

Supplemental Characterization Data

Furoxans (oxadiazole-4N-oxides) with Attenuated Reactivity are Neuroprotective, Cross the Blood Brain Barrier, and Improve Passive Avoidance Memory

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Kalee Royster[†], Maxwell Ducharme[†], Katelyn Hagood[†], Megan Post[†], Zahoor A. Shah[†], Isaac T.
Schiefer^{†*}*

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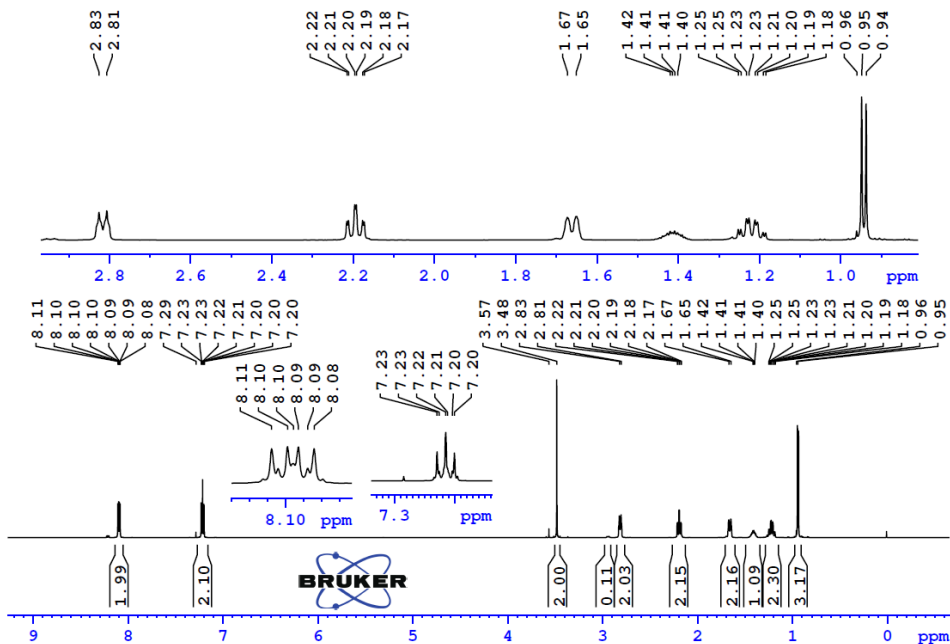
[‡]Department of Pharmacology and Experimental Therapeutics, College of Pharmacy and Pharmaceutical Sciences, University of Toledo, Toledo, OH 43614

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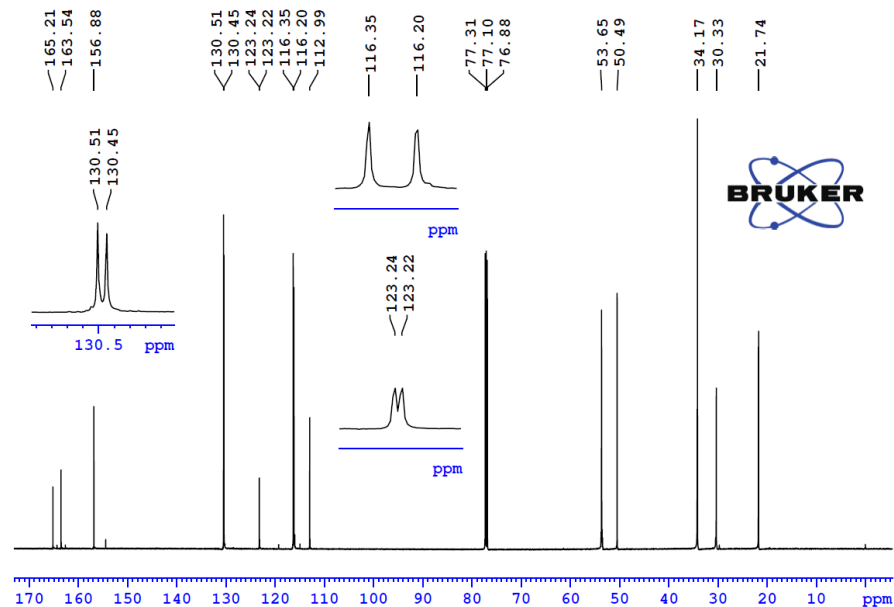
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Analysis Report

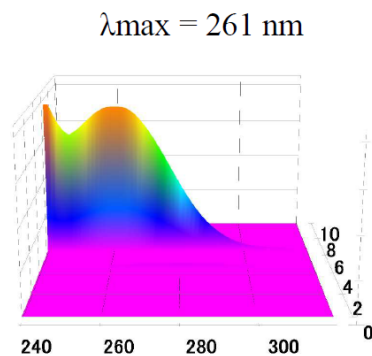
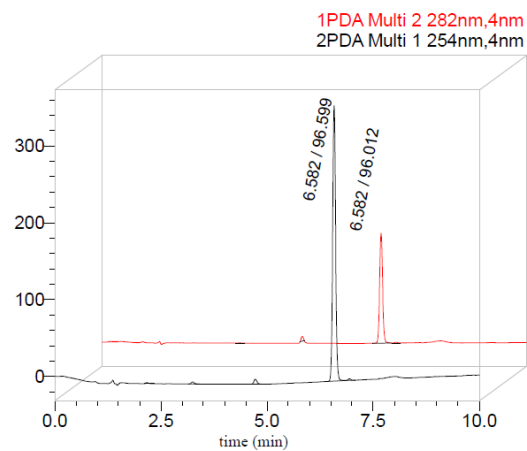
¹H NMR



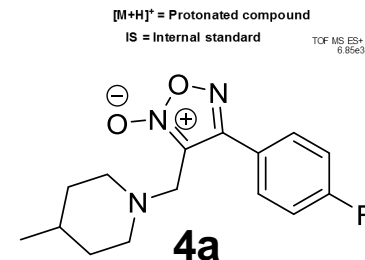
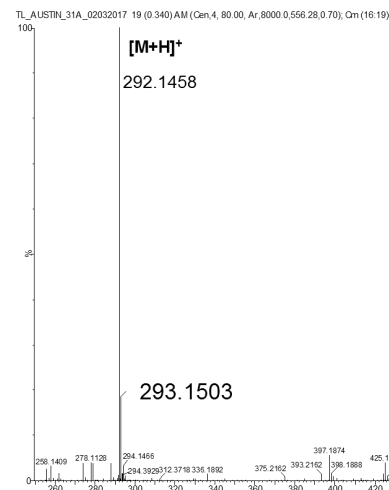
¹³C NMR



HPLC purity (2 wavelength)



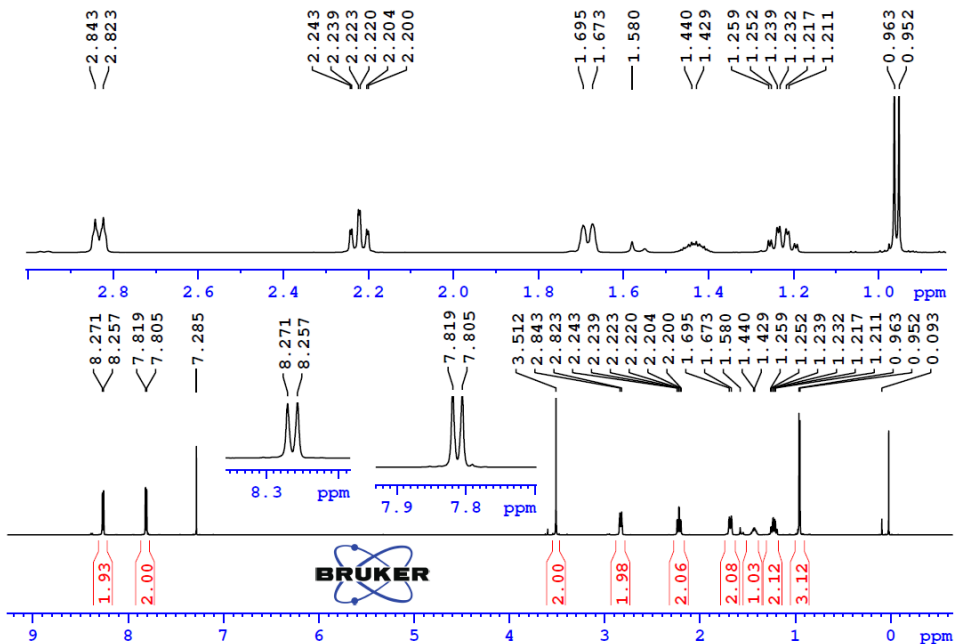
S3



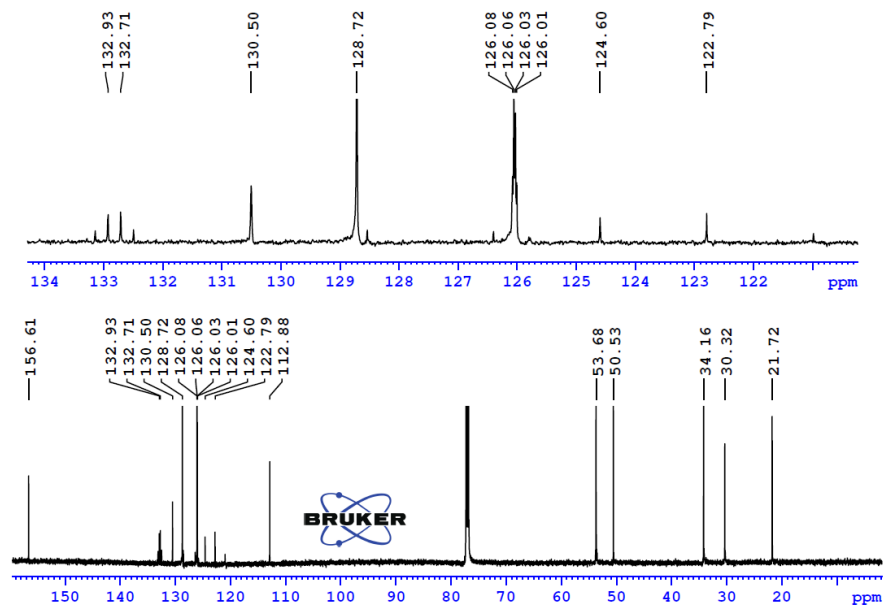
Mass Accuracy = ((292.1458-292.1461)/292.1461) * 10⁶ = -1.0 ppm

Analysis Report

¹H NMR

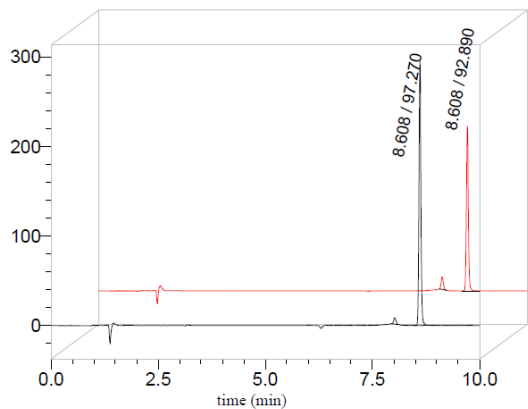


¹³C NMR

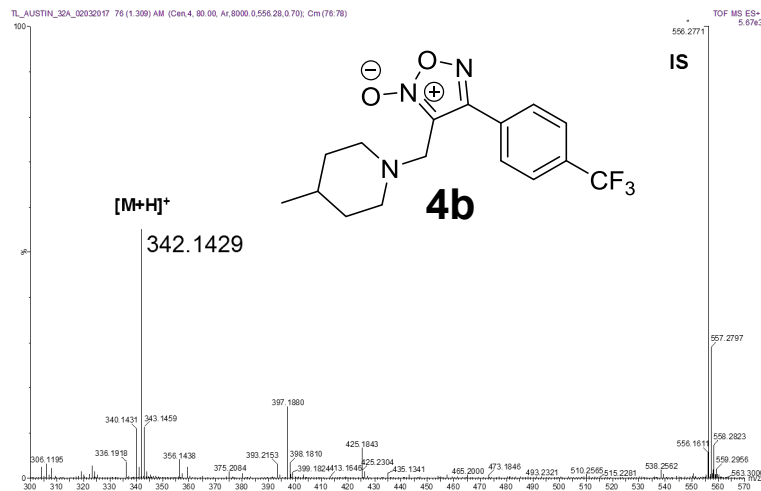
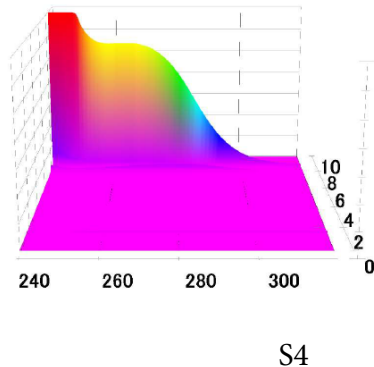


HPLC purity (2 wavelength)

1PDA Multi 2 282nm,4nm
2PDA Multi 1 254nm,4nm



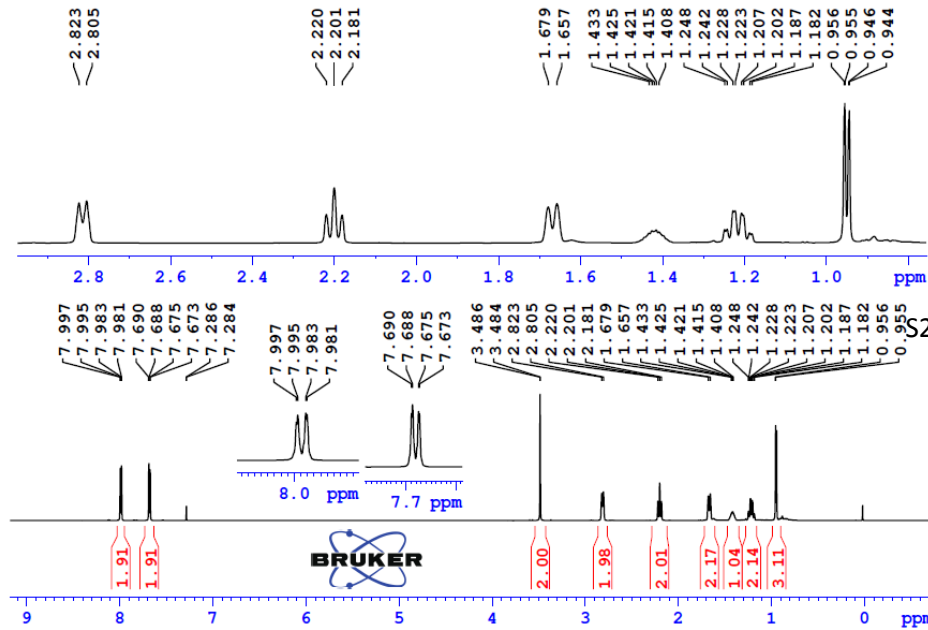
$\lambda_{max} = 263 \text{ nm}$



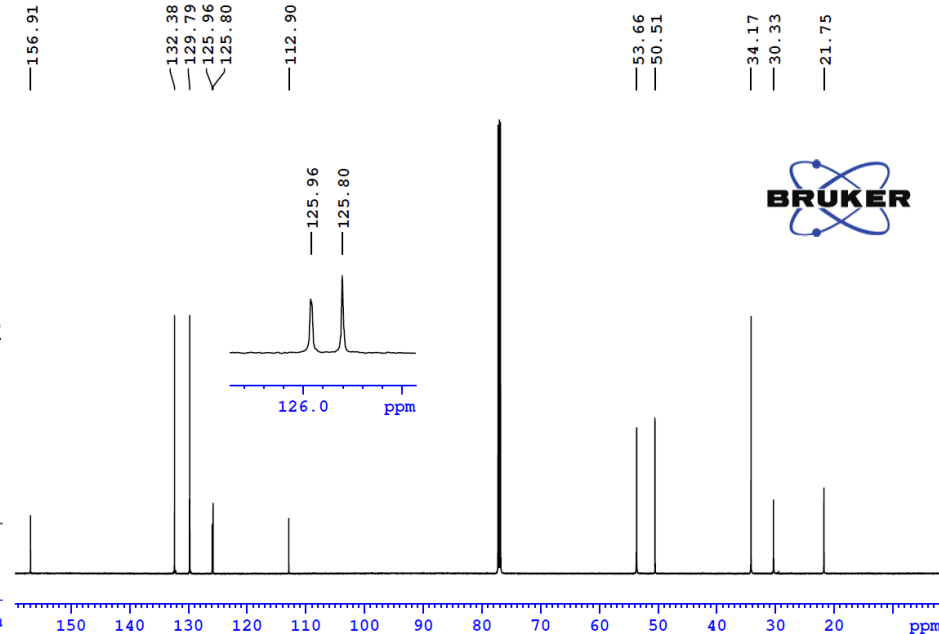
Mass Accuracy = $((342.1429-342.1429)/342.1429) \times 10^6 = 0 \text{ ppm}$

Analysis Report

¹H NMR

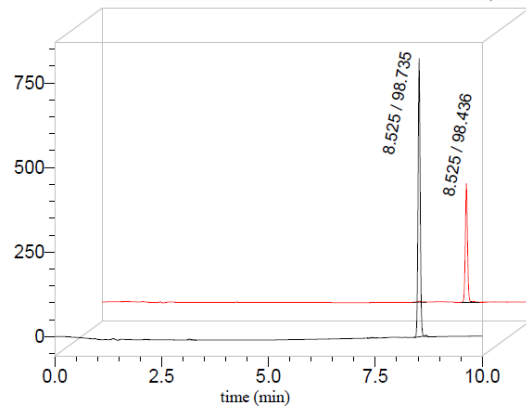


¹³C NMR

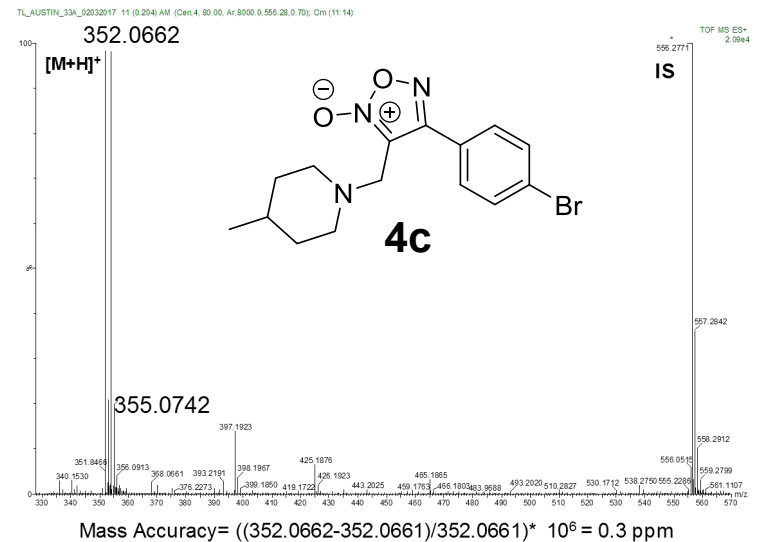
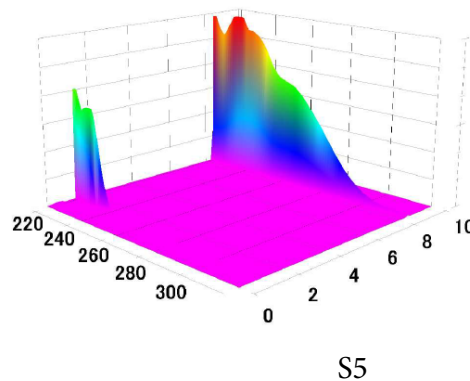


HPLC purity (2 wavelength)

