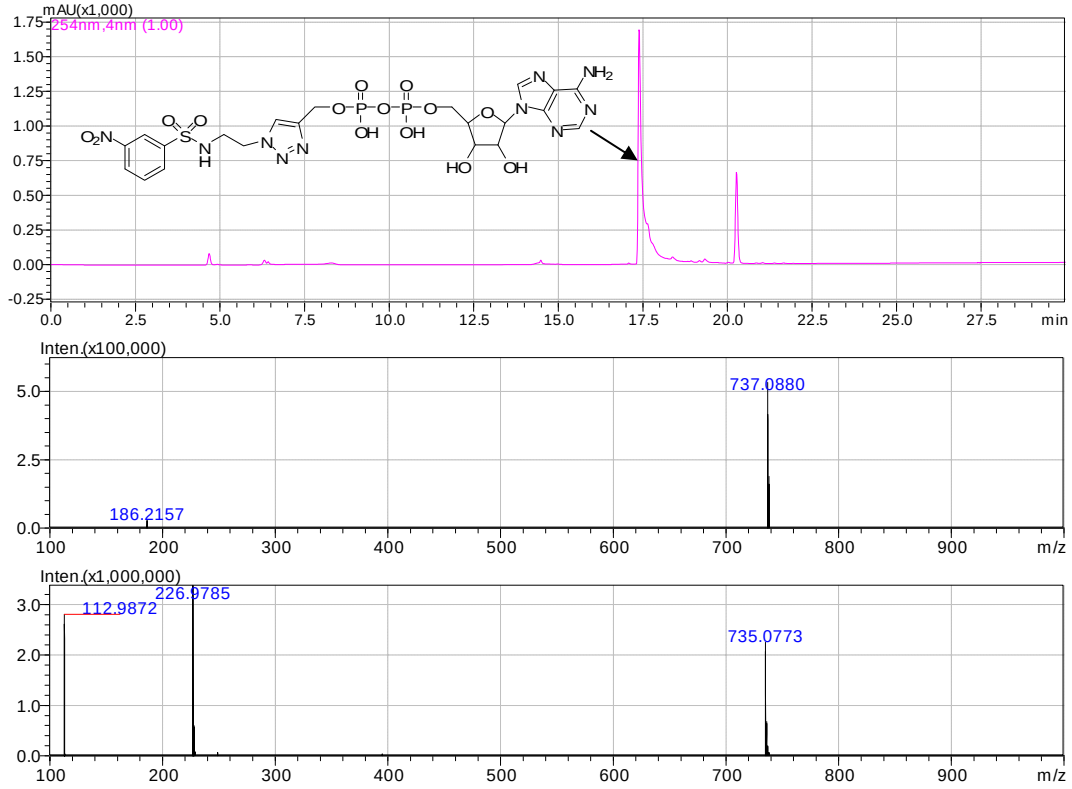
SA-B6-2C



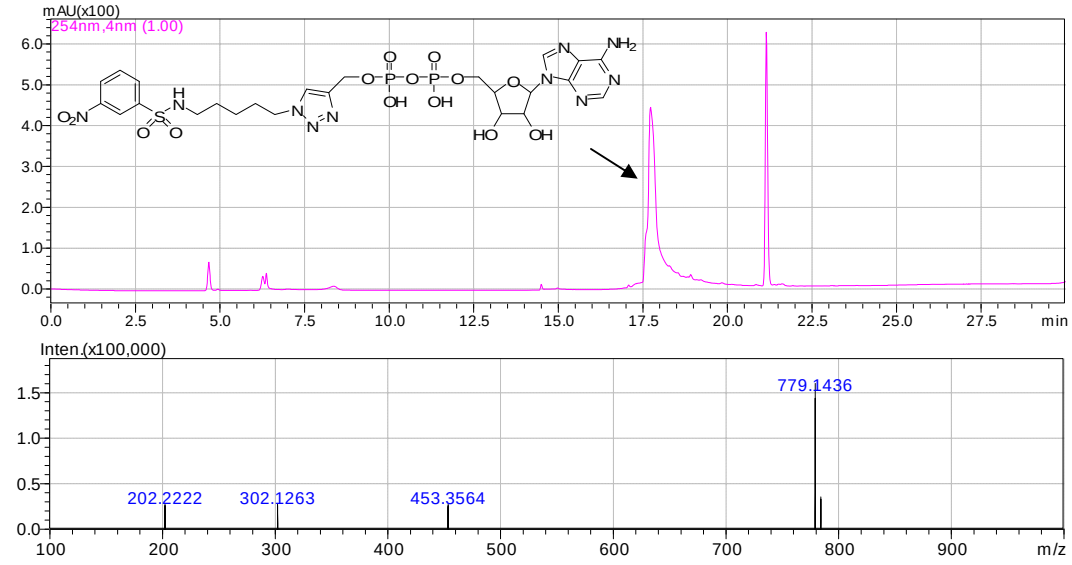
SA-B6-5C

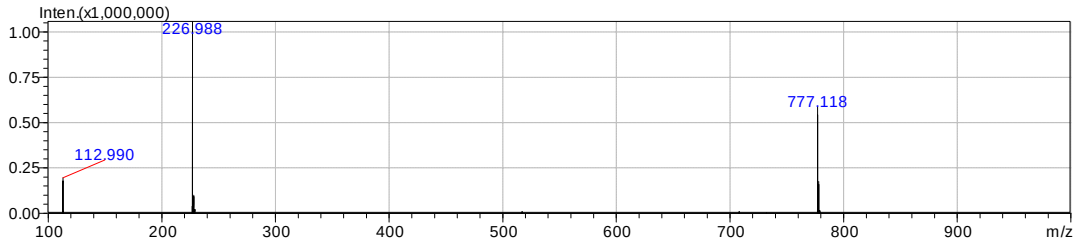


SA-B7-2C

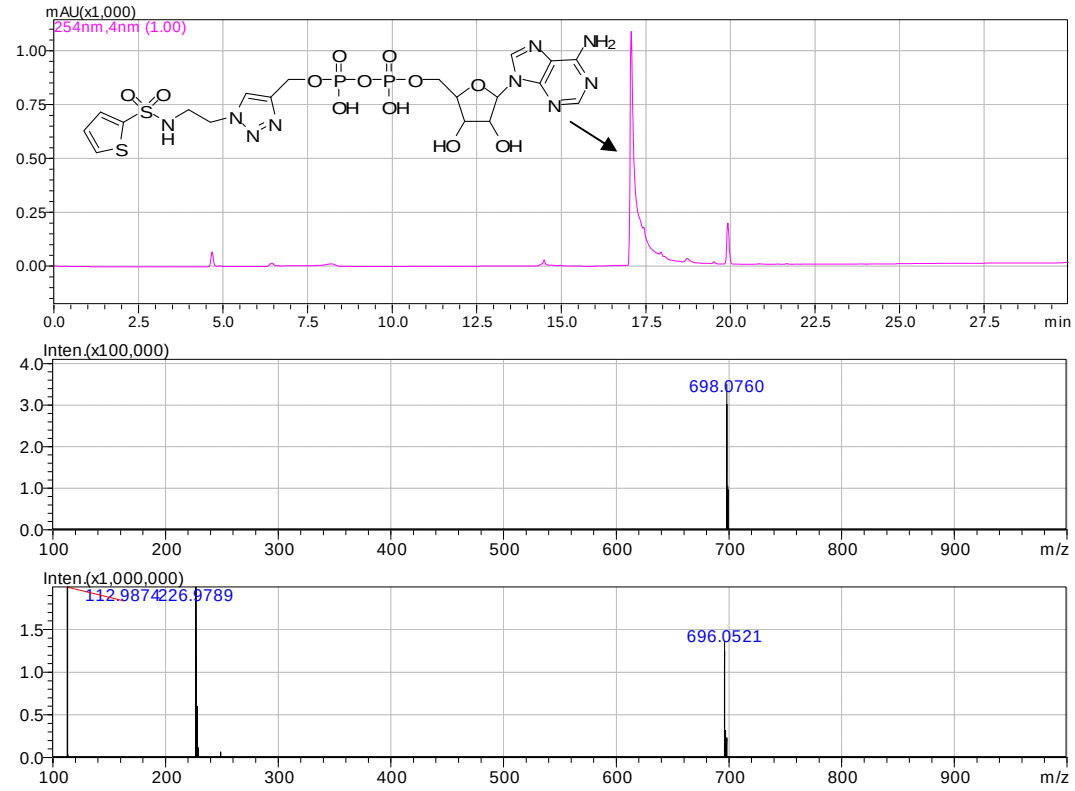


SA-B7-5C

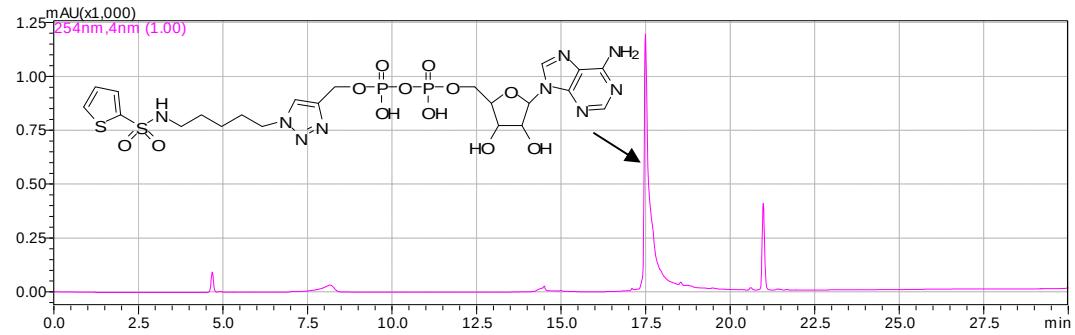


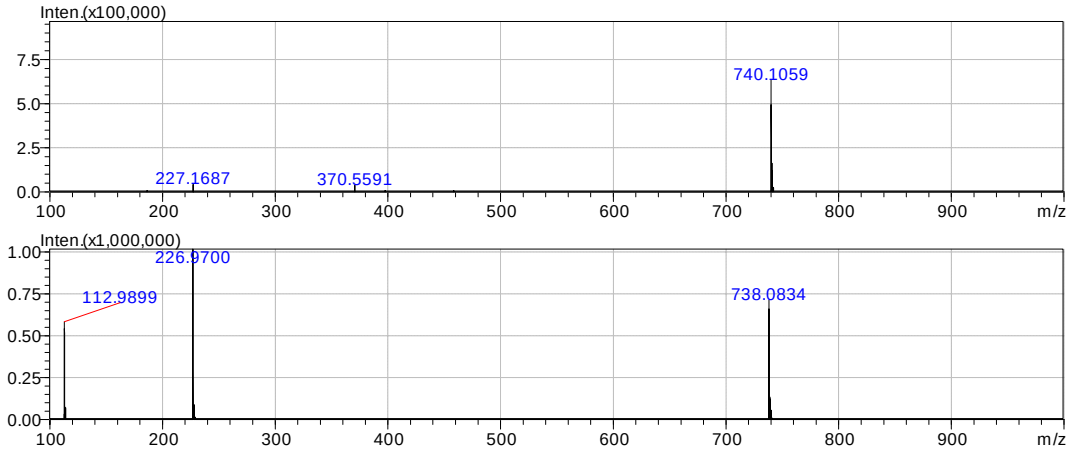


SA-B10-2C

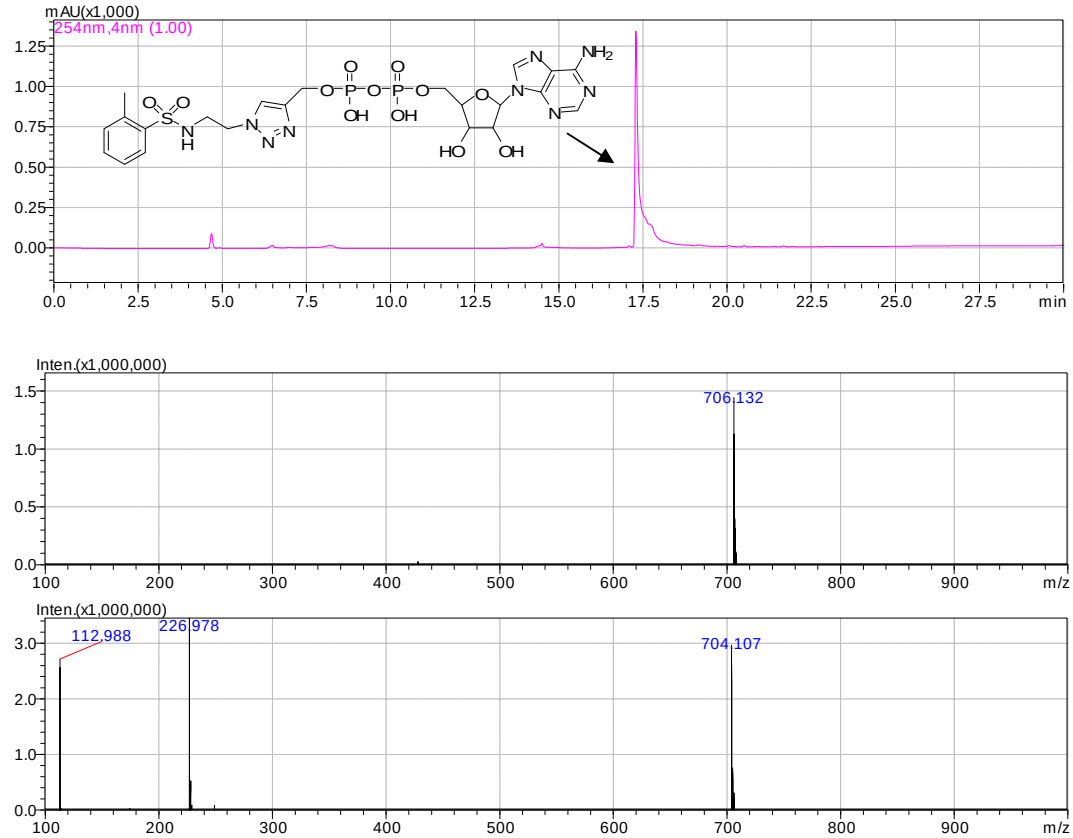


SA-B10-5C

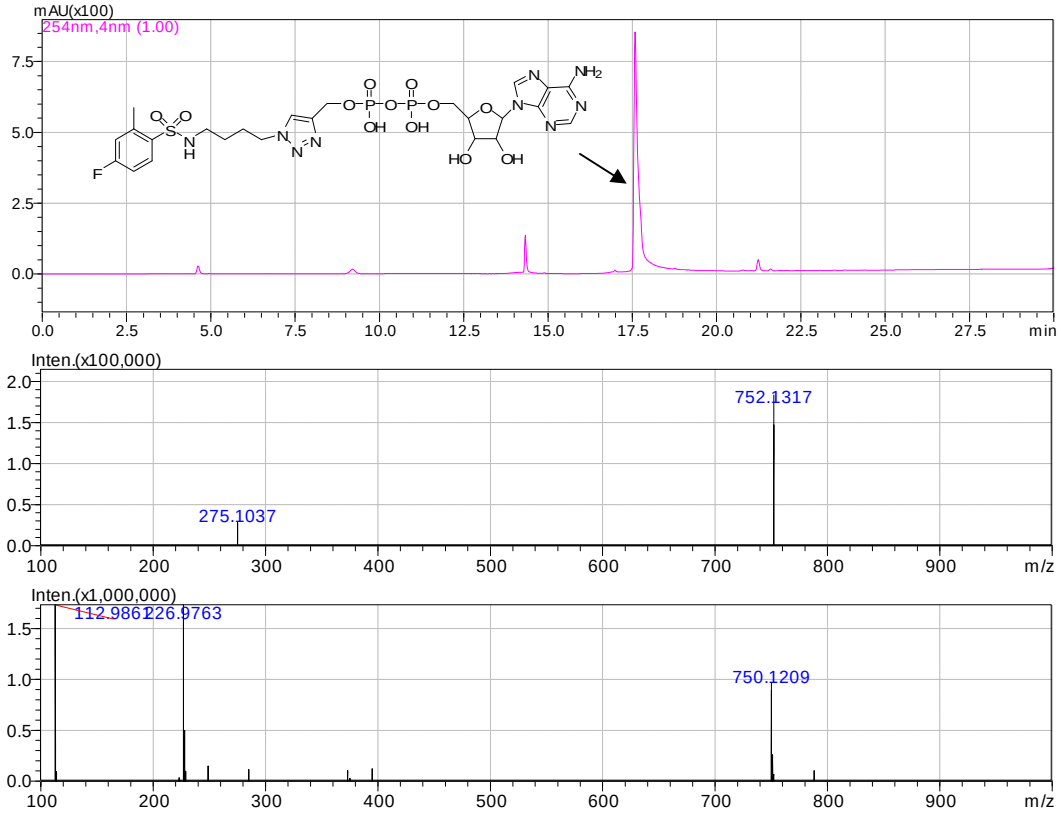



Inten.(x100,000)
740.1059
227.1687
370.5591
m/z
Inten.(x1,000,000)
226.9700
112.9899
738.0834
m/z

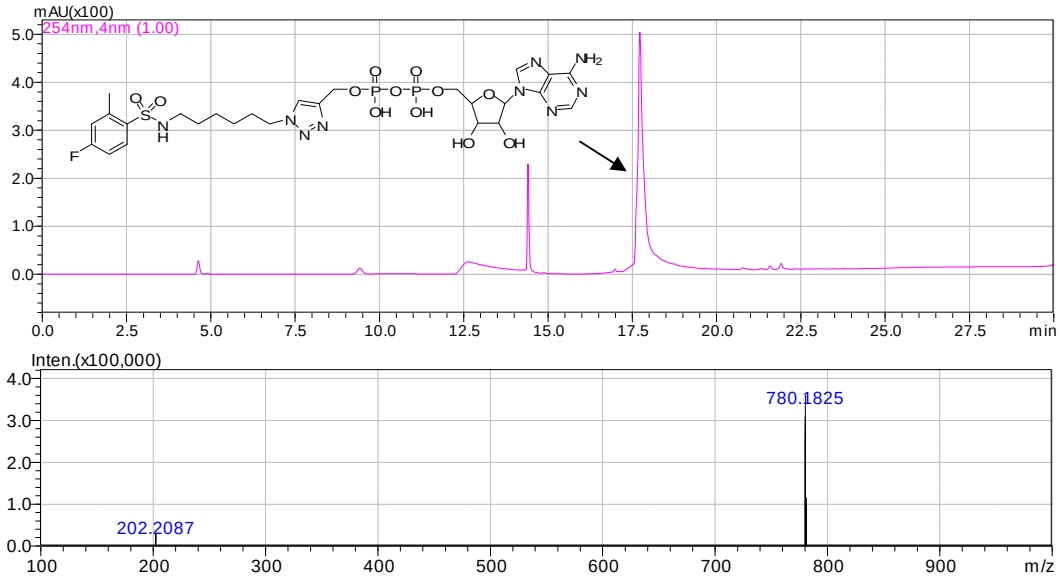
SA-B11-2C

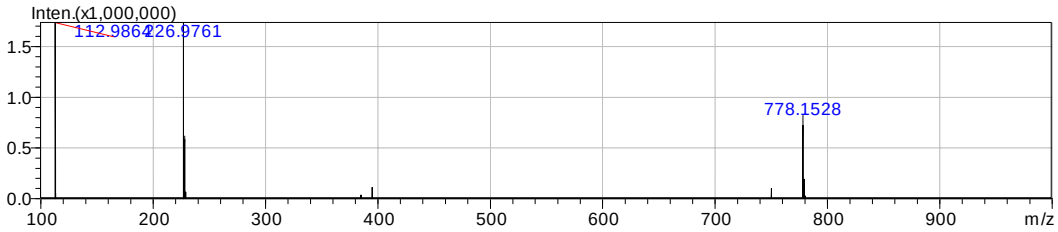

mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
706.132
m/z
Inten.(x1,000,000)
112.988
226.978
704.107
m/z

SA-B1-4C

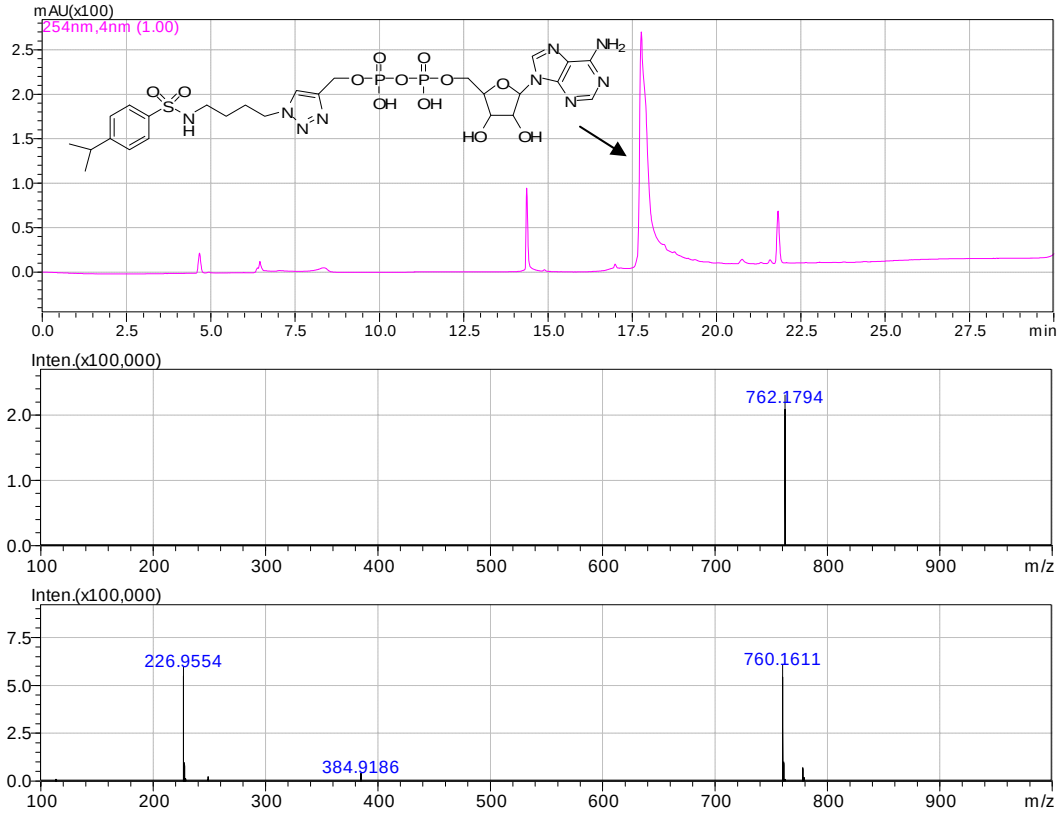


SA-B1-6C

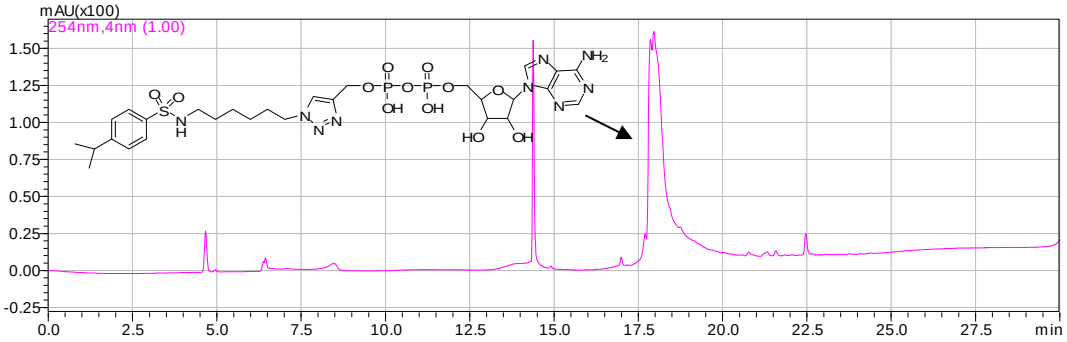


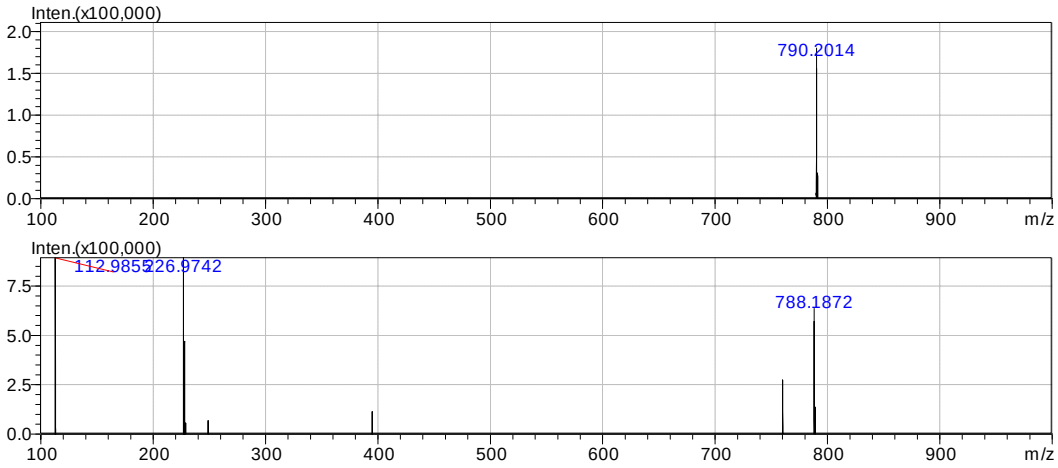


SA-B2-4C



SA-B2-6C




Inten.(x100,000)
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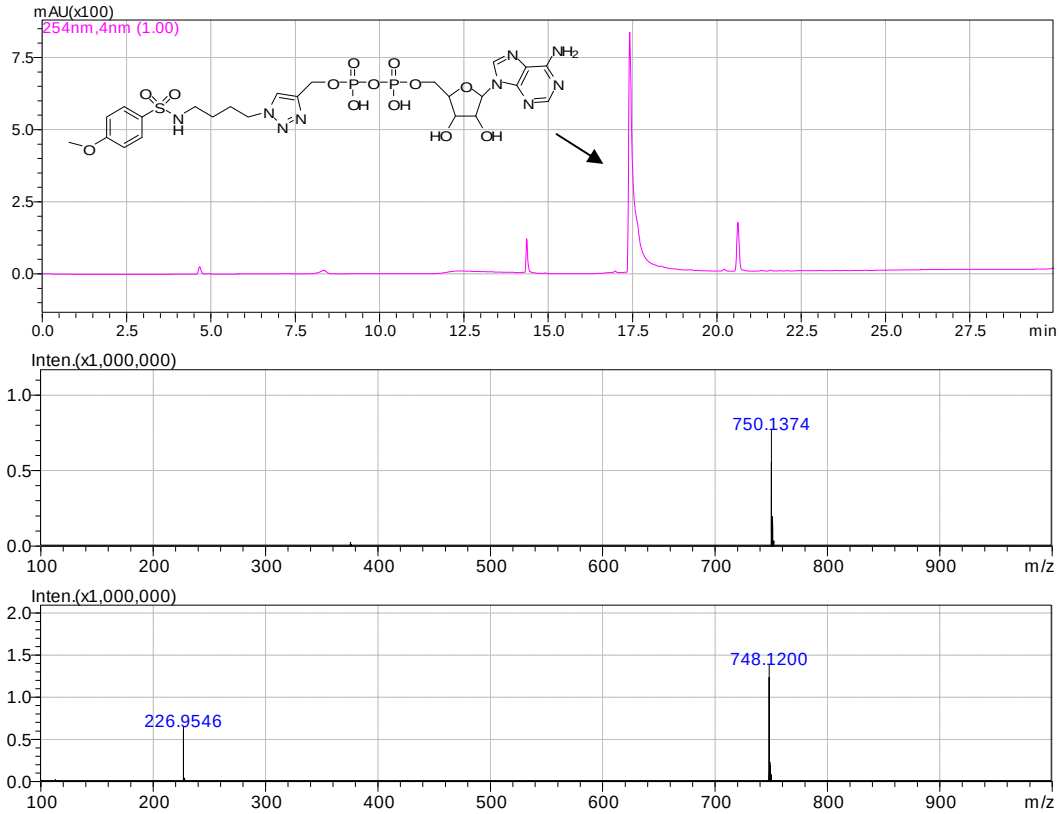
m/z
Inten.(x100,000)
112.9855
226.9742
788.1872
m/z

SA-B3-4C


mAU(x100)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
750.1374
m/z
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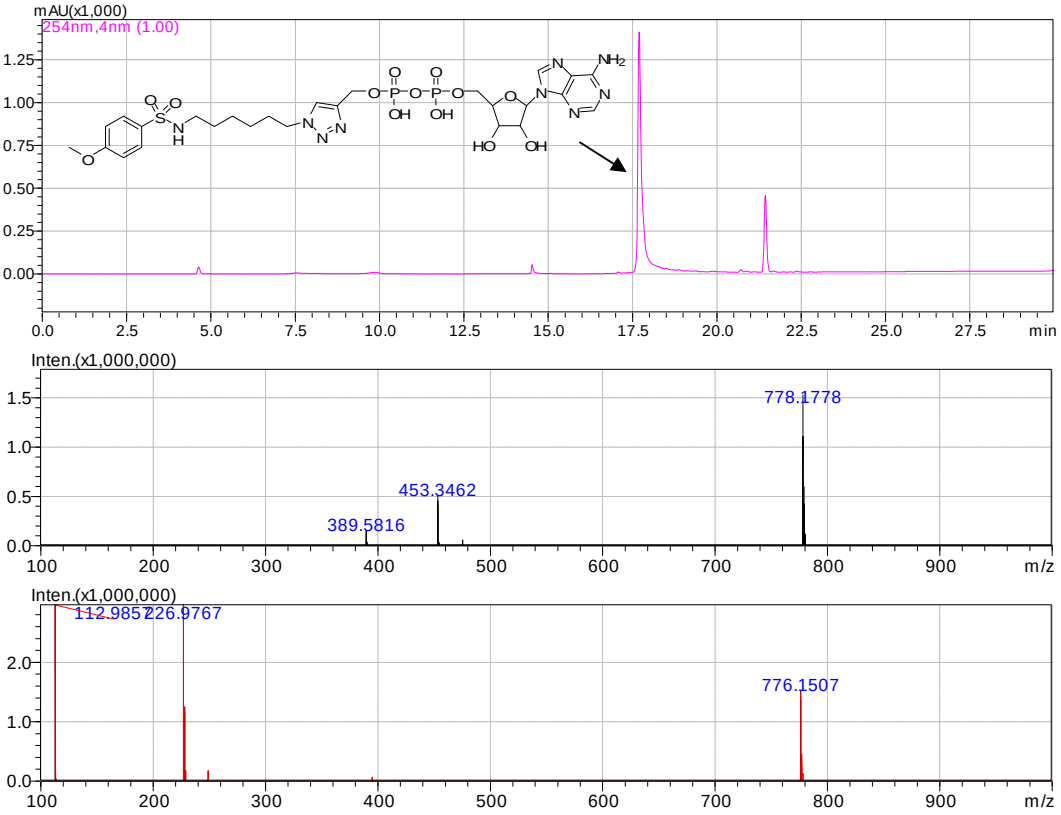
748.1200
226.9546
m/z

SA-B3-6C



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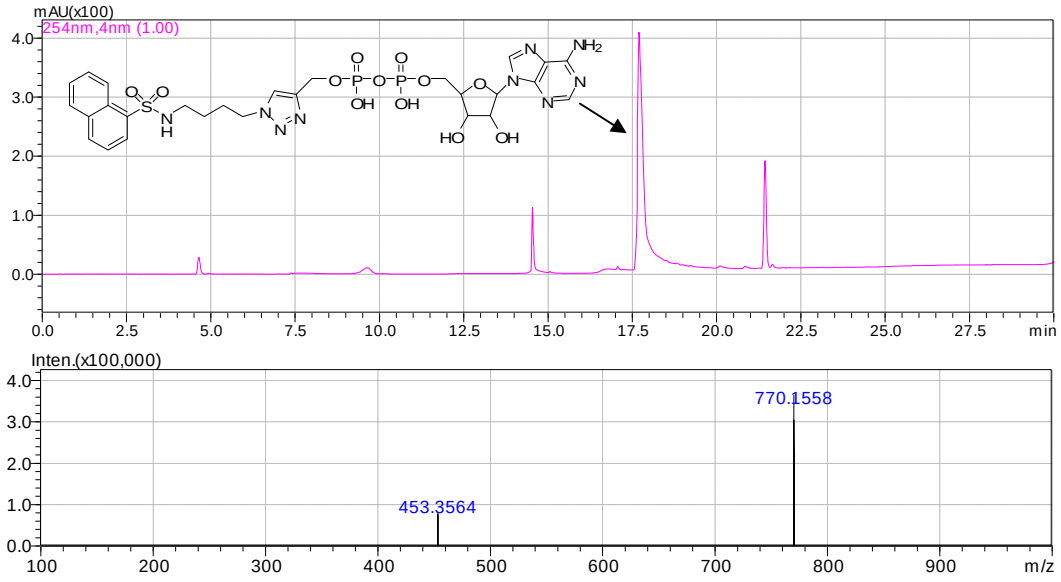