1PDA Multi 2 282nm,4nm
2PDA Multi 1 254nm,4nm

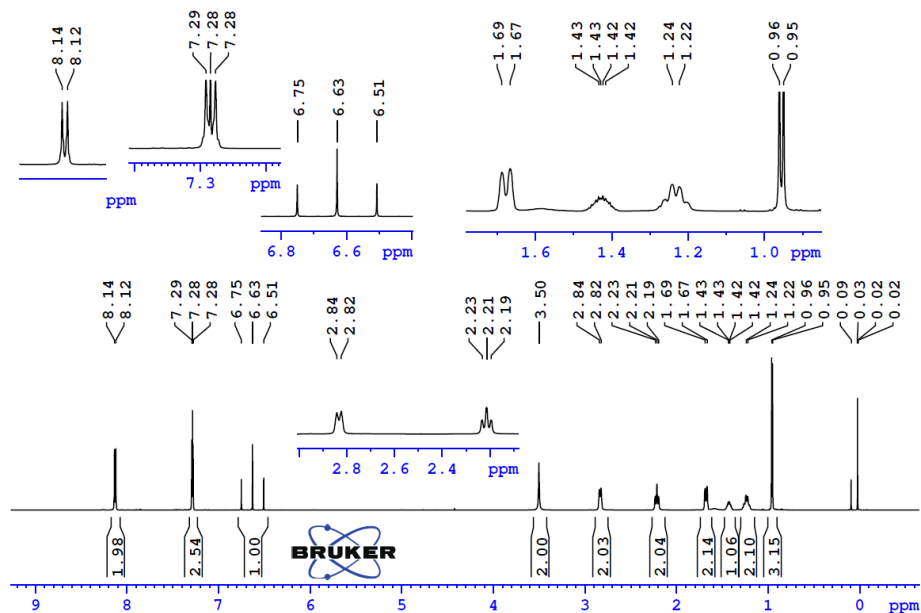


$\lambda_{max} = 233 \text{ nm}$

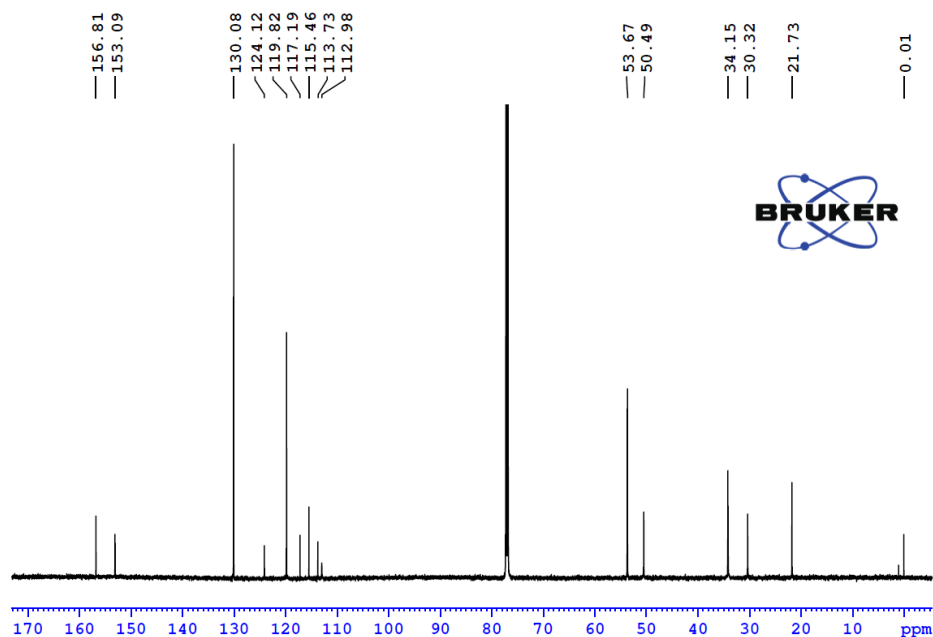


Analysis Report

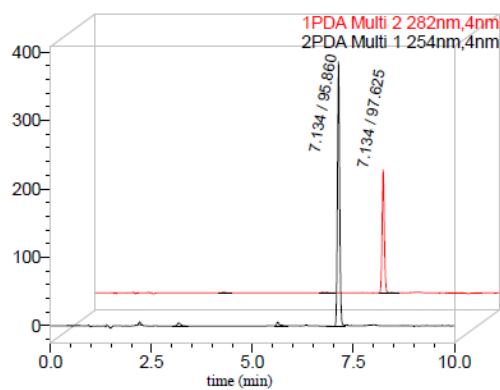
¹H NMR



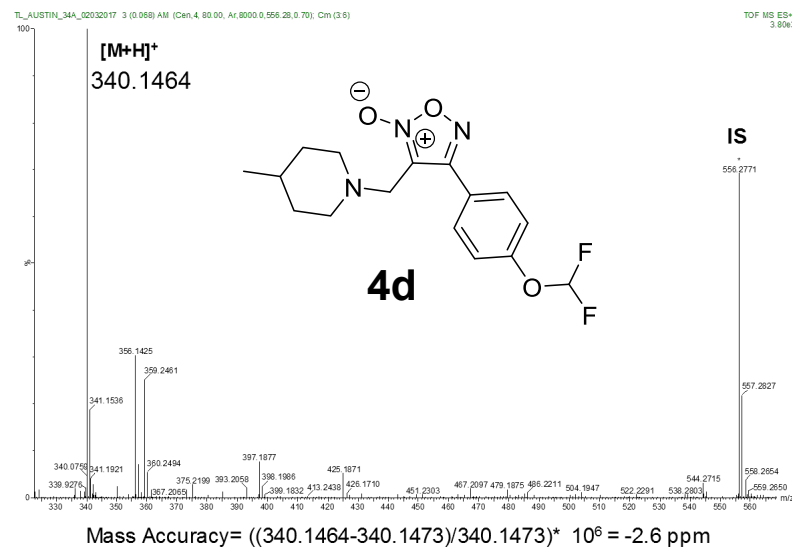
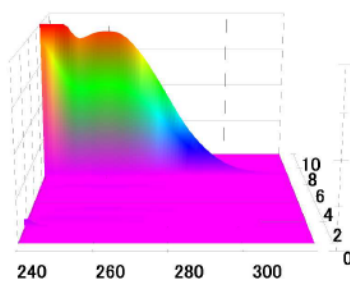
¹³C NMR



HPLC purity (2 wavelength)



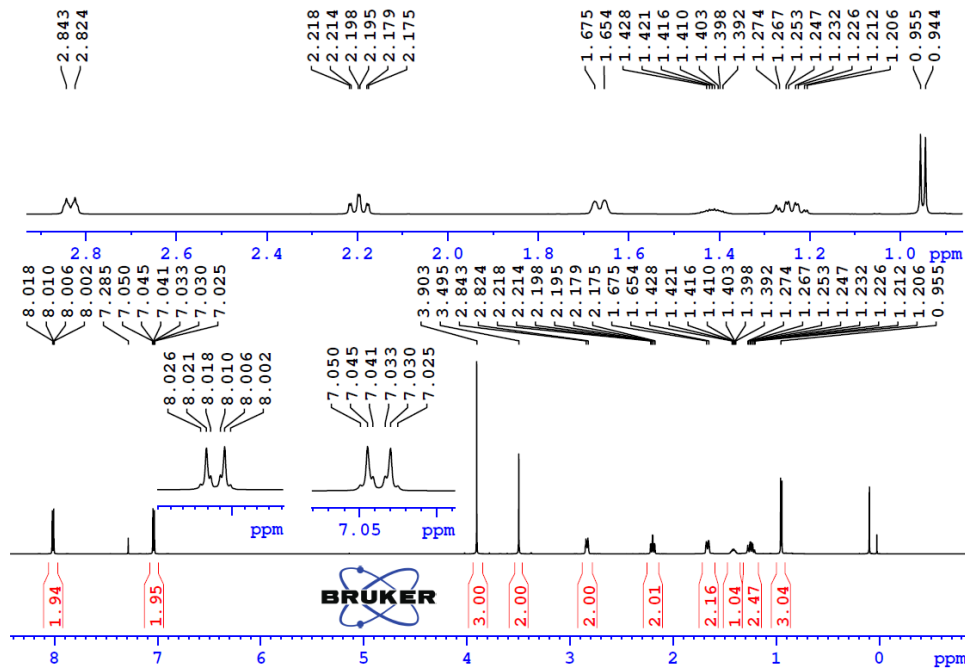
$\lambda_{max} = 261 \text{ nm}$



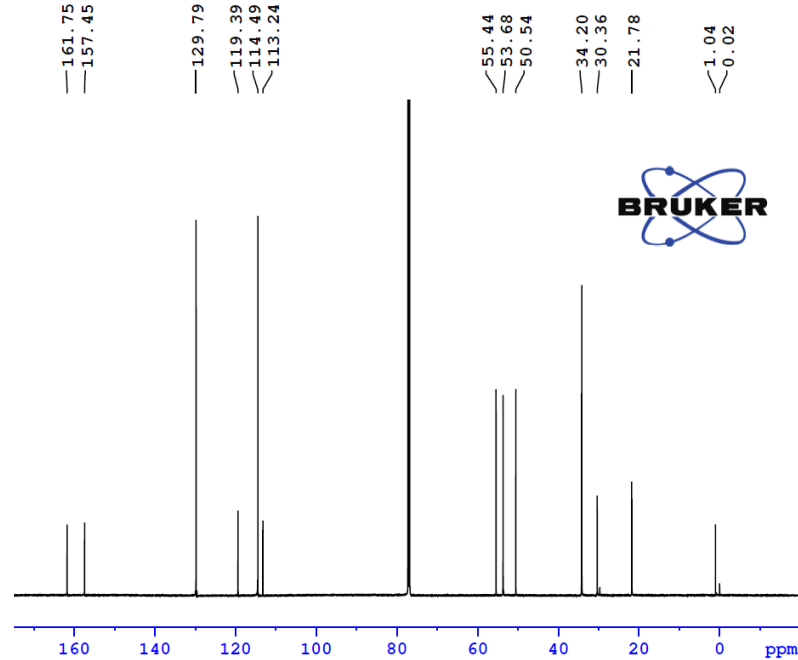
Mass Accuracy = $\left(\frac{340.1464 - 340.1473}{340.1473}\right) \times 10^6 = -2.6 \text{ ppm}$

Analysis Report

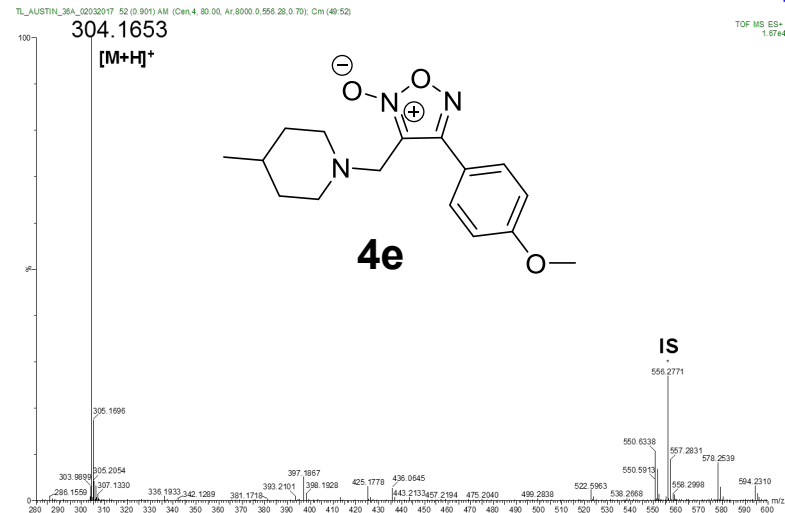
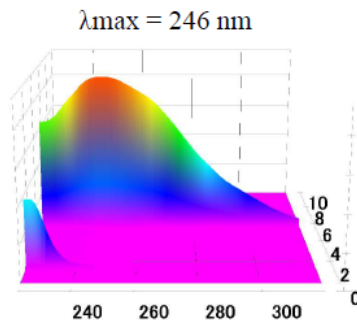
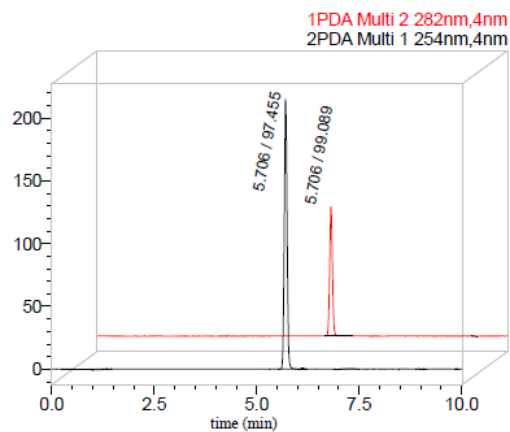
¹H NMR



¹³C NMR

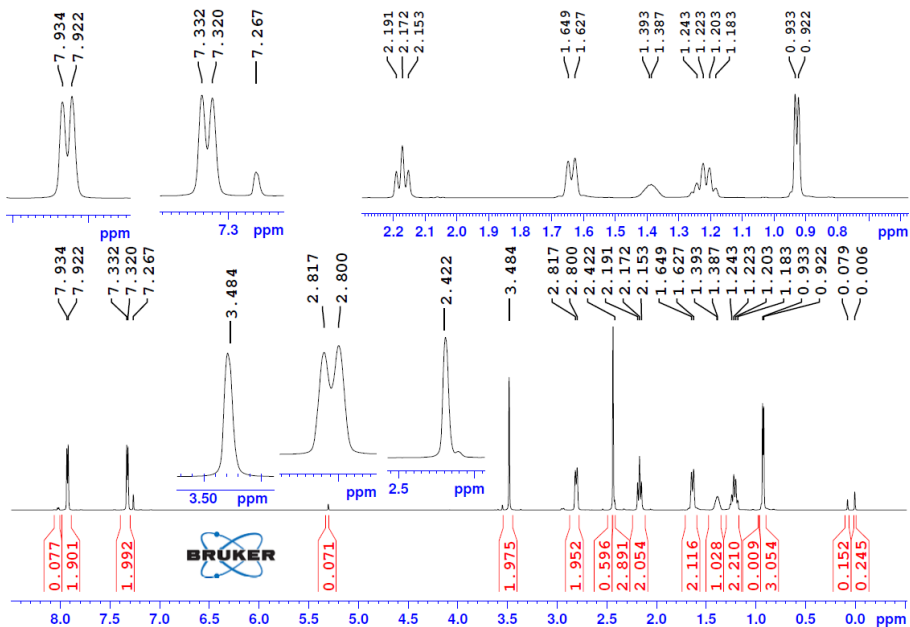


HPLC purity (2 wavelength)

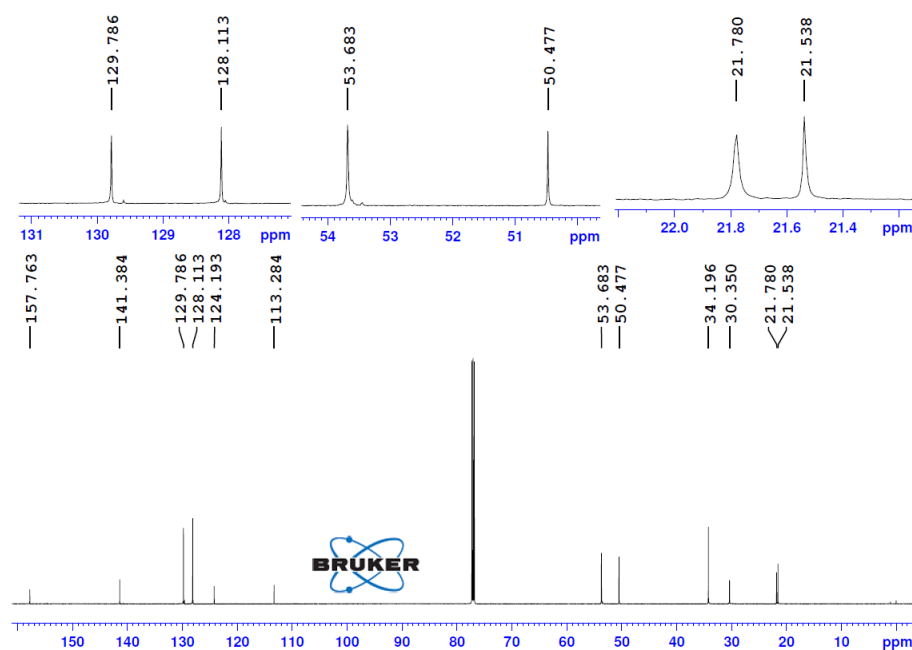


Analysis Report

¹H NMR

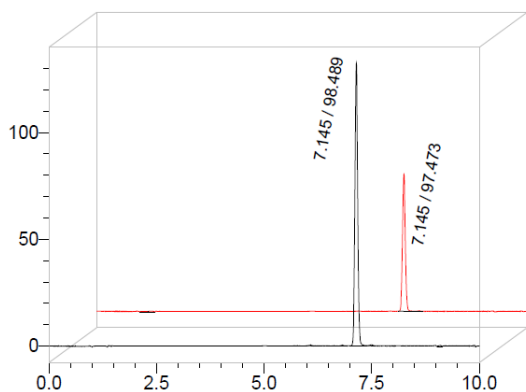


¹³C NMR

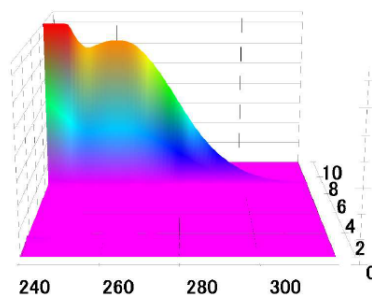


HPLC purity (2 wavelength)

1PDA Multi 2 282nm,4nm
1PDA Multi 2 254nm,4nm

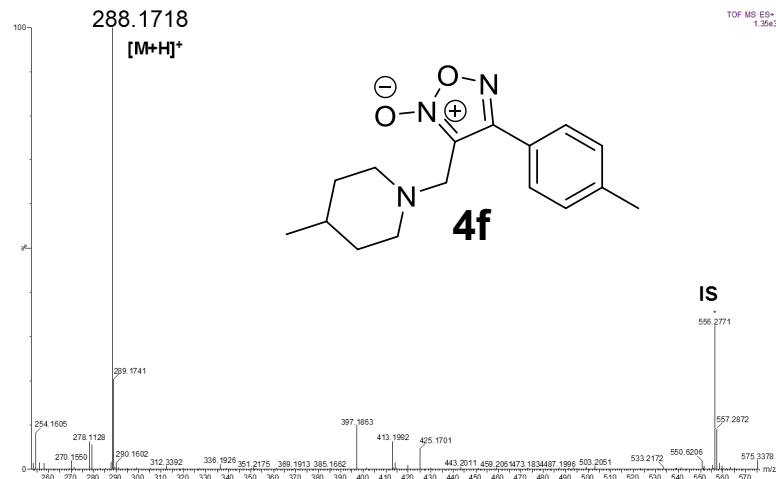


$\lambda_{max} = 233 \text{ nm}$



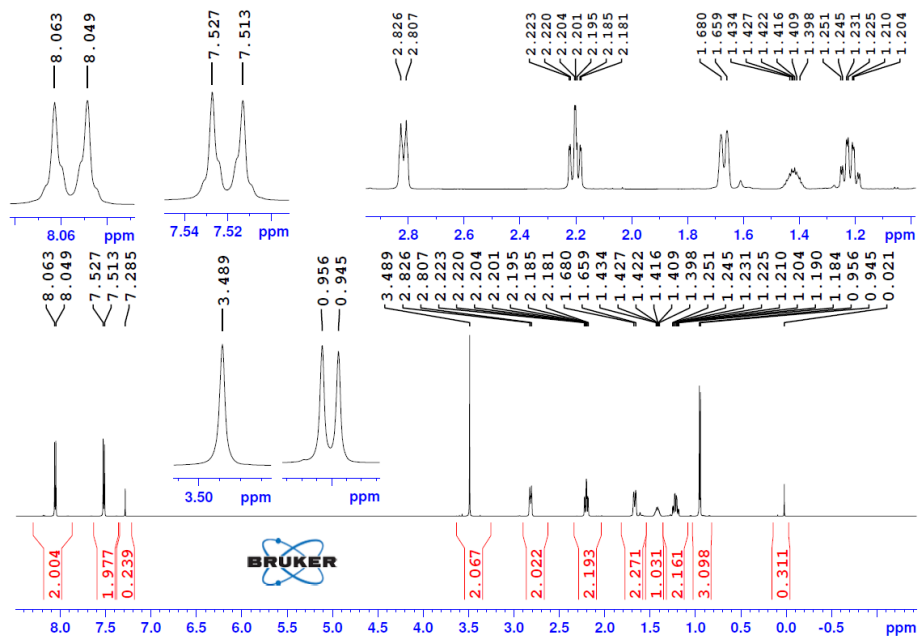
S8

TL_AUSTIN_38A_02032017 39 (0.680) AM (C₁₆H₁₈N₂O₂, Ar: 8000, 0.556, 28.070), Cm (37.40)