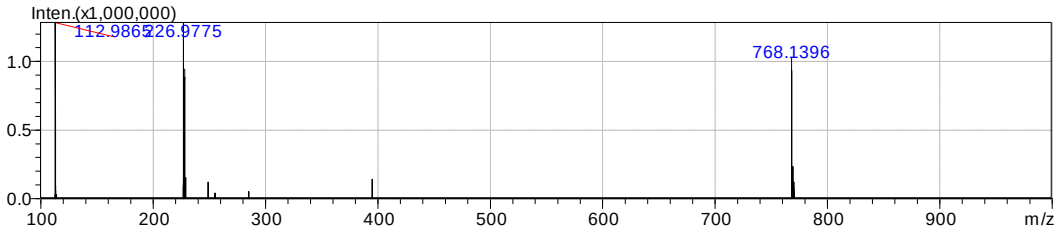

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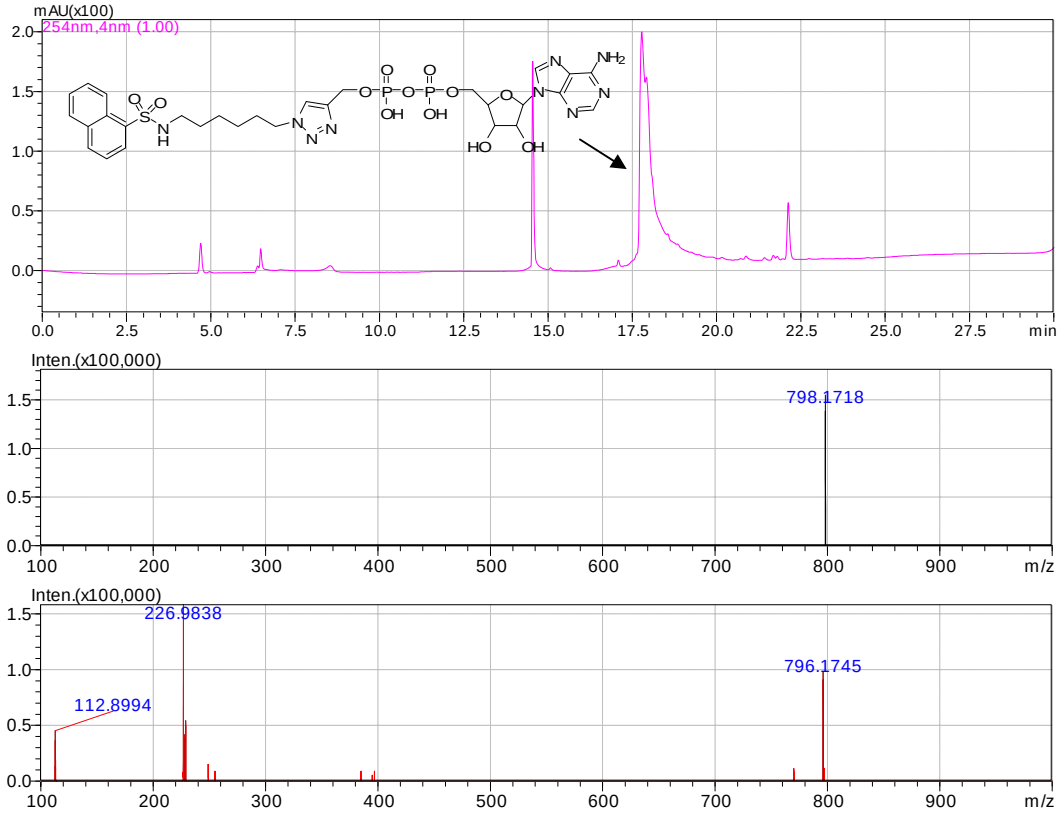

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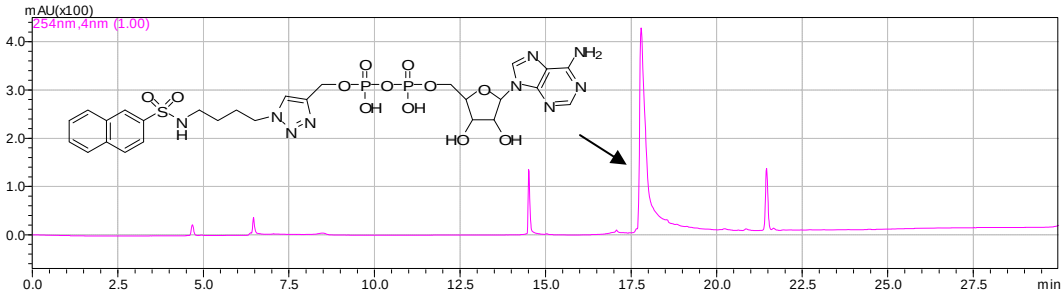

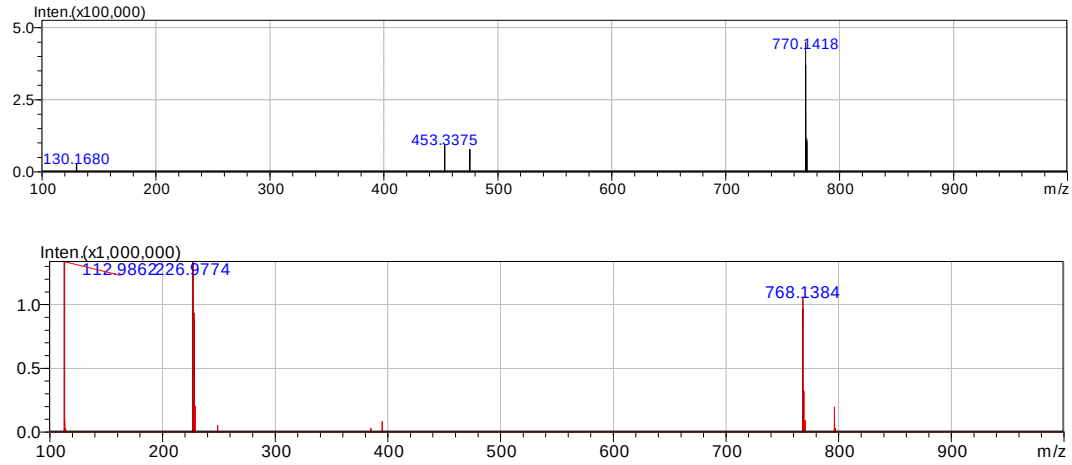
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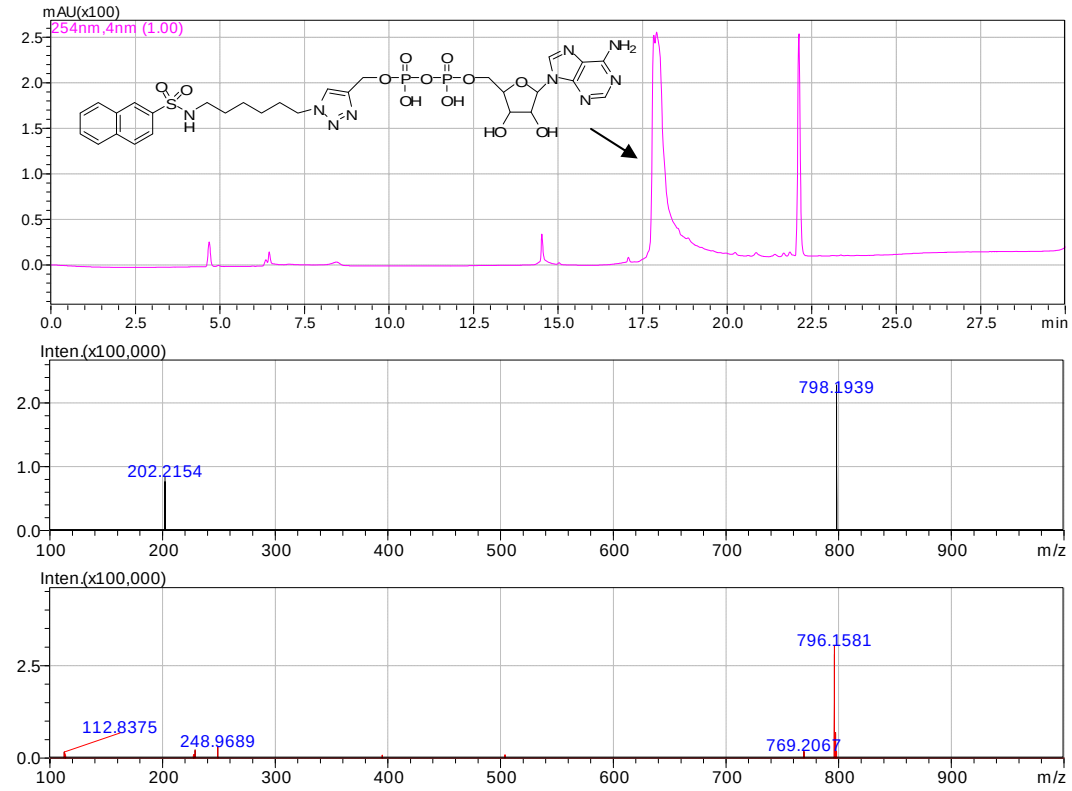
770.1418
453.3375
130.1680
m/z
Inten.(x1,000,000)
112.9862
226.9774
768.1384
m/z

SA-B6-6C


mAU(x100)
254nm,4nm (1.00)
min
Inten.(x100,000)
798.1939
202.2154
m/z
Inten.(x100,000)
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112.8375
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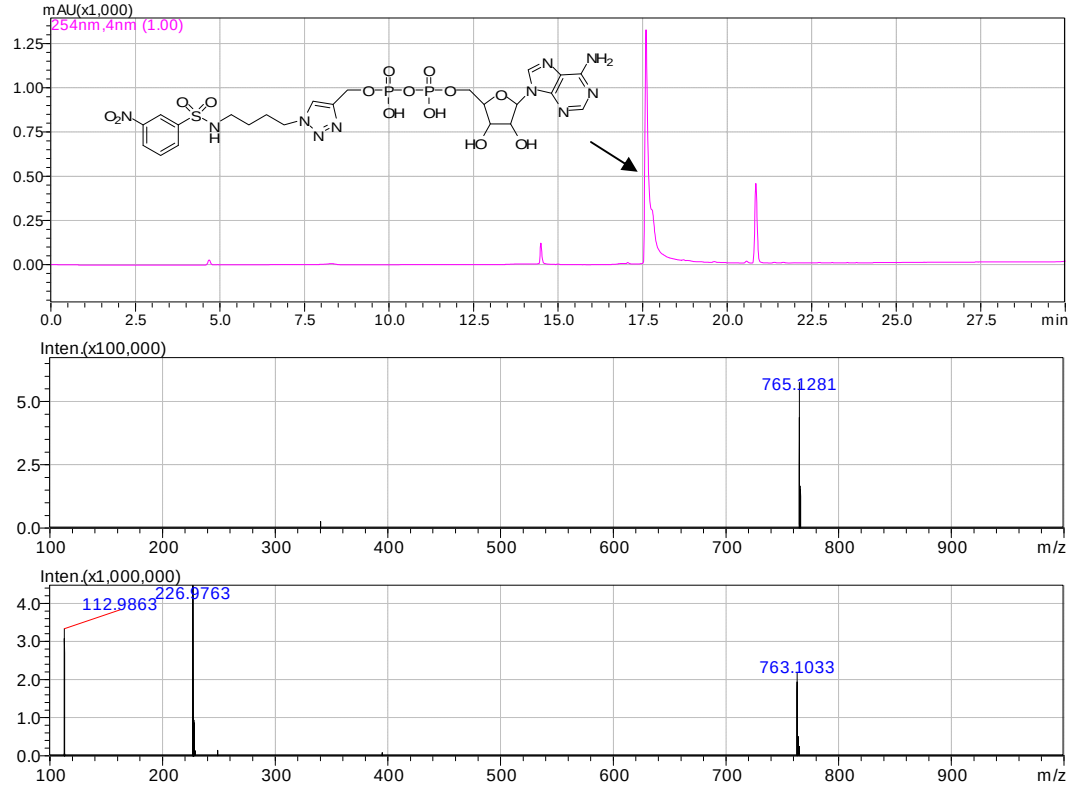
769.2067
m/z

SA-B7-4C



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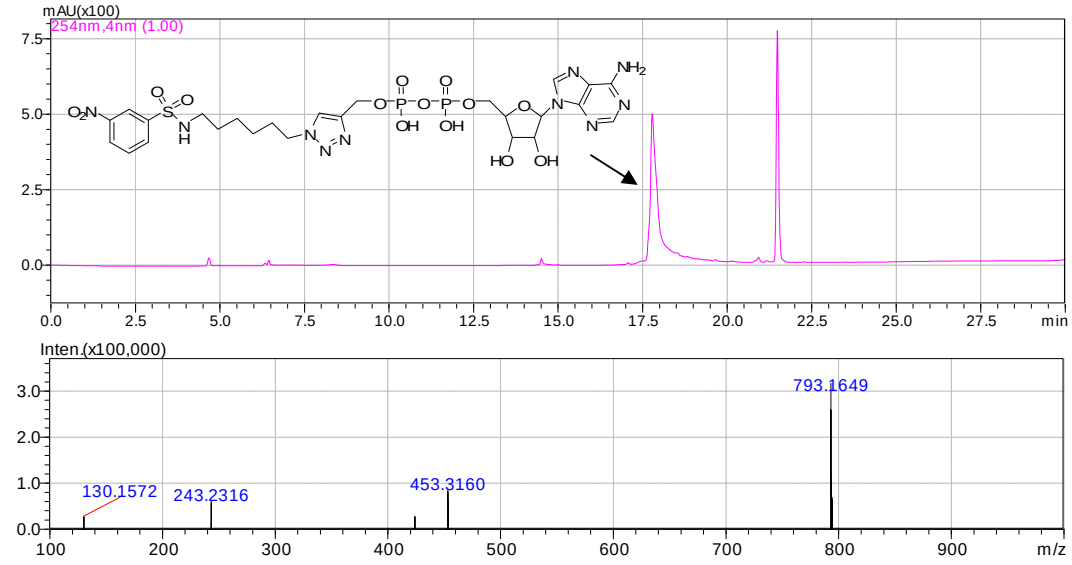

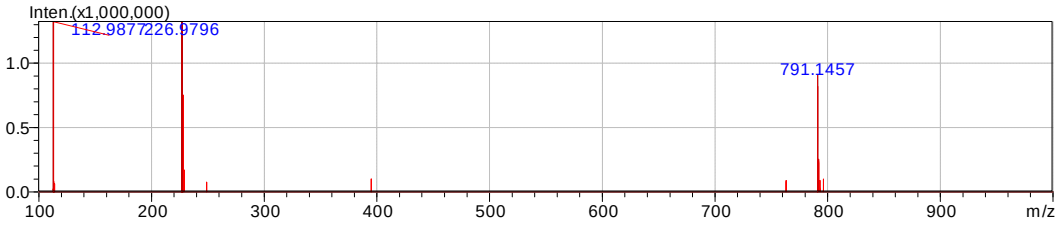

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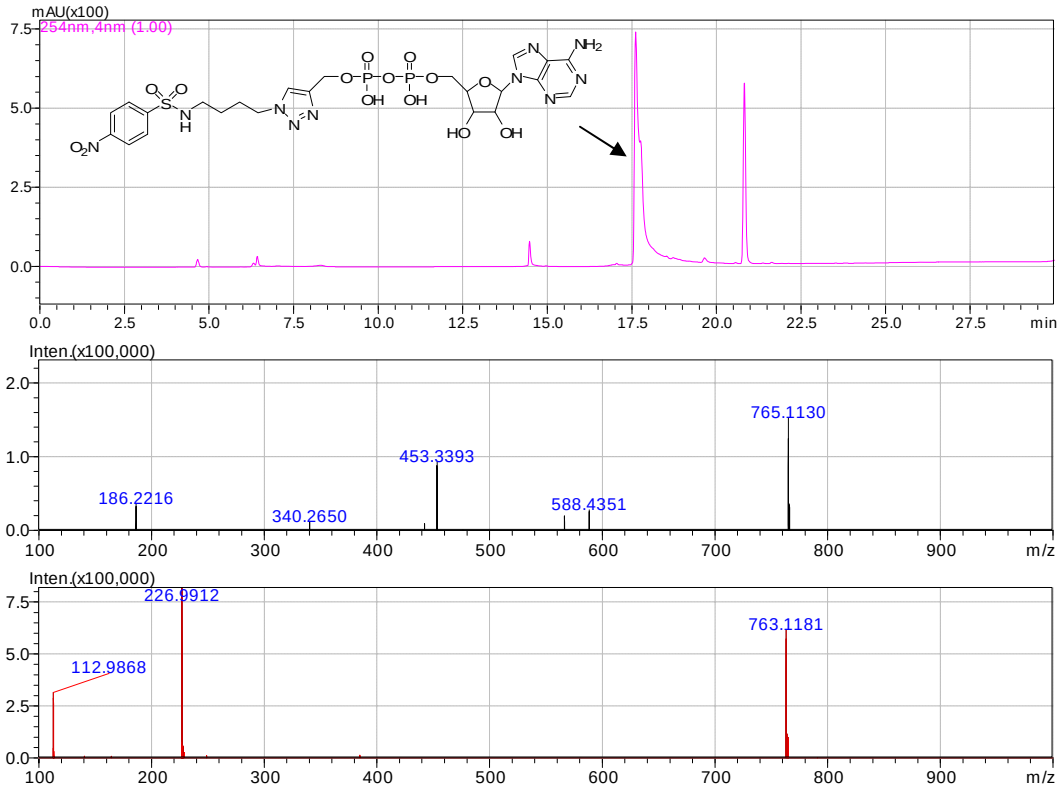

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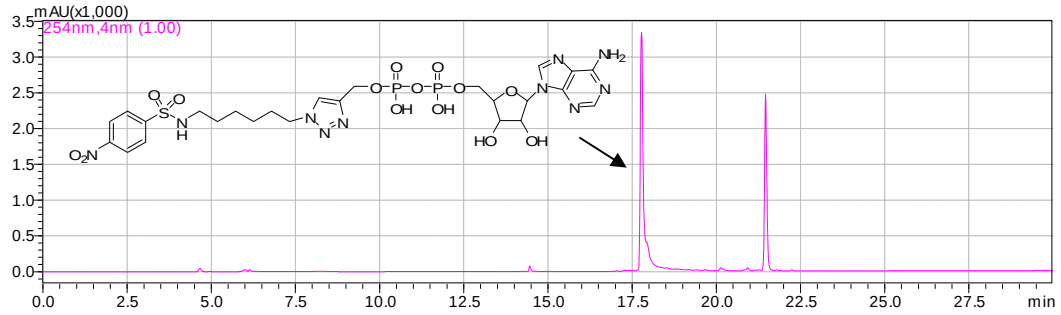

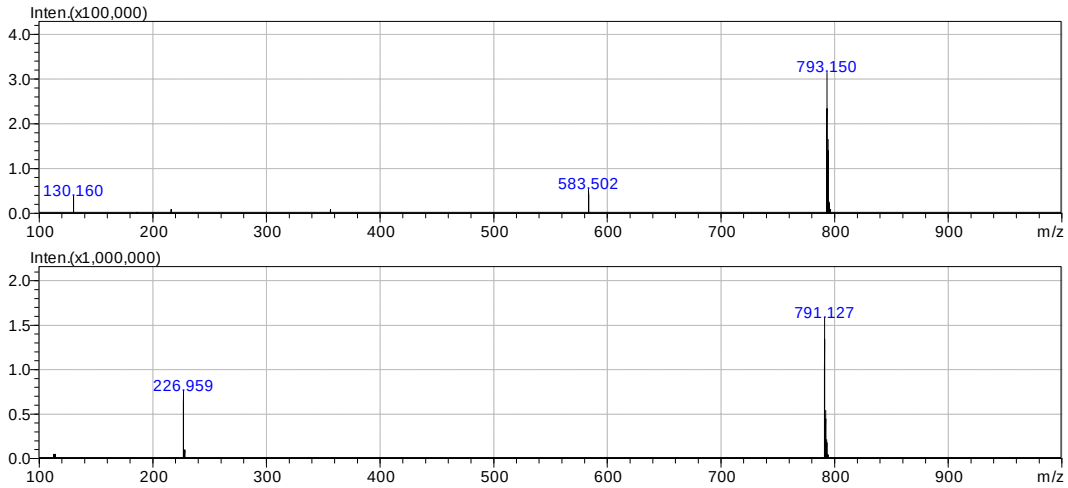
Inten.(x100,000)
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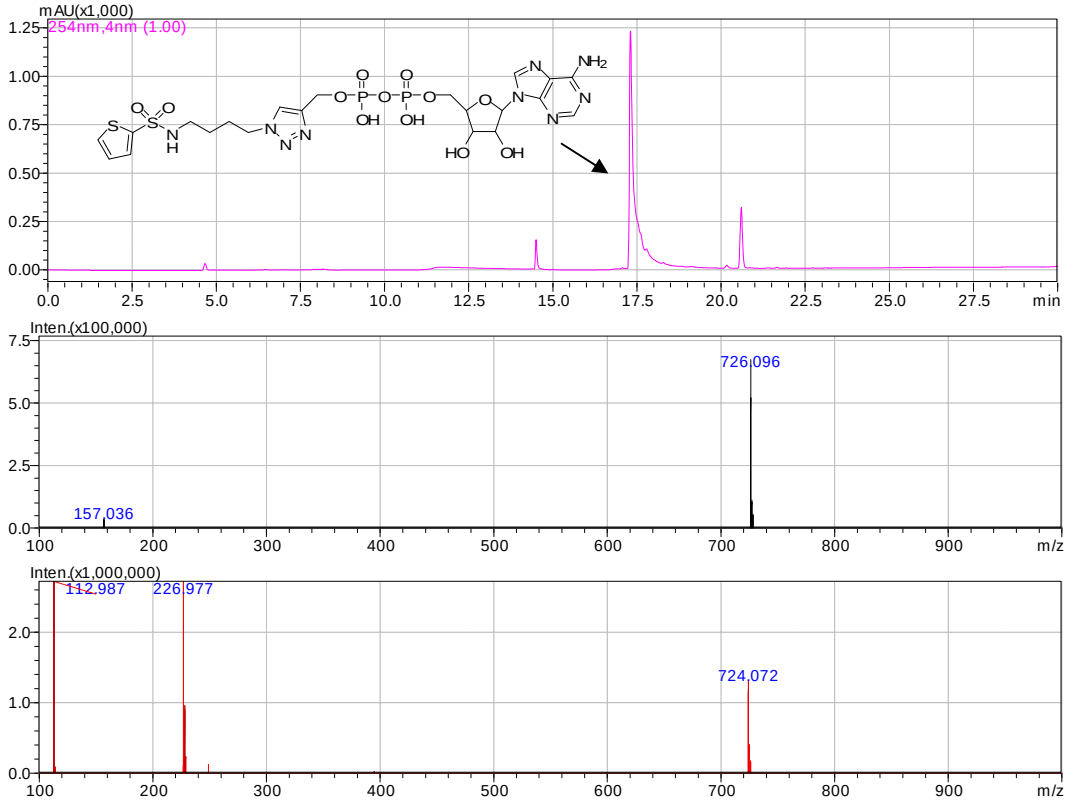
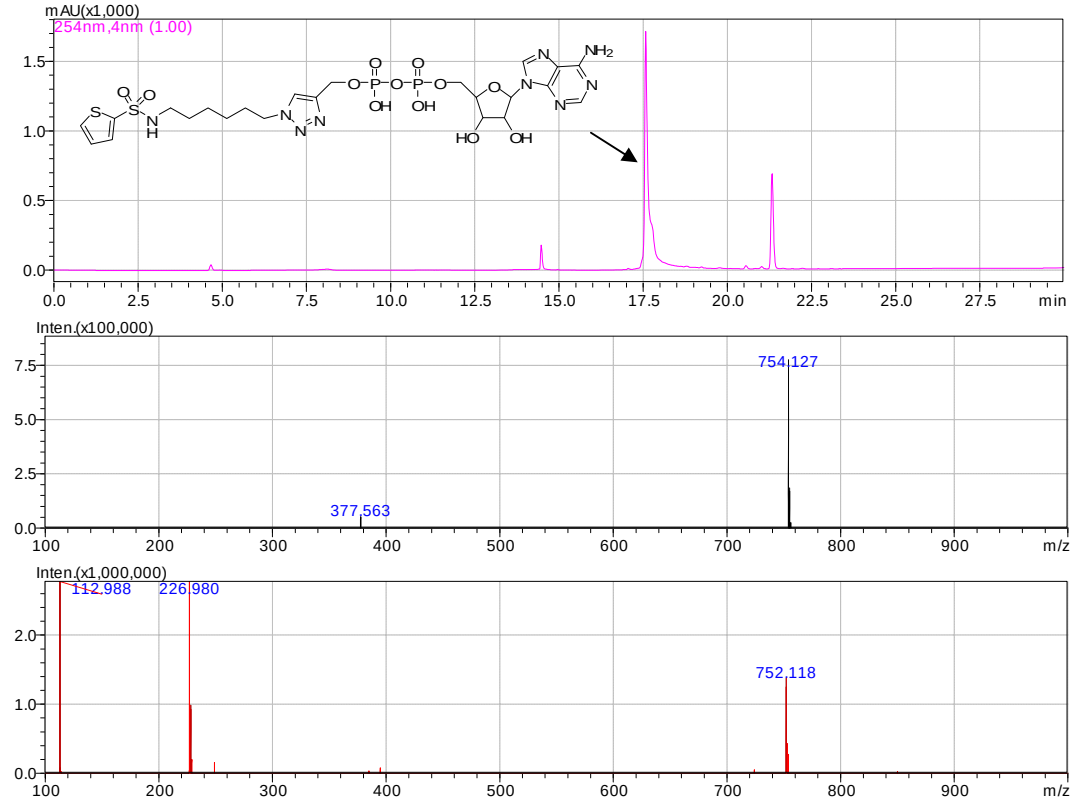
583,502
130,160
m/z
Inten.(x1,000,000)
791,127
226,959
m/z

SA-B10-4C


mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x100,000)
726,096
157,036
m/z
Inten.(x1,000,000)
112,987
226,977
724,072
m/z

SA-B10-6C



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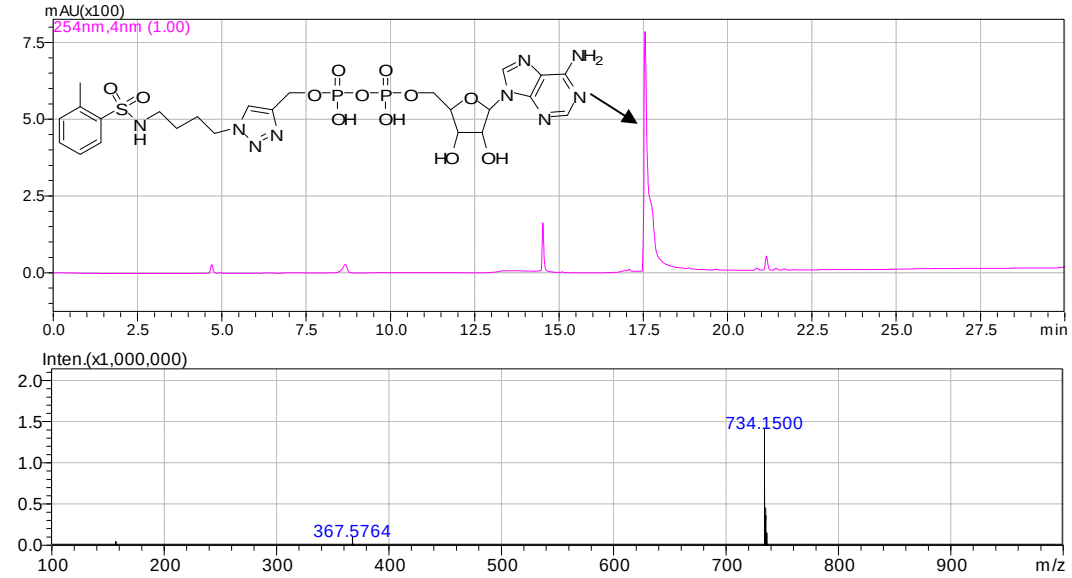
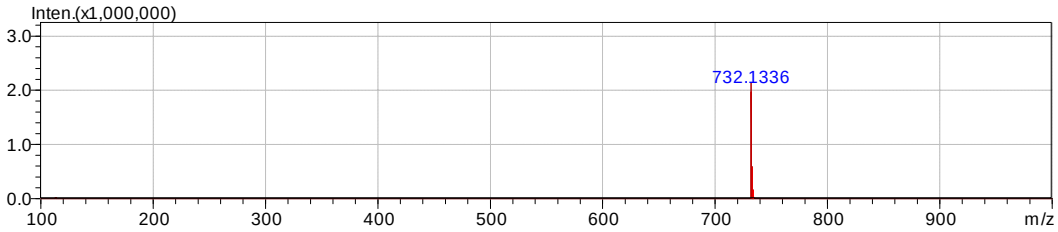
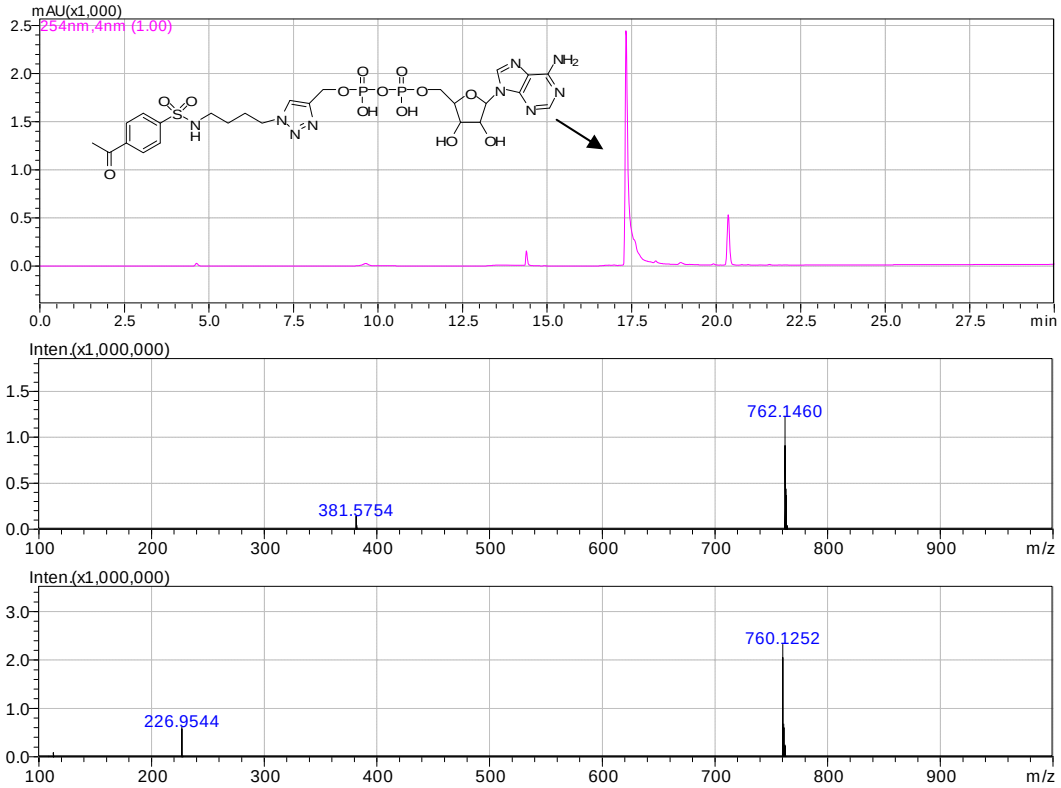
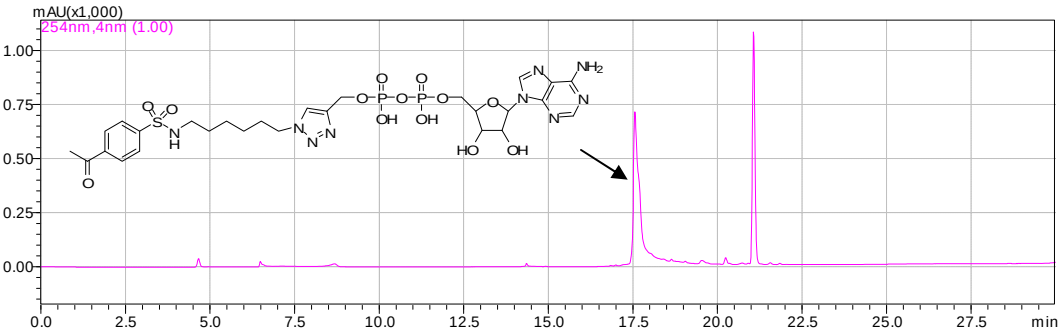


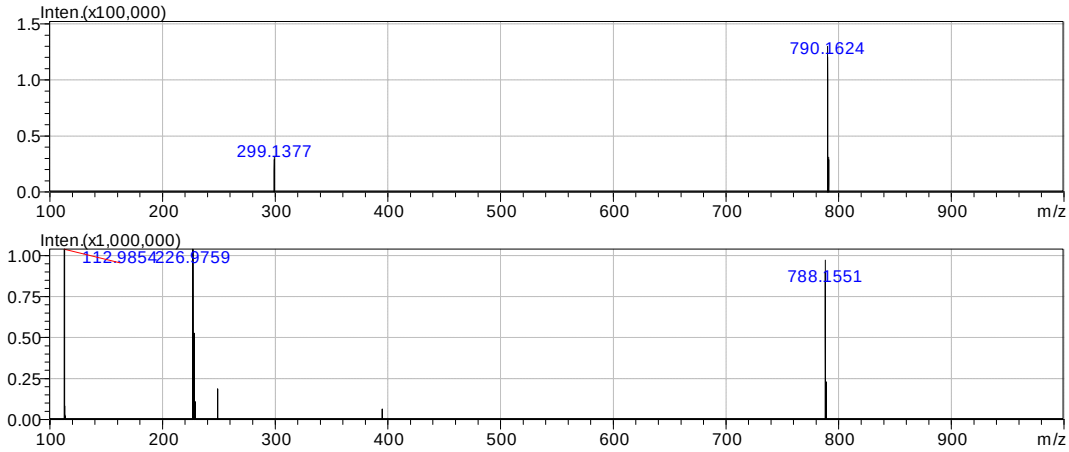


SA-A1-4C

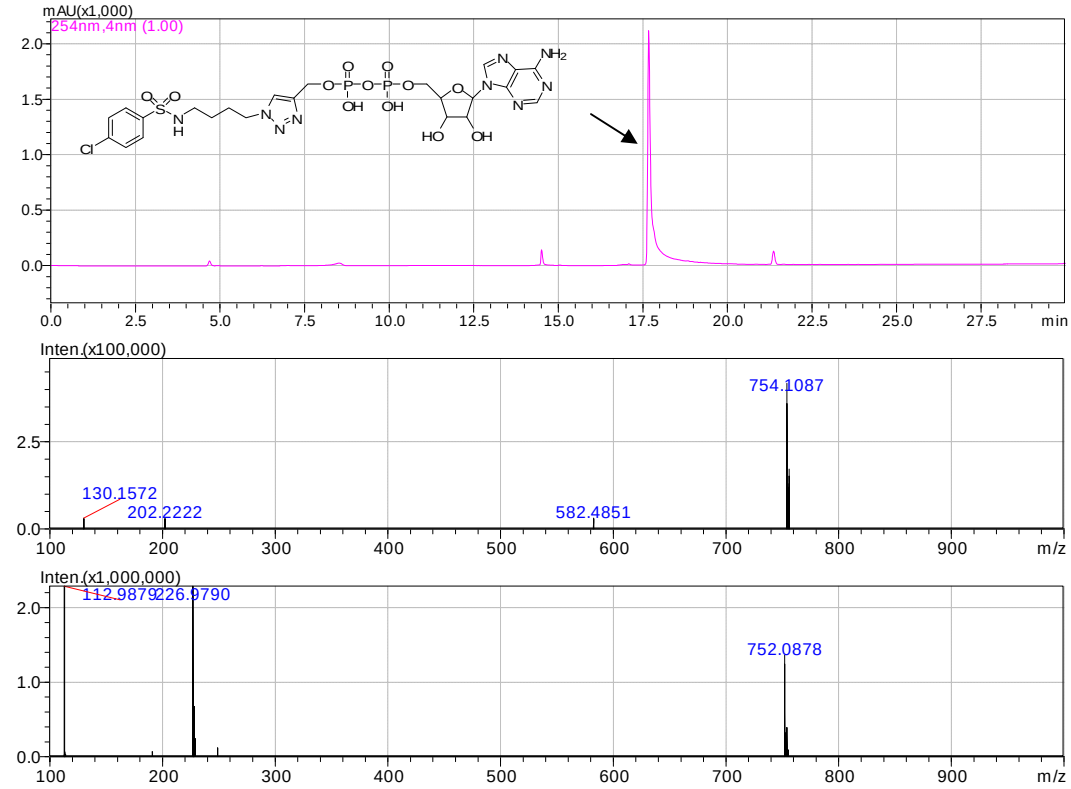


SA-A1-6C




Inten.(x100,000)
790.1624
299.1377
m/z
Inten.(x1,000,000)
112.9854
226.9759
788.1551
m/z

SA-A3-4C


mAU(x1,000)
254nm,4nm (1.00)
min
Inten.(x100,000)
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130.1572
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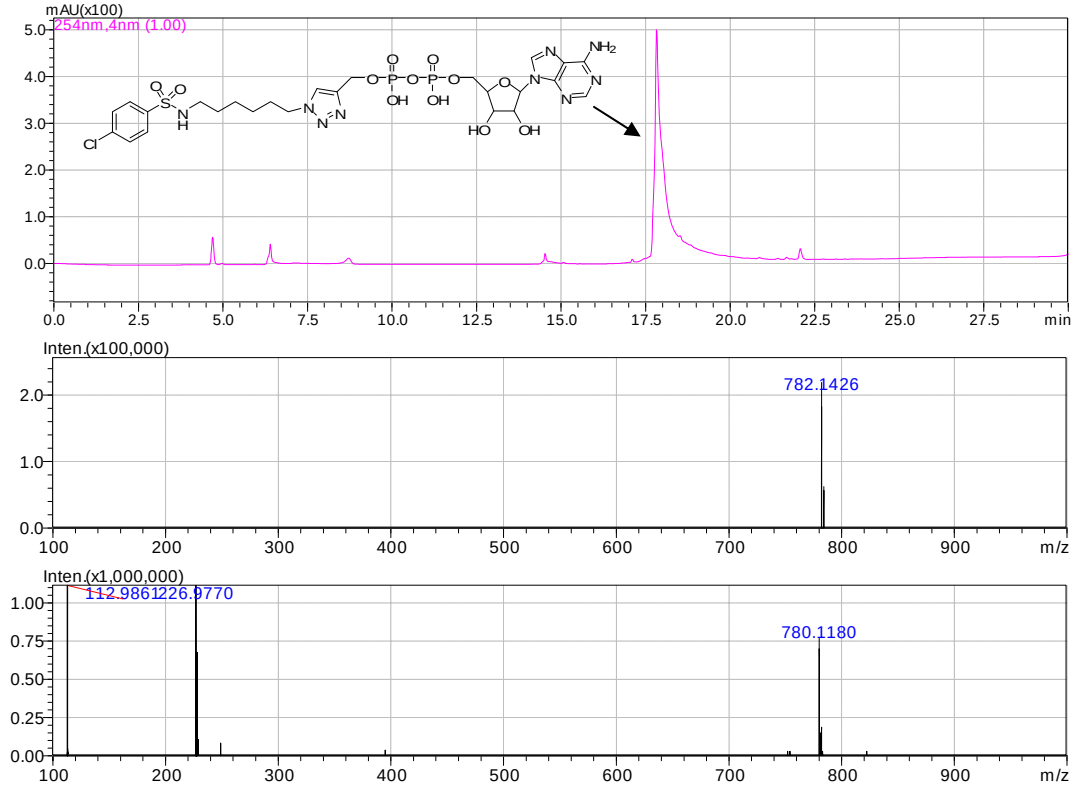
m/z
Inten.(x1,000,000)
112.9879
226.9790
752.0878
m/z

SA-A3-6C



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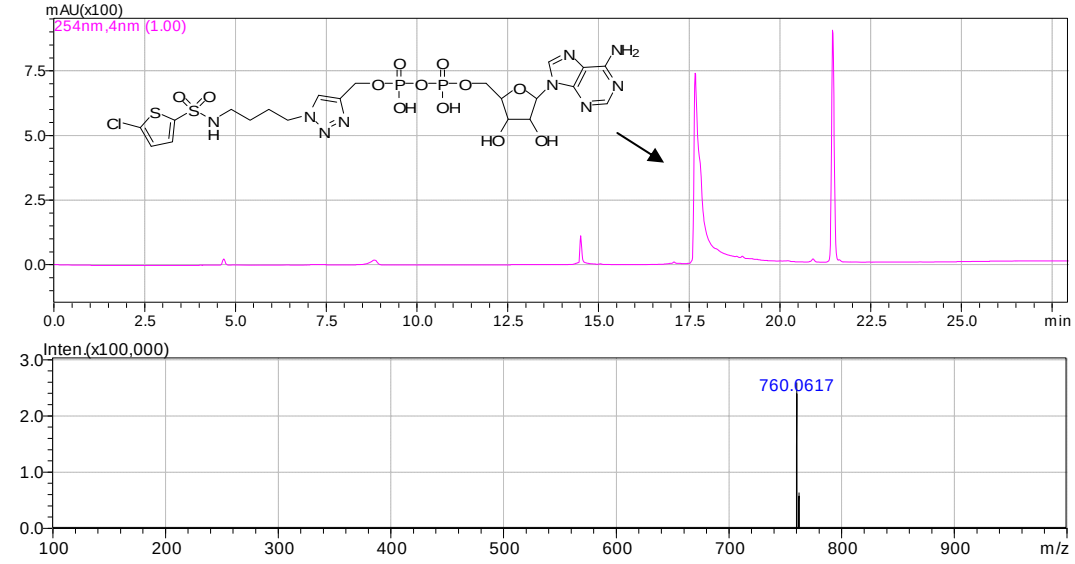

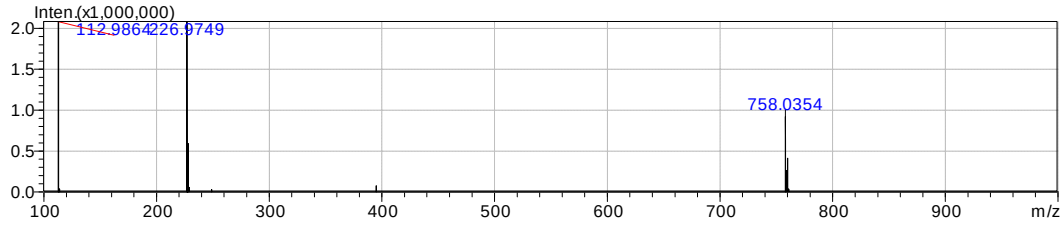

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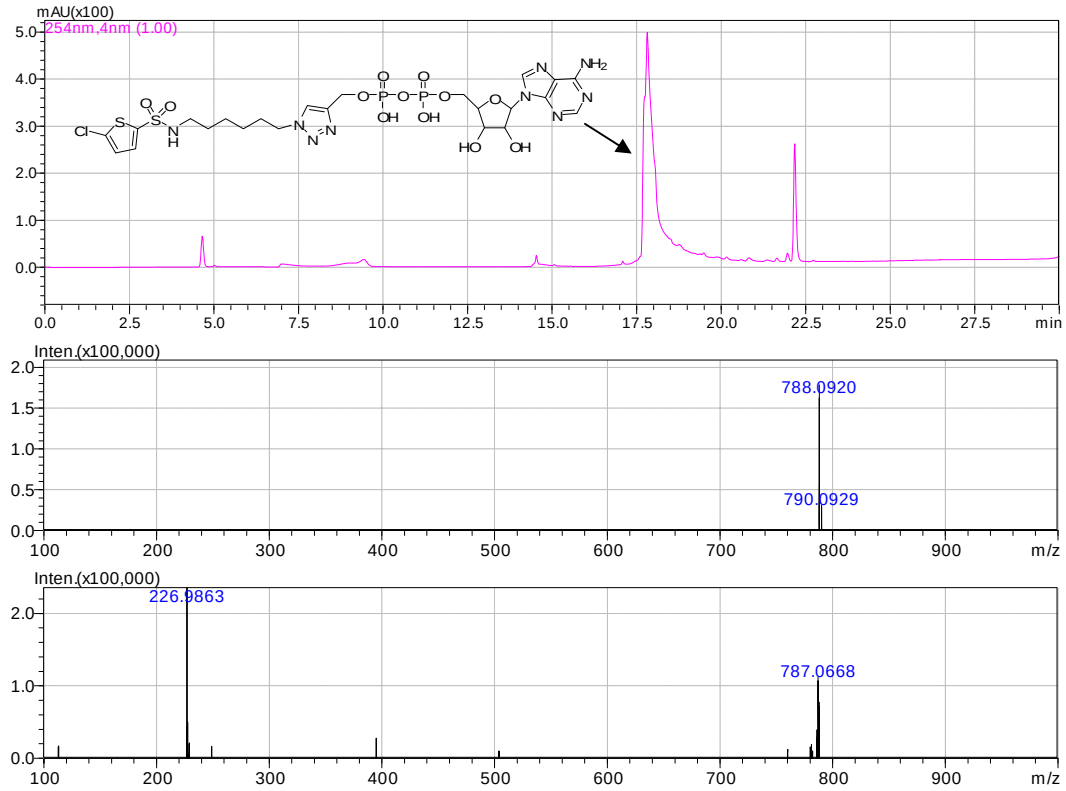

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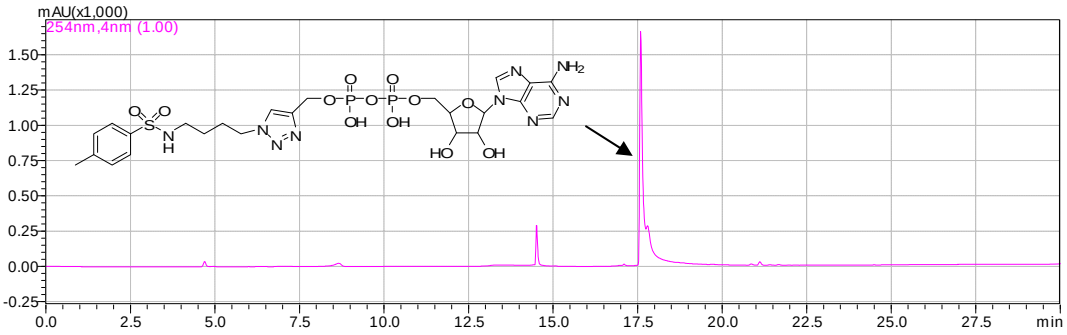

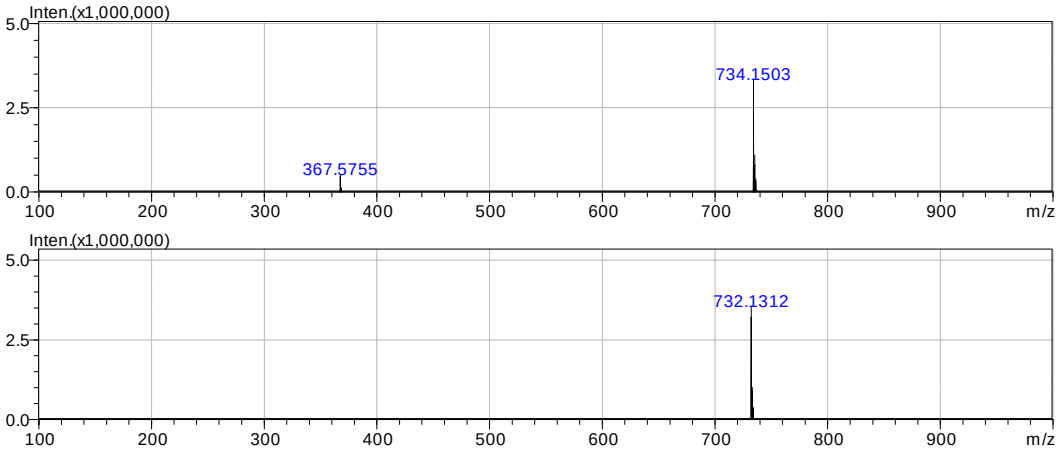
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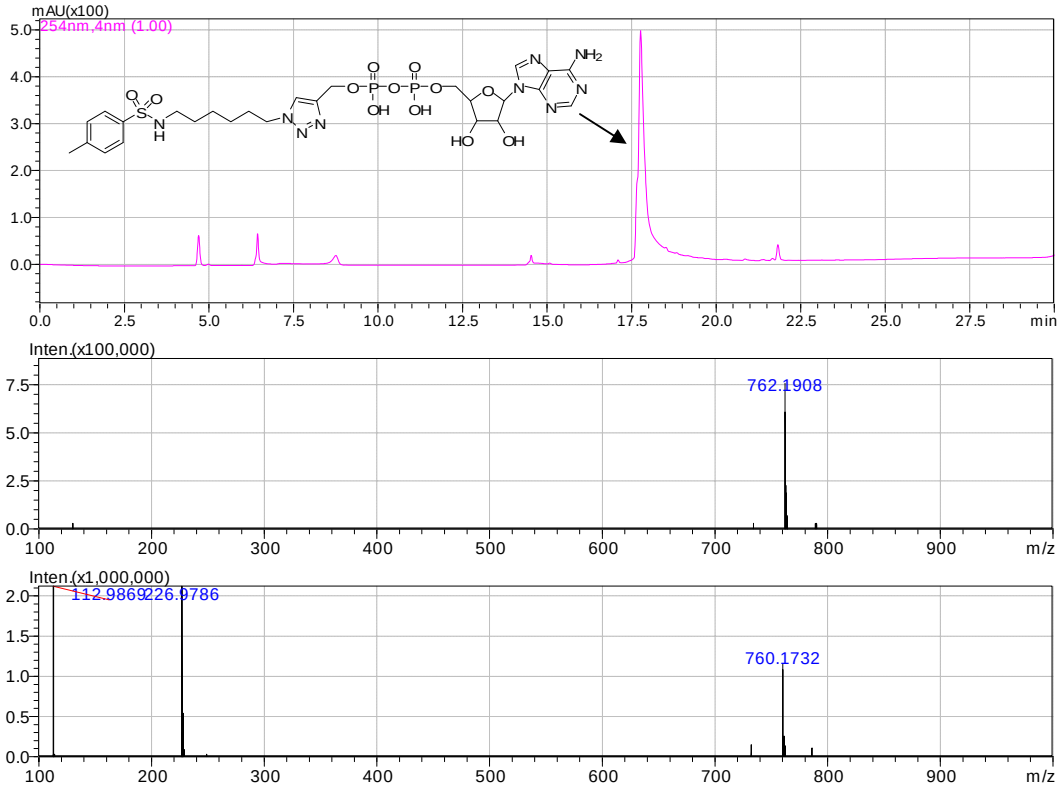
m/z
Inten.(x1,000,000)
732.1312
m/z

SA-A5-6C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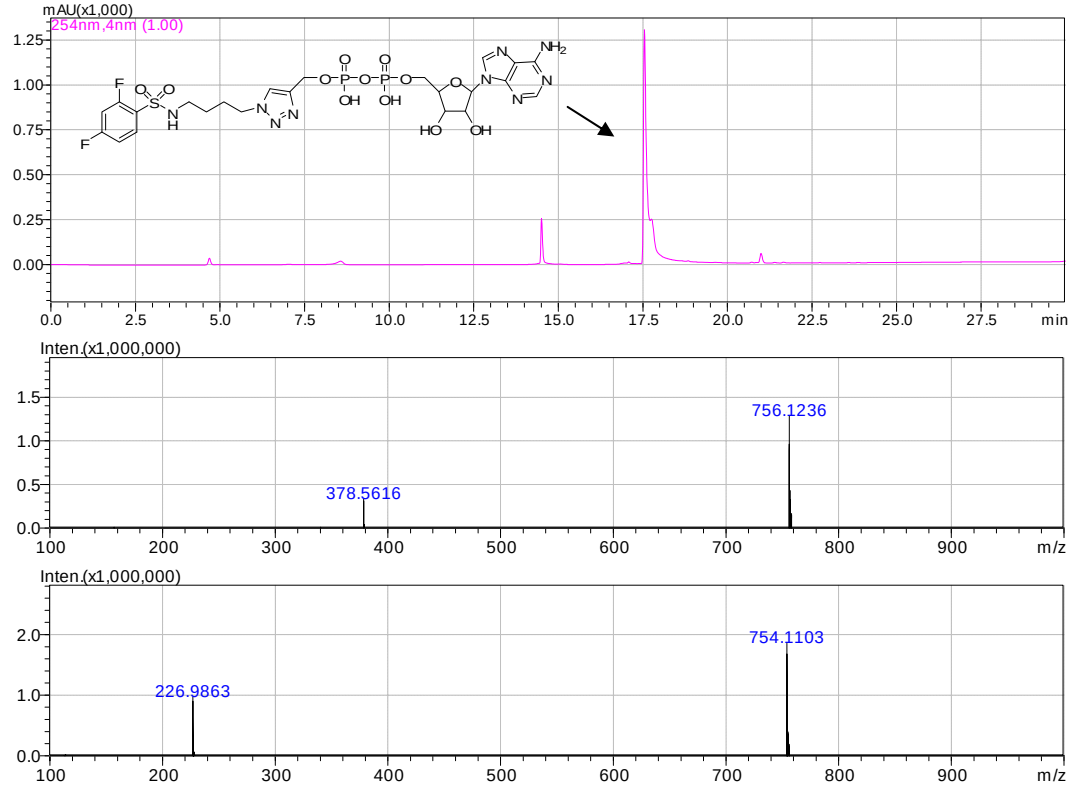
254nm,4nm (1.00)
min
Inten.(x100,000)
762.1908
m/z
Inten.(x1,000,000)
112.9869
226.9786
760.1732
m/z

SA-A6-4C



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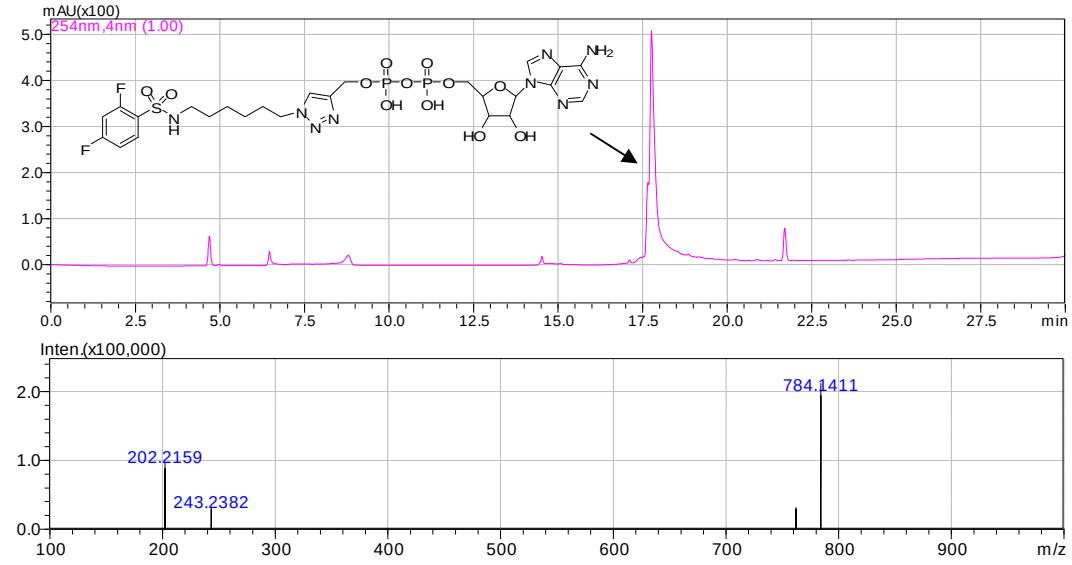

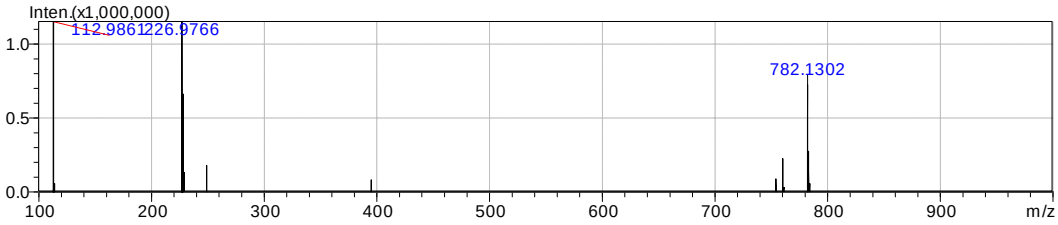

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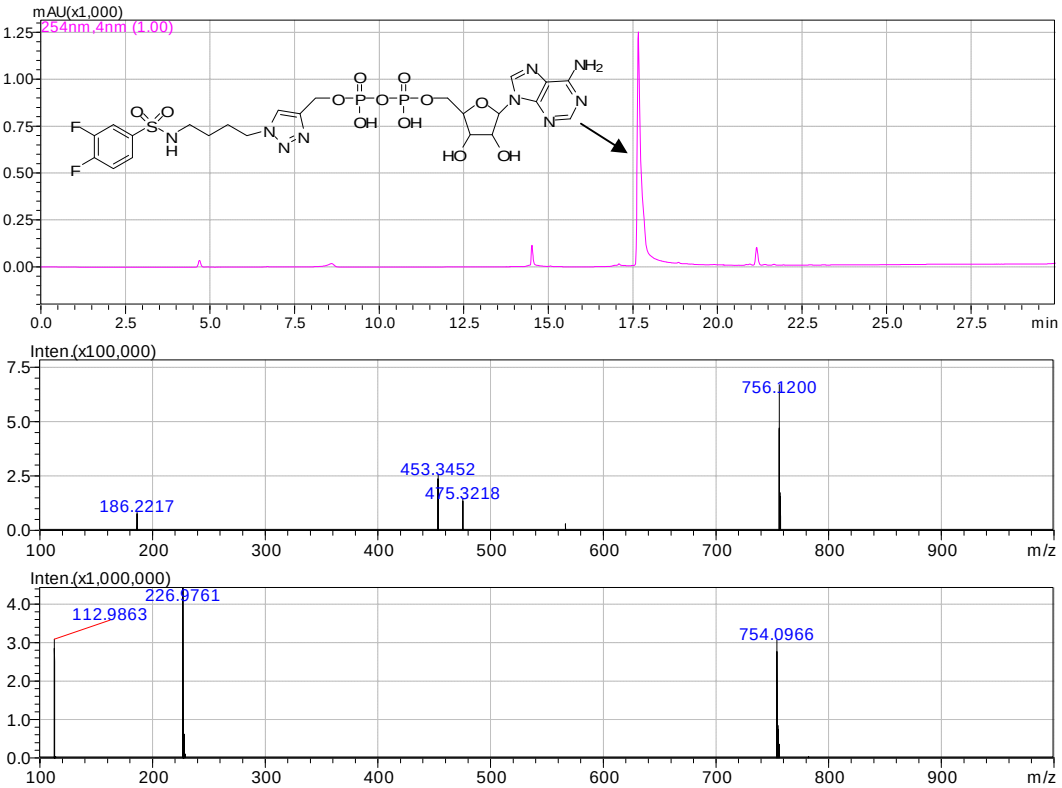
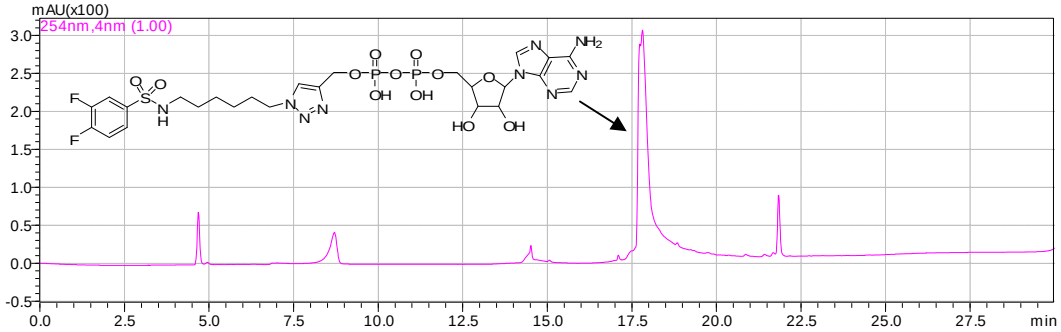
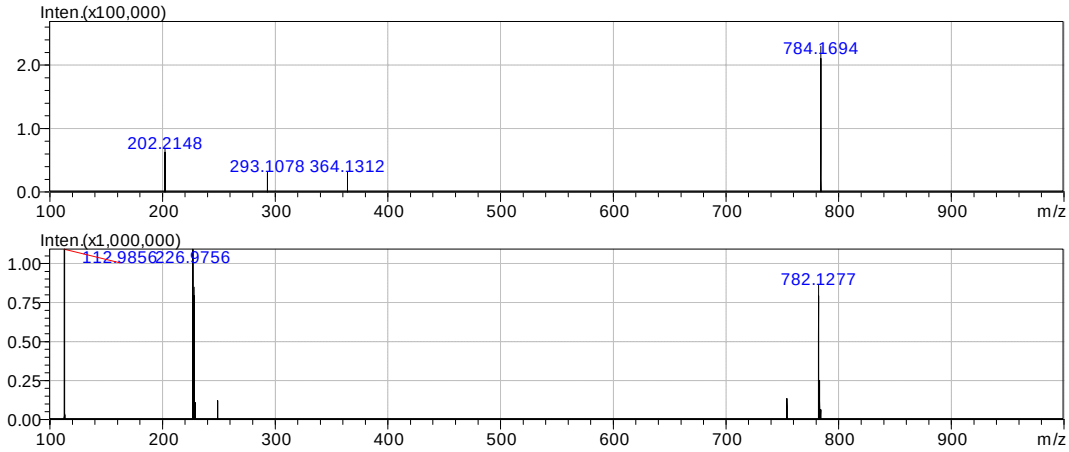


SA-A7-6C

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784.1694
202.2148
293.1078 364.1312
m/z
Inten.(x1,000,000)
112.9856226.9756
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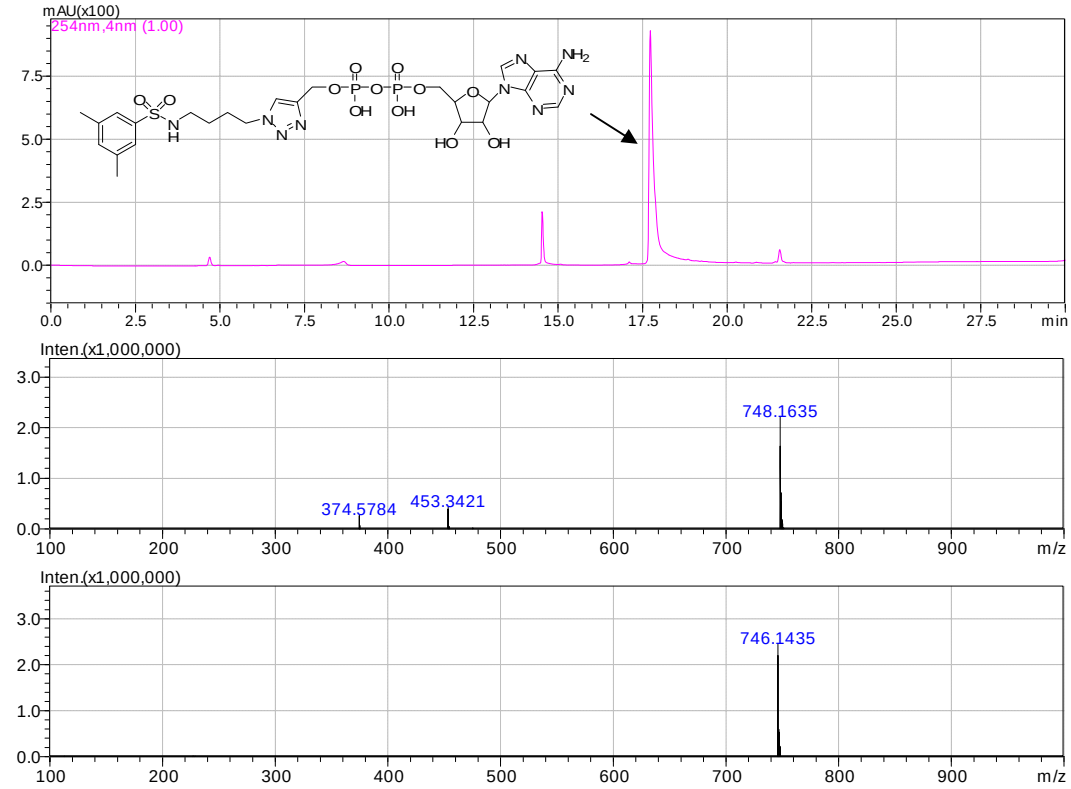
m/z

SA-A8-4C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254nm,4nm (1.00)
min
Inten.(x1,000,000)
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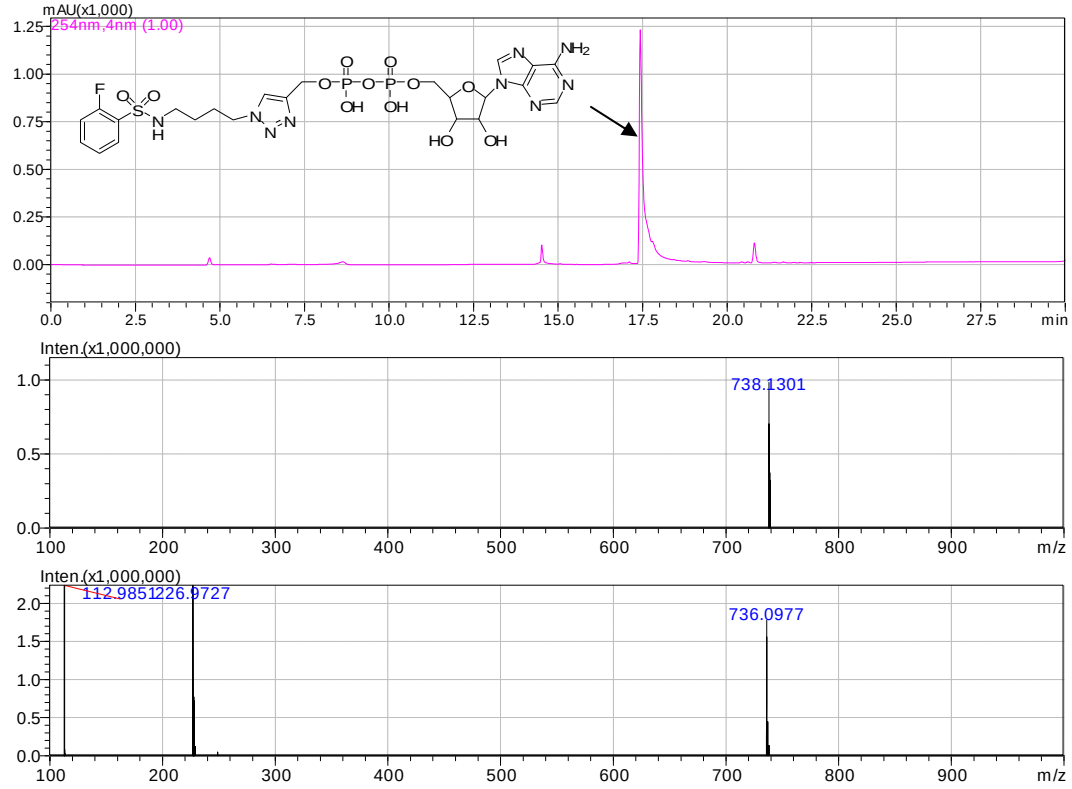
374.5784
453.3421
m/z
Inten.(x1,000,000)
746.1435
m/z

SA-A9-4C



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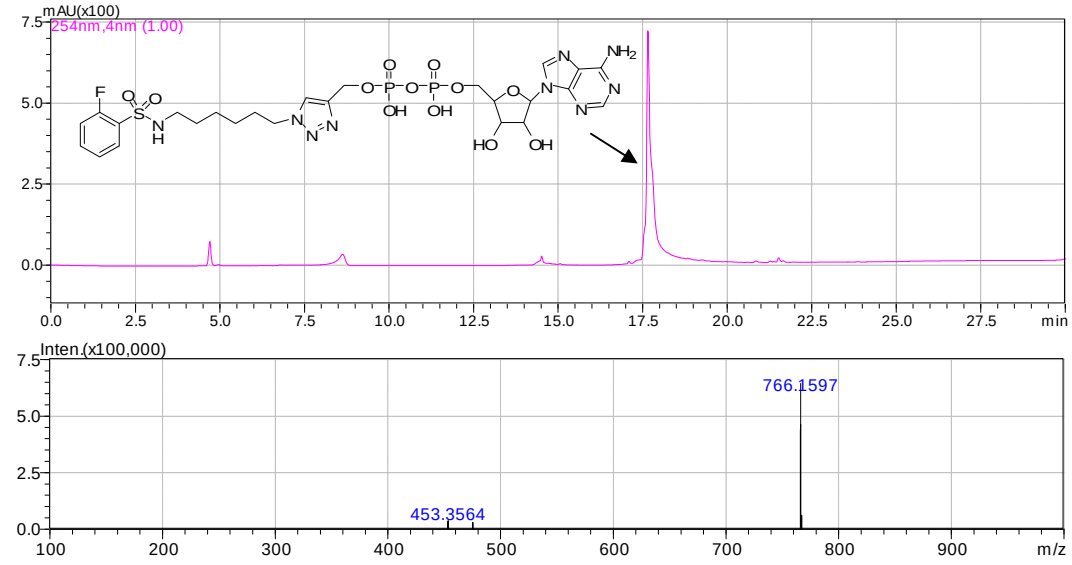