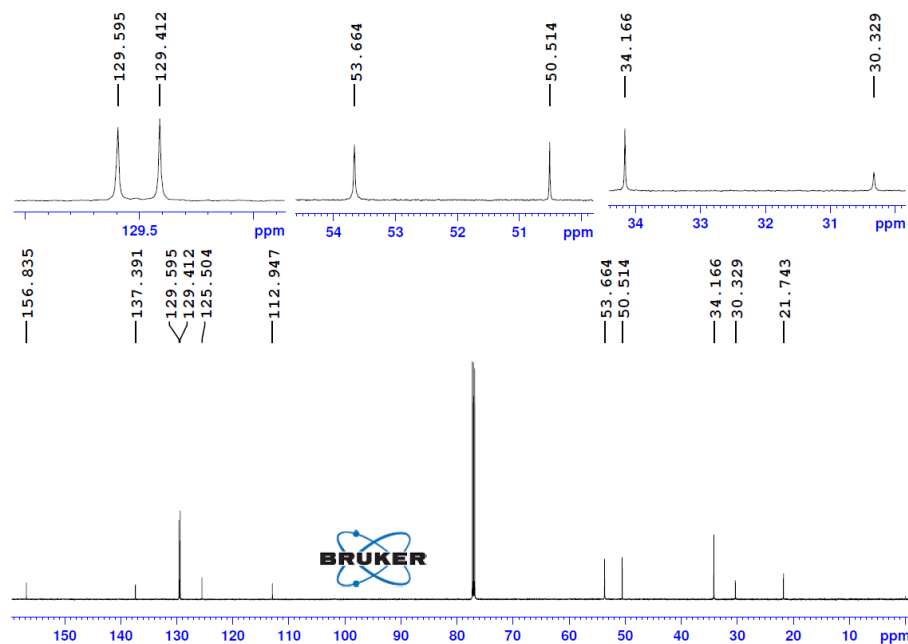


Analysis Report

¹H NMR

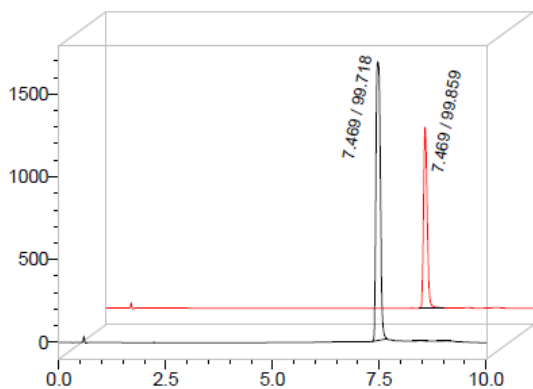


¹³C NMR

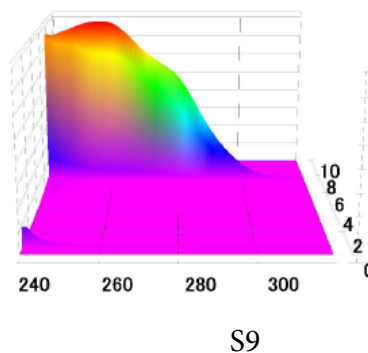


HPLC purity (2 wavelength)

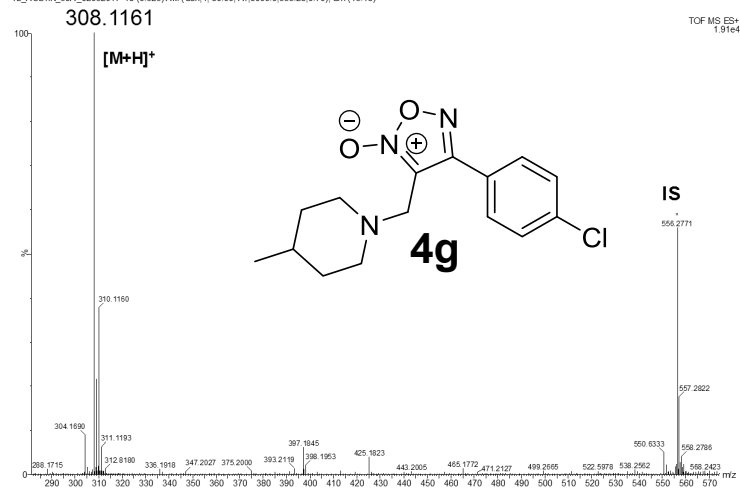
1PDA Multi 2 282nm,4nm
2PDA Multi 1 254nm,4nm



$\lambda_{max} = 256 \text{ nm}$

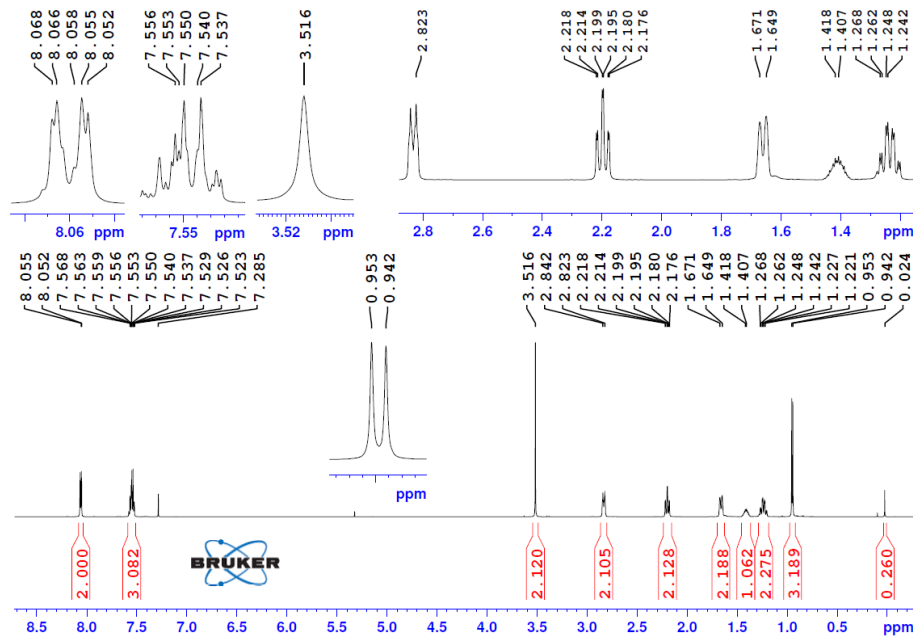


TL_AUSTIN_30A_02032017 18 (0.323)AM (Cm.4, 80.00, Ar,8000,0.556,28.070), Cm (15:18)

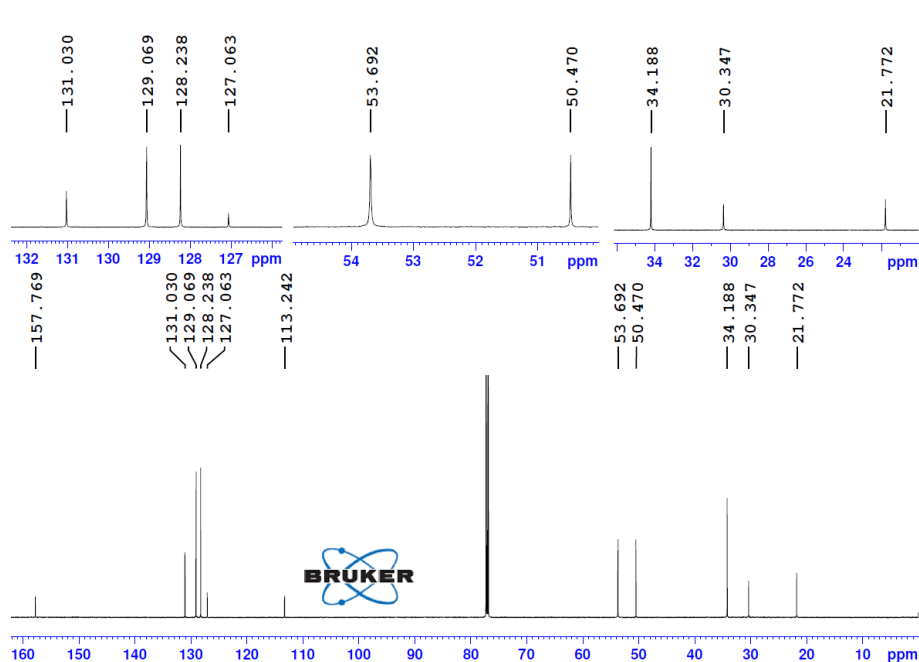


Analysis Report

¹H NMR

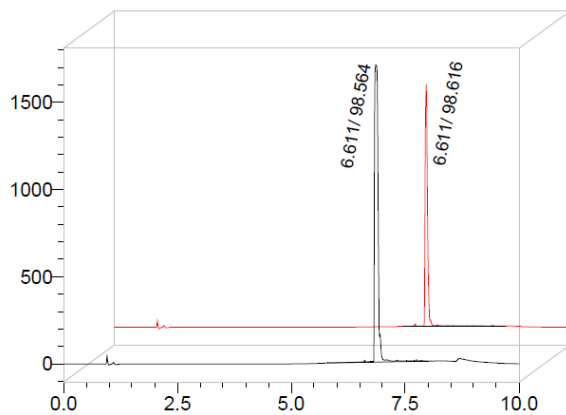


¹³C NMR

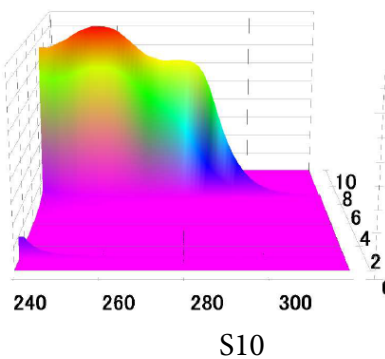


HPLC purity (2 wavelength)

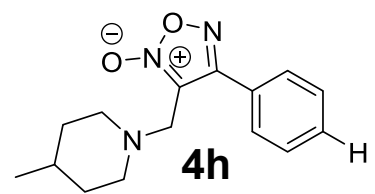
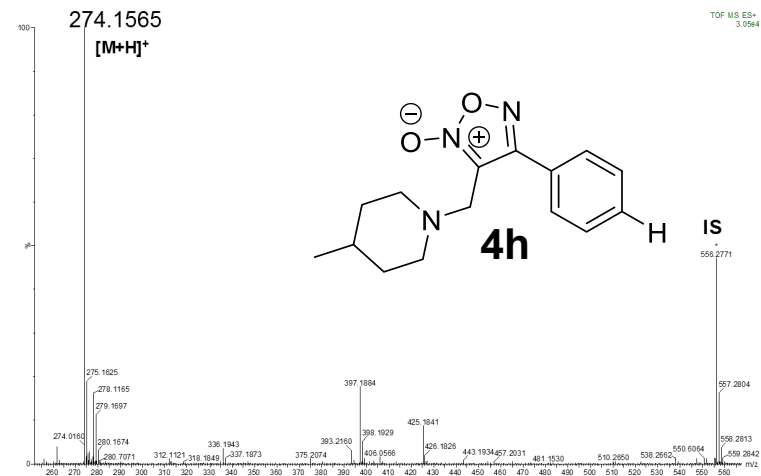
1PDA Multi 2 282nm,4nm
2PDA Multi 1 254nm,4nm



$\lambda_{max} = 257 \text{ nm}$



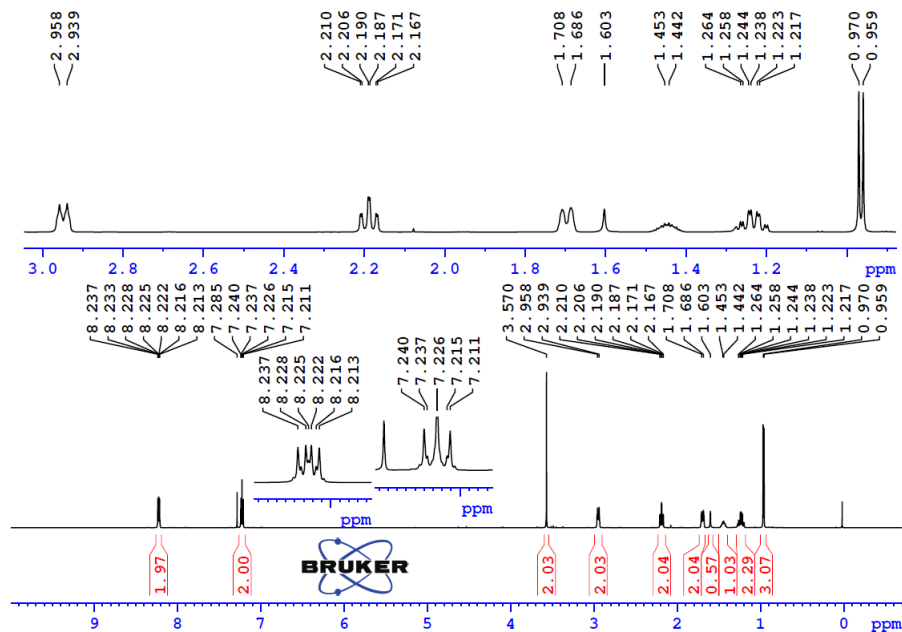
TL_AUSTIN_45A_02032017 3 (0.68) AM (Cen.4, 80.00, Ar:8000.0,566.28,0.70); Cm (2:4)



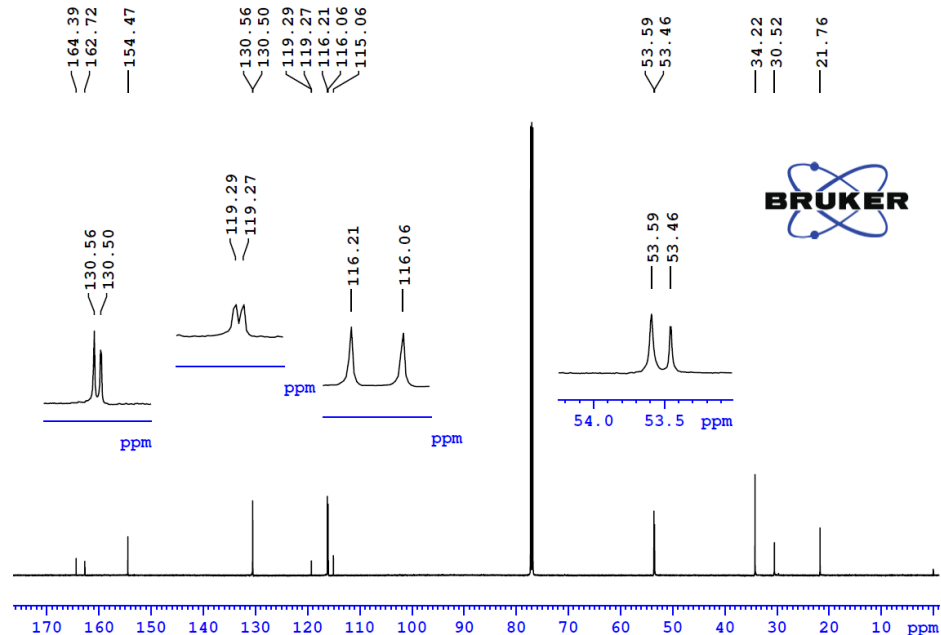
Mass Accuracy = $\frac{(274.1565 - 274.1556)}{274.1556} \times 10^6 = -3.3 \text{ ppm}$

Analysis Report

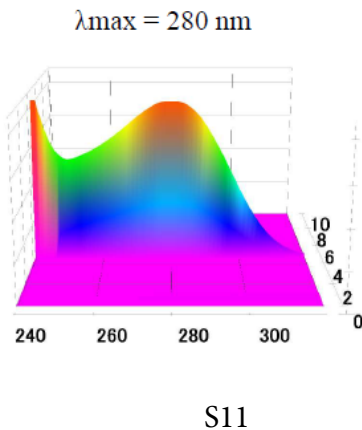
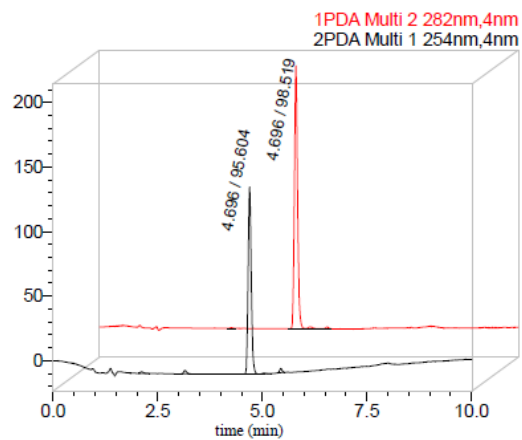
¹H NMR



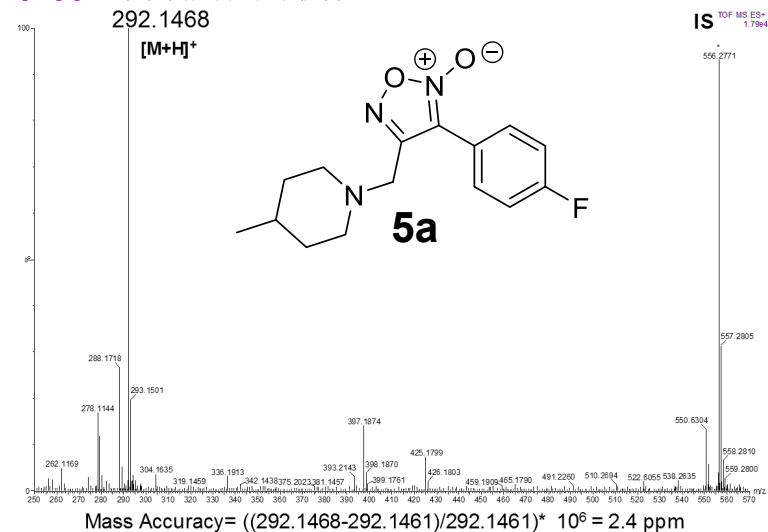
¹³C NMR



HPLC purity (2 wavelength)

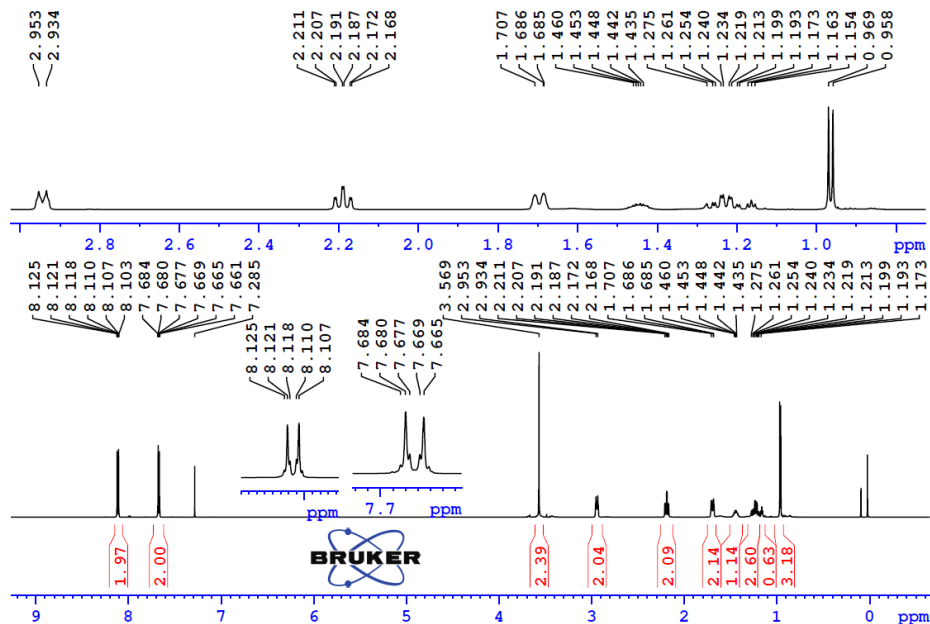


TL_AUSTIN_31B_02032017 1 (0.034) AM (Gen4, 80.00, Ar, 8000.0, 556.28, 0.70), Cm (1.4)

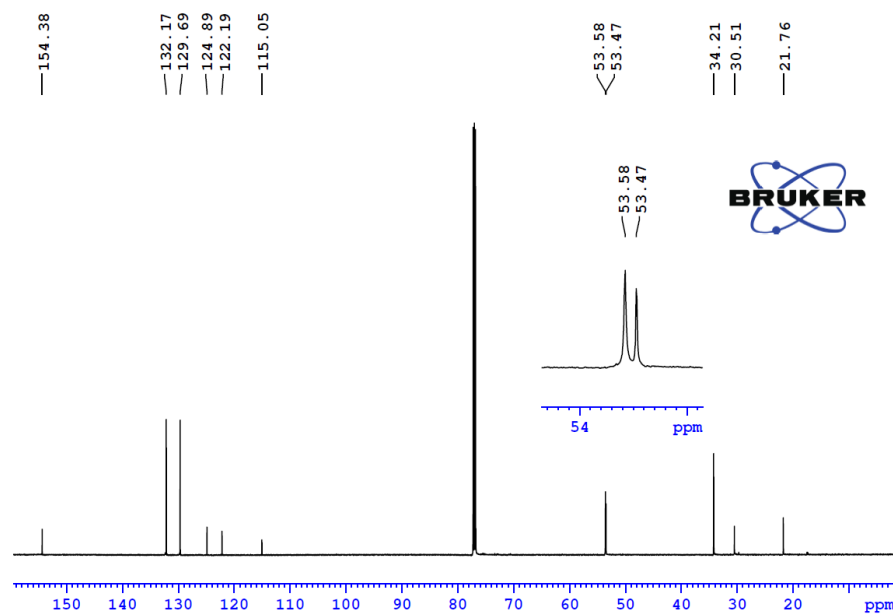


Analysis Report

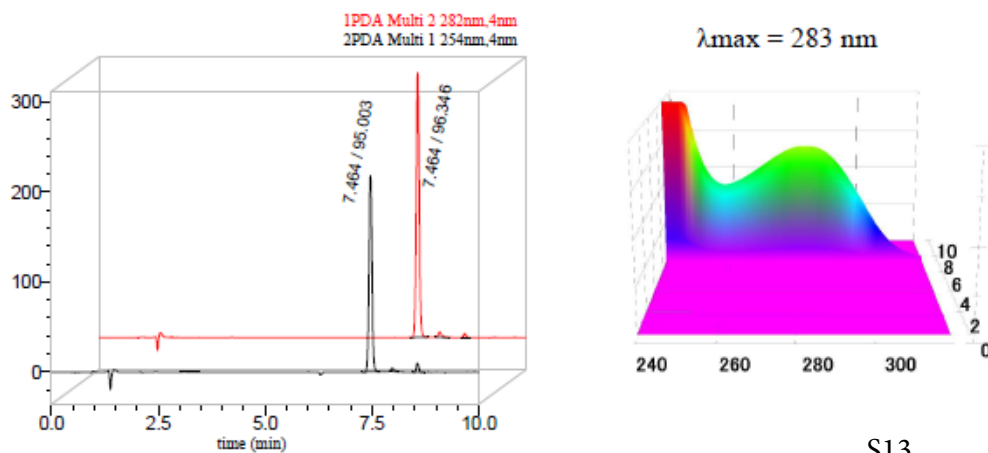
^1H NMR



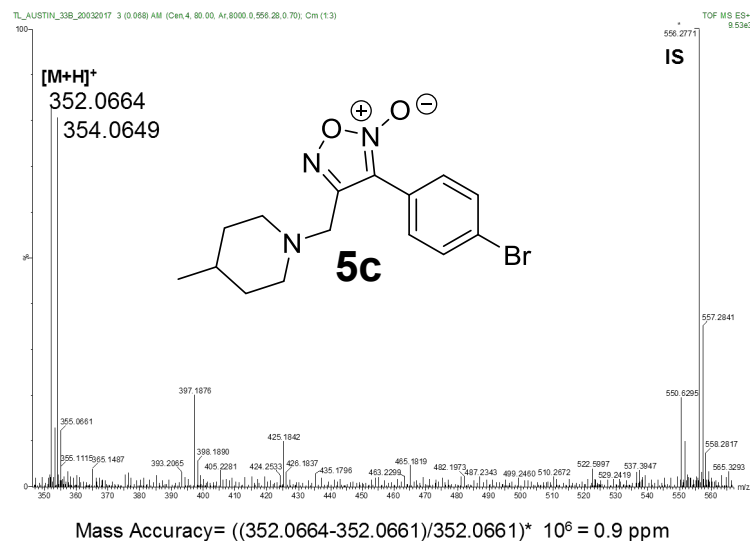
^{13}C NMR



HPLC purity (2 wavelength)

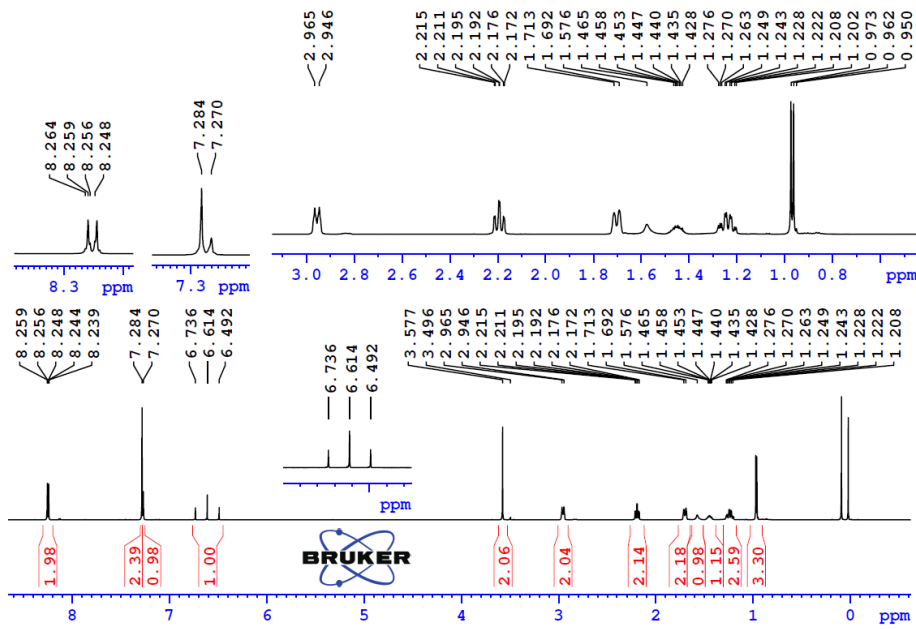


S13

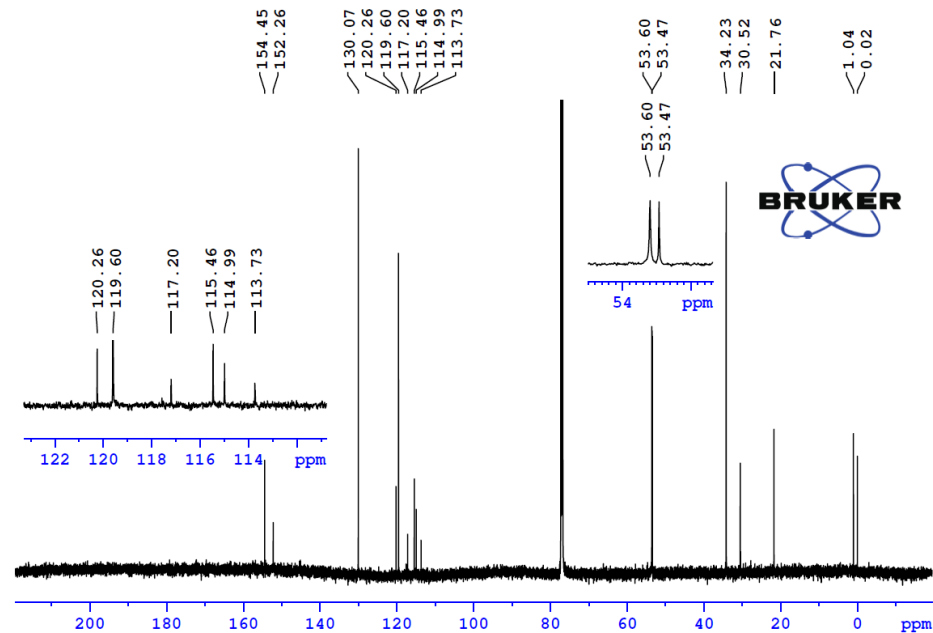


Analysis Report

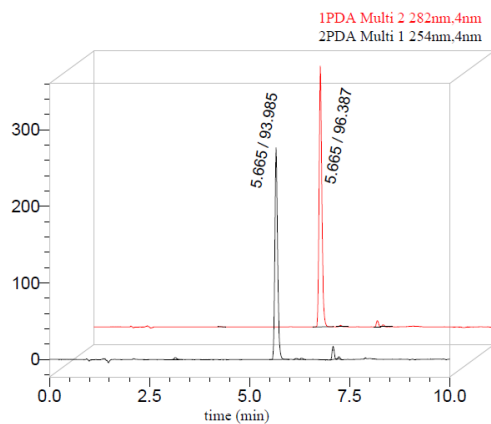
¹H NMR



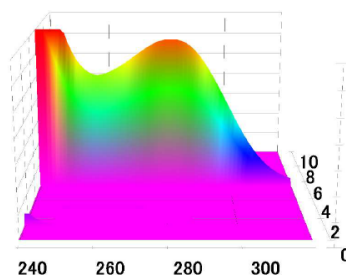
¹³C NMR



HPLC purity (2 wavelength)

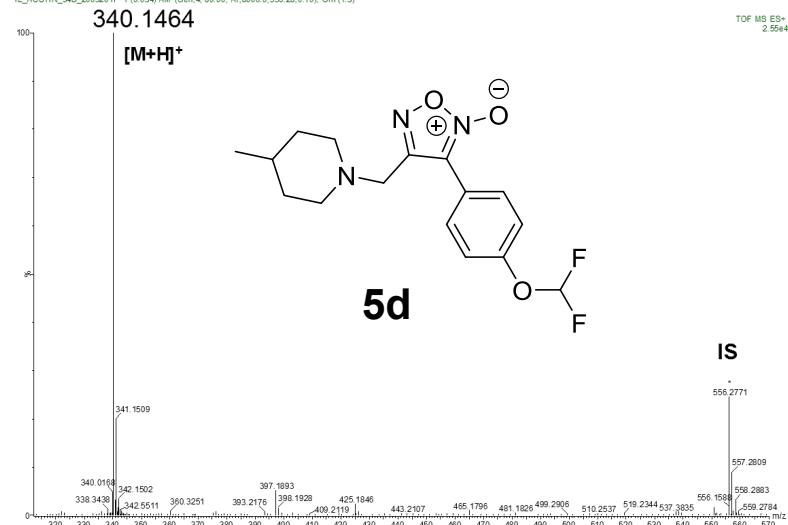


$\lambda_{max} = 281 \text{ nm}$

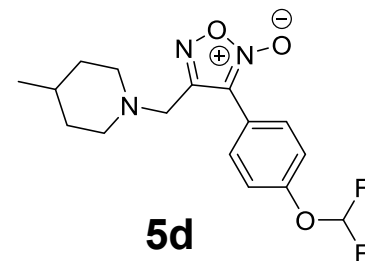


S14

TL_AUSTIN_34B_200202017 1 (0.034 AM) (Cen:4.80.00, Ar:8000.0,556.28,0.70); Cm (1.3)



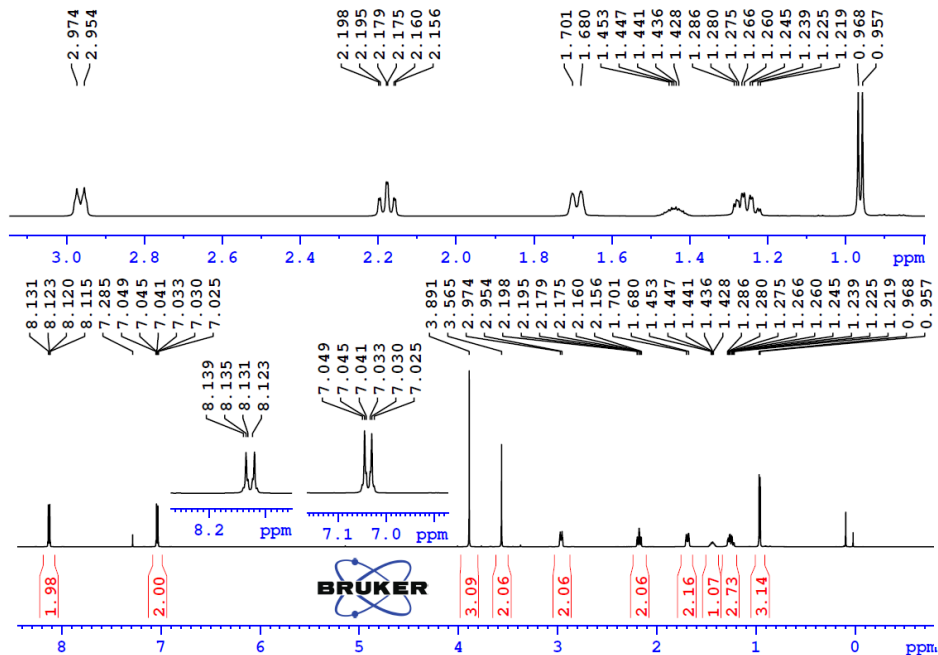
Mass Accuracy = $\left(\frac{340.1764 - 340.1473}{340.1473}\right) \times 10^6 = -2.6 \text{ ppm}$



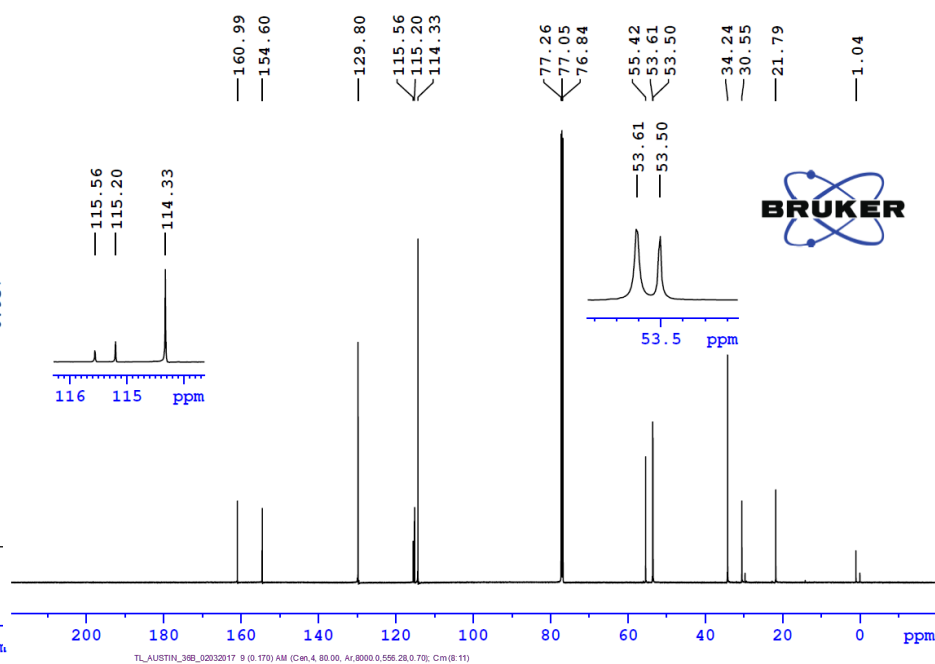
IS

Analysis Report

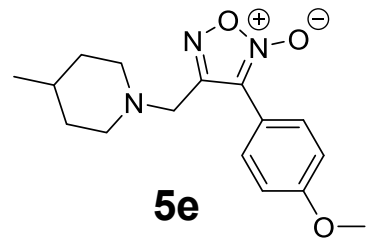
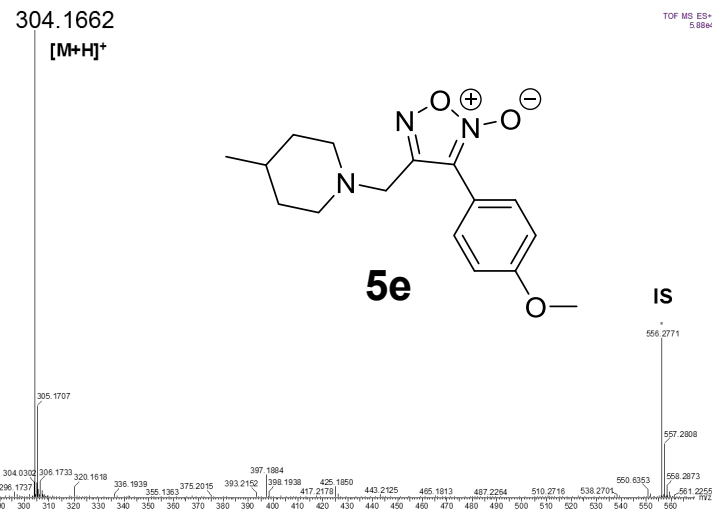
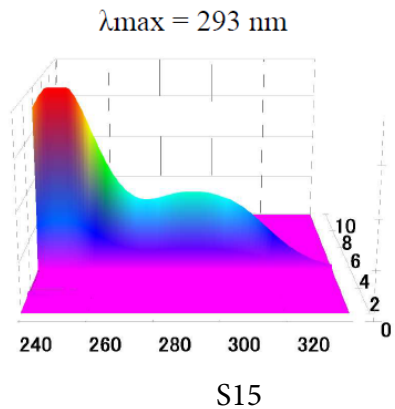
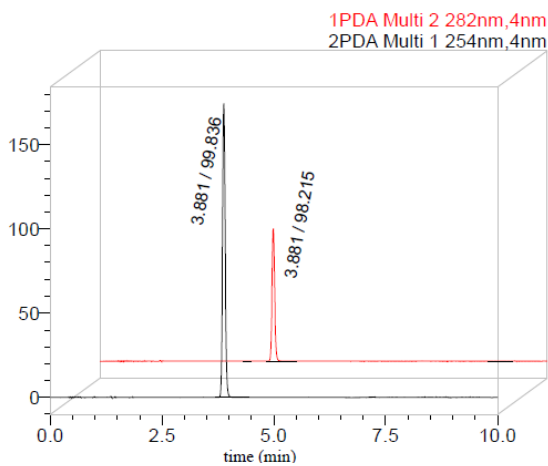
¹H NMR