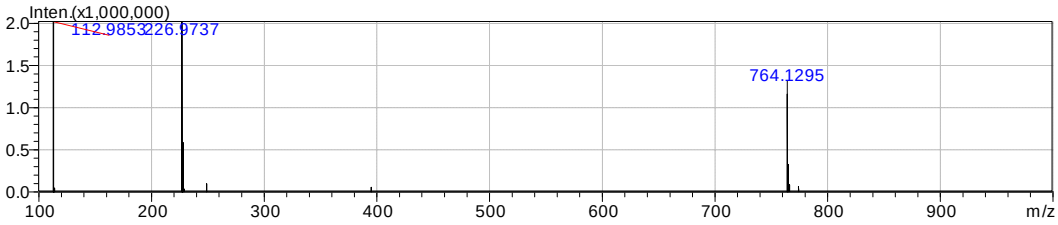

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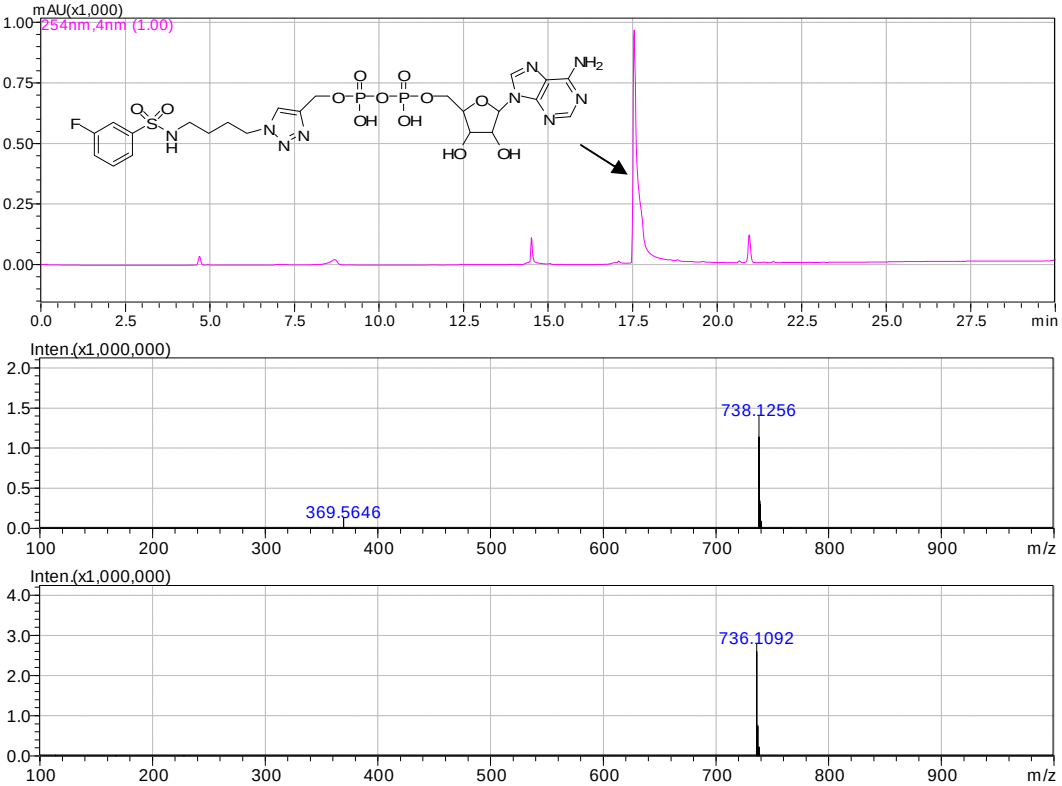

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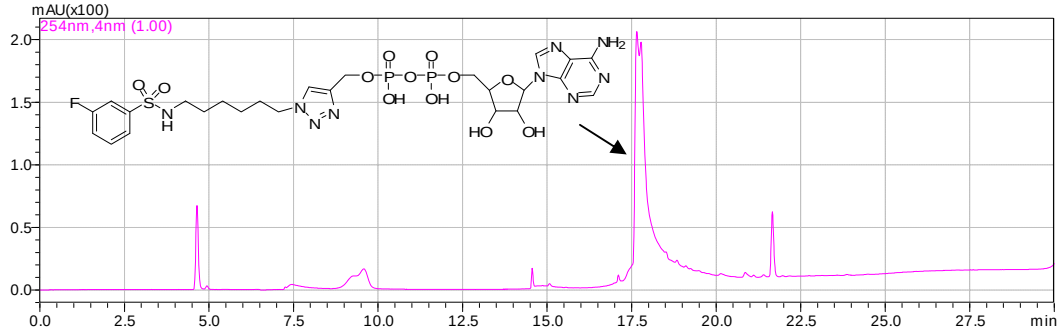
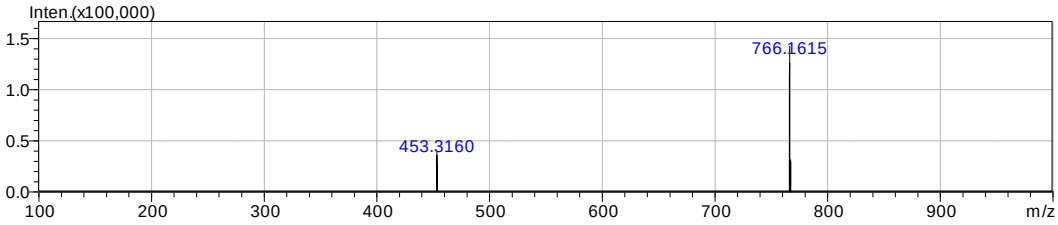
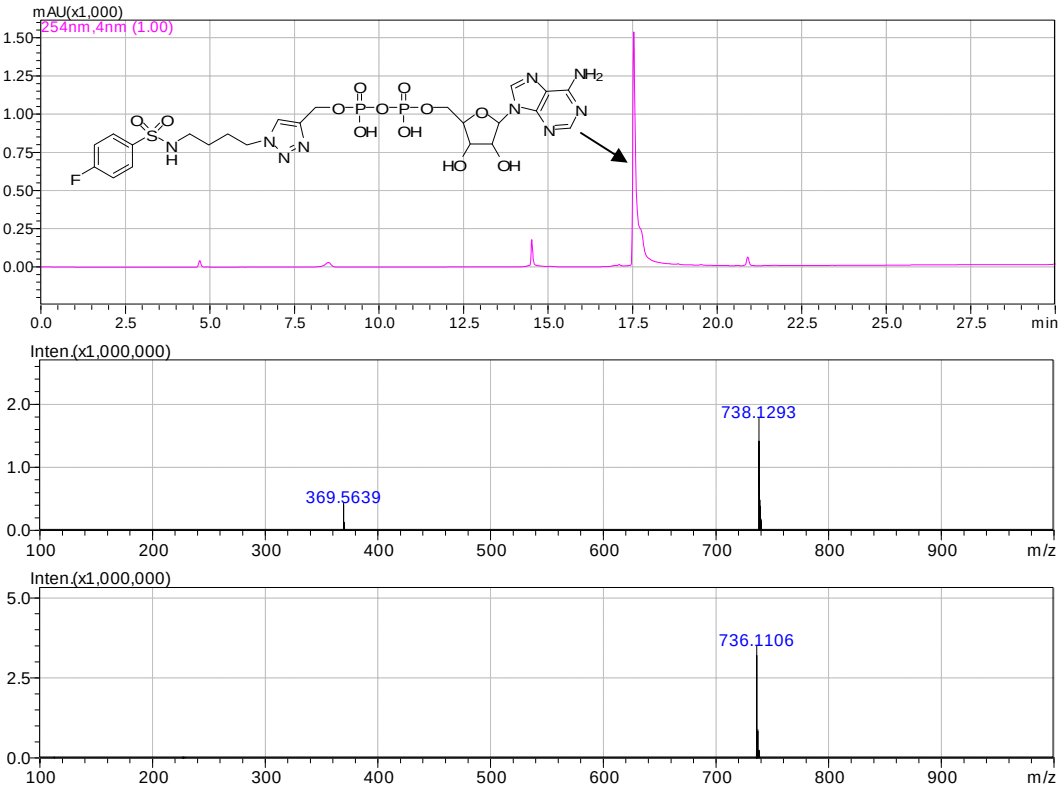
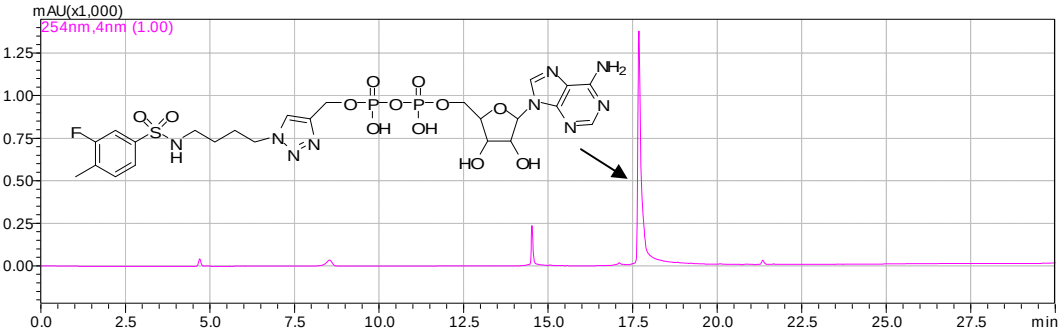


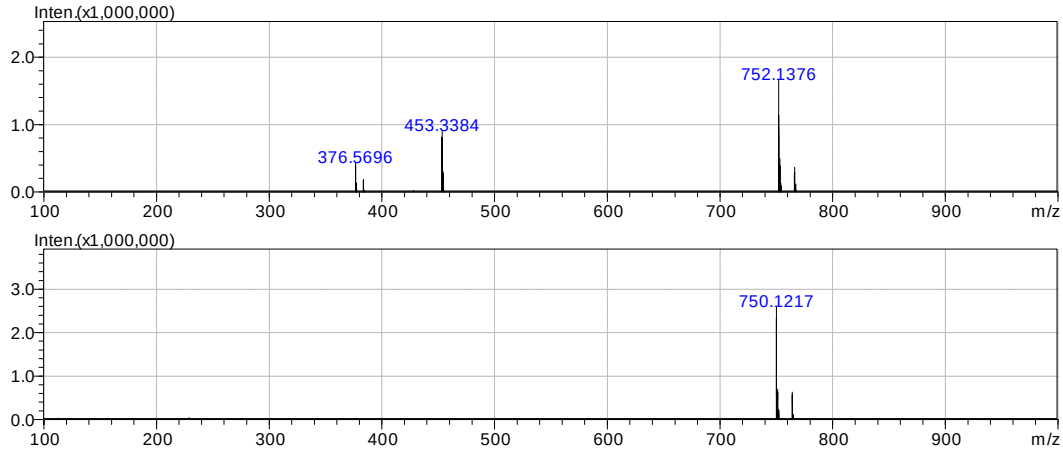


SA-A11-4C



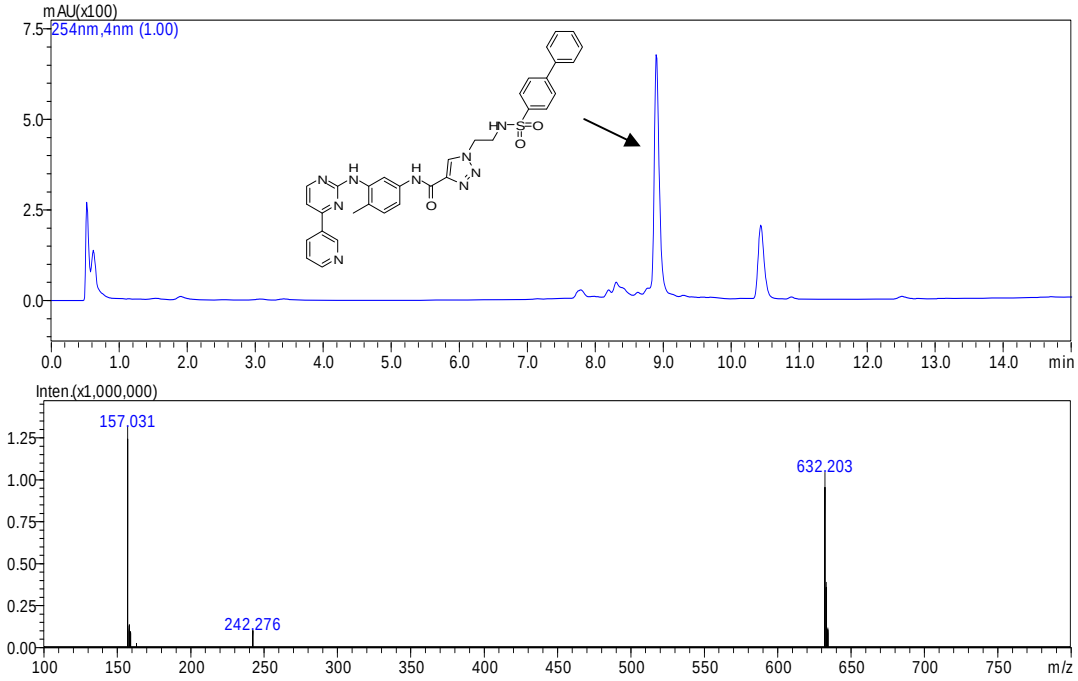
SA-A12-4C



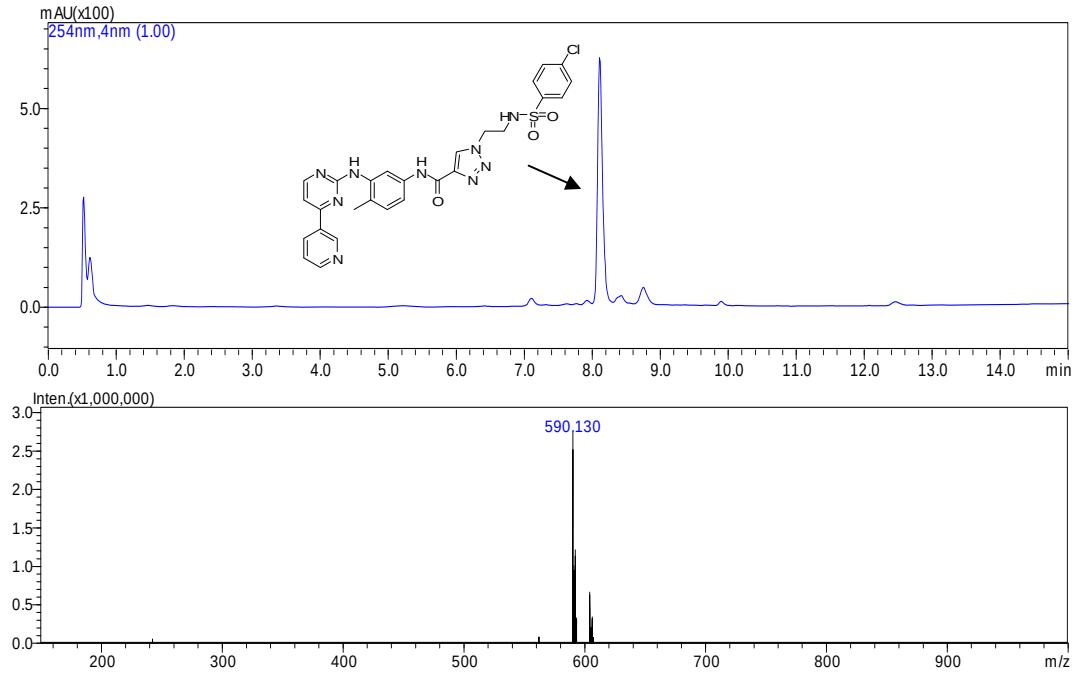


1. 3. LC-MS profiles of the click-library of Imatinib analogue and the traceless azides

W1-SA2



W1-SA3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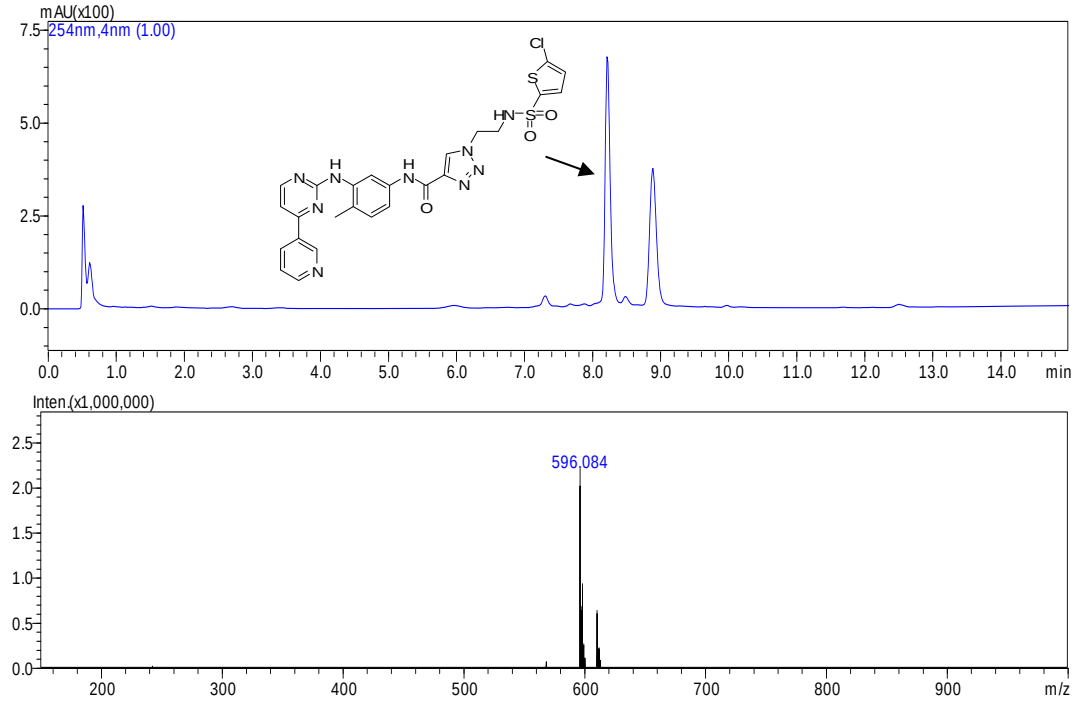
min
Inten.(x1,000,000)
590.130
m/z

W1-SA4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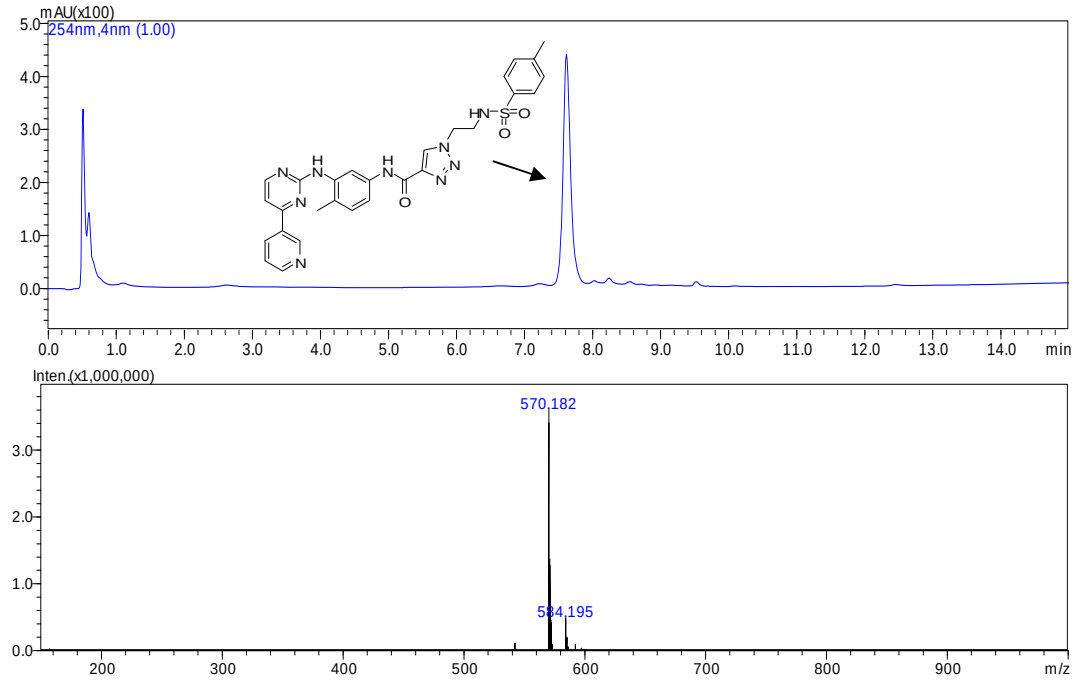
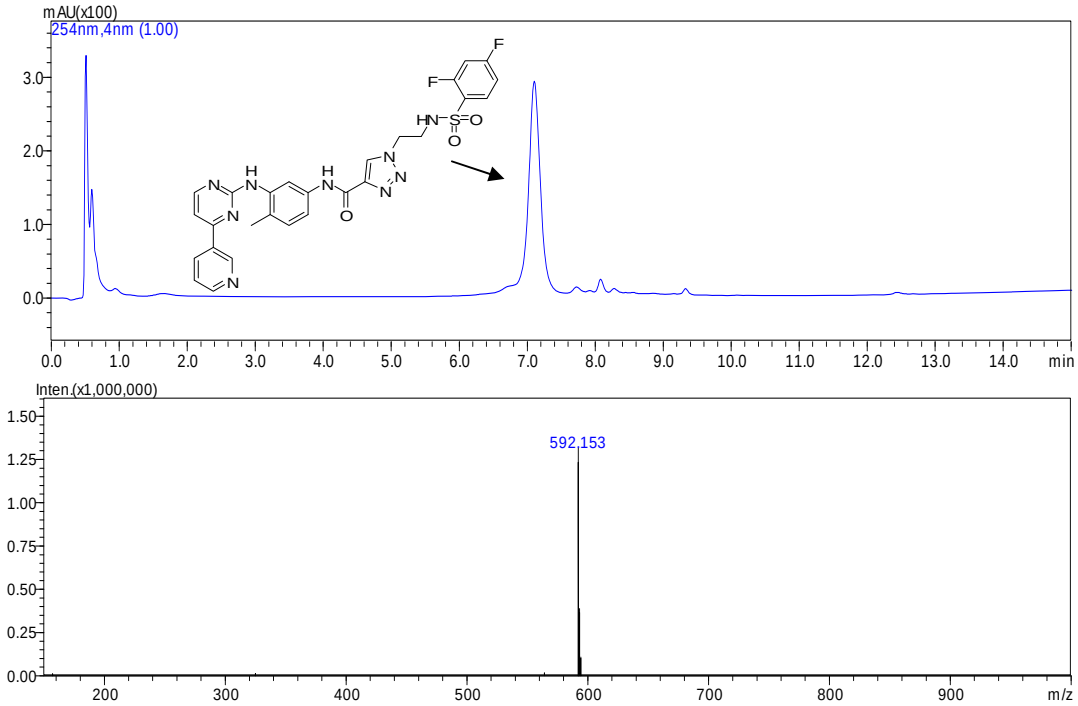
min
Inten.(x1,000,000)
596.084
m/z

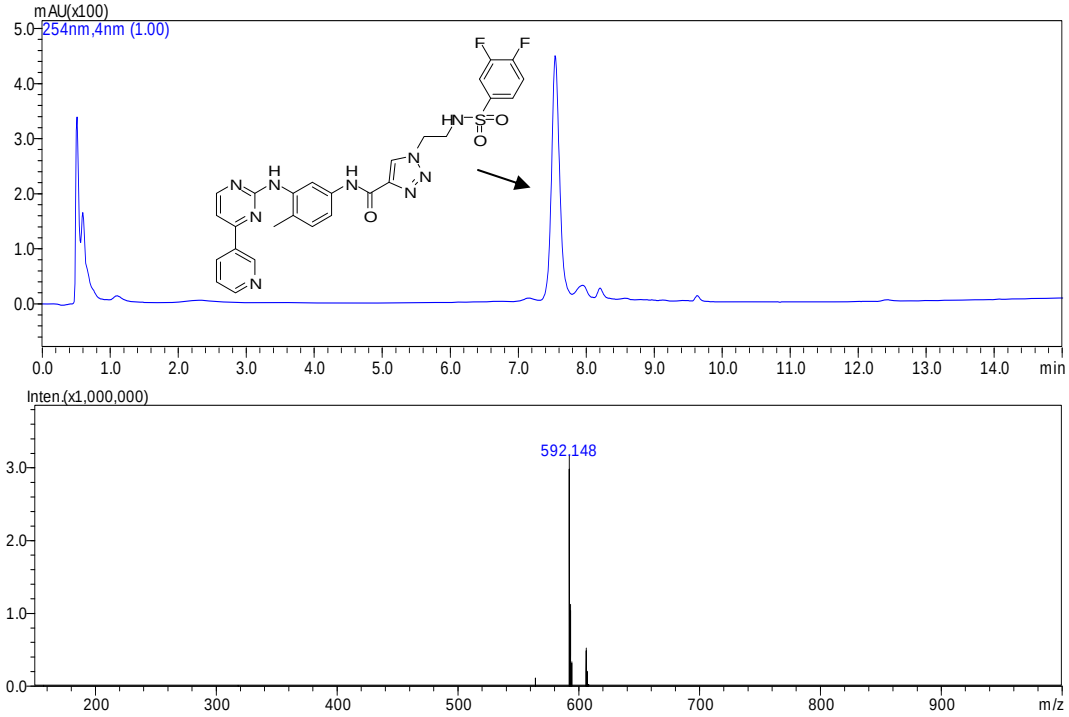
W1-SA5


mAU(x100)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
570.182
584.195
m/z