¹³C NMR



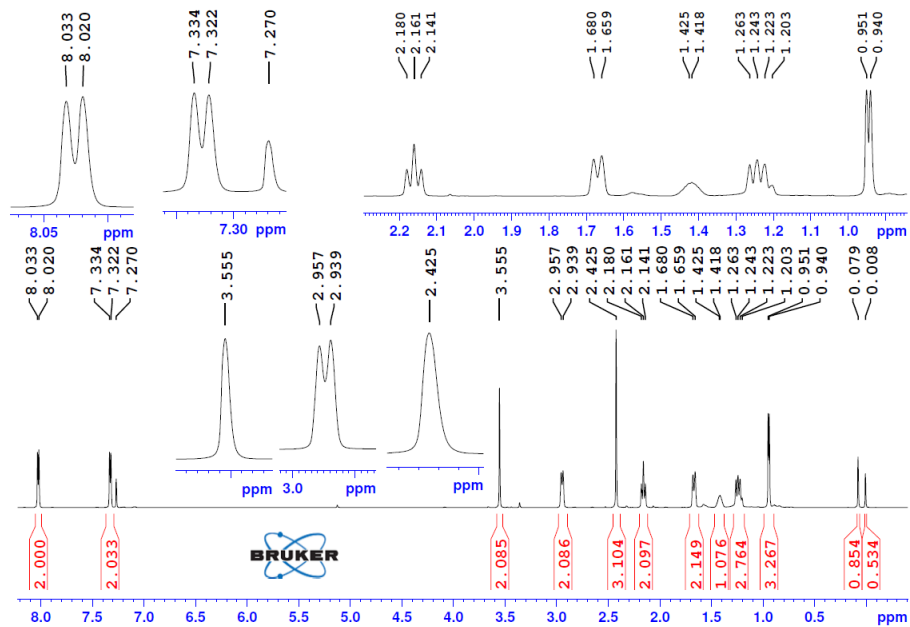
HPLC purity (2 wavelength)



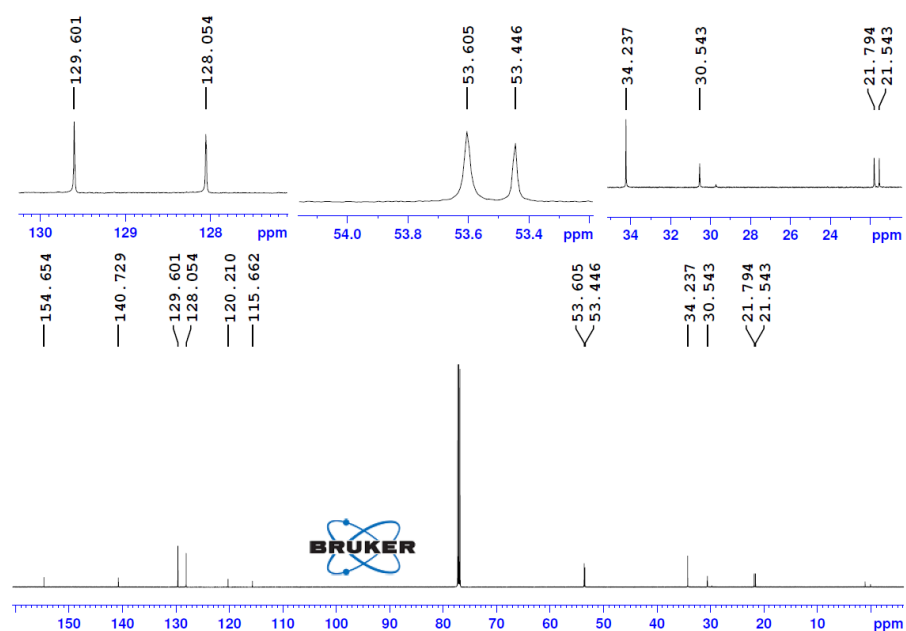
Mass Accuracy = ((304.1662-304.1661)/304.1661) * 10⁶ = 0.3 ppm

Analysis Report

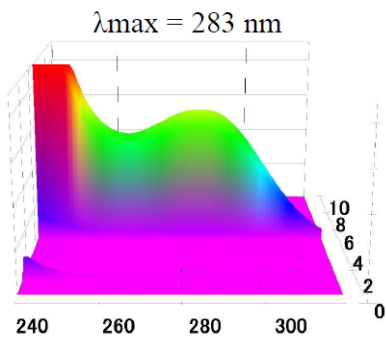
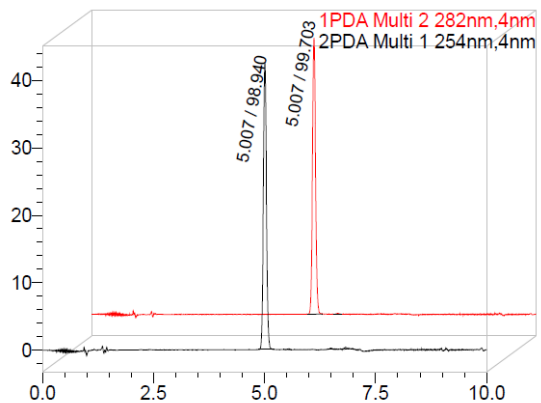
¹H NMR



¹³C NMR

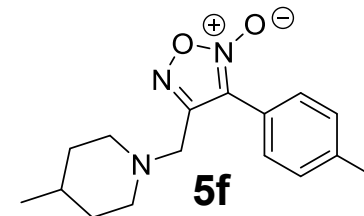
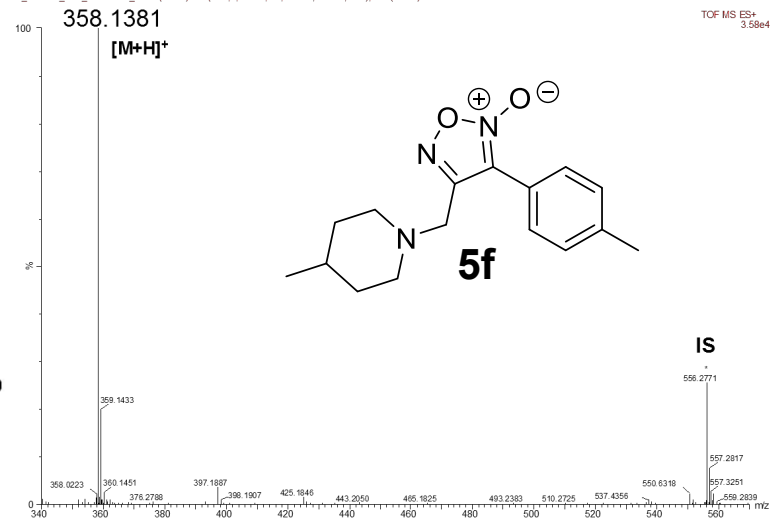


HPLC purity (2 wavelength)



S16

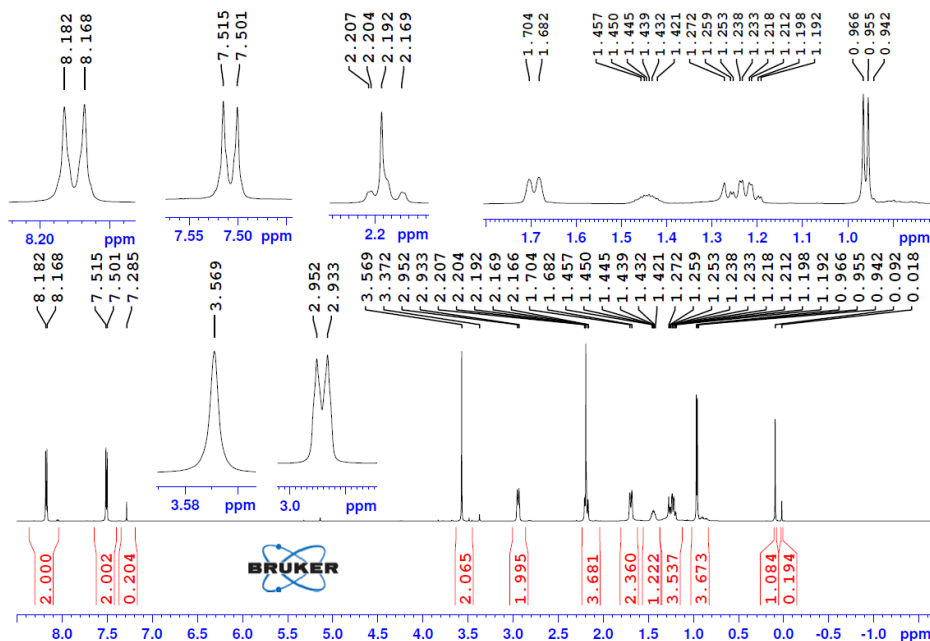
TL_AUSTIN_37B_20032017_2_53 (0.918) AM (Cen.4, 80.00, Ar.8000,0.556,28.0,70), Cm (53.54)



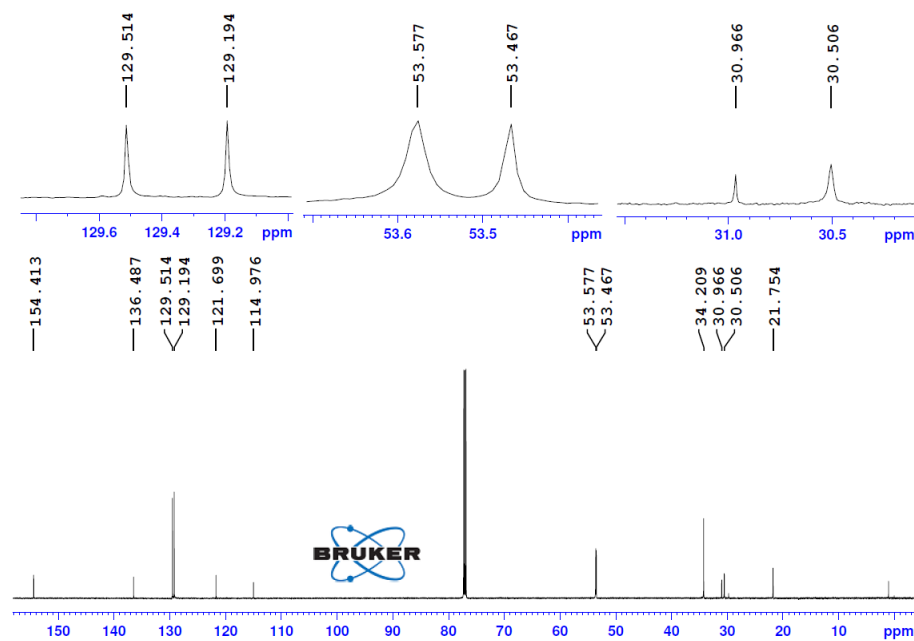
Mass Accuracy = $\frac{(358.1381 - 358.1379)}{358.1379} \times 10^6 = 0.6 \text{ ppm}$

Analysis Report

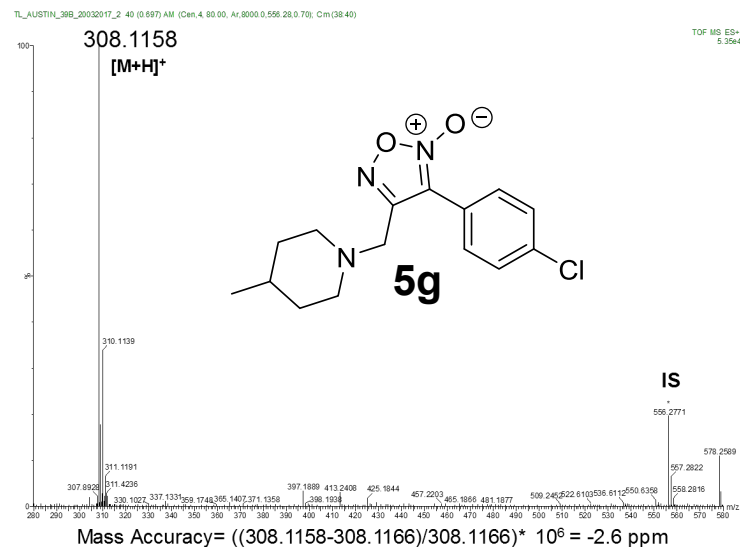
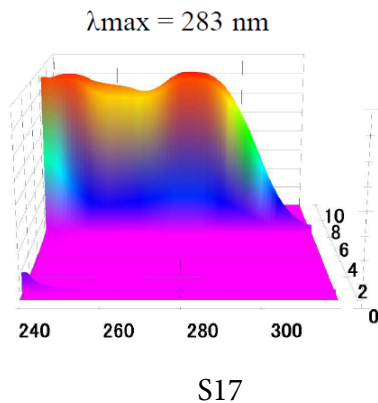
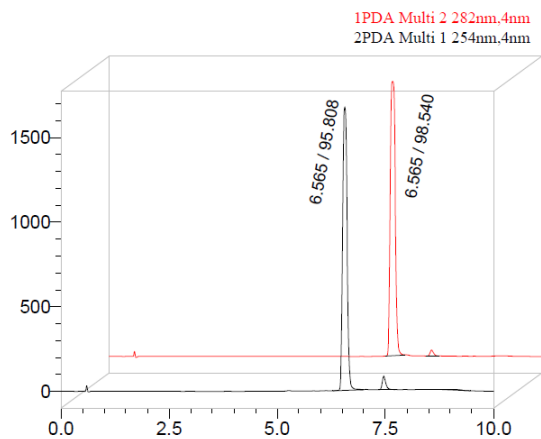
¹H NMR



¹³C NMR

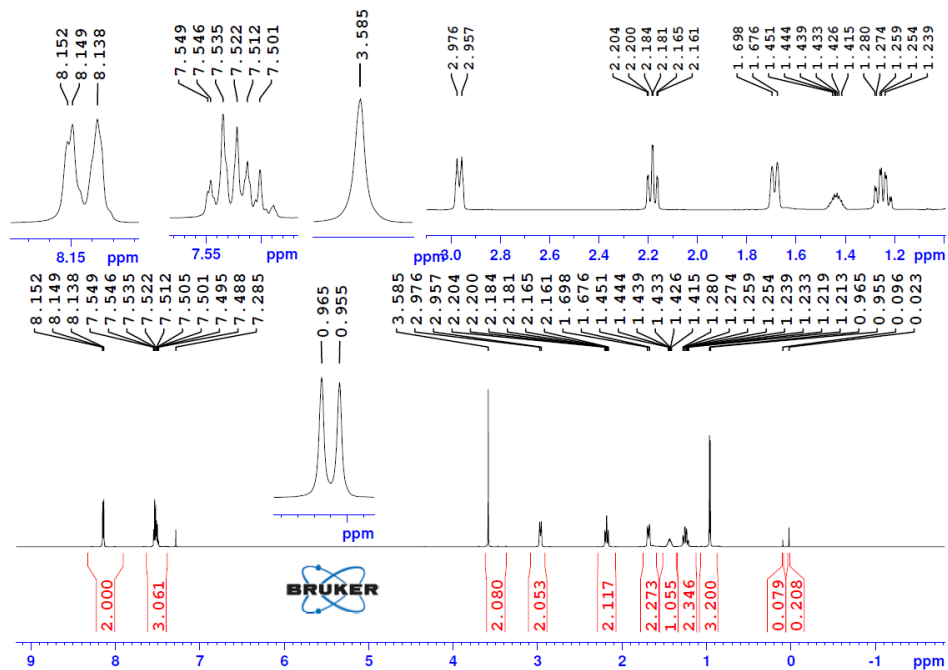


HPLC purity (2 wavelength)

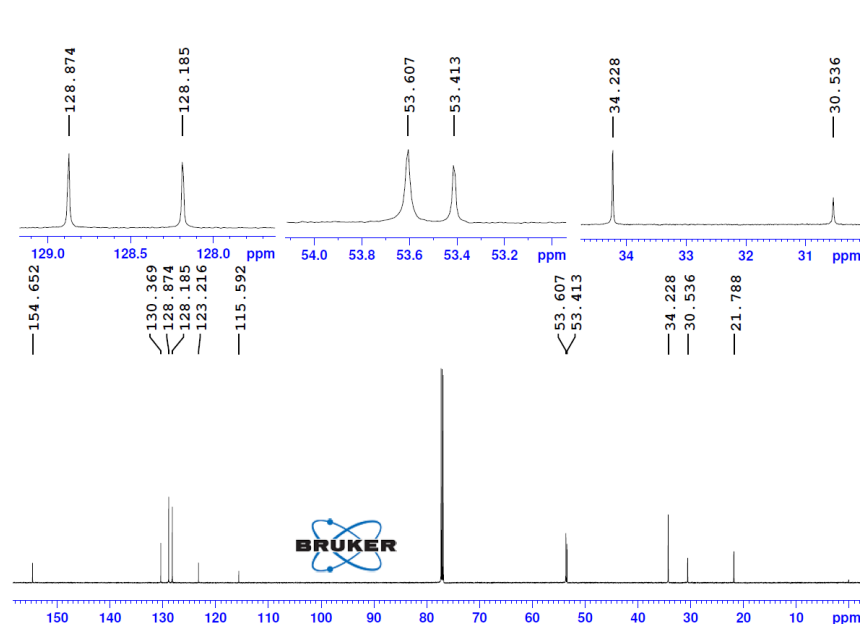


Analysis Report

¹H NMR

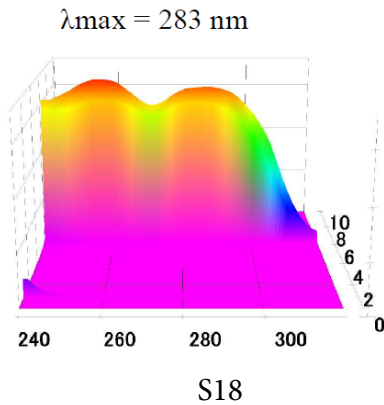
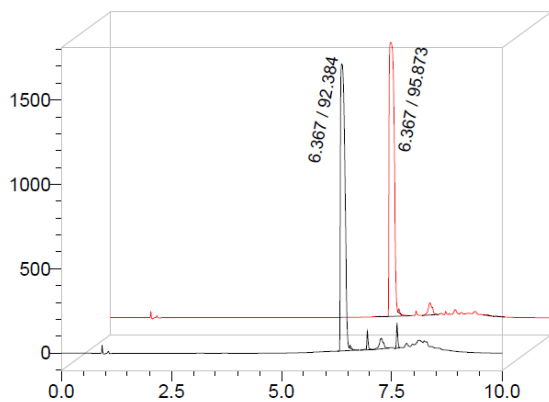


¹³C NMR

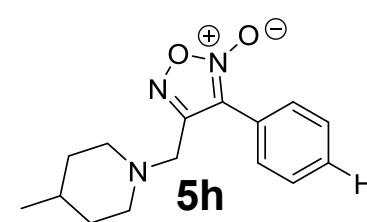
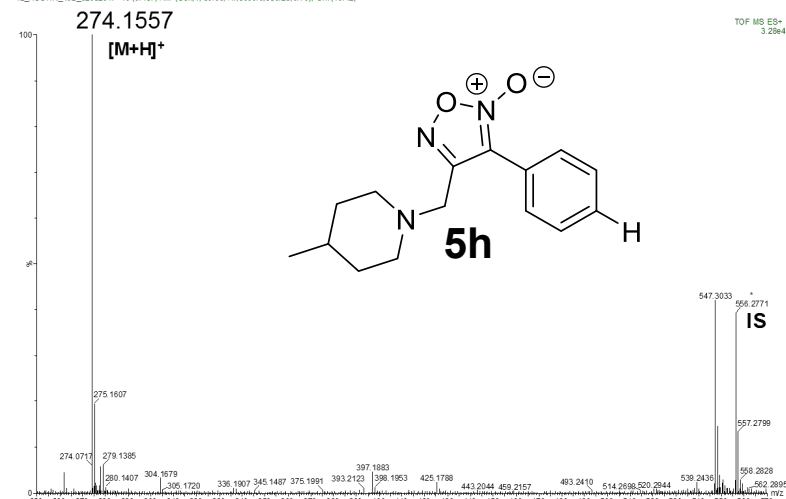


HPLC purity (2 wavelength)