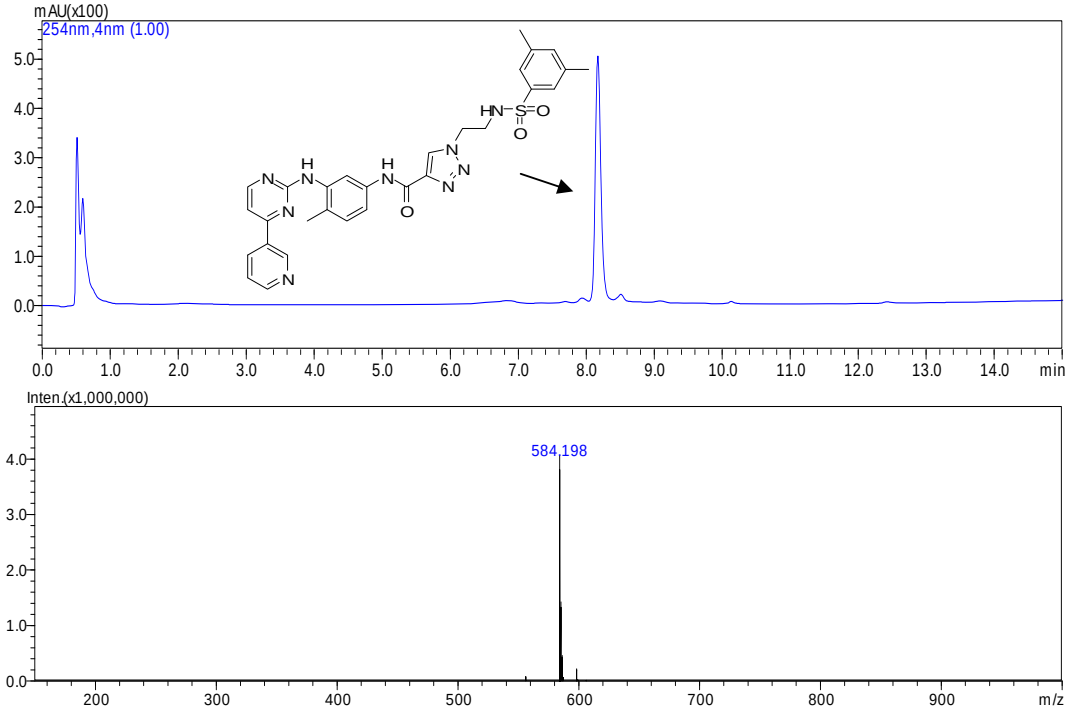
W1-SA6


mAU(x100)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
592.153
m/z

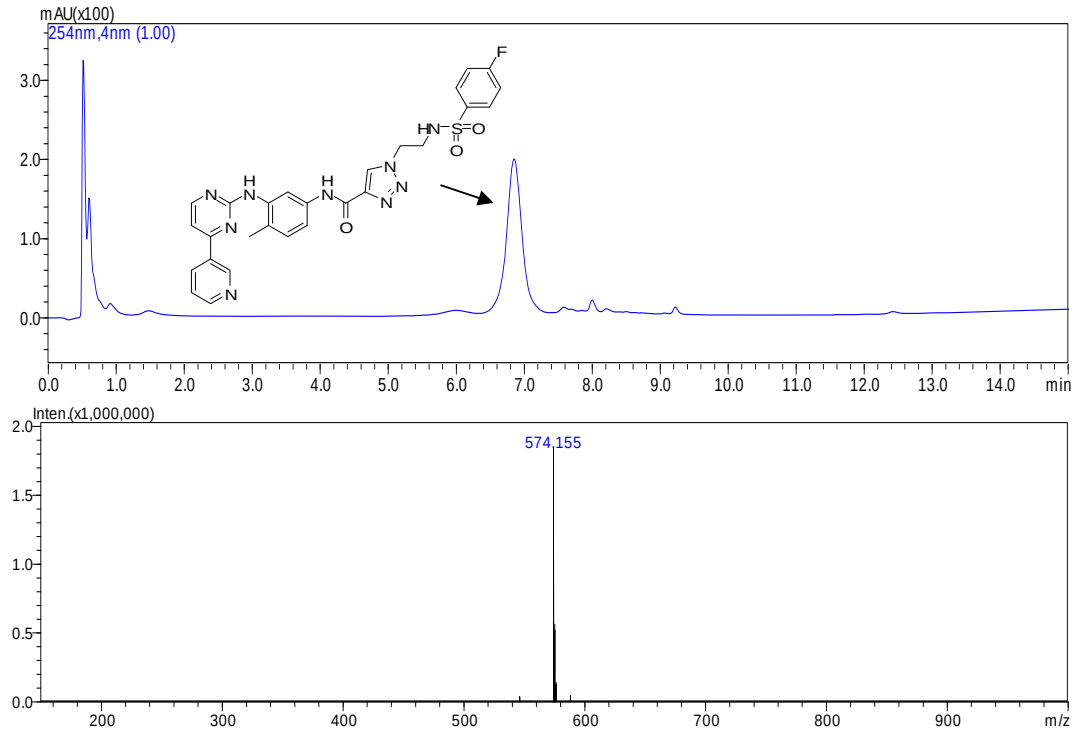
W1-SA7


mAU(x100)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
592.148
m/z

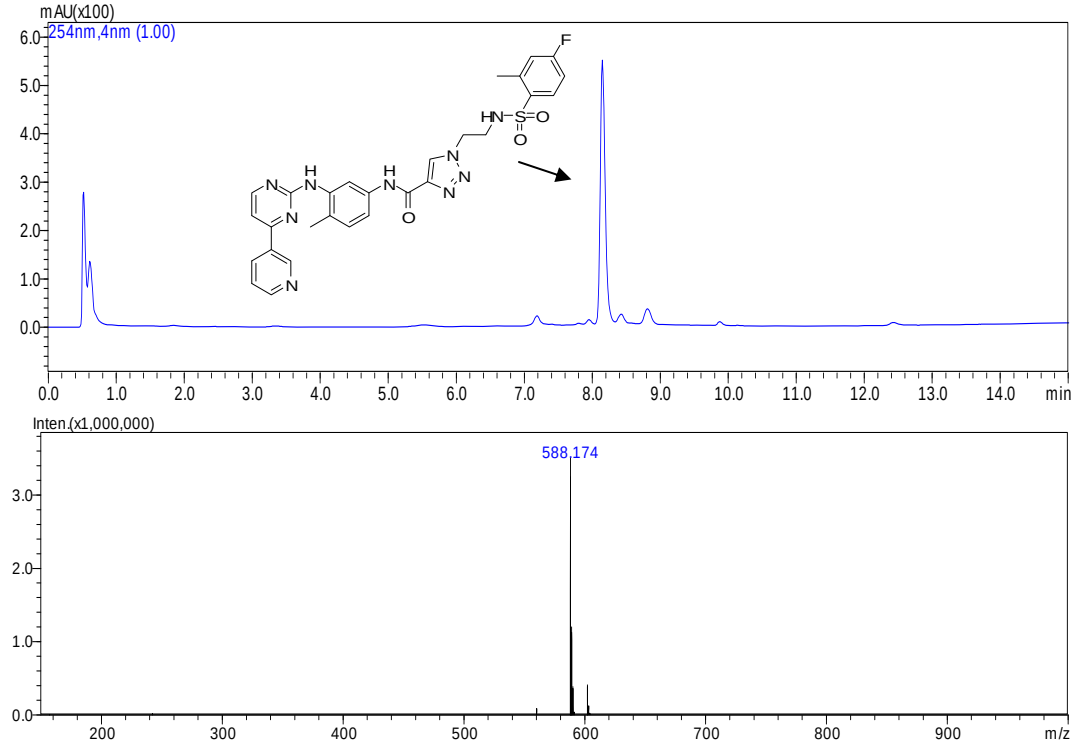
W1-SA8


mAU(x100)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
584.198
m/z

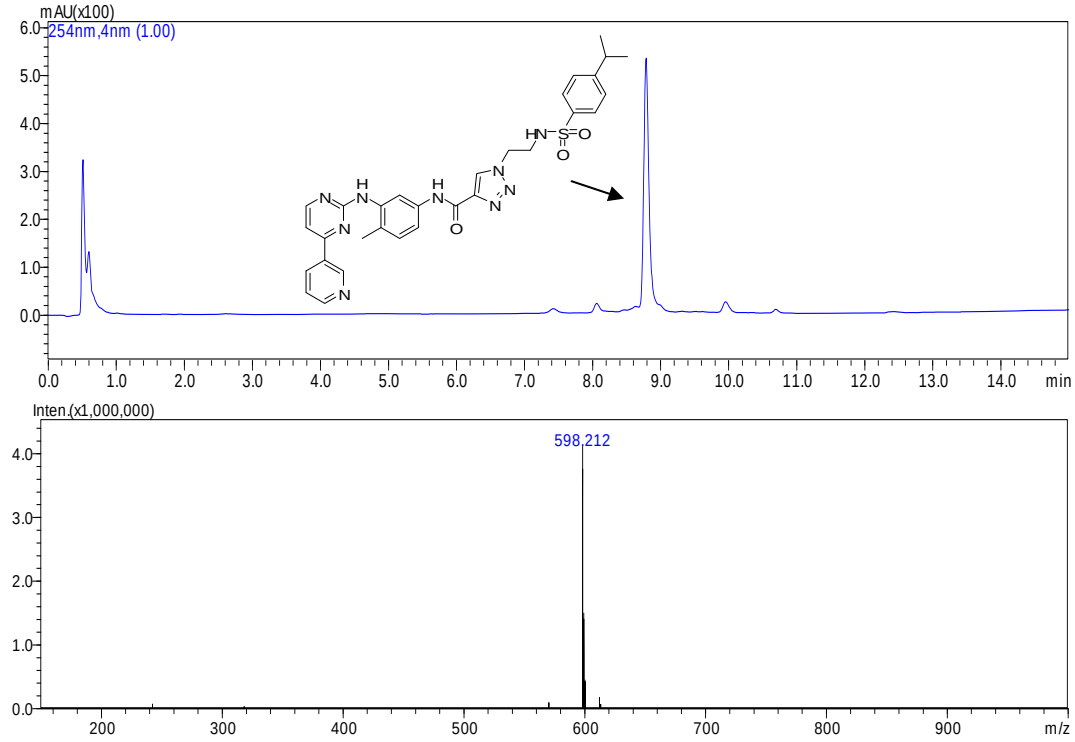
W1-SA11



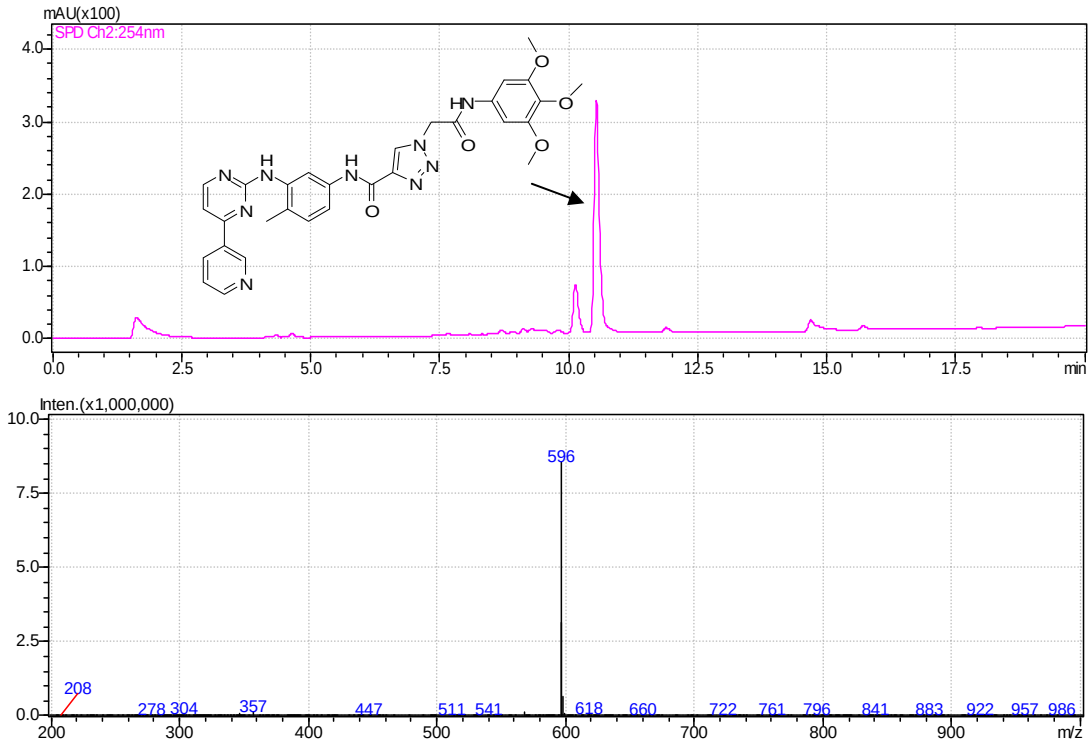
W1-SA13



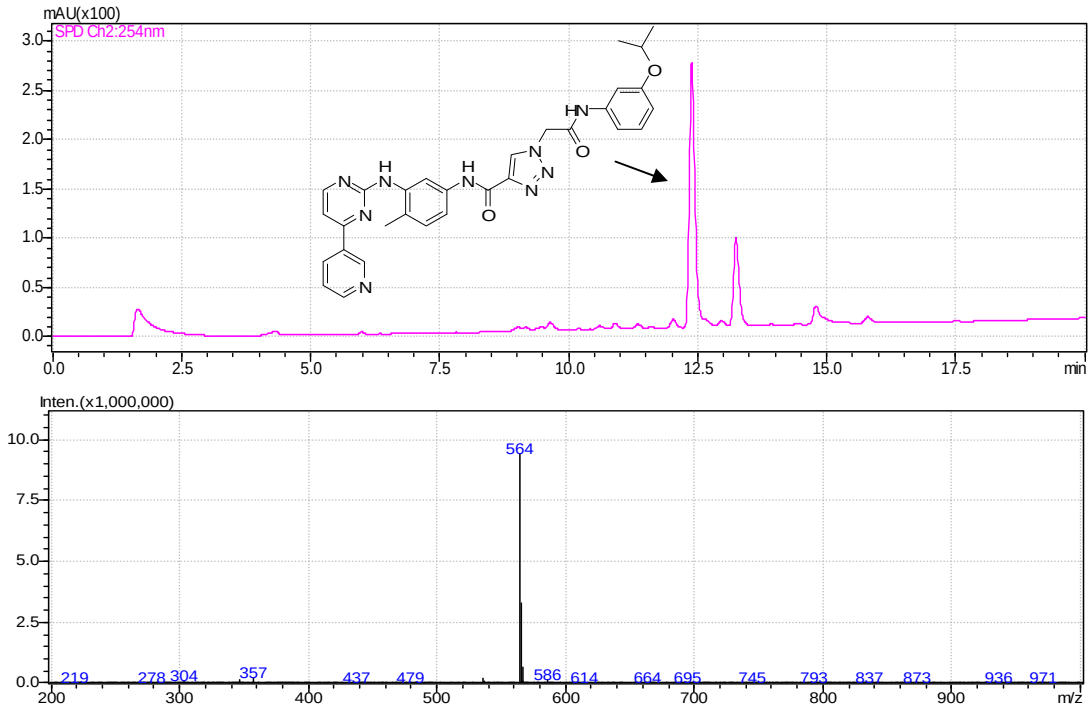
W1-SA14



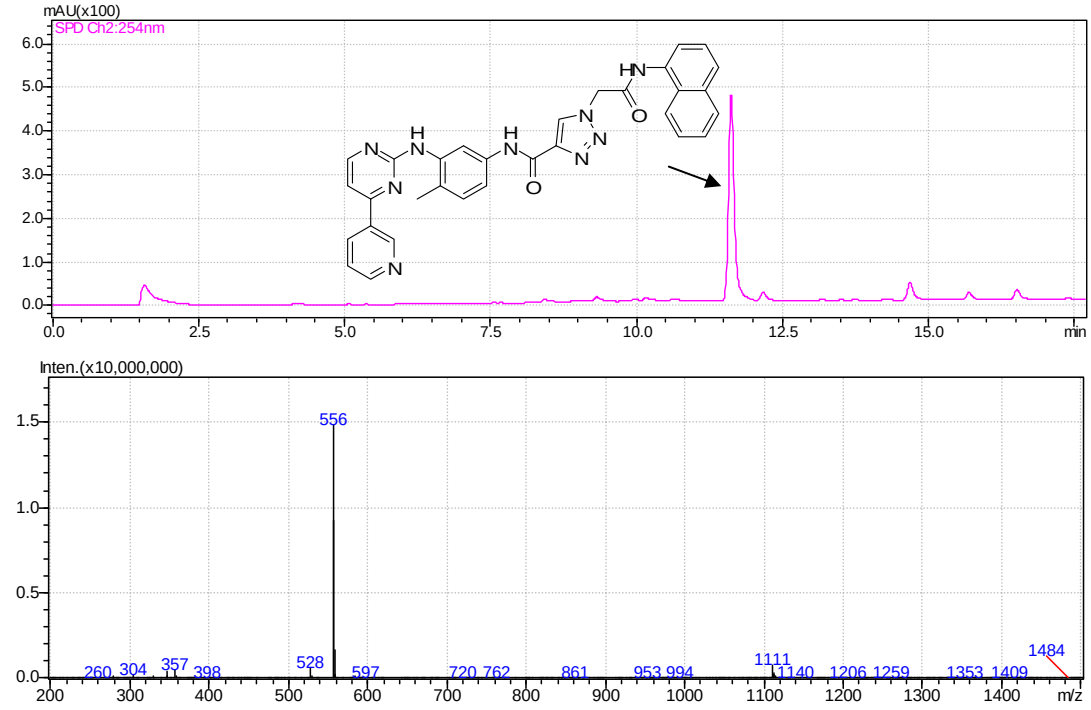
W1-A31



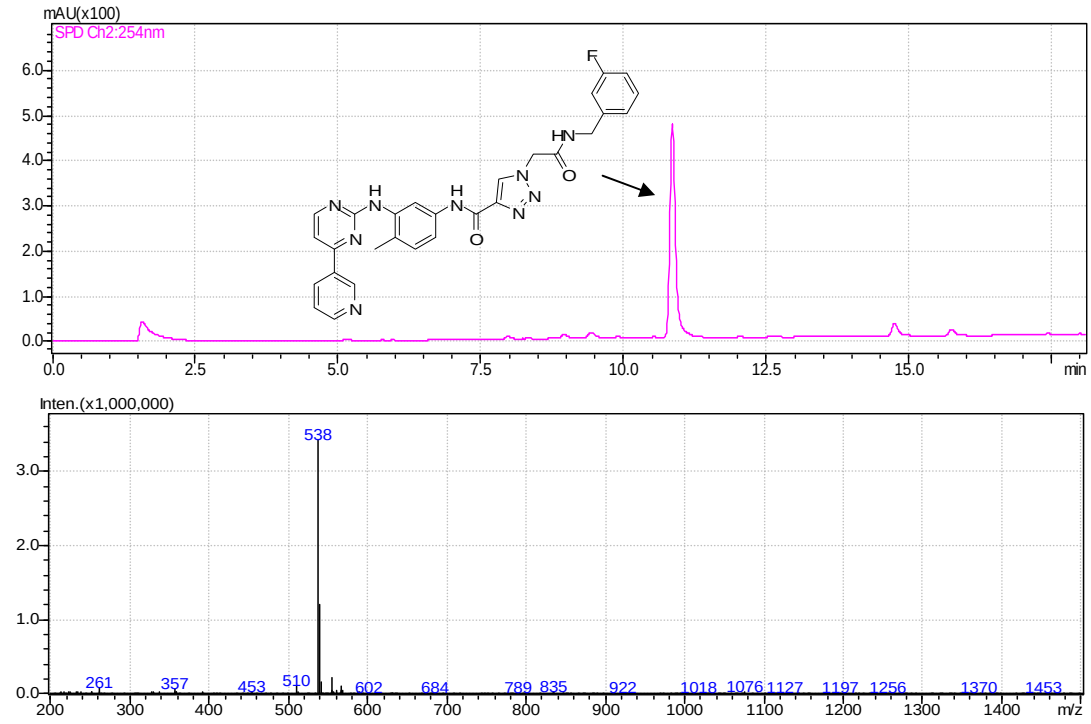
W1-A32


mAU(x100)
SPD Ch2:254nm
min
Inten.(x1,000,000)
564
m/z

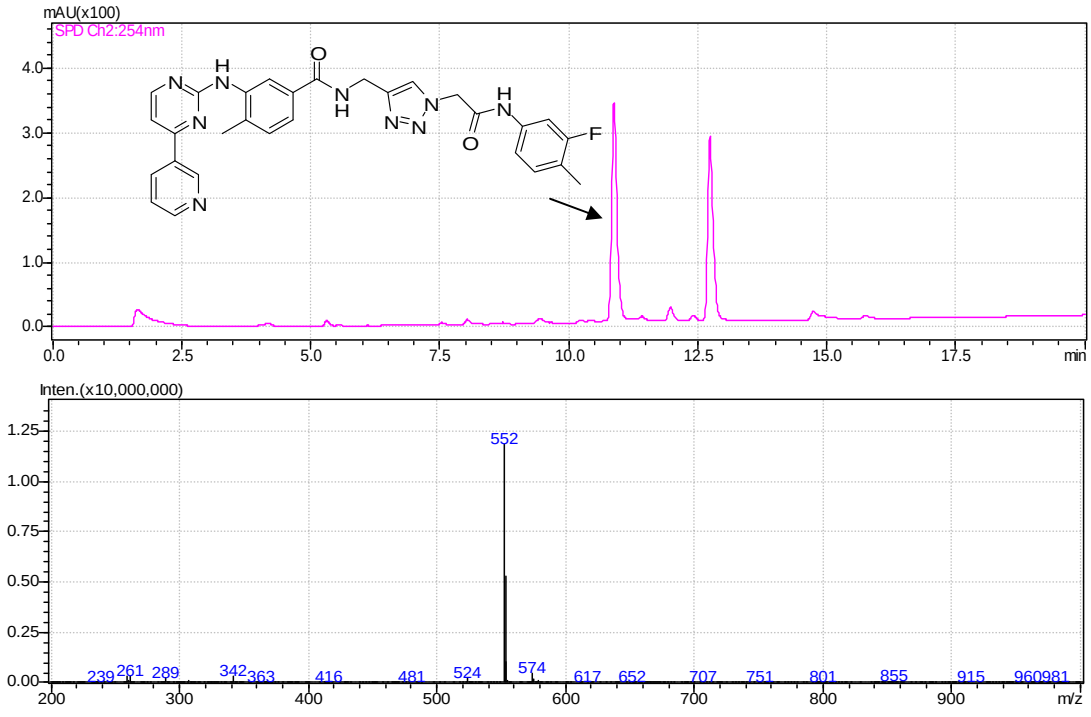
W1-A41


mAU(x100)
SPD Ch2:254nm
min
Inten.(x10,000,000)
556
1484
m/z

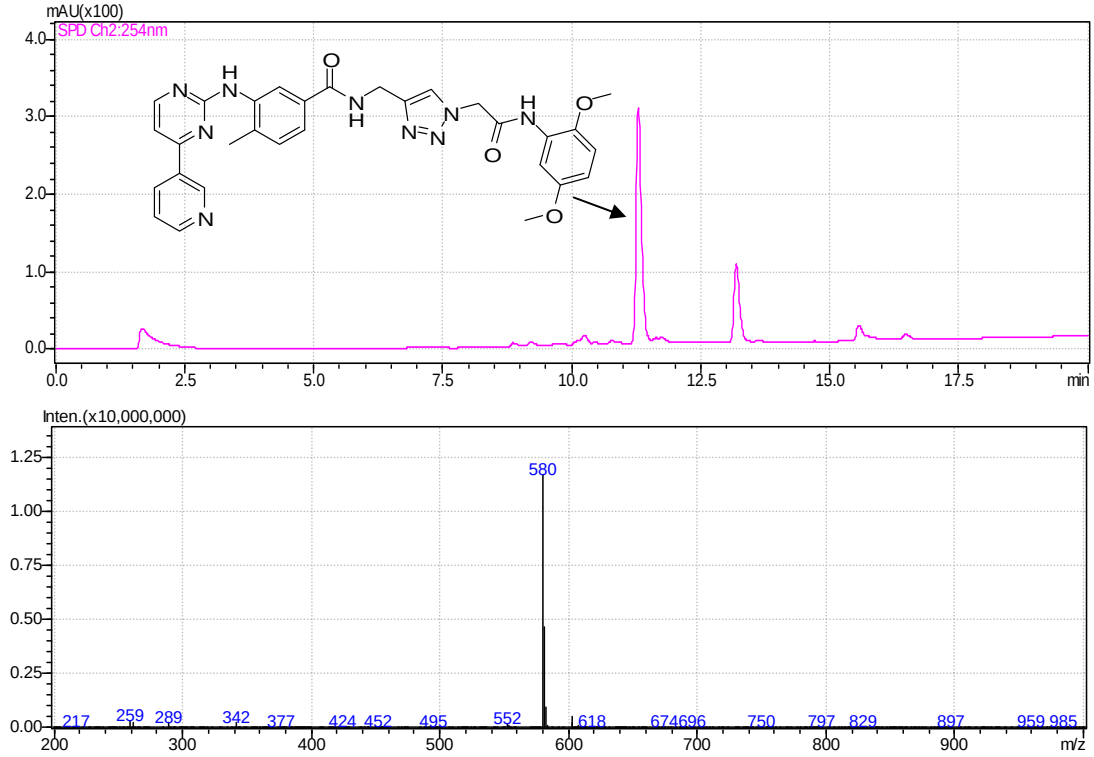
W1-A43


mAU(x100)
SPD Ch2:254nm
min
Inten.(x1,000,000)
538
261
357
453
510
602
684
789
835
922
1018
1076
1127
1197
1256
1370
1453
m/z

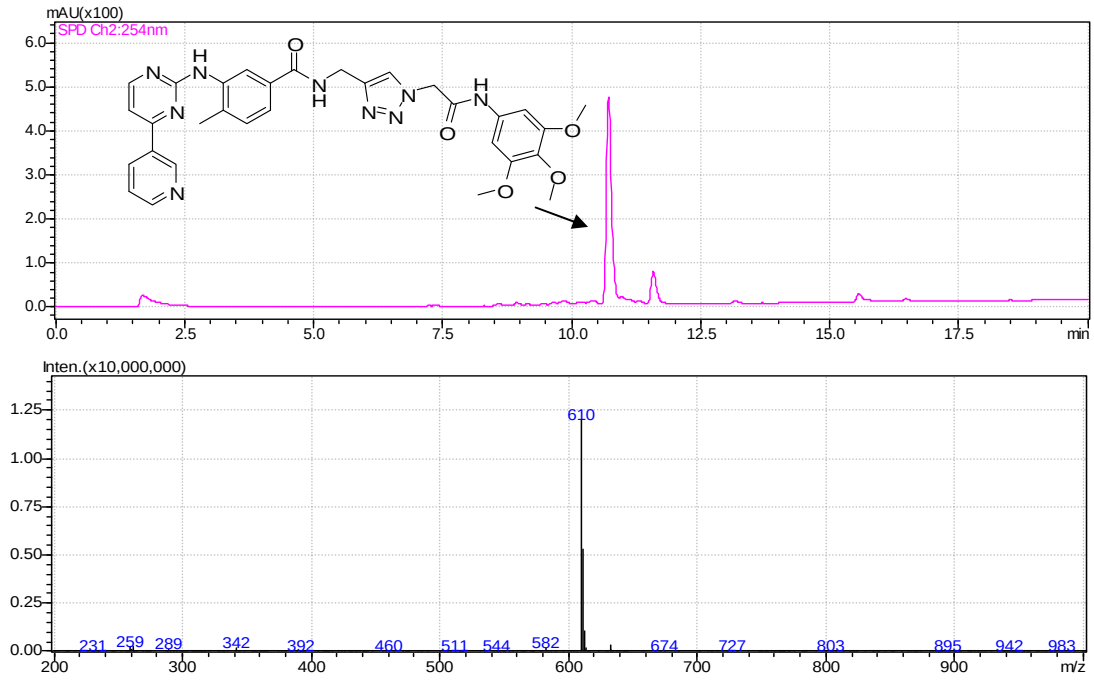
W2-A27


mAU(x100)
SPD Ch2:254nm
min
Inten.(x10,000,000)
552
239
261
289
342
363
416
481
524
574
617
652
707
751
801
855
915
960
981
m/z

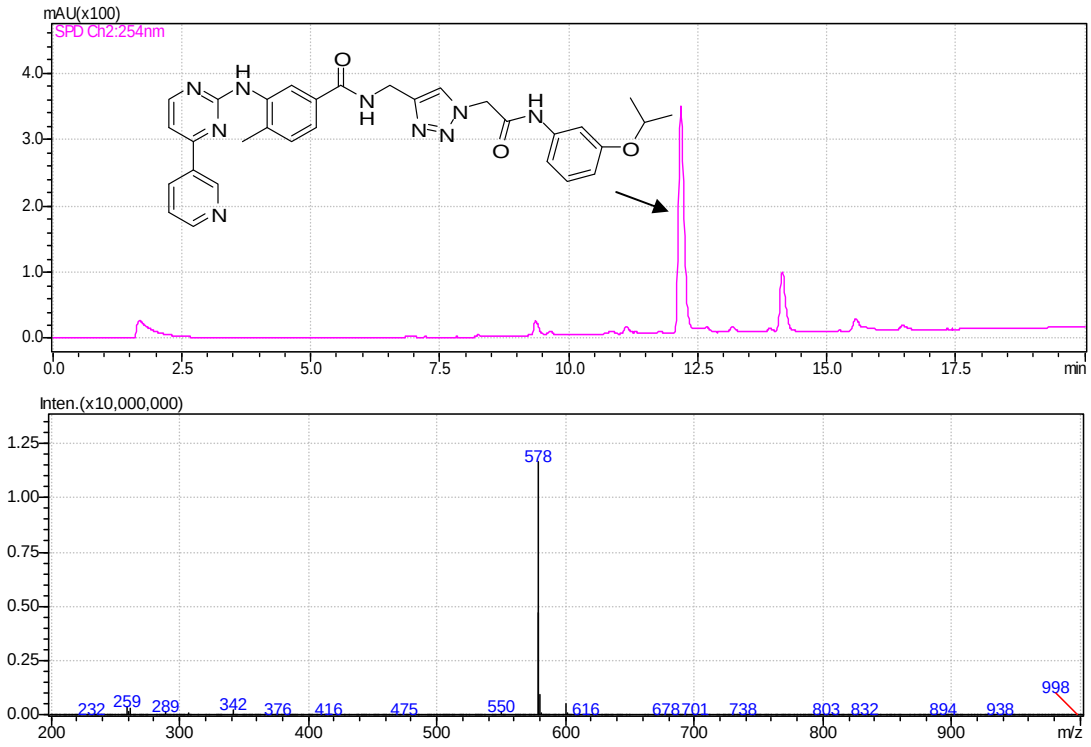
W2-A30


mAU(x100)
SPD Ch2:254nm
min
Inten.(x10,000,000)
580
m/z

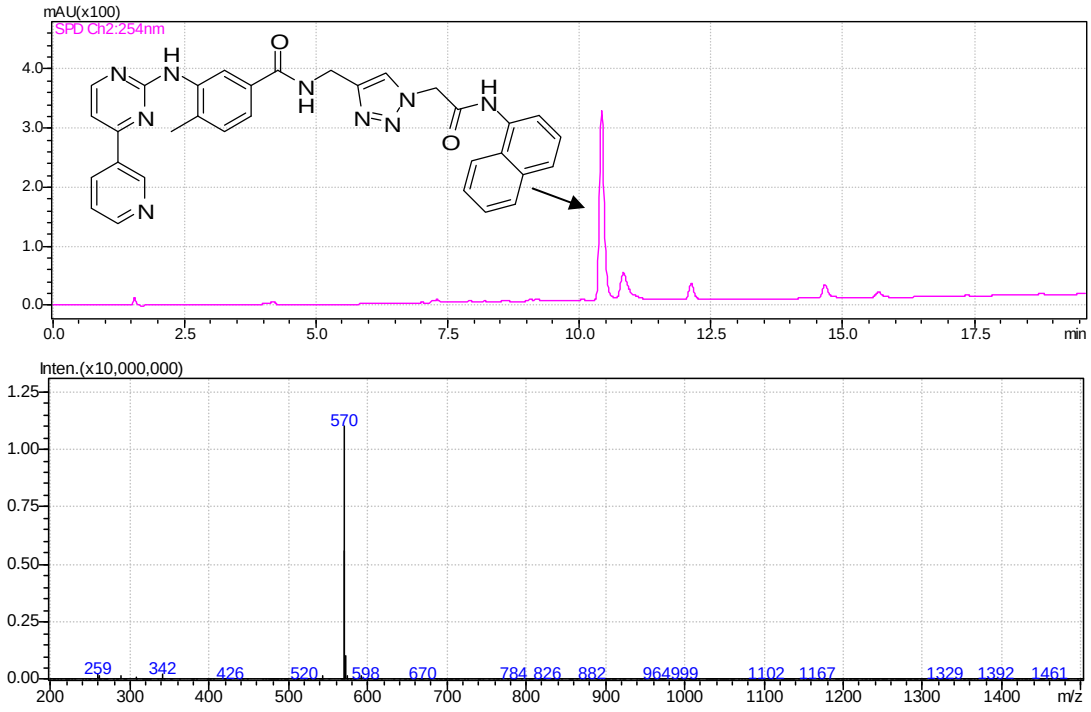
W2-A31


mAU(x100)
SPD Ch2:254nm
min
Inten.(x10,000,000)
610
m/z

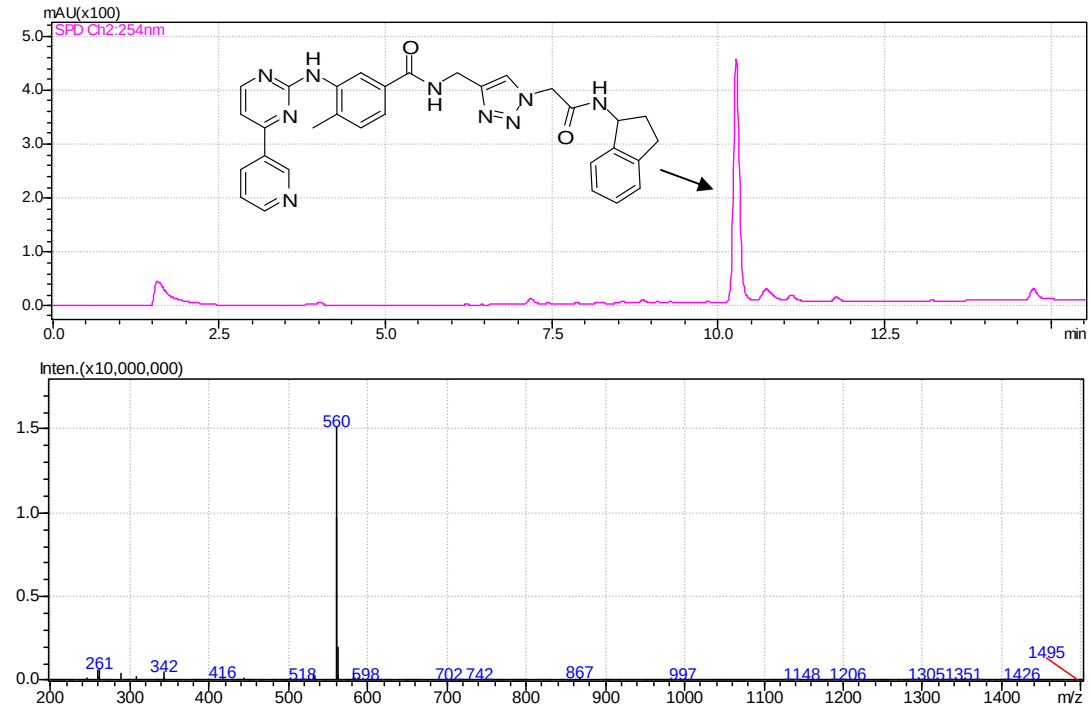
W2-A32


mAU(x100)
SPD Ch2:254nm
4.0
3.0
2.0
1.0
0.0
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
min
Inten.(x10,000,000)
1.25
1.00
0.75
0.50
0.25
0.00
578
232
259
289
342
376
416
475
550
616
678
701
738
803
832
894
938
998
200
300
400
500
600
700
800
900
m/z

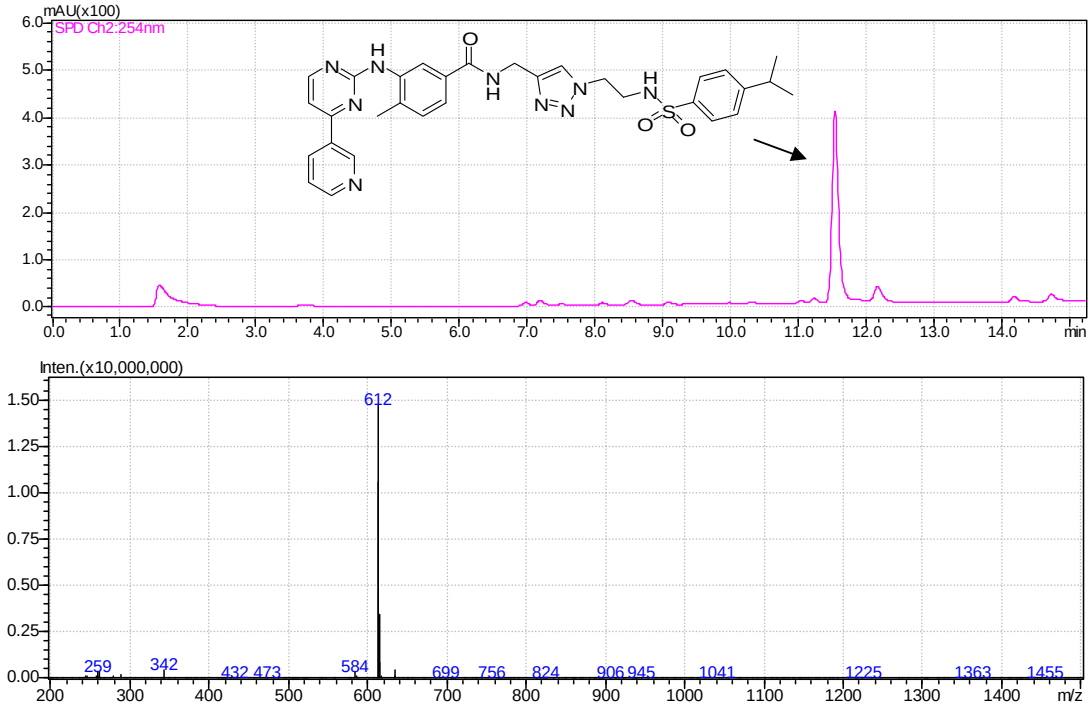
W2-A41


mAU(x100)
SPD Ch2:254nm
4.0
3.0
2.0
1.0
0.0
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
min
Inten.(x10,000,000)
1.25
1.00
0.75
0.50
0.25
0.00
570
259
342
426
520
598
670
784
826
882
964
999
1102
1167
1329
1392
1461
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
m/z

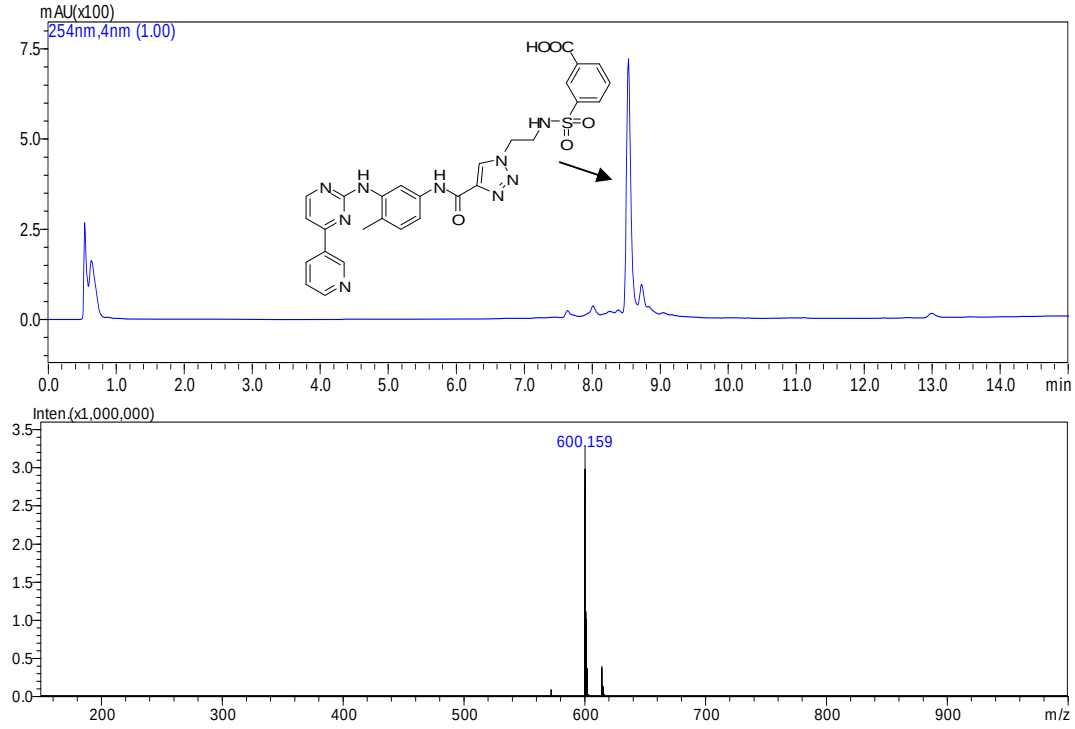
W2-A42



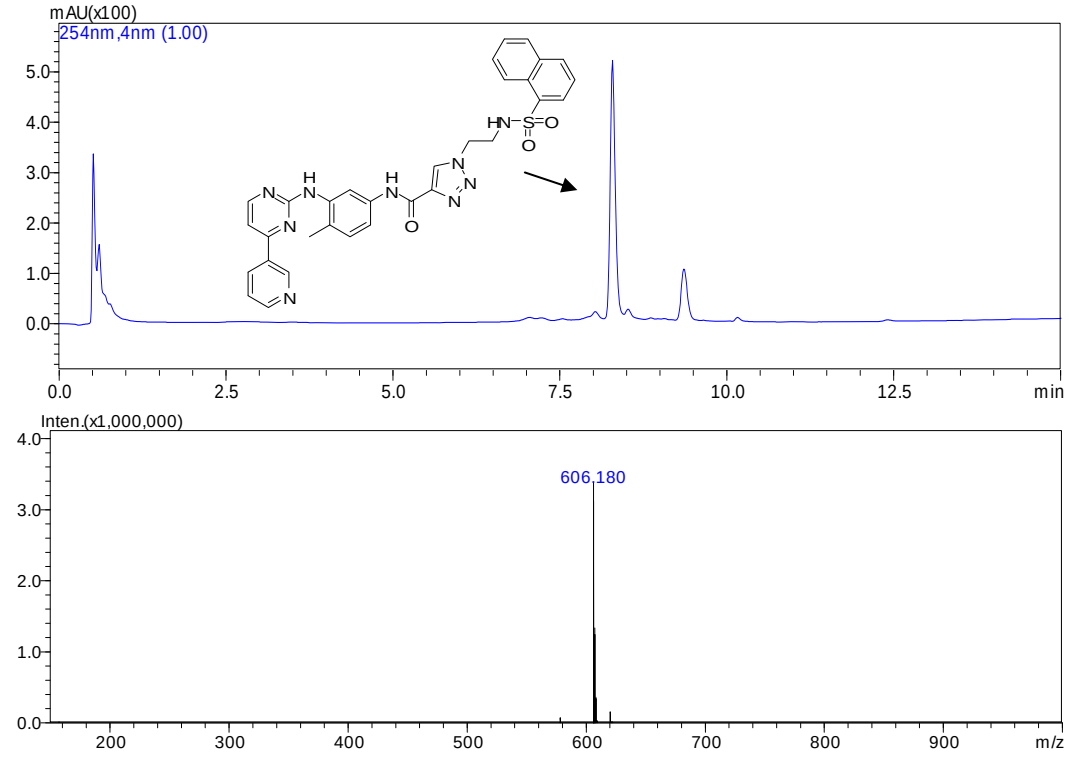
W2-SA14



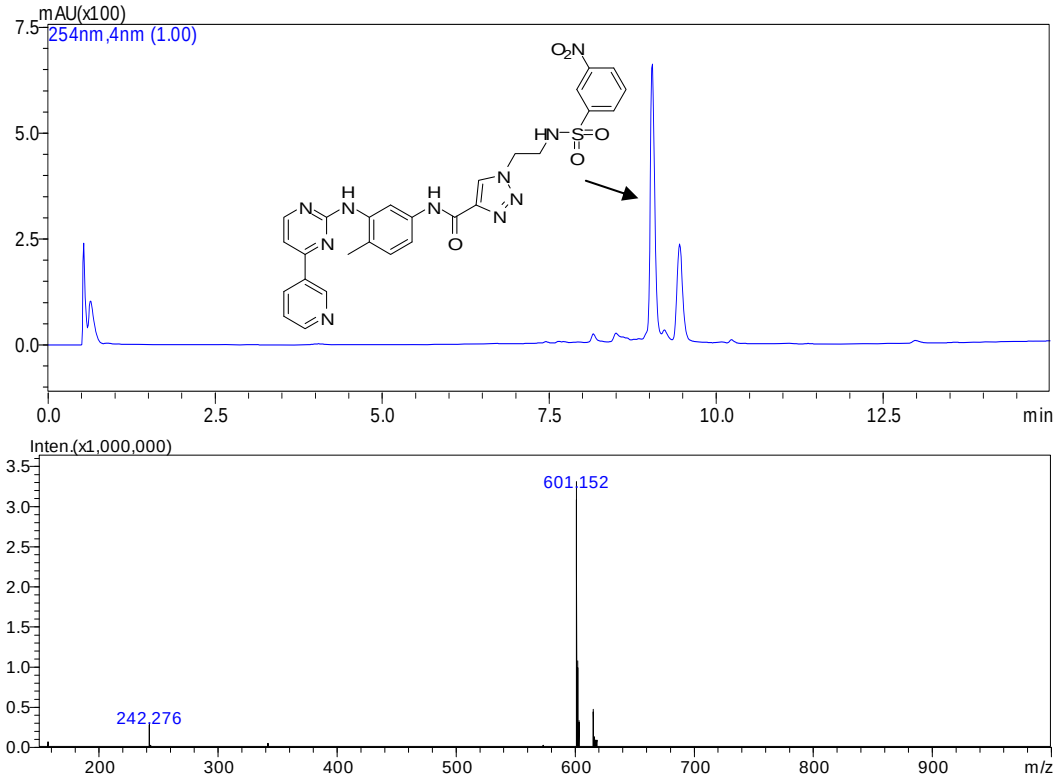
W1-SA16



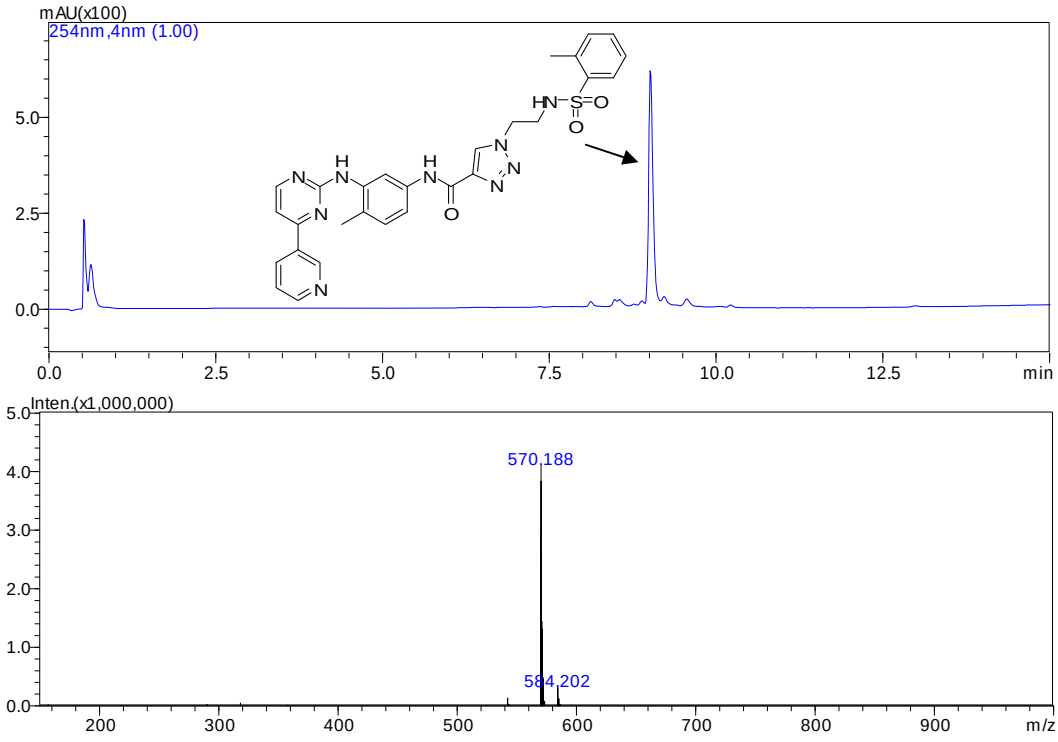
W1-SA18



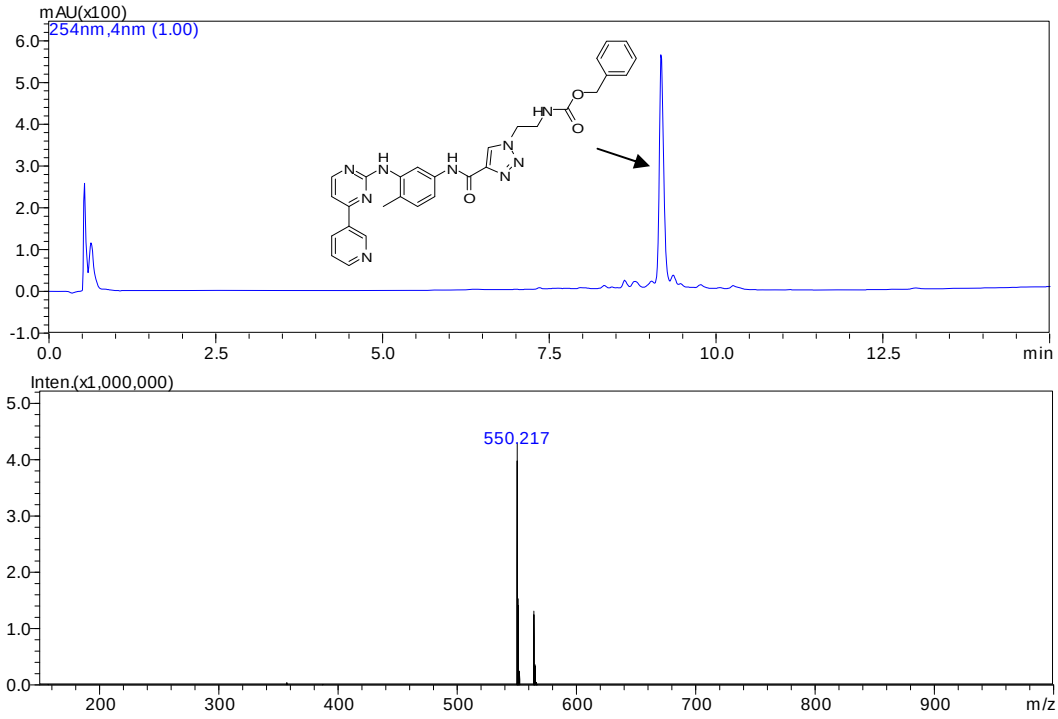
W1-SA19



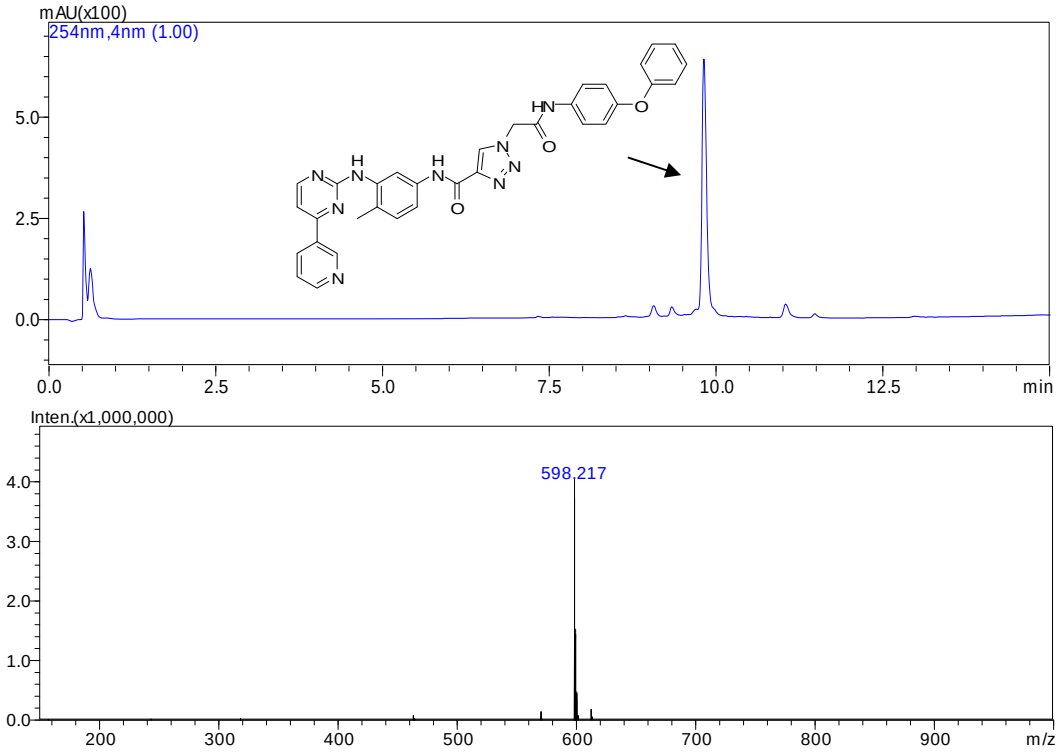
W1-SA20



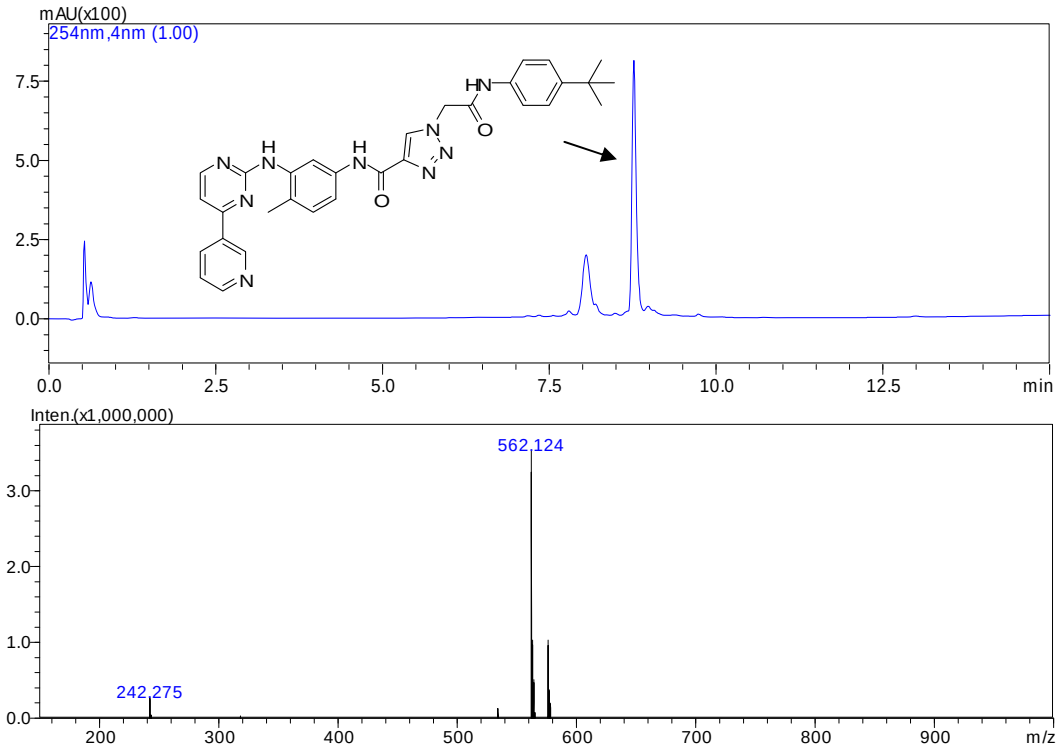
W1-SA25



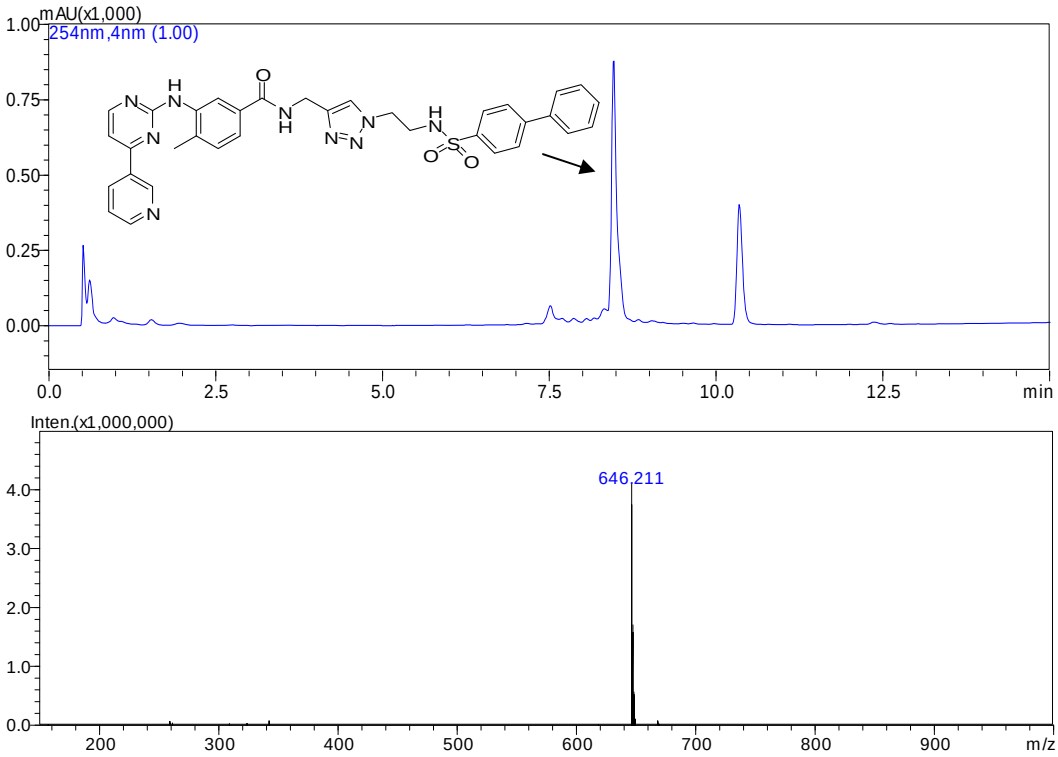
W1-A37



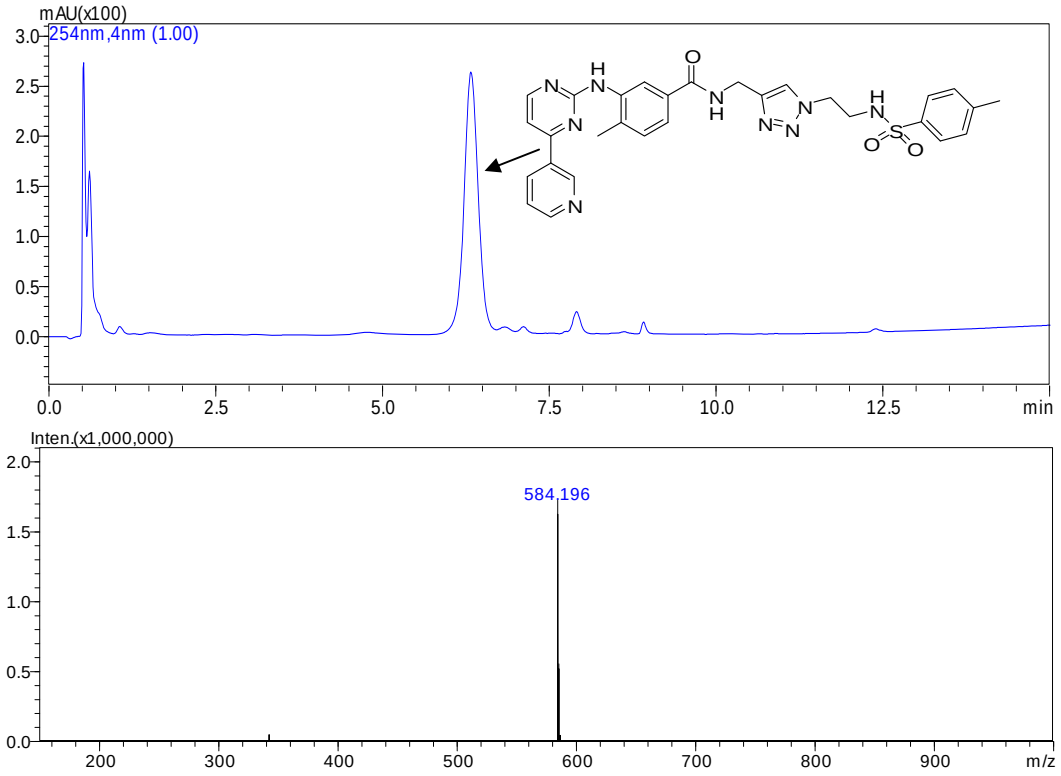
W1-A40


mAU(x100)
254nm,4nm (1.00)
7.5
5.0
2.5
0.0
0.0
2.5
5.0
7.5
10.0
12.5
min
Inten.(x1,000,000)
562.124
242.275
3.0
2.0
1.0
0.0
200
300
400
500
600
700
800
900
m/z

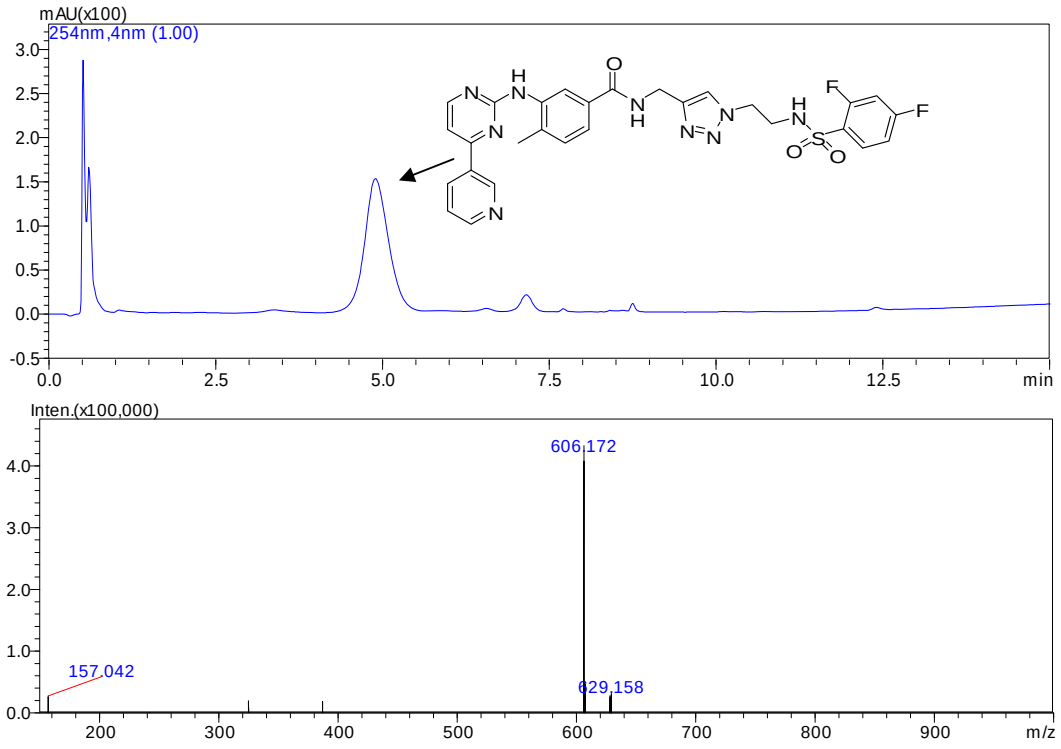
W2-SA2


mAU(x1,000)
254nm,4nm (1.00)
1.00
0.75
0.50
0.25
0.00
0.0
2.5
5.0
7.5
10.0
12.5
min
Inten.(x1,000,000)
646.211
4.0
3.0
2.0
1.0
0.0
200
300
400
500
600
700
800
900
m/z