1PDA Multi 2 282nm,4mm
2PDA Multi 1 254nm,4mm



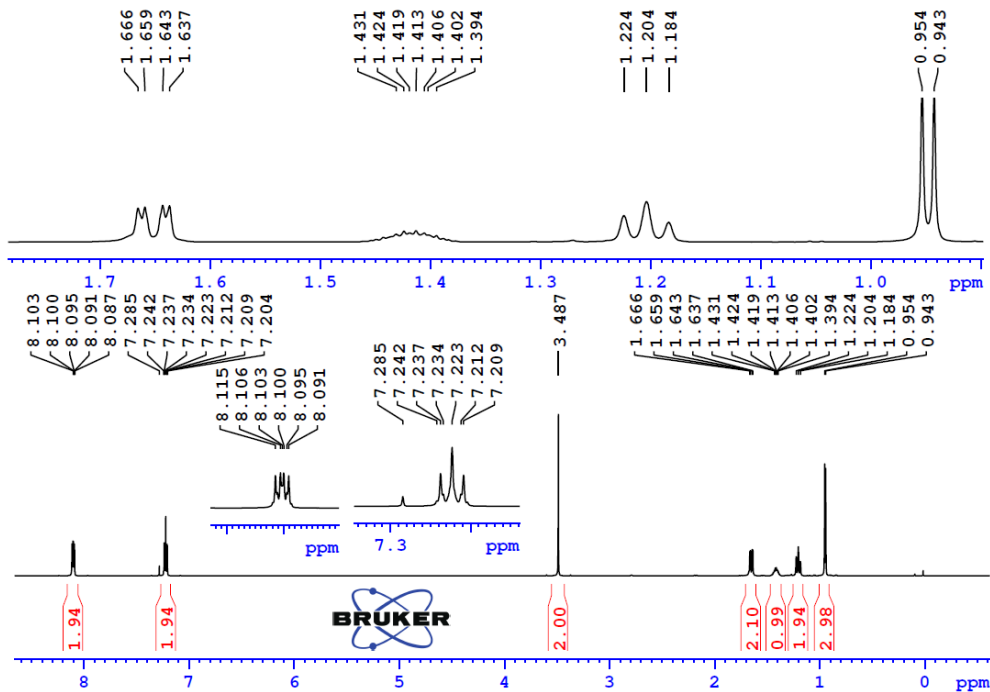
TL_AUSTIN_408_02032017 10 (0.187) AM (C16H4, 80.00, Ar:8000 0.556,28.0,70), Cm(10:12)



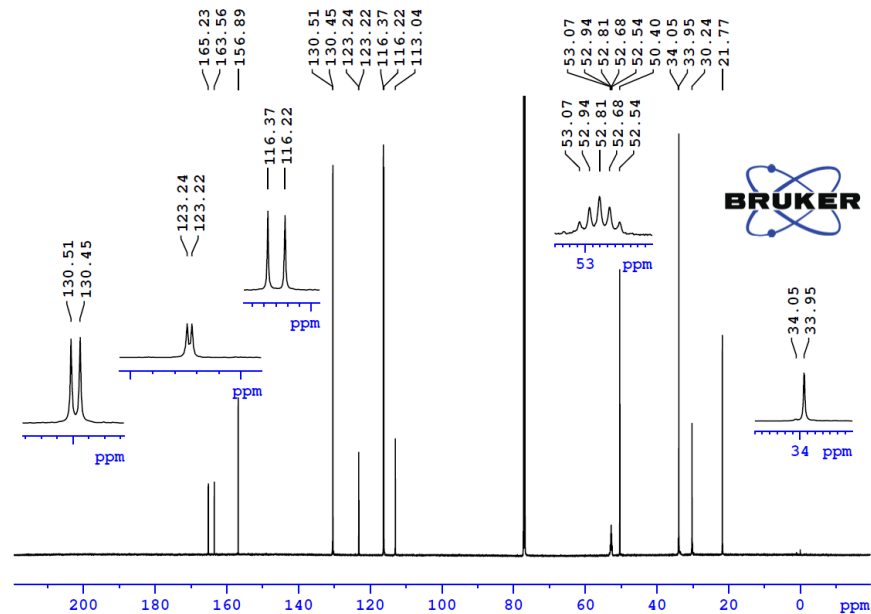
Mass Accuracy = ((274.1557-274.1556)/274.1556) * 10⁶ = 0.4 ppm

Analysis Report

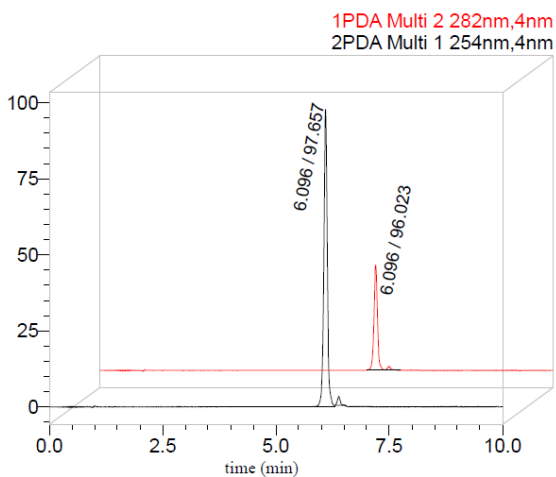
¹H NMR



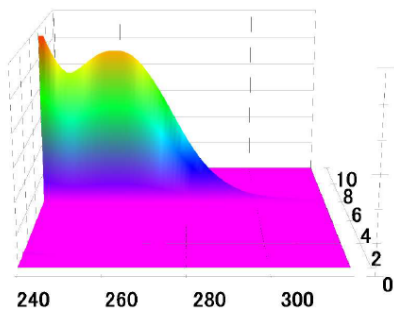
¹³C NMR



HPLC purity (2 wavelength)



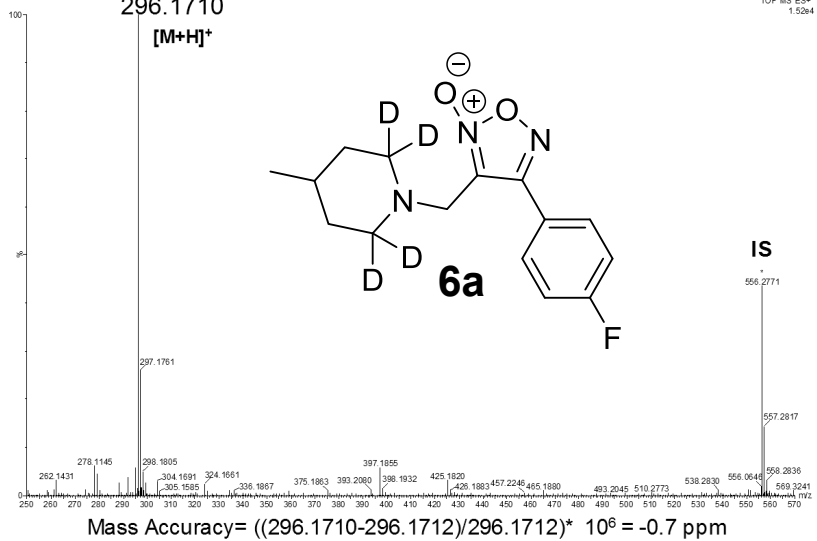
$\lambda_{max} = 260 \text{ nm}$



S19

296.1710

[M+H]⁺



BRUKER

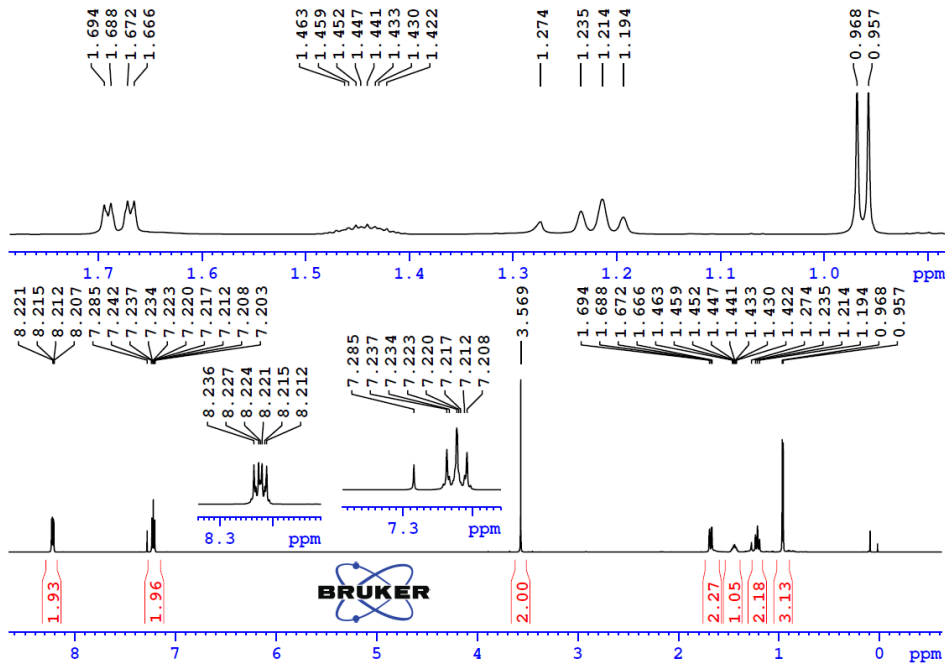
BRUKER

TOF MS ES+
1.52e4

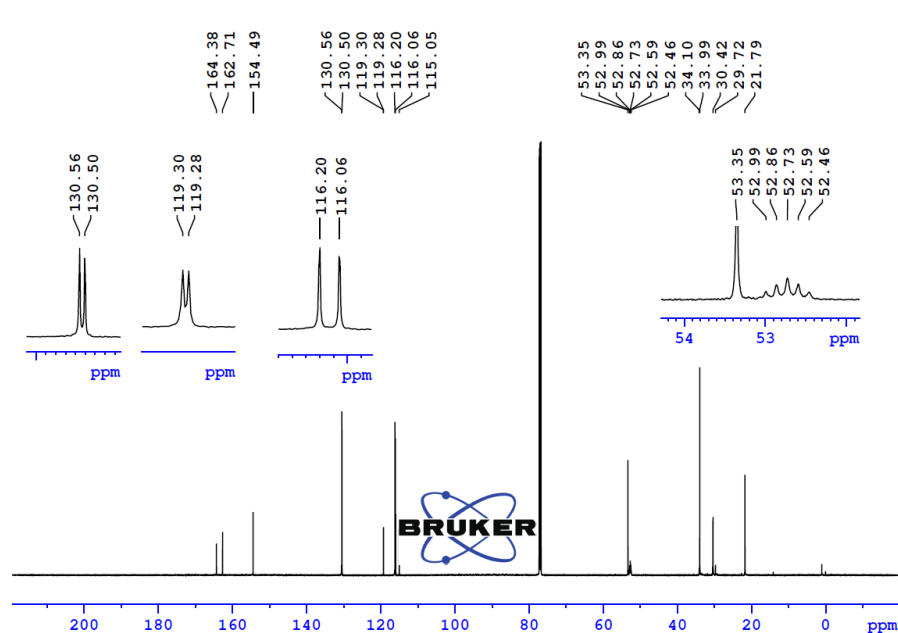
IS

Analysis Report

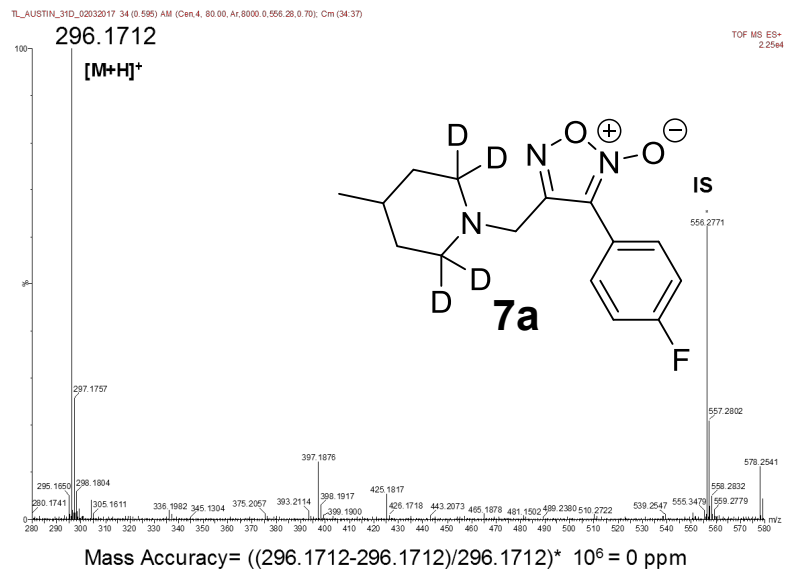
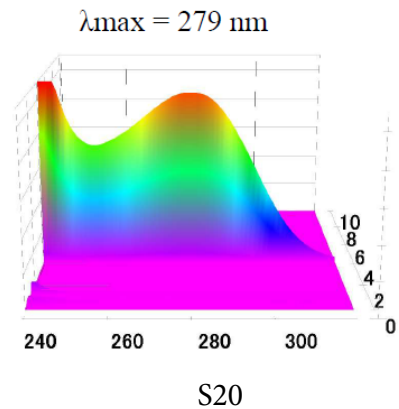
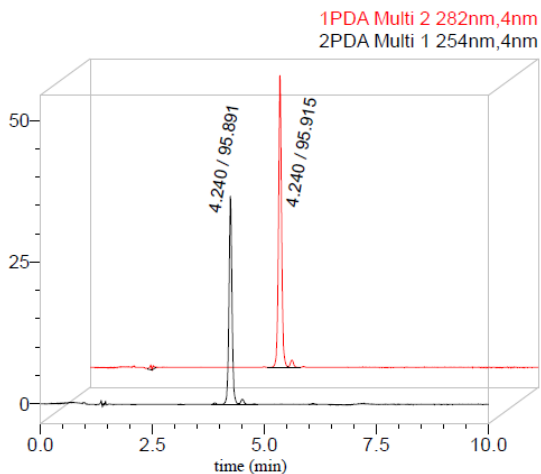
¹H NMR



¹³C NMR



HPLC purity (2 wavelength)



Supplemental LC-MS/MS Data

Furoxans (oxadiazole-4N-oxides) with Attenuated Reactivity are Neuroprotective, Cross the Blood Brain Barrier, and Improve Passive Avoidance Memory

*Austin Horton[†], Kevin Nash[‡], Ethel Tackie-Yarboi[†], Alexander Kostrevski[†], Adam Novak[†],
Aparna Raghavan[†], Jatin Tulsulkar[†], Qasim Alhadidi[†], Nathan Wamer[†], Bryn Langenderfer[†],
Kalee Royster[†], Maxwell Ducharme[†], Katelyn Hagood[†], Megan Post[†], Zahoor A. Shah[†], Isaac T.
Schiefer^{†*}*

[†]Department of Medicinal and Biological Chemistry, College of Pharmacy and Pharmaceutical Sciences, University of Toledo, Toledo, OH, 43614

[‡]Department of Pharmacology and Experimental Therapeutics, College of Pharmacy and Pharmaceutical Sciences, University of Toledo, Toledo, OH 43614

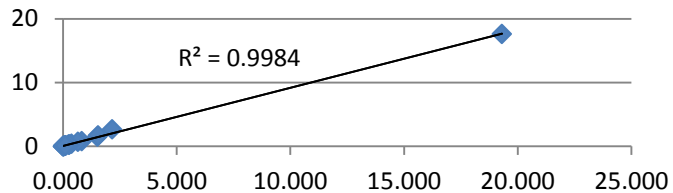
List of Contents

- S3 Data compilation for all data from LC-MS/MS analysis of **5a** in brain and plasma
- S4 Raw data compilation for LC-MS/MS analysis of **5a** in brain, extraction 1
- S5 Raw data compilation for LC-MS/MS analysis of **5a** in brain, extraction 2
- S6 Raw data compilation for LC-MS/MS analysis of **5a** in plasma
- S7-59 MRM chromatograms reported in raw data compilations (S4-S6)

Data compilation

Treatment	5a (uM) BRAIN EXTRACTION 1	5a (uM) BRAIN EXTRACTION 2	5a (uM) Average	5a (uM) PLASMA	Brain:Plasma ratio	Cohort average
1h A po	5.021404692	7.570475142	6.295939917	1.152172646	6.570608291	1.902184
1h B po	0.438005541	0.496247619	0.46712658	1.504803625	0.329775667	
1h C po	0.18573551	0.191764773	0.188750141	0.746087117	0.257027321	
1h D po	0.304083271	0.375337329	0.3397103	0.83163151	0.451326489	
2h A po	0.234814764	0.176872844	0.205843804	0.491709233	0.359710235	2.143243
2h B po	0.319784173	0.343704818	0.331744496	0.656694293	0.523386333	
2h C po	3.496903256	5.308982024	4.40294264	0.784998351	6.763048632	
2h D po	0.40976202	0.460532135	0.435147078	0.496891309	0.926826706	
12h A po	0.203863481	0.195914571	0.199889026	0.479731977	0.408383389	0.428112
12h B po	0.190676356	0.188929416	0.189802886	0.50597177	0.373399124	
12h C po	0.283623444	0.262208379	0.272915912	0.47450688	0.552591311	
12h D po	0.238651466	0.179023128	0.208837297	0.473514035	0.378073541	
1h A ip	0.929929189	1.367733691	1.14883144	3.959449899	0.345435282	0.740835
1h B ip	33.79972295	66.75282608	50.27627451	120.4377418	0.554251724	
1h C ip	2.028460029	2.77090799	2.39968401	1.793674967	1.544821688	
1h D ip	1.829281108	2.470738824	2.150009966	4.762129032	0.518830718	
2h A ip	3.298339546	5.901326053	4.599832799	5.201636318	1.13451339	0.695345
2h B ip	0.746475489	1.113685354	0.930080421	1.956476171	0.569230216	
2h C ip	0.619481016	0.875068739	0.747274878	2.429136944	0.360238537	
2h D ip	0.62765278	1.064356716	0.846004748	1.483635842	0.717397549	
12h A ip	0.456982172	0.516527212	0.486754692	0.567720034	0.909827345	0.665269
12h B ip	0.328336552	0.309402532	0.318869542	0.84678724	0.365384028	
12h C ip	0.408506456	0.63185246	0.520179458	0.645084262	0.979488258	
12h D ip	0.351659445	0.486566094	0.419112769	1.197328758	0.406376353	

Removed from interpretation as outlier



Correlation for brain extraction 1 versus brain extraction 2_{S3}

Calculations based on ratio of AUC of **5a:7a** from raw data shown on subsequent pages.

Forebrain Extraction 1

	5a TIC Extraction 1 Forebrain Run 1	7a TIC Extraction 2 Forebrain Run 1	5a TIC Extraction 2 Forebrain Run 2	7a TIC Extraction 2 Forebrain Run 2	5a:7a Forebrain Run 1	5a:7a Forebrain Run 2	31b:41b Average	Concentration in 100 uL load solvent	Forebrain Weight	5a (µM) in Forebrain	Cohort Average Brain (µM)
1h A po	779347	4701470	1416954	4101943	0.166	0.345434834	0.256	0.308736491	0.332	0.929929189	9.646848318
1h B po	28833485	3617342	61522339	4626808	7.971	13.29692933	10.634	10.98490996	0.325	33.79972295	
1h C po	3335096	6711663	2583986	4985591	0.497	0.51829081	0.508	0.567968808	0.28	2.028460029	
1h D po	2906672	6743284	2172793	4857855	0.431	0.447274157	0.439	0.497564461	0.272	1.829281108	
2h A po	6704560	6518573	5309932	4996548	1.029	1.062720102	1.046	1.121435446	0.34	3.298339546	1.322987208
2h B po	825194	4253708	862977	4956202	0.194	0.174120627	0.184	0.235139779	0.315	0.746475489	
2h C po	637230	4658609	468954	3430703	0.137	0.136693267	0.137	0.186463786	0.301	0.619481016	
2h D po	793817	5997856	640887	4749837	0.132	0.134928209	0.134	0.183274612	0.292	0.62765278	
12h A po	402876	5210222	326855	4240963	0.077	0.077070939	0.077	0.125213115	0.274	0.456982172	0.386371156
12h B po	242646	5797943	183557	4427289	0.042	0.041460361	0.042	0.088650869	0.27	0.328336552	
12h C po	420880	5658467	337511	4282496	0.074	0.078811749	0.077	0.124594469	0.305	0.408506456	
12h D po	412869	6176968	337853	4797744	0.067	0.070419139	0.069	0.116399276	0.331	0.351659445	
1h A ip	7272318	4782264	6063018	3878786	1.521	1.563122585	1.542	1.631956525	0.325	5.021404692	1.487307254
1h B ip	341196	4637403	286498	3577714	0.074	0.080078508	0.077	0.124831579	0.285	0.438005541	
1h C ip	80231	6564810	66415	5170861	0.012	0.012844089	0.013	0.058692421	0.316	0.18573551	
1h D ip	212498	5246856	178873	4040679	0.041	0.044268055	0.042	0.089400482	0.294	0.304083271	
2h A ip	103651	4987592	86691	3841547	0.021	0.02256669	0.022	0.068096281	0.29	0.234814764	1.115316053
2h B ip	256979	4994341	212791	4025713	0.051	0.052857966	0.052	0.099452878	0.311	0.319784173	
2h C ip	3349998	3291223	2701203	2464891	1.018	1.095871176	1.057	1.132996655	0.324	3.496903256	
2h D ip	355031	4948924	271467	3737264	0.072	0.072637898	0.072	0.120060272	0.293	0.40976202	
12h A ip	69549	4498797	52679	3215395	0.015	0.016383368	0.016	0.062178362	0.305	0.203863481	0.229203687
12h B ip	79150	5221270	60415	4188312	0.015	0.014424666	0.015	0.061016434	0.32	0.190676356	
12h C ip	143336	5438582	102936	3911626	0.026	0.026315399	0.026	0.072891225	0.257	0.283623444	
12h D ip	114567	4187649	138709	4812100	0.027	0.028825045	0.028	0.074697909	0.313	0.238651466	

Assuming tissue density = 1

Forebrain Extraction 2

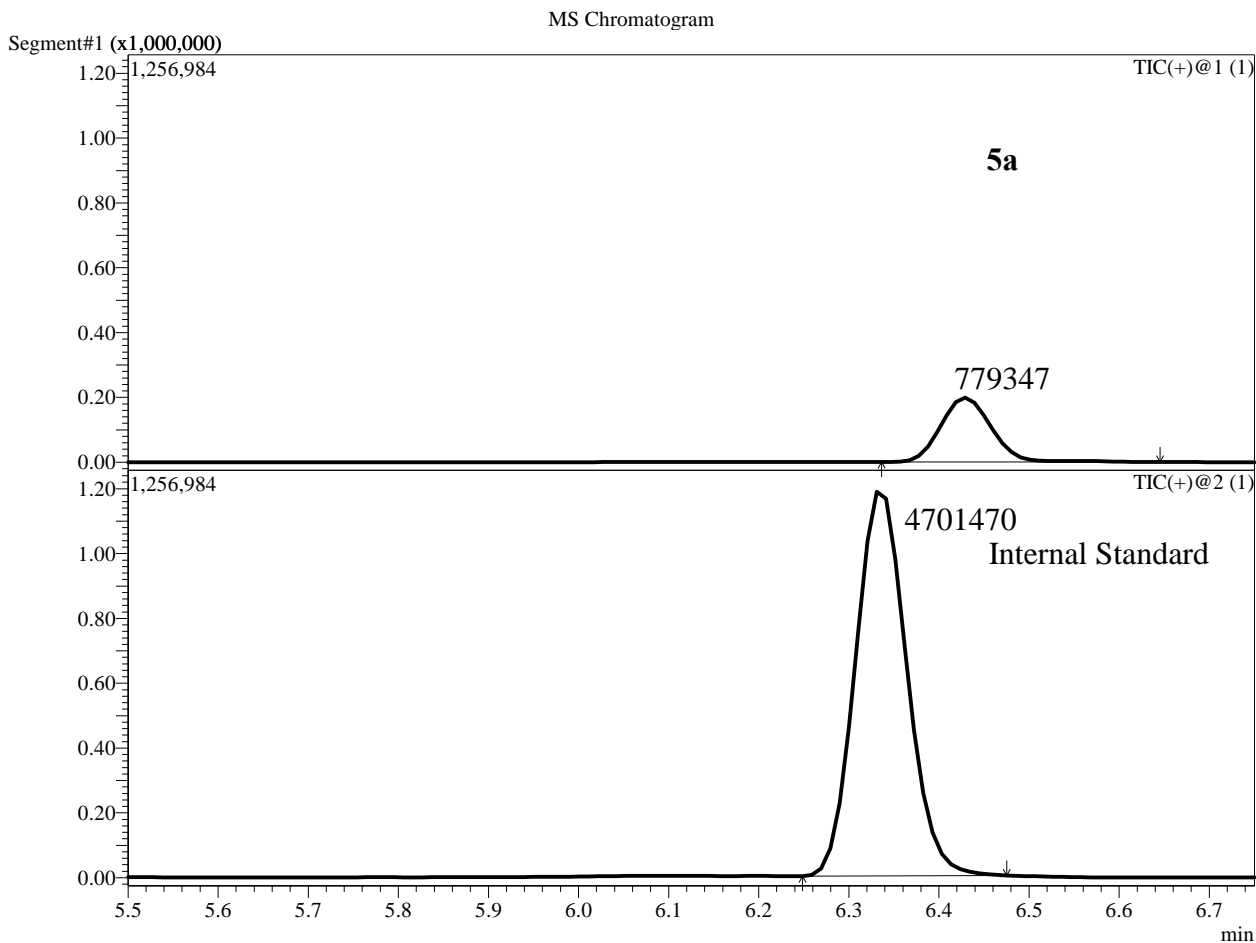
	5a TIC Extraction 1 Forebrain Run 1	7a TIC Extraction 2 Forebrain Run 1	5a TIC Extraction 2 Forebrain Run 2	7a TIC Extraction 2 Forebrain Run 2	5a:7a Forebrain Run 1	5a:7a Forebrain Run 2	31b:41b Average	Concentration in 100 uL load solvent	Forebrain Weight	5a (µM) in Forebrain	Cohort Average Brain (µM)
1h A po	5977020	2759730	6141928	2333818	2.166	2.631708214	2.399	2.513397747	0.332	7.570475142	2.158456216
1h B po	292507	2668536	272899	2375017	0.110	0.11490402	0.112	0.161280476	0.325	0.496247619	
1h C po	25436	2933832	17519	2623429	0.009	0.006677901	0.008	0.053694136	0.28	0.191764773	
1h D po	152439	2730977	148097	2761766	0.056	0.053624022	0.055	0.102091754	0.272	0.375337329	
2h A po	36528	2712517	35960	2495991	0.013	0.014407103	0.014	0.060136767	0.34	0.176872844	1.572522955
2h B po	159645	2683537	156009	2517982	0.059	0.061957949	0.061	0.108267018	0.315	0.343704818	
2h C po	4185007	2755530	3748330	2500504	1.519	1.499029796	1.509	1.598003589	0.301	5.308982024	
2h D po	199599	2474028	224150	2443716	0.081	0.091725061	0.086	0.134475383	0.292	0.460532135	
12h A po	12881	1744456	19722	2484663	0.007	0.007937495	0.008	0.053680592	0.274	0.195914571	0.206518873
12h B po	13743	2713069	12945	2555452	0.005	0.00506564	0.005	0.051010942	0.27	0.188929416	
12h C po	77824	2426256	77919	2267426	0.032	0.034364517	0.033	0.079973556	0.305	0.262208379	
12h D po	28540	2298942	32820	2387249	0.012	0.013748042	0.013	0.059256655	0.331	0.179023128	
1h A ip	945282	2496297	963363	2429633	0.379	0.396505563	0.388	0.444513449	0.325	1.367733691	2.203126835
1h B ip	44142396	2286375	44884226	2551428	19.307	17.59180584	18.449	19.02455543	0.285	66.75282608	
1h C ip	1927865	2325073	1817727	2318090	0.829	0.784148588	0.807	0.875606925	0.316	2.77090799	
1h D ip	1255381	1904408	1648445	2482521	0.659	0.664020566	0.662	0.726397214	0.294	2.470738824	
2h A ip	3769513	2443467	4040845	2383218	1.543	1.695541491	1.619	1.711384555	0.29	5.901326053	2.238609215
2h B ip	572336	2029841	625088	2067222	0.282	0.302380683	0.292	0.346356145	0.311	1.113685354	
2h C ip	511351	2198383	533855	2325388	0.233	0.229576742	0.231	0.283522272	0.324	0.875068739	
2h D ip	603096	2213597	370398	1512960	0.272	0.244816783	0.259	0.311856518	0.293	1.064356716	
12h A ip	253486	2251485	254211	2428911	0.113	0.104660484	0.109	0.1575408	0.305	0.516527212	0.486087075
12h B ip	94468	1928442	129539	2378523	0.049	0.05446195	0.052	0.09900881	0.32	0.309402532	
12h C ip	253352	2215015	262466	2337447	0.114	0.112287466	0.113	0.162386082	0.257	0.63185246	
12h D ip	233487	2196476	248146	2463052	0.106	0.100747365	0.104	0.152295187	0.313	0.486566094	

Assuming tissue density = 1

Plasma Extraction

	5a TIC Extraction Plasma Run 1	7a TIC Extraction Plasma Run 1	5a TIC Extraction Plasma Run 2	7a TIC Extraction Plasma Run 2	5a:7a Plasma Run 1	5a:7a Plasma Run 2	5a:7a Average	Concentration in 100 uL load solvent	Plasma volume (ml)	5a (µM) in Plasma	Cohort Average Plasma (µM)
1h A po	47339	1602760	52848	1718260	0.030	0.030756696	0.030	0.07681151	0.1	1.152172646	1.058673725
1h B po	54222	996223	59588	1155461	0.054	0.051570758	0.053	0.100320242	0.1	1.504803625	
1h C po	5309	1415864	6167	1577710	0.004	0.00390883	0.004	0.049739141	0.1	0.746087117	
1h D po	93448	2514127	105524	2974826	0.037	0.035472327	0.036	0.083163151	0.1	0.83163151	
2h A po	7829	1860480	5257	2241122	0.004	0.0023457	0.003	0.049170923	0.1	0.491709233	0.607573297
2h B po	39748	2039735	47444	2478357	0.019	0.019143328	0.019	0.065669429	0.1	0.656694293	
2h C po	89652	2700075	101756	3350373	0.033	0.030371544	0.032	0.078499835	0.1	0.784998351	
2h D po	10090	2366111	9453	2867263	0.004	0.003296872	0.004	0.049689131	0.1	0.496891309	
12h A po	5158	2055674	5970	3479059	0.003	0.001715981	0.002	0.047973198	0.1	0.479731977	0.483431165
12h B po	11477	2763038	17700	3421667	0.004	0.005172917	0.005	0.050597177	0.1	0.50597177	
12h C po	4403	2511109	4686	3218713	0.002	0.001455861	0.002	0.047450688	0.1	0.47450688	
12h D po	3690	1966545	3079	2701224	0.002	0.001139854	0.002	0.047351404	0.1	0.473514035	
1h A ip	911119	2647505	1159548	3444783	0.344	0.336609882	0.340	0.39594499	0.1	3.959449899	3.505084632
1h B ip	31977557	2689738	41393319	3619008	11.889	11.43775283	11.663	12.04377418	0.1	120.4377418	
1h C ip	356622	2638480	433347	3480134	0.135	0.124520205	0.130	0.179367497	0.1	1.793674967	
1h D ip	1244440	2847130	1407472	3521113	0.437	0.39972361	0.418	0.476212903	0.1	4.762129032	
2h A ip	558145	1171861	934405	2095224	0.476	0.445969023	0.461	0.520163632	0.1	5.201636318	2.767721319
2h B ip	449711	2997634	533305	3773955	0.150	0.141311966	0.146	0.195647617	0.1	1.956476171	
2h C ip	456163	2221701	584815	3287191	0.205	0.177907216	0.192	0.242913694	0.1	2.429136944	
2h D ip	290795	2782072	353790	3728829	0.105	0.094879653	0.100	0.148363584	0.1	1.483635842	
12h A ip	37150	2925522	30010	3476117	0.013	0.008633196	0.011	0.056772003	0.1	0.567720034	0.814230074
12h B ip	105672	2701833	130864	3587591	0.039	0.036476845	0.038	0.084678724	0.1	0.84678724	
12h C ip	40048	2133356	52906	3005912	0.019	0.017600648	0.018	0.064508426	0.1	0.645084262	
12h D ip	240618	3214133	304325	4418325	0.075	0.068877912	0.072	0.119732876	0.1	1.197328758	

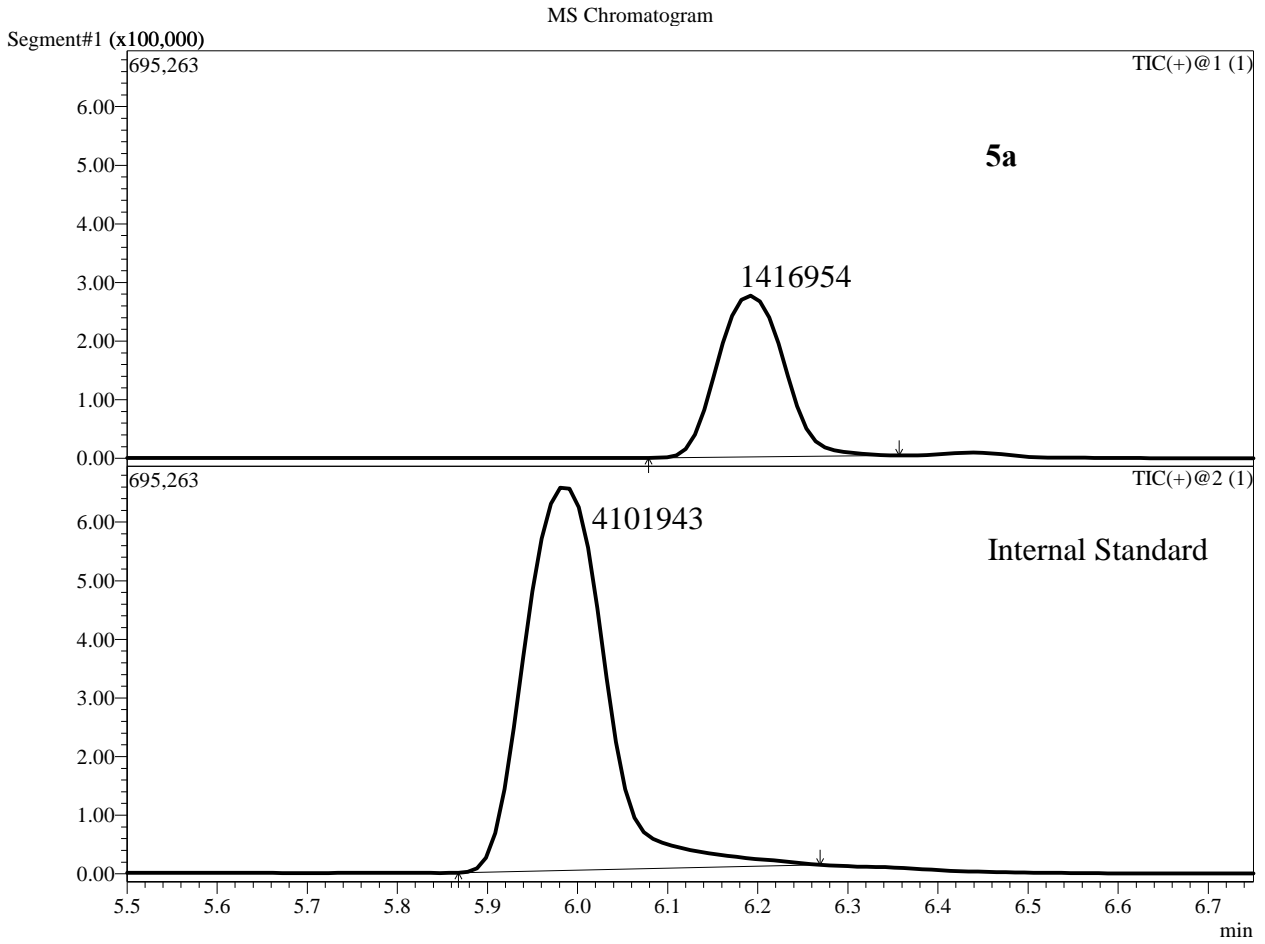
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 Injection Volume : 10
 Data File : 1.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.429	TIC	779347		1-1
2	6.335	TIC	4701470		1-2

Date Acquired : 3/31/2016 9:31:19 AM
 Sample ID : 1h ipA Plasma
 Injection Volume : 25.lcd
 Data File : V1.lcm
 Method File :

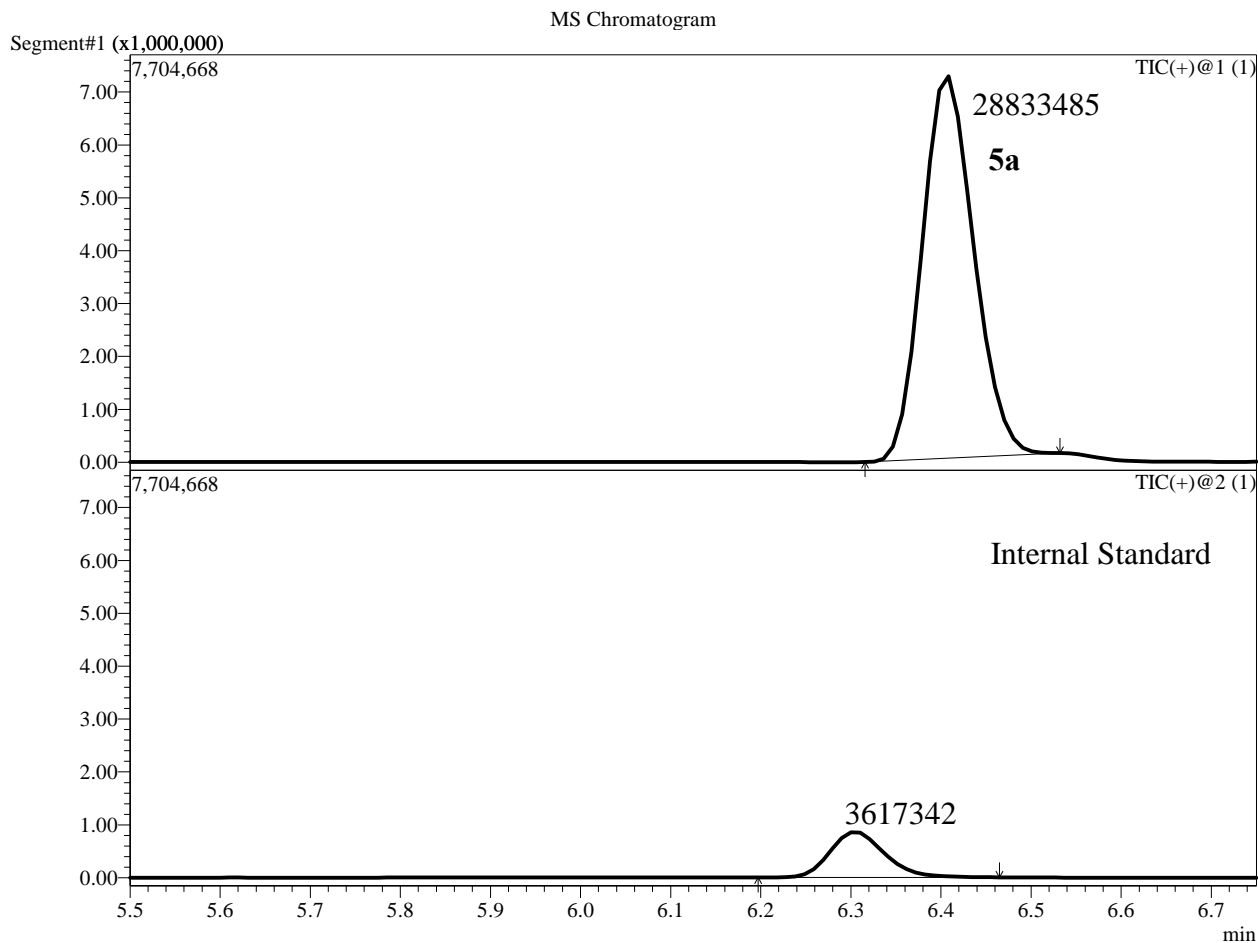


MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.191	TIC	1416954		1-1
2	5.986	TIC	4101943		1-2