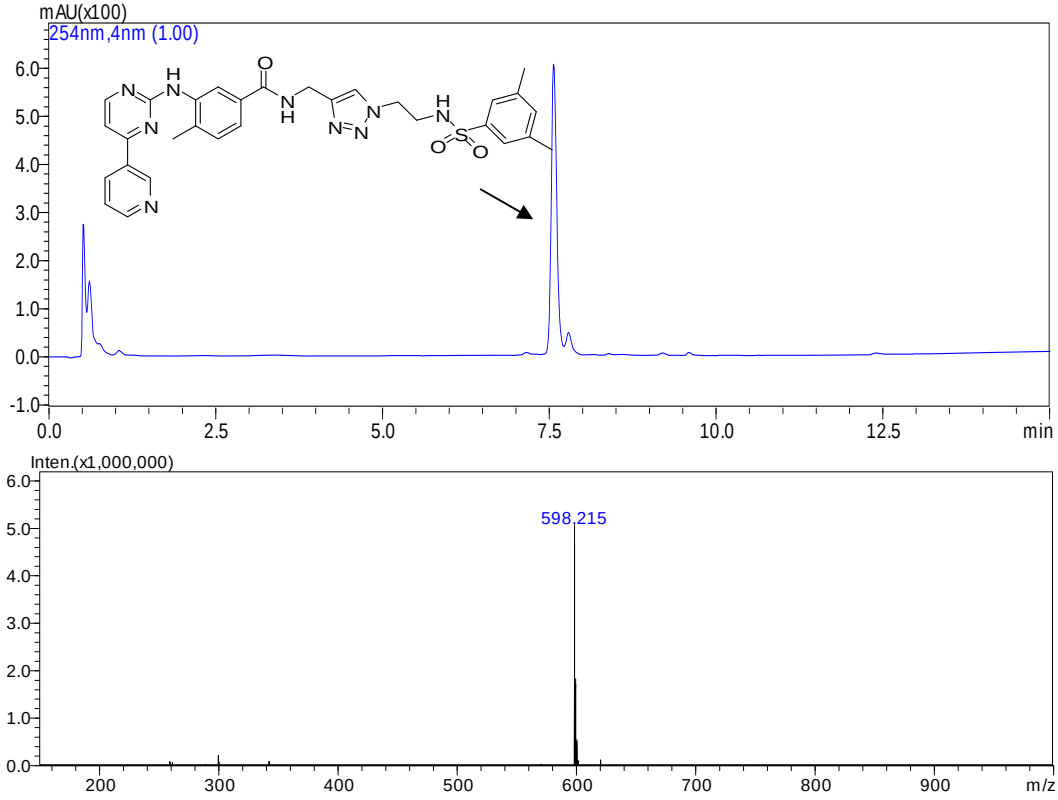
W2-SA5


mAU(x100)
254nm,4nm (1.00)
min
Inten.(x1,000,000)
584.196
m/z

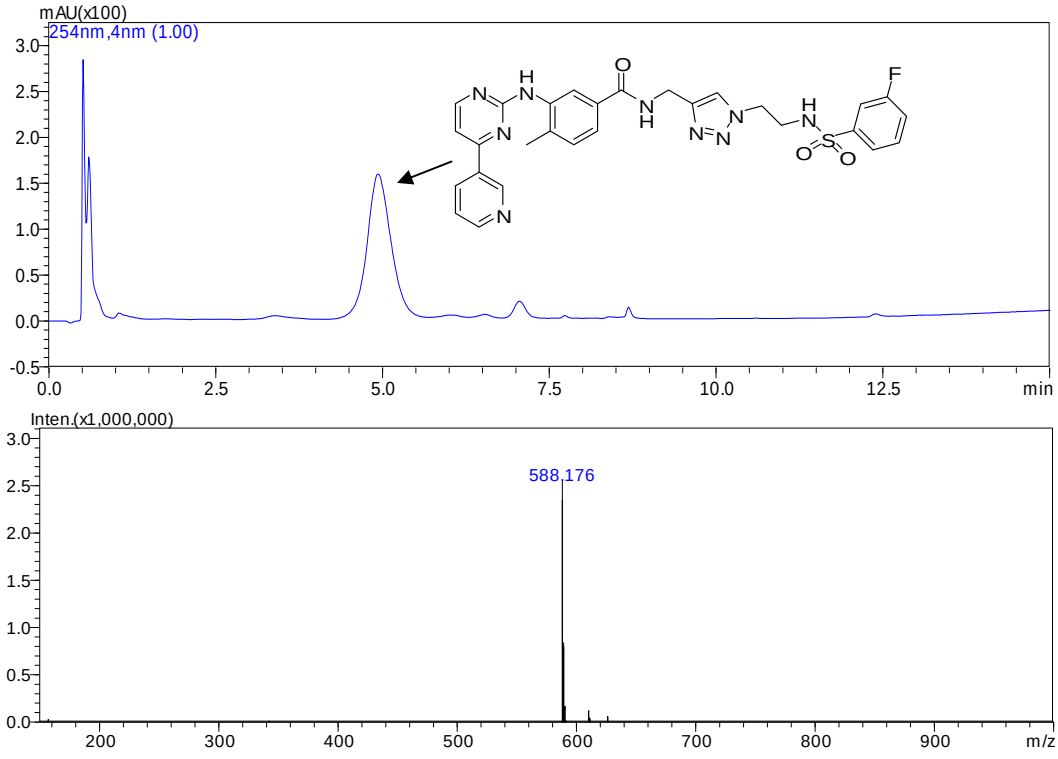
W2-SA6


mAU(x100)
254nm,4nm (1.00)
min
Inten.(x100,000)
606.172
157.042
629.158
m/z

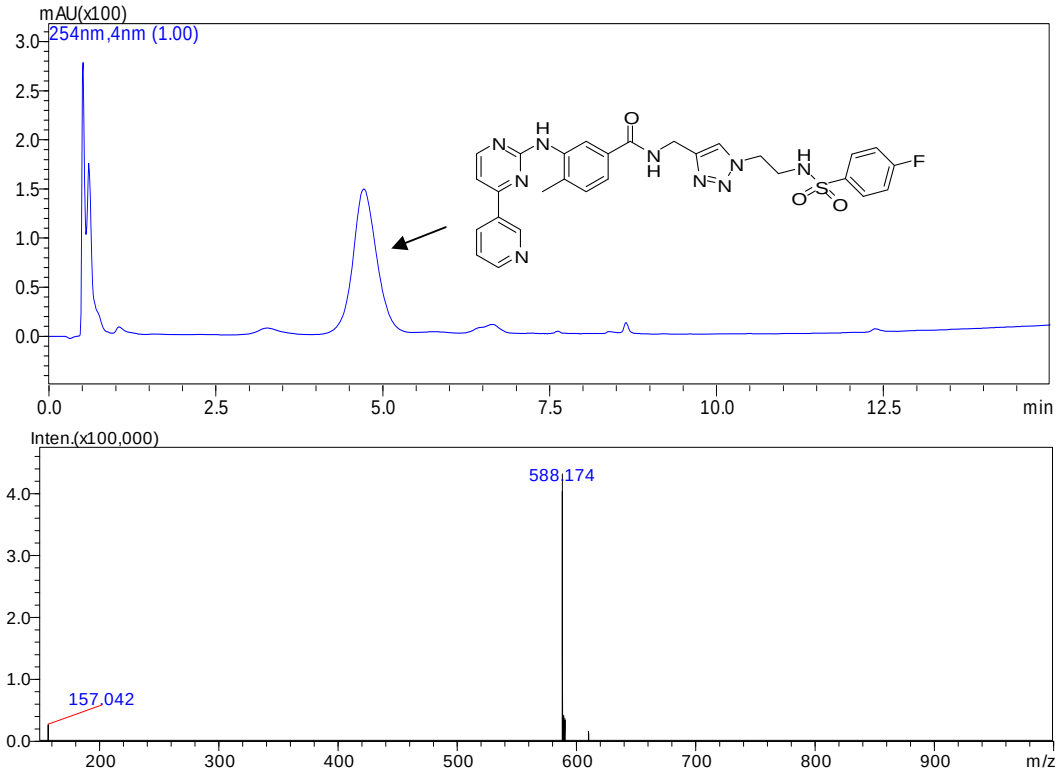
W2-SA8



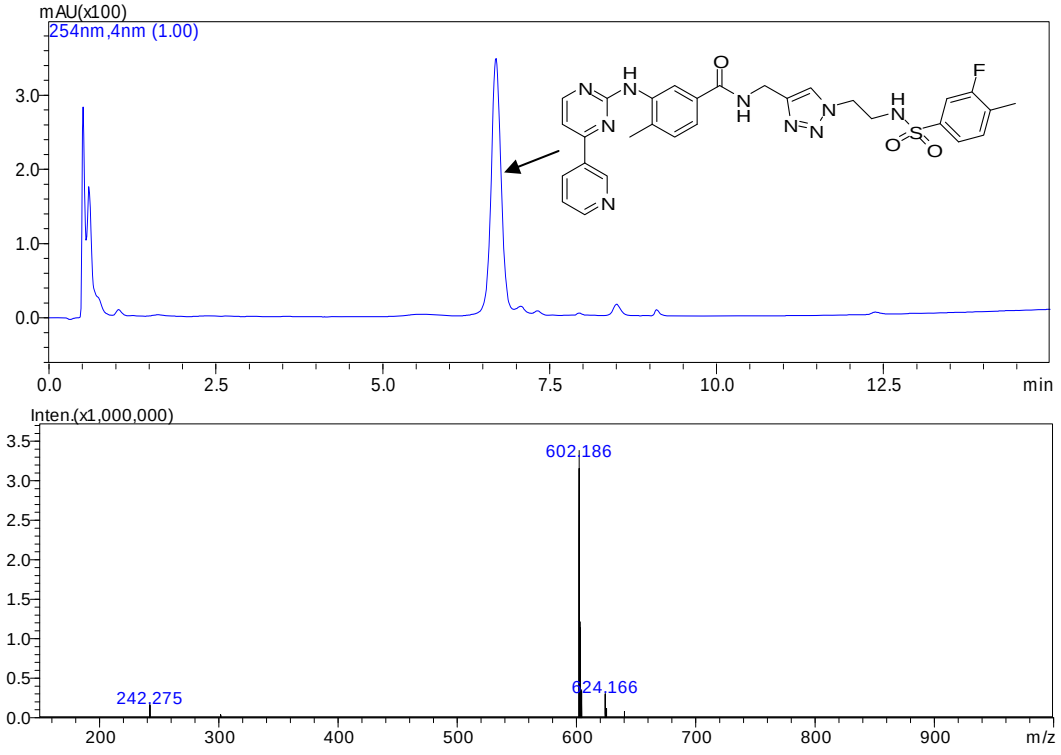
W2-SA10



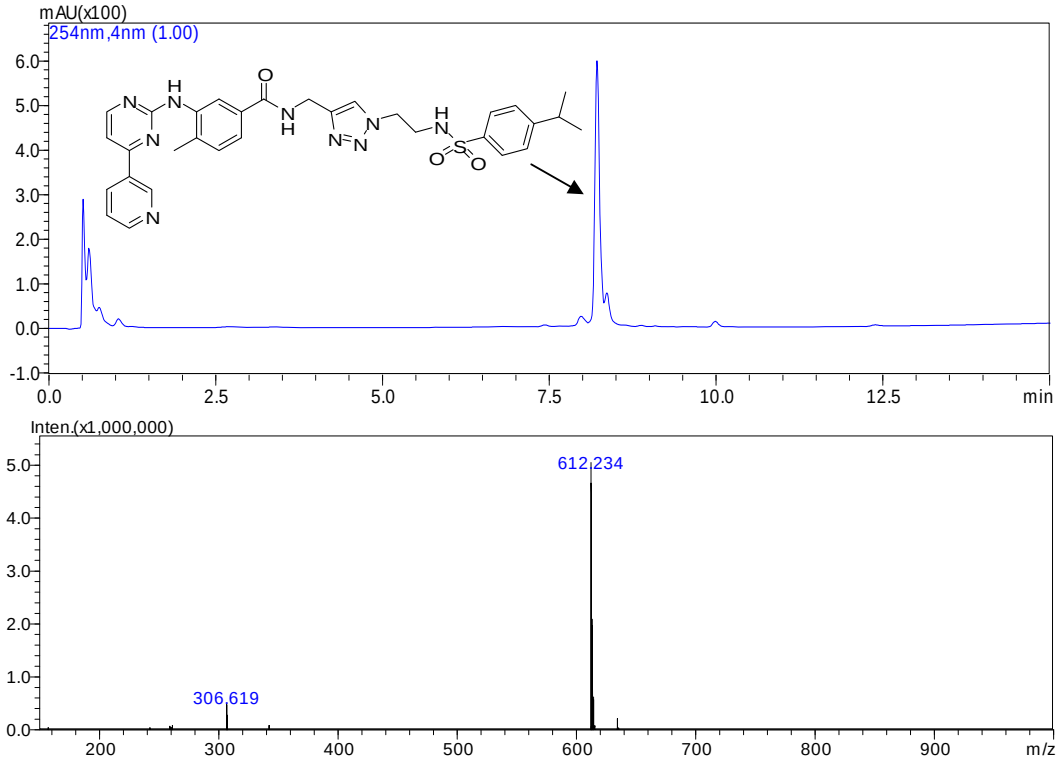
W2-SA11



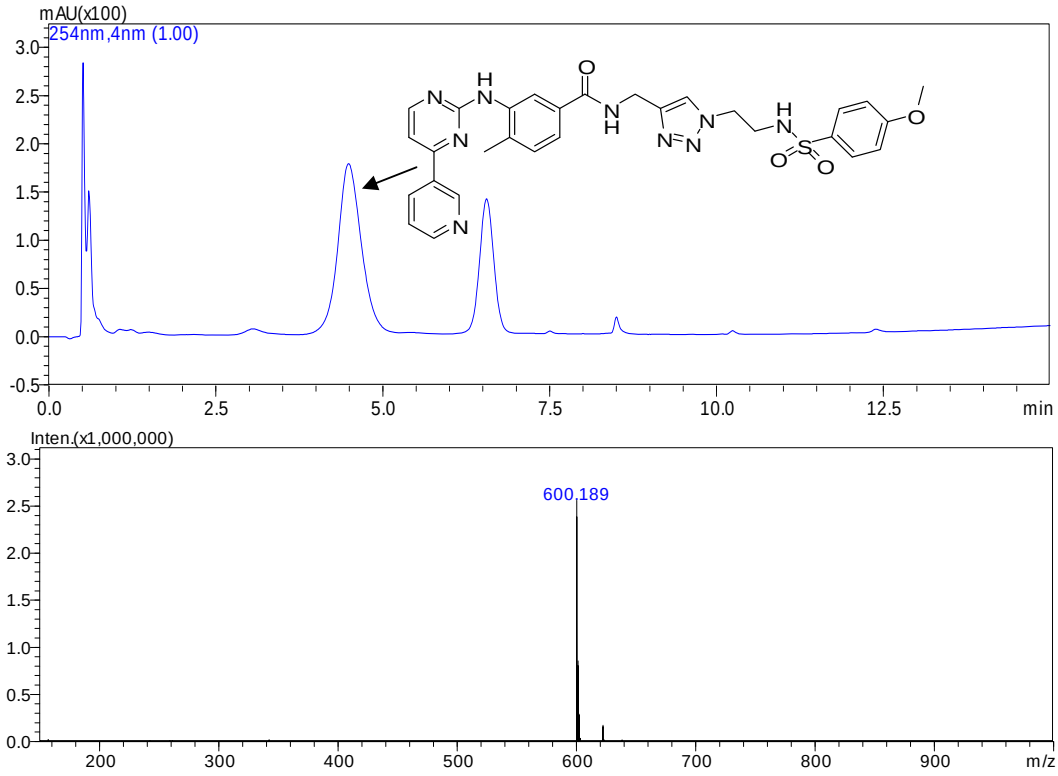
W2-SA12



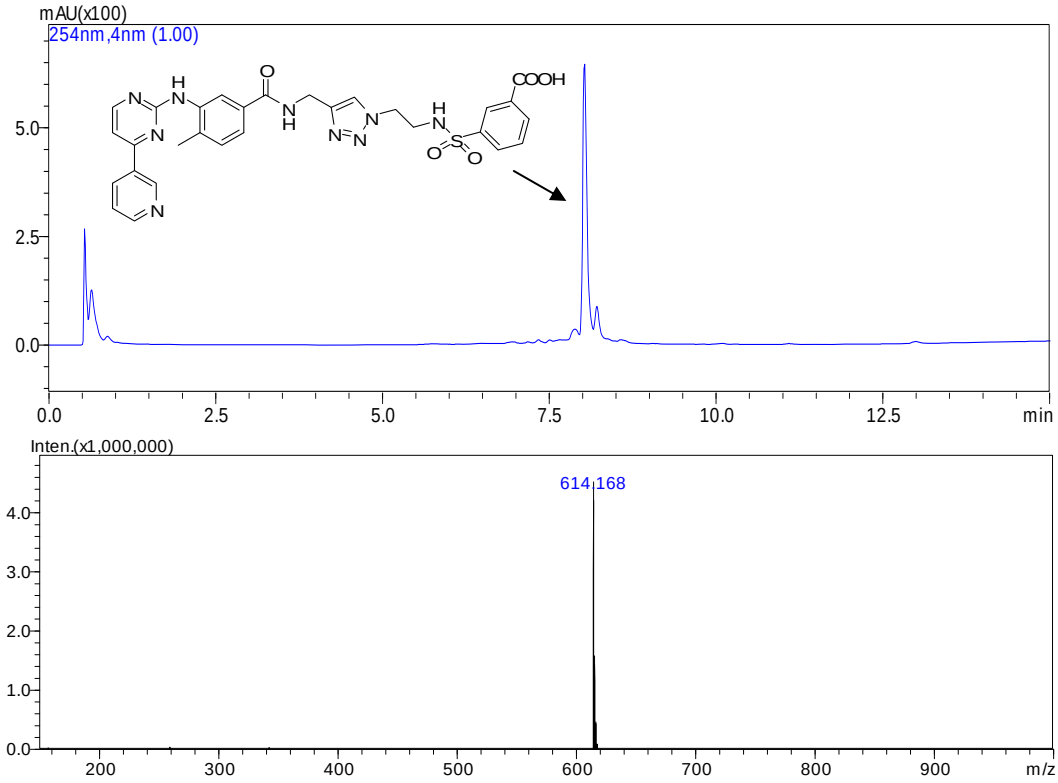
W2-SA14



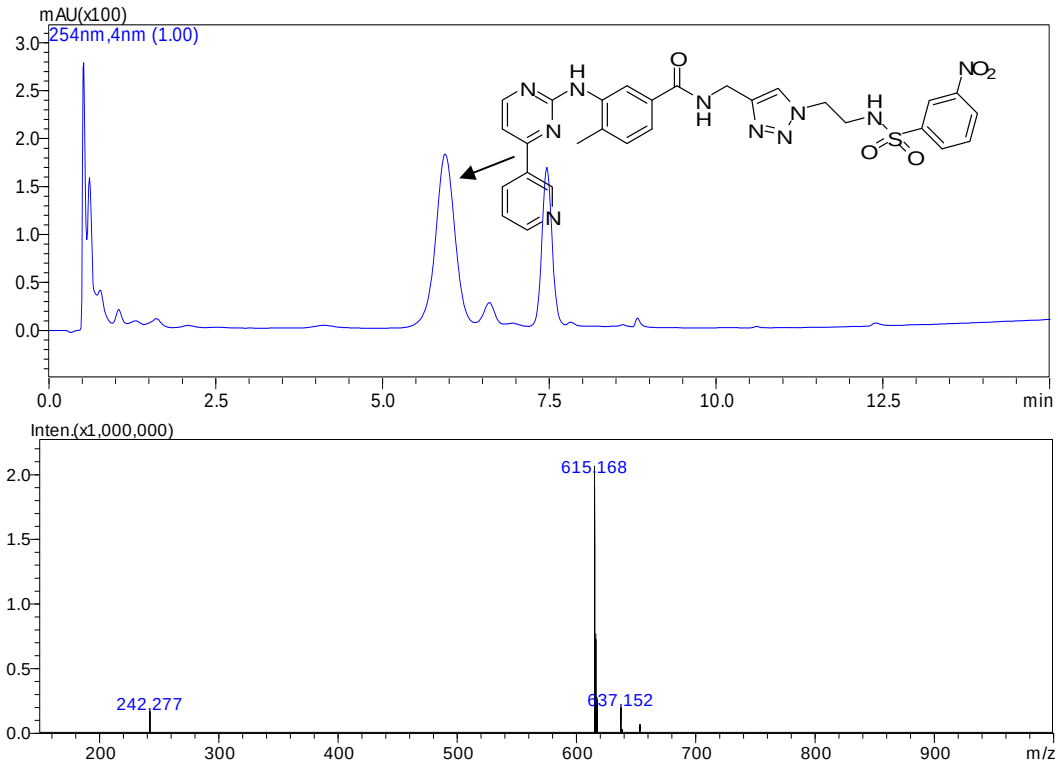
W2-SA15



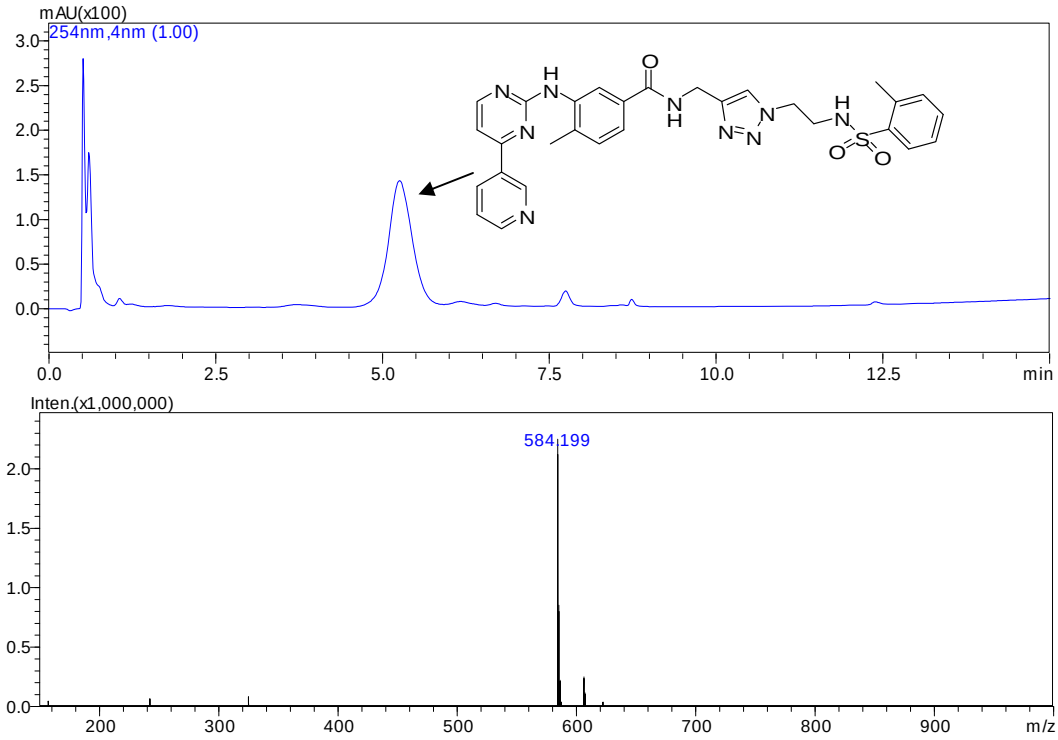
W2-SA16



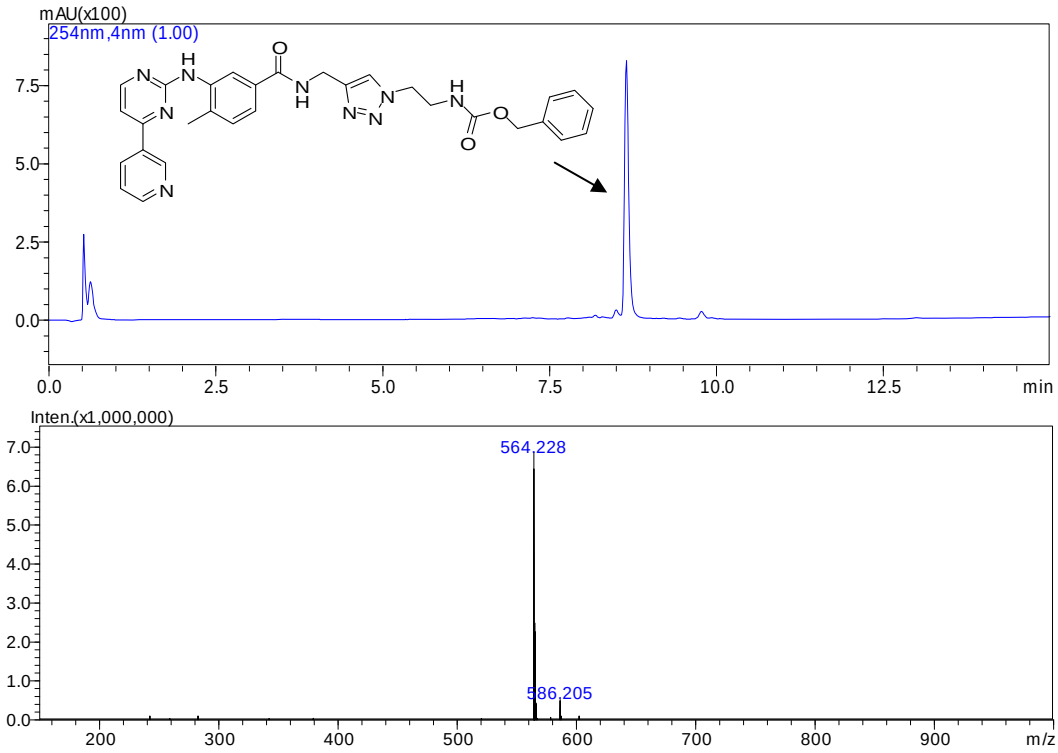
W2-SA19



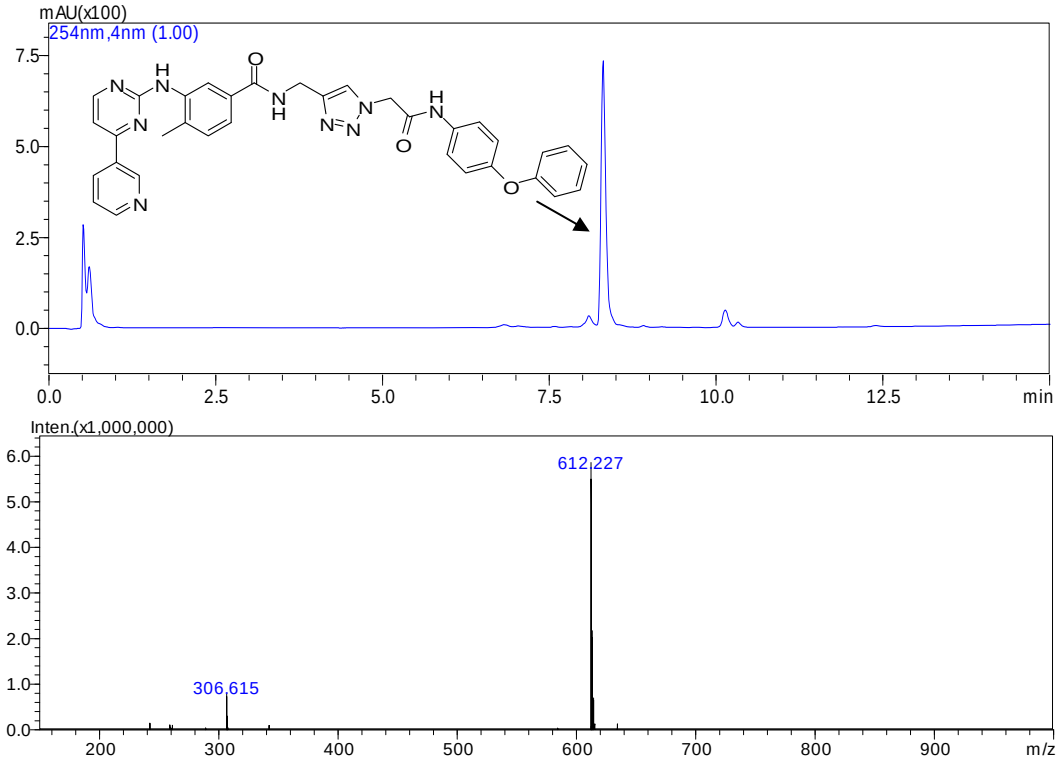
W2-SA20



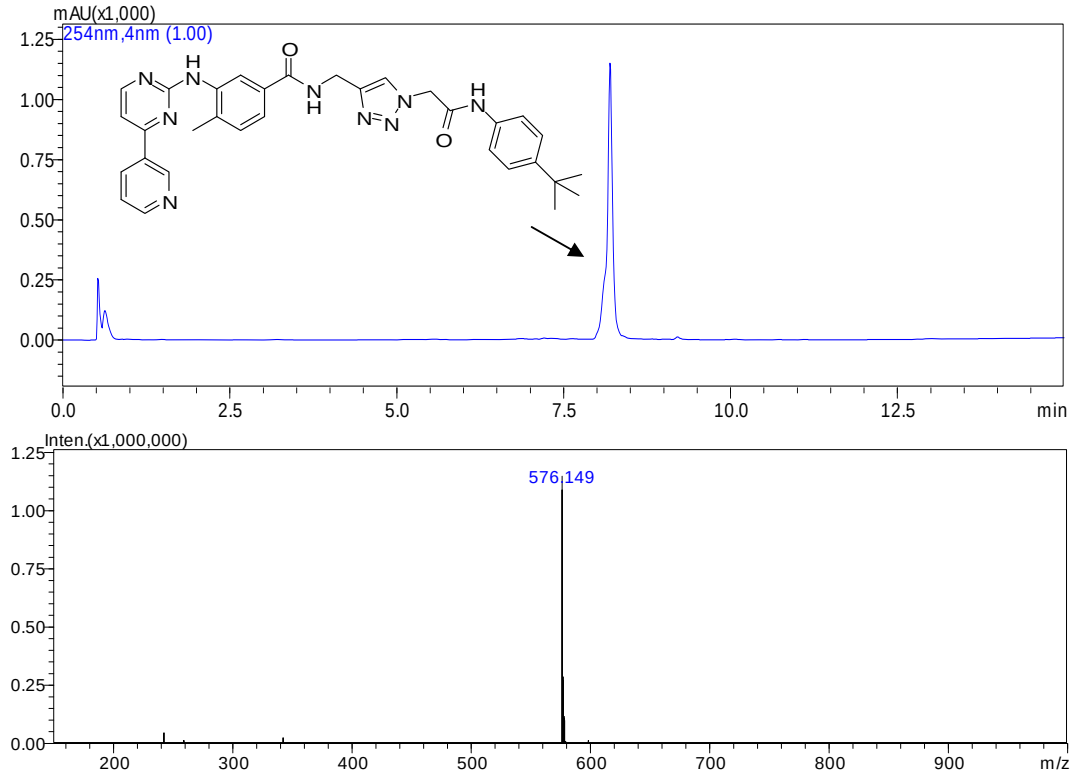
W2-SA25



W2-A37

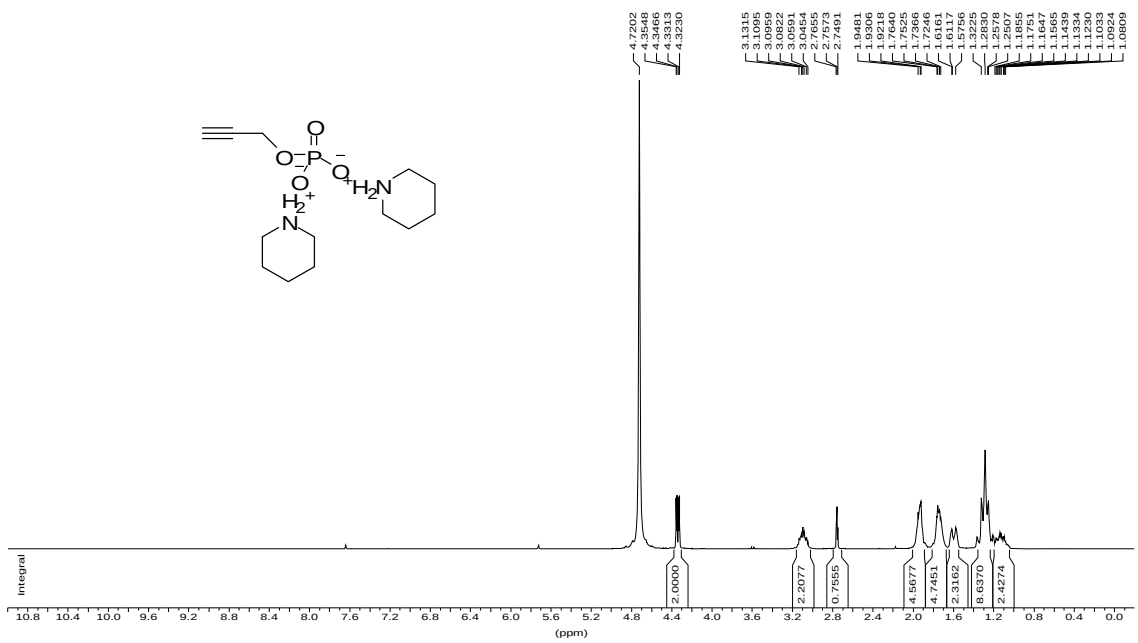

mAU(x100)
254nm,4nm (1.00)
7.5
5.0
2.5
0.0
0.0
2.5
5.0
7.5
10.0
12.5
min
Inten.(x1,000,000)
612.227
306.615
6.0
5.0
4.0
3.0
2.0
1.0
0.0
200
300
400
500
600
700
800
900
m/z

W2-A40

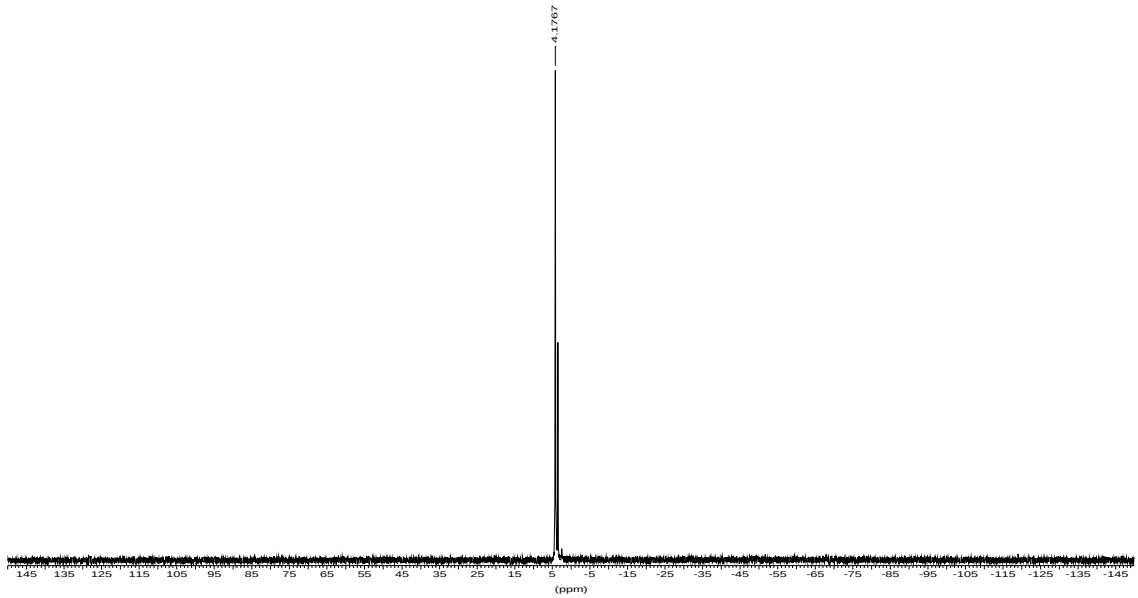

mAU(x1,000)
254nm,4nm (1.00)
1.25
1.00
0.75
0.50
0.25
0.00
0.0
2.5
5.0
7.5
10.0
12.5
min
Inten.(x1,000,000)
576.149
1.25
1.00
0.75
0.50
0.25
0.00
200
300
400
500
600
700
800
900
m/z

2. NMR Spectra

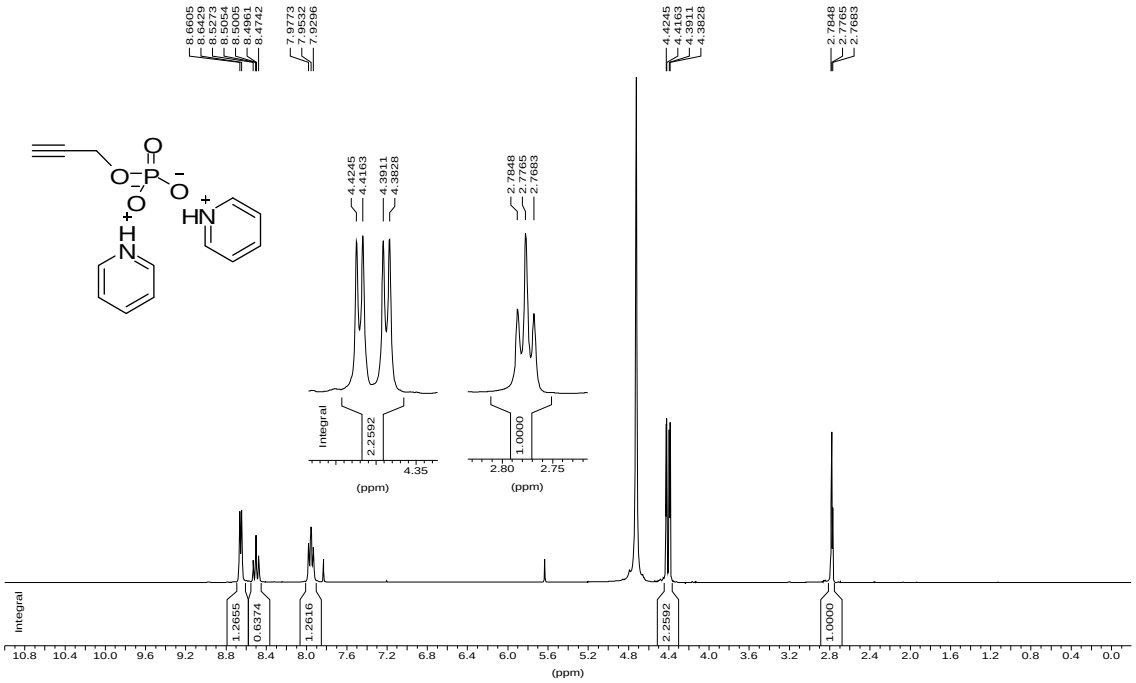
1H normal range AV300, 106



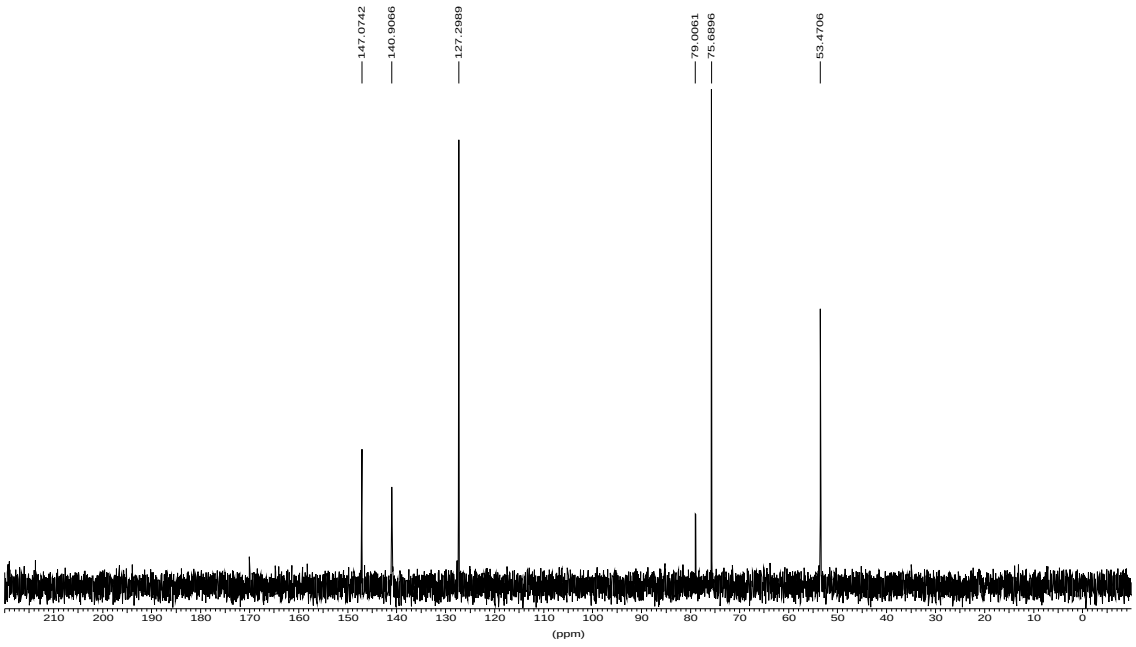
31P AV300



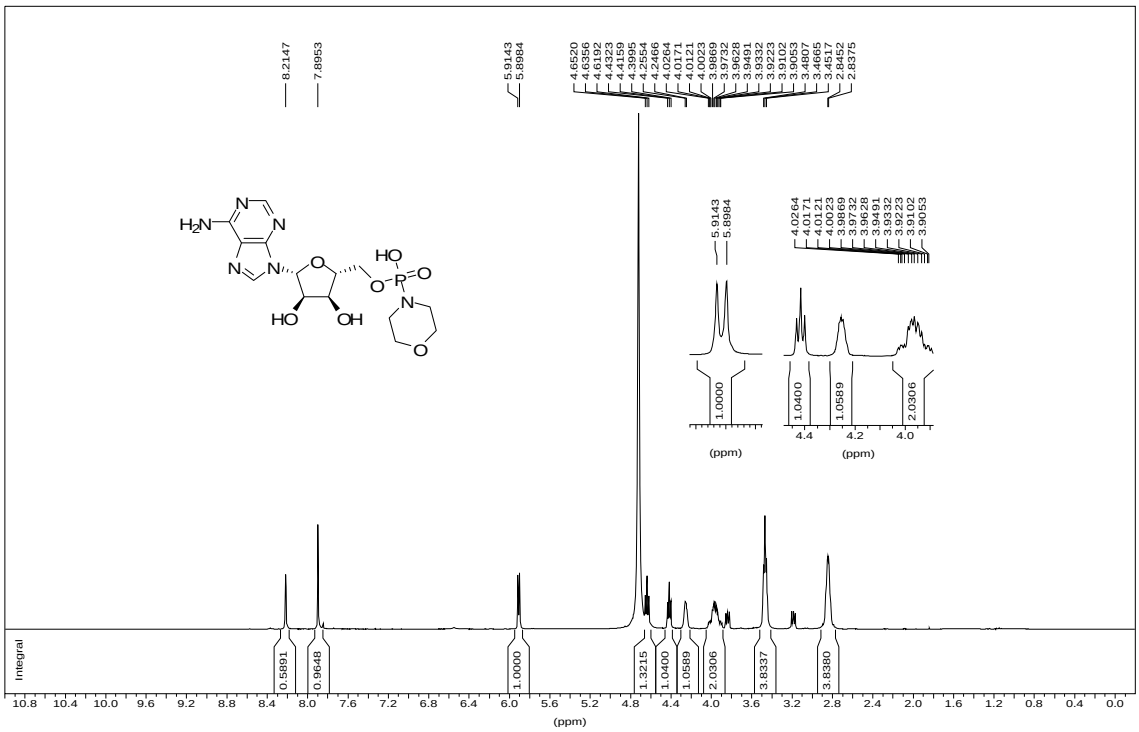
1H normal range AV300, 106, water elution



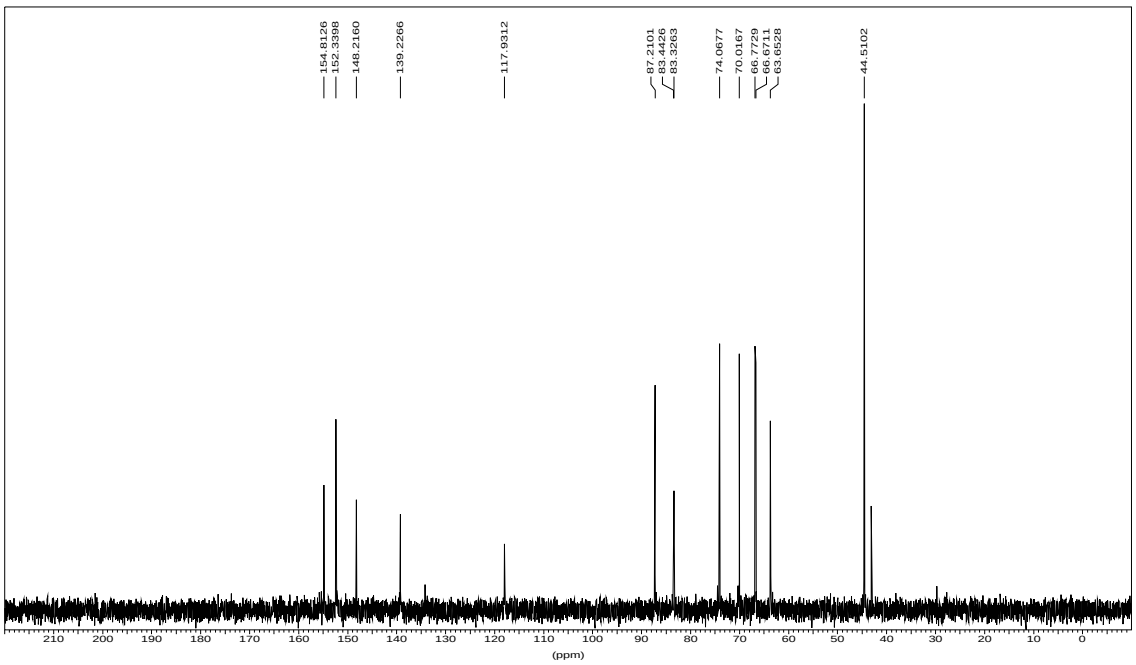
13C Standard AC300, Propa.Phos(Pyr),slow, 5%



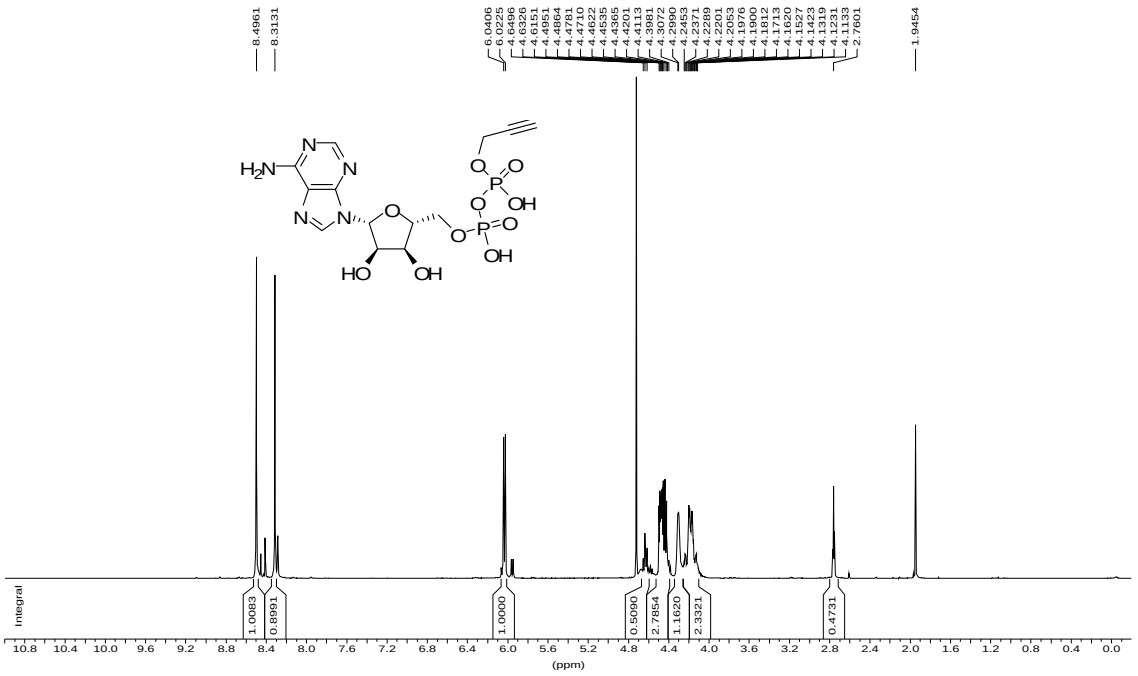
1H normal range AC300



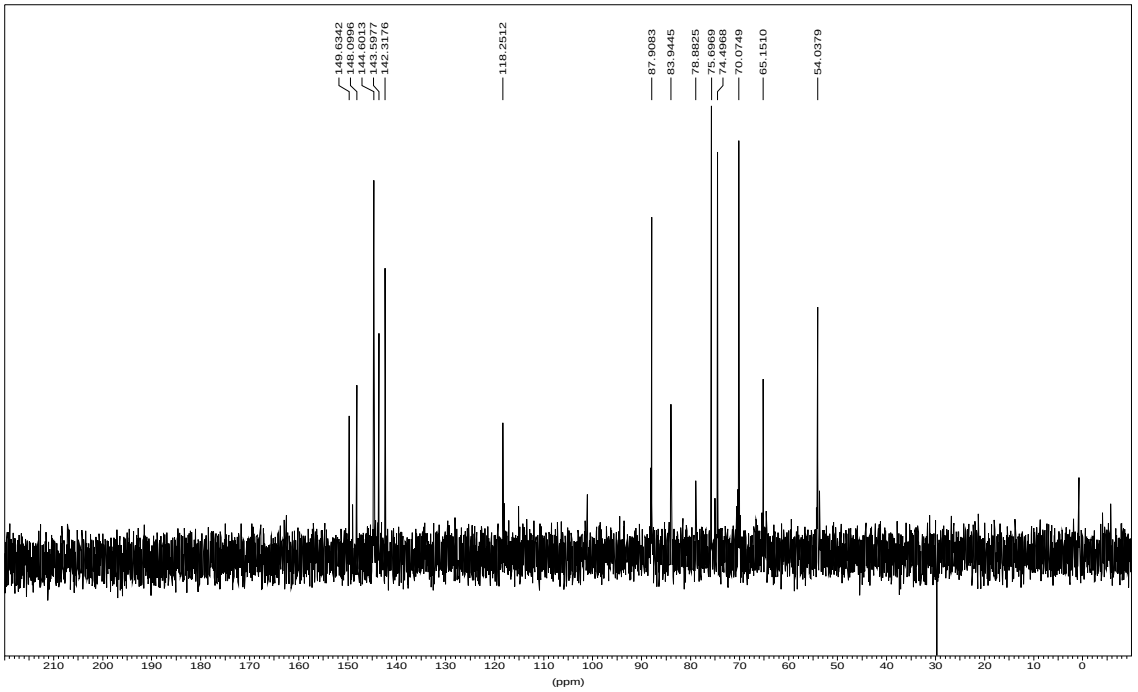
13C Standard AC300



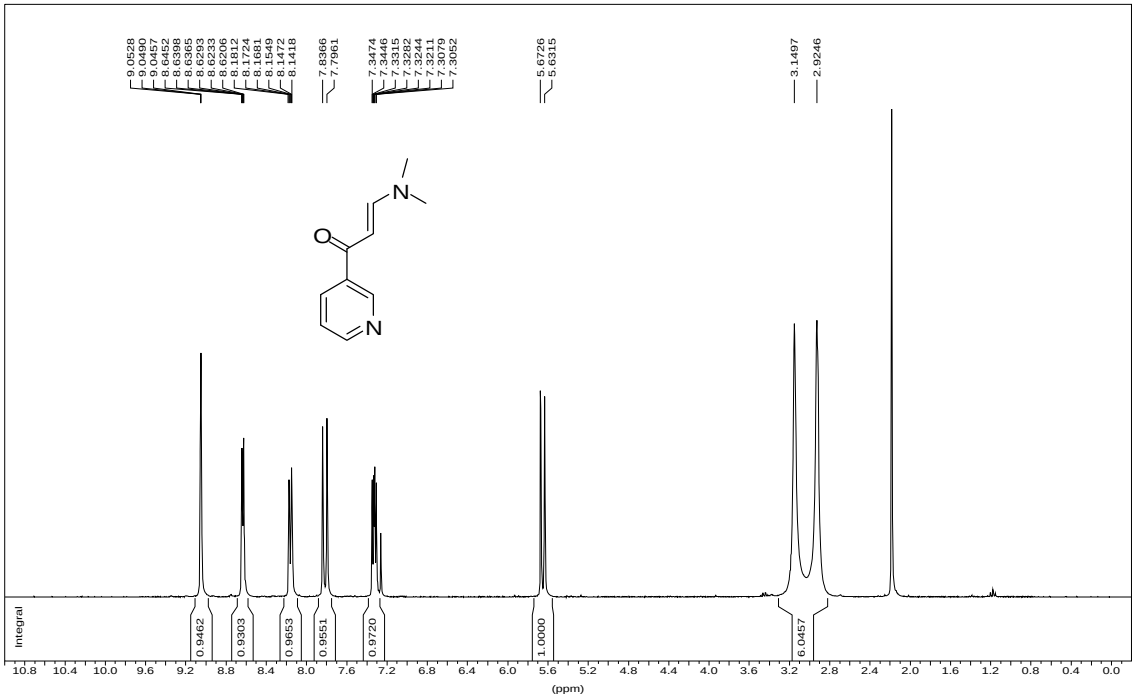
1H Water suppression



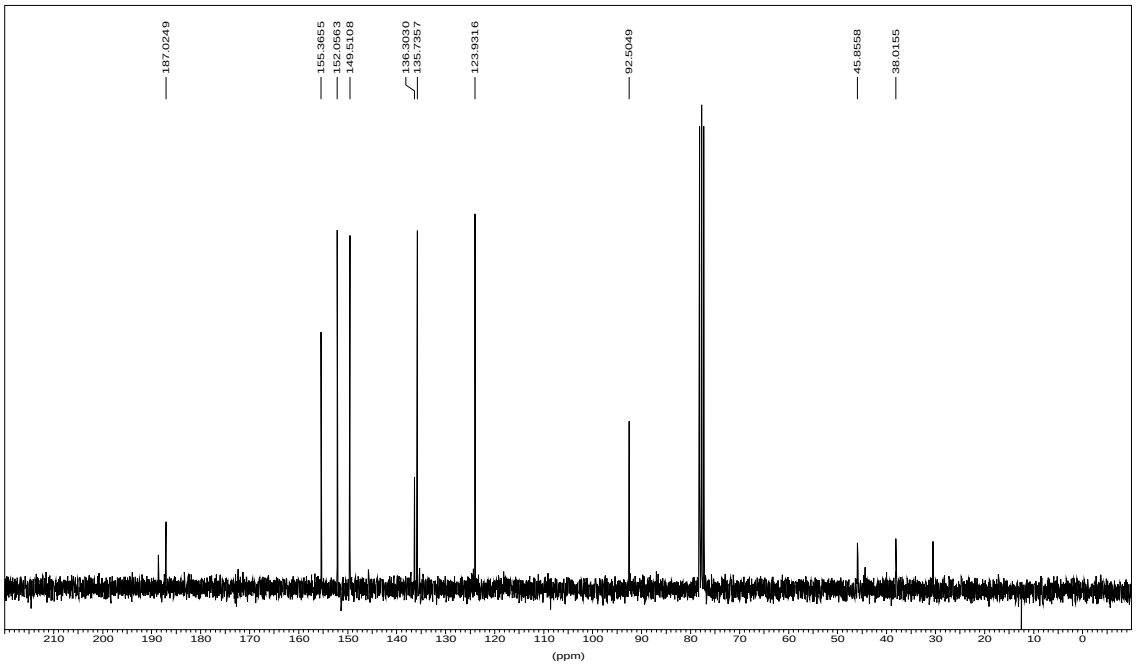
13C Standard AC300



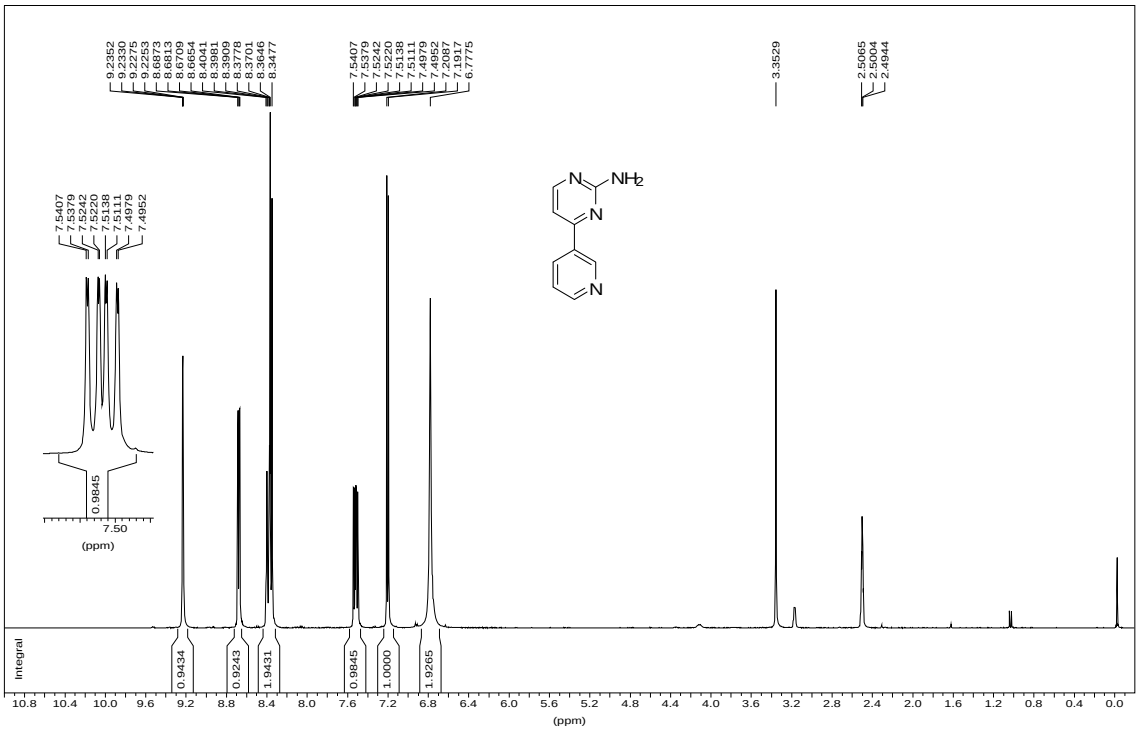
1H normal range AC300, 256



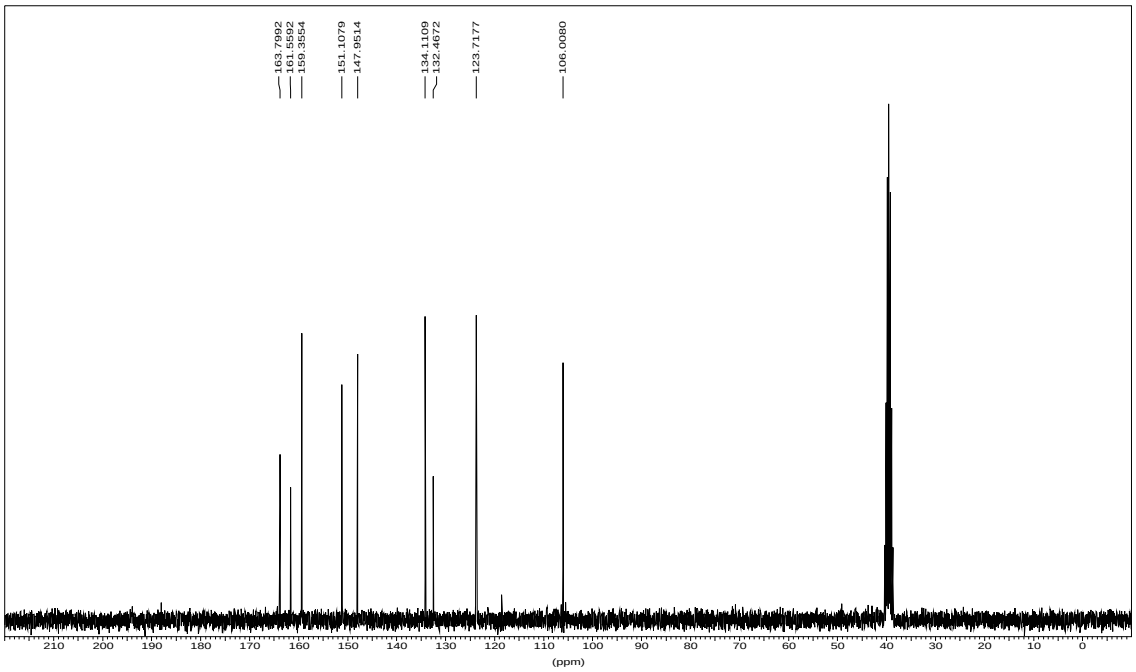
13C Standard AC300, 256



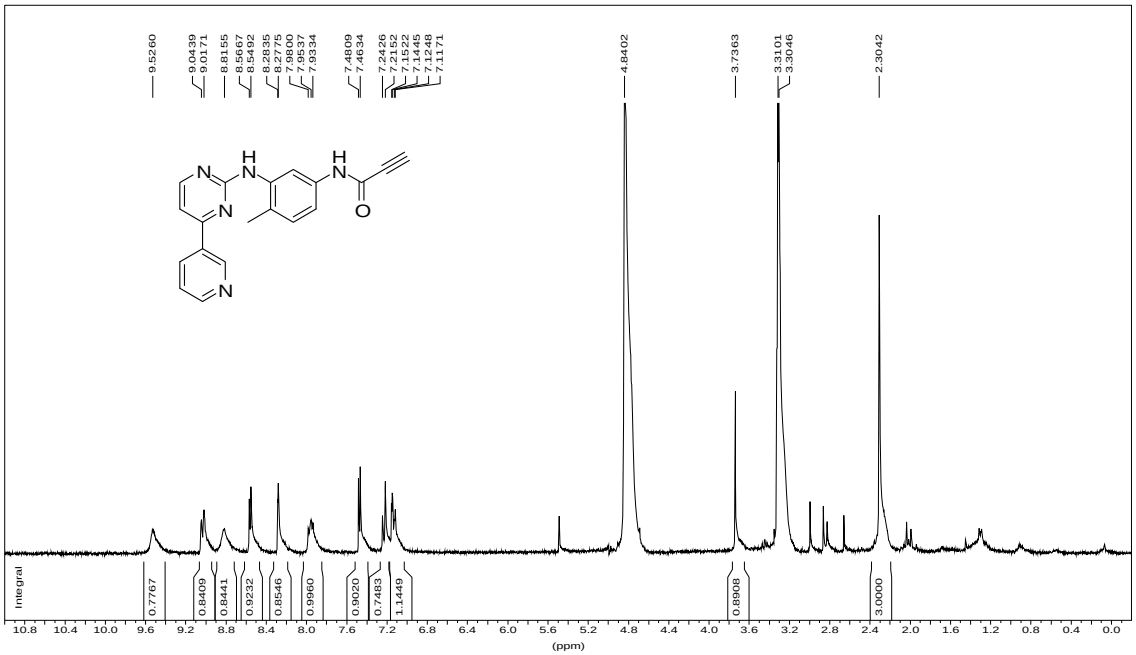
1H normal range AC300



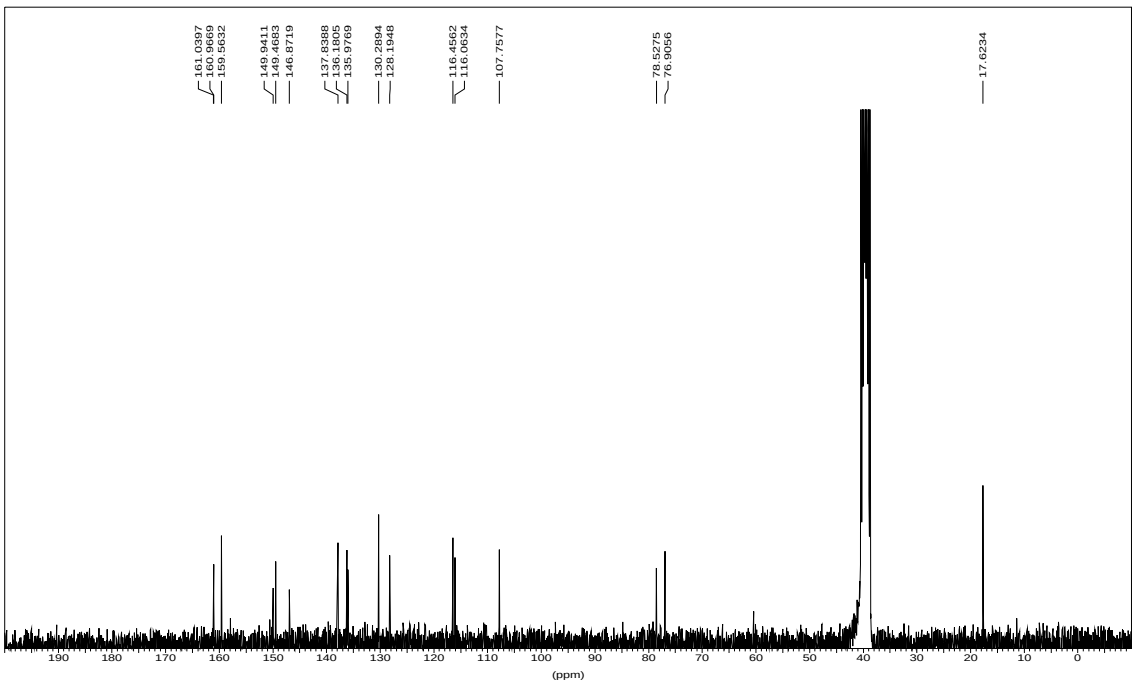
13C Standard AC300



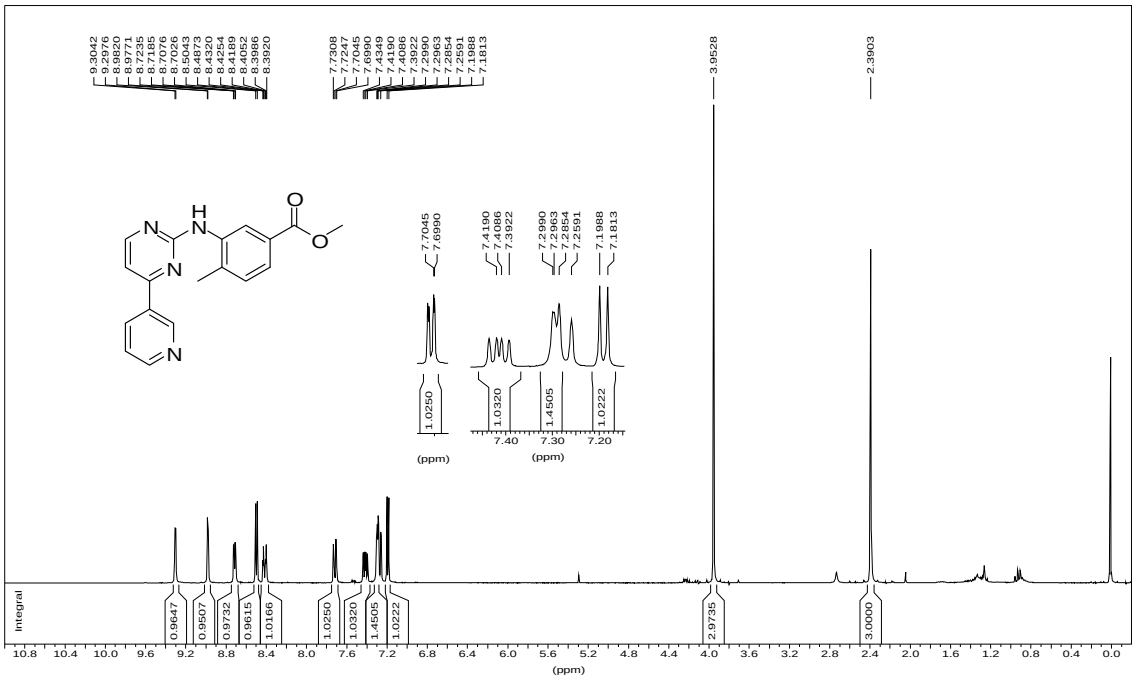
1H normal range AC300, B3-217



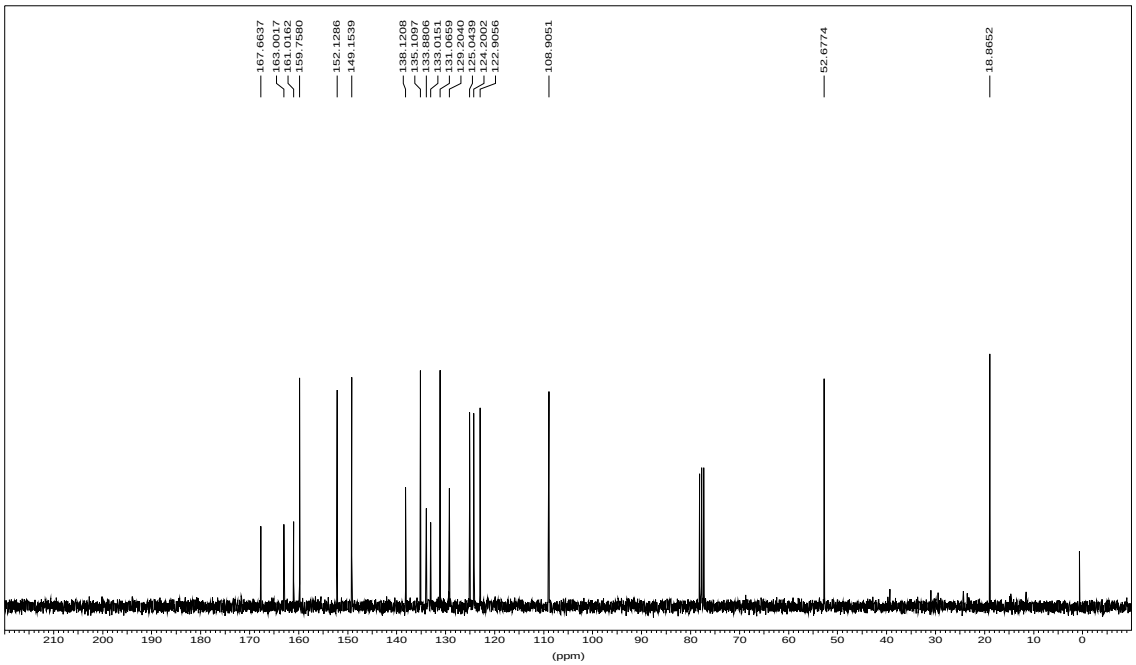
13C Standard AC300, W1



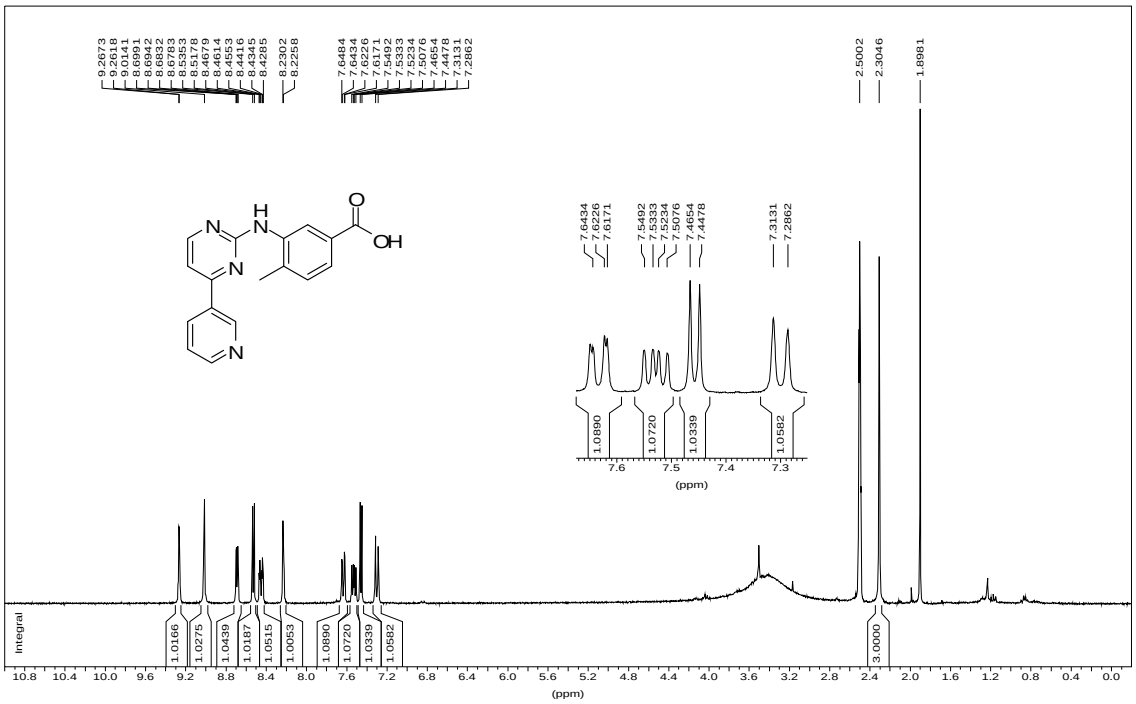
1H normal range AC300



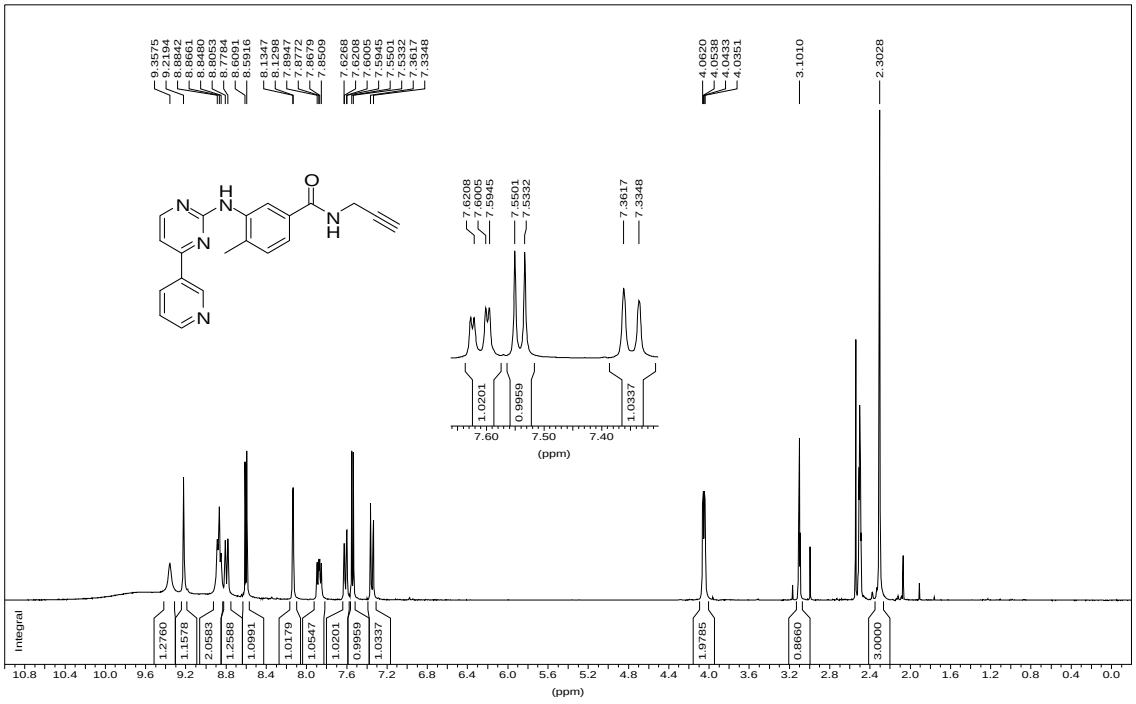
13C Standard AC300



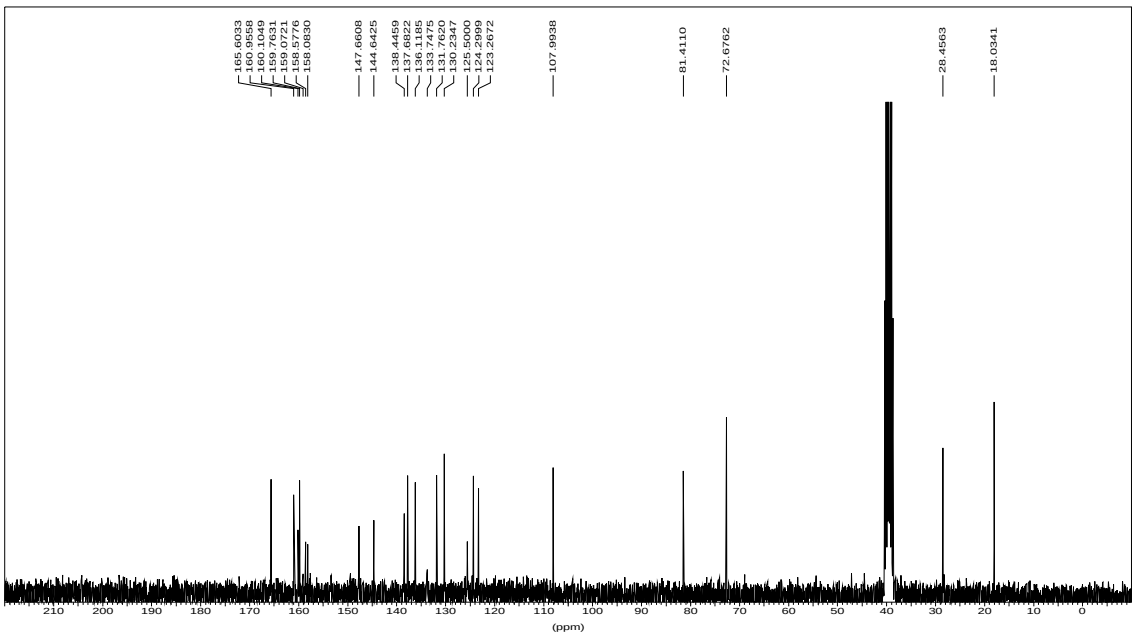
1H normal range AC300

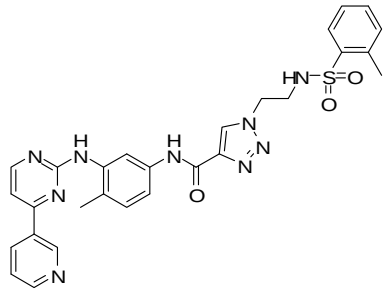


1H normal range AC300, W2

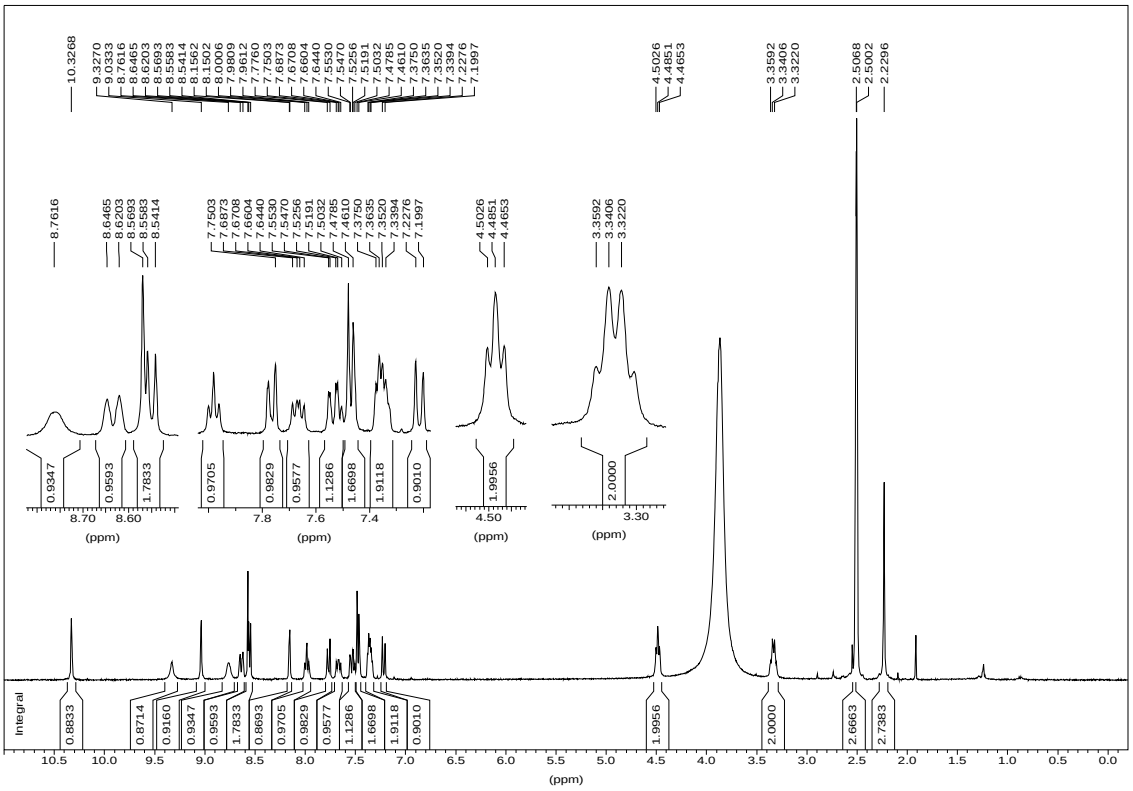


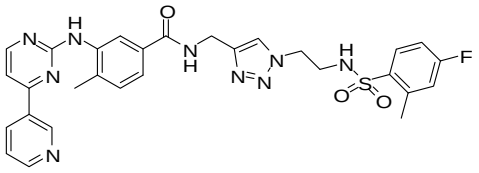
13C Standard AC300, W2





1H normal range AC300, W1-SA20





1H normal range AC300, W2-SA13