Sample Information

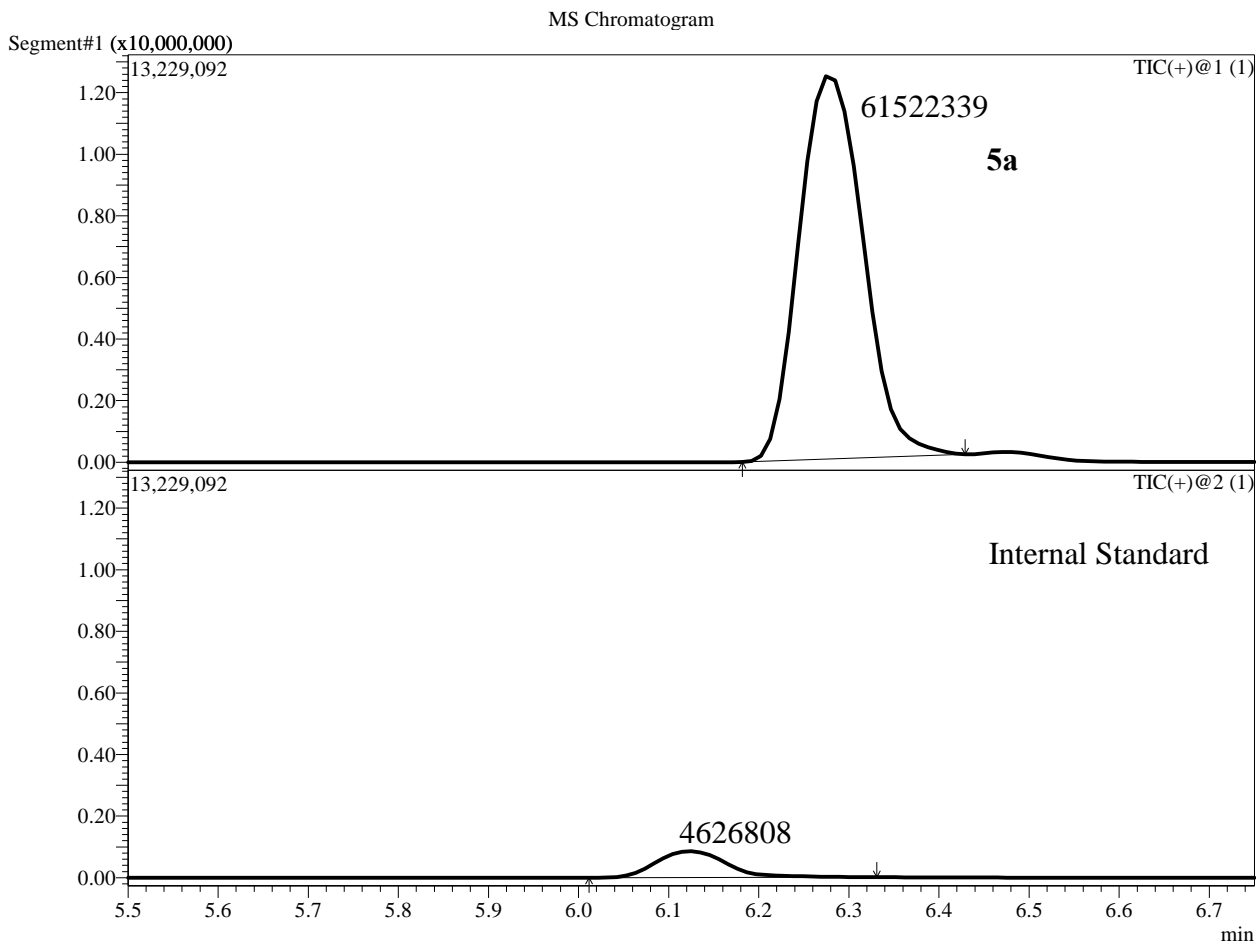
Date Acquired : 3/30/2016 5:32:50 PM
 Sample ID : 1h ipB Brain
 Injection Volume : 10
 Data File : 2.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.406	TIC	28833485		1-1
2	6.305	TIC	3617342		1-2

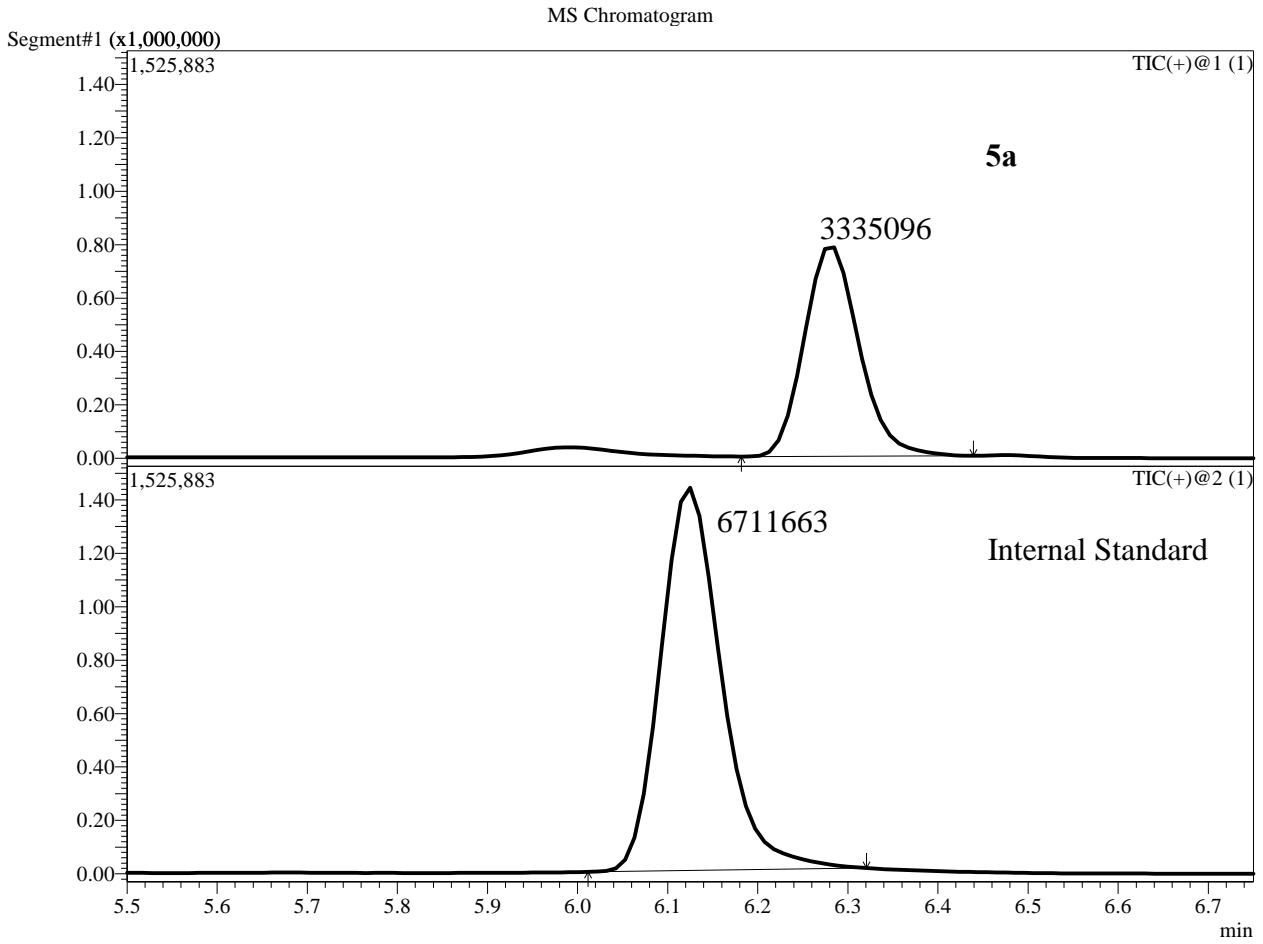
Date Acquired : 3/31/2016 9:41:51 AM
 Sample ID : 1h ipB Plasma
 Injection Volume : 10
 Data File : 26.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.278	TIC	61522339		1-1
2	6.124	TIC	4626808		1-2

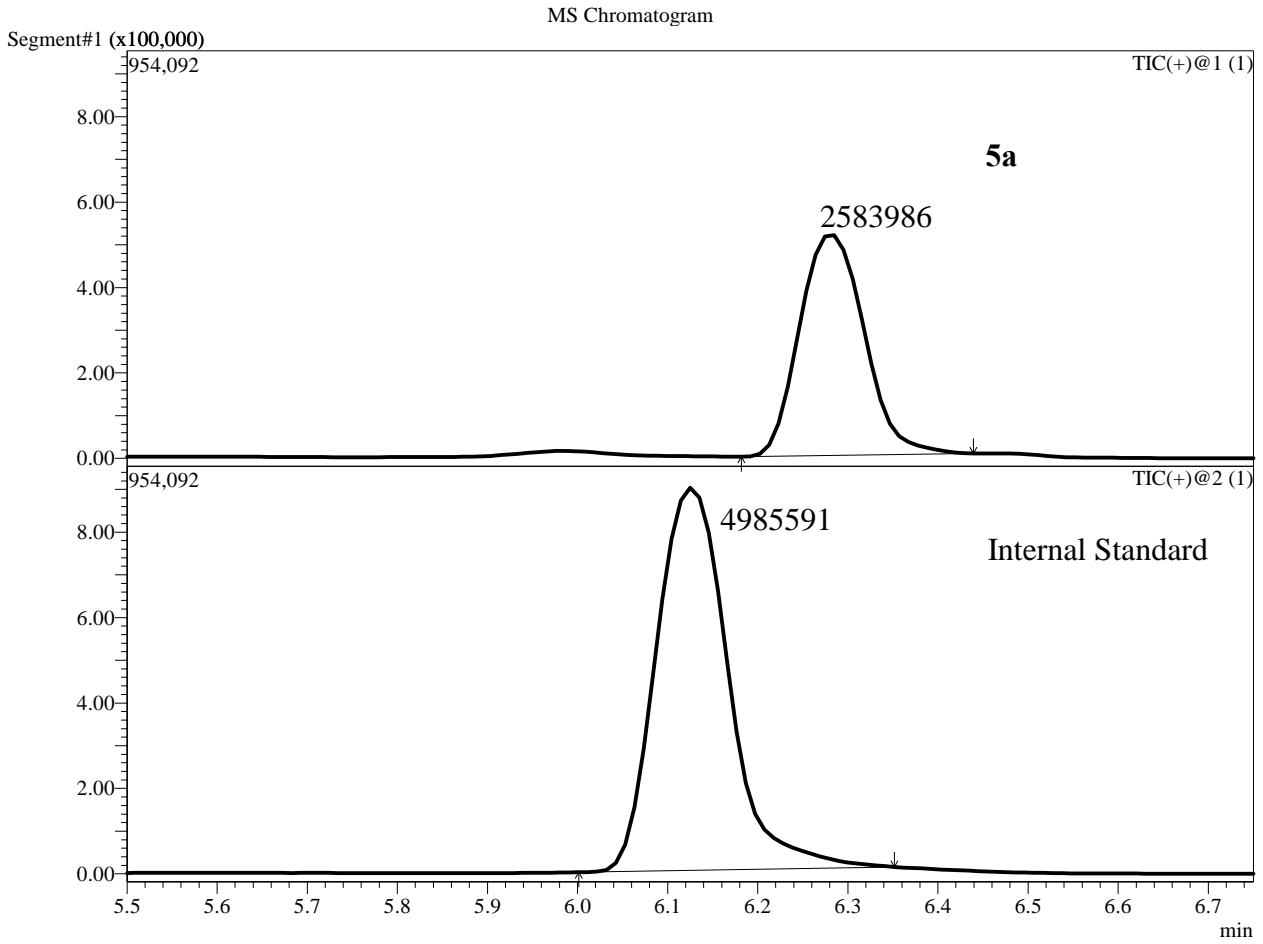
Date Acquired : 3/30/2016 5:43:20 PM
 Sample ID : 1h ipC Brain
 Injection Volume : 10
 Data File : 3.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.280	TIC	3335096		1-1
2	6.123	TIC	6711663		1-2

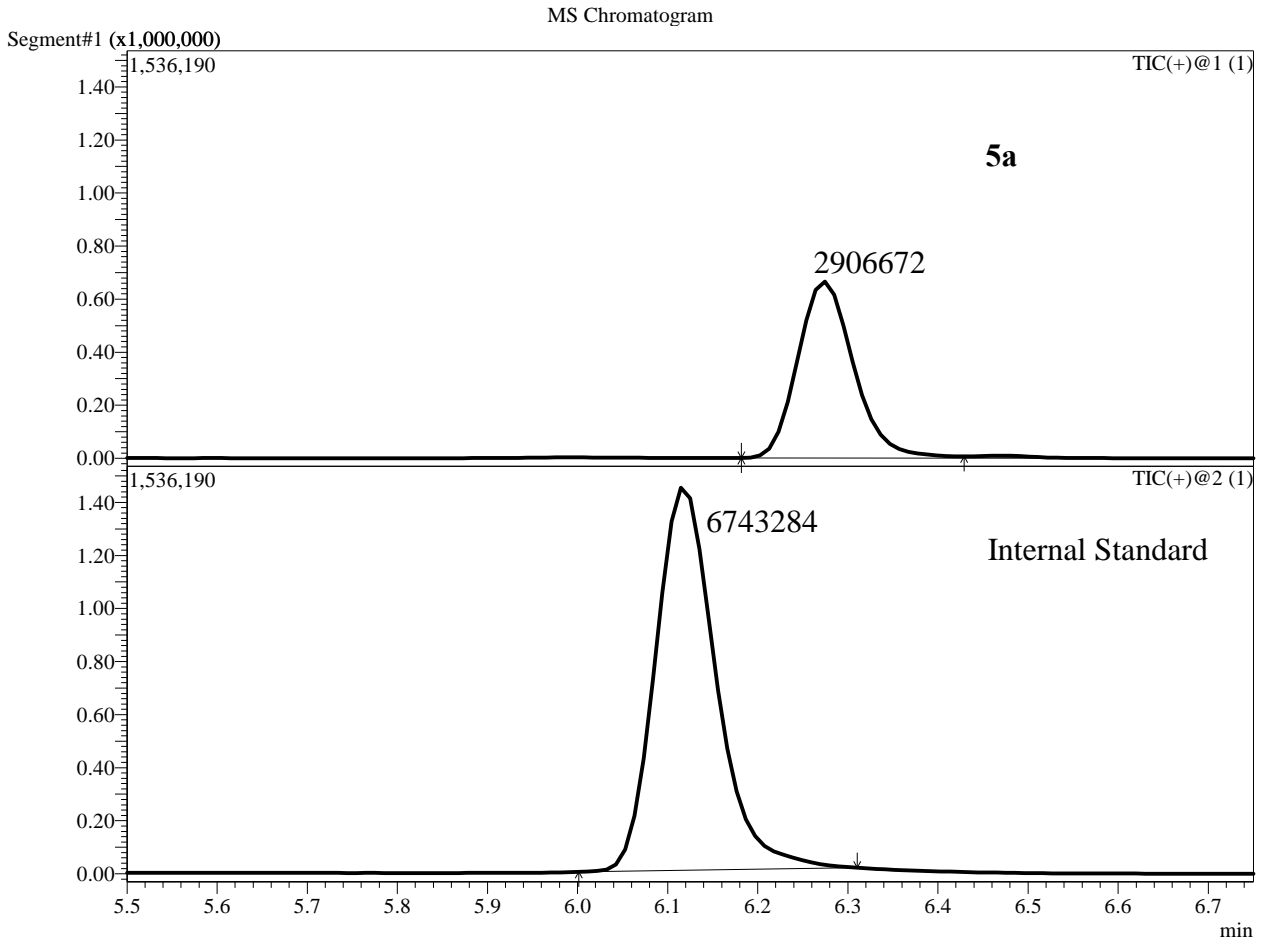
Date Acquired : 3/31/2016 9:52:21 AM
 Sample ID : 1h ipC Plasma
 Injection Volume : 10
 Data File : 27.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.280	TIC	2583986		1-1
2	6.126	TIC	4985591		1-2

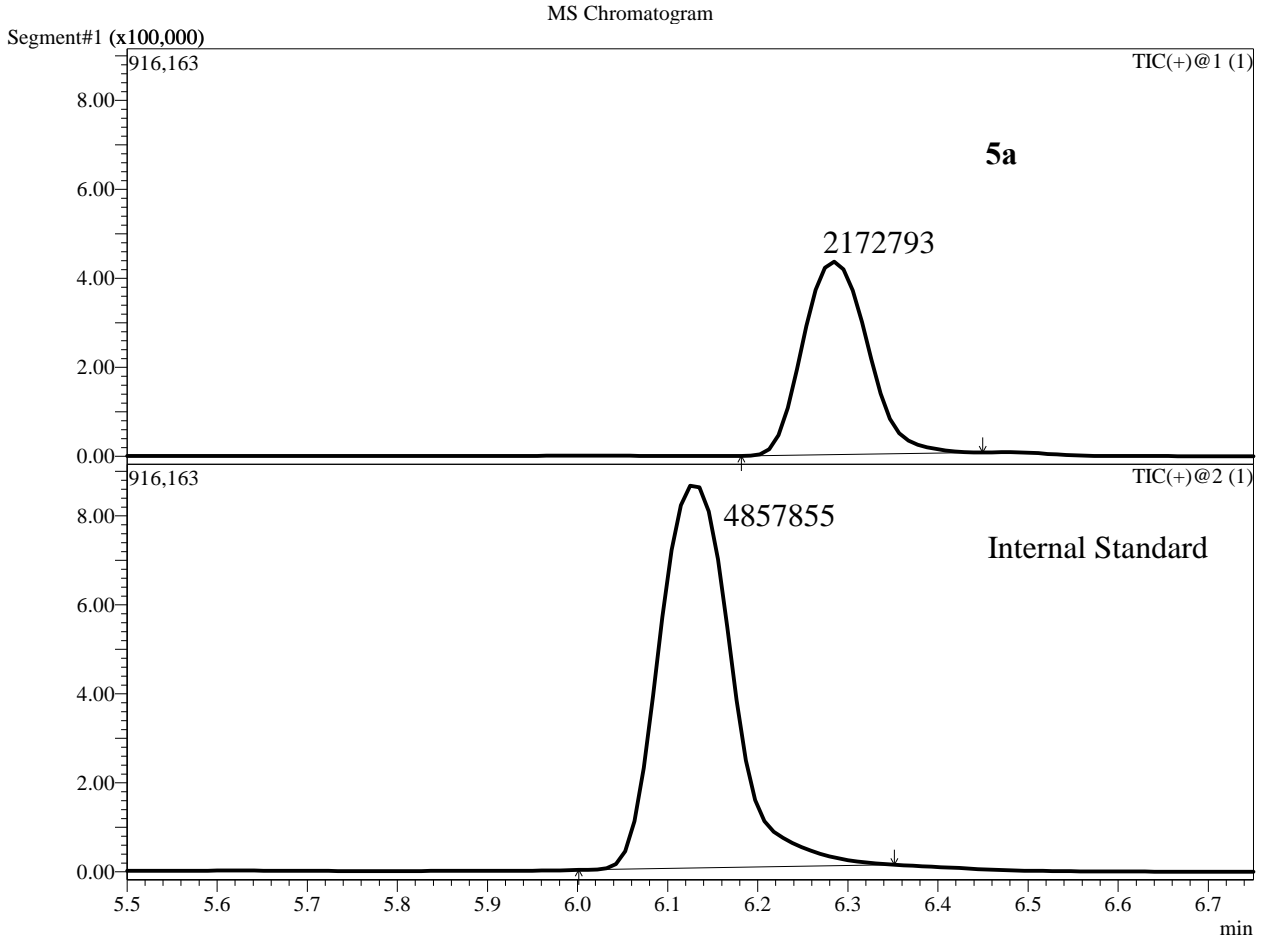
Date Acquired : 3/30/2016 5:53:50 PM
 Sample ID : 1h ipD Brain
 Injection Volume : 10
 Data File : 4.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.273	TIC	2906672		1-1
2	6.118	TIC	6743284		1-2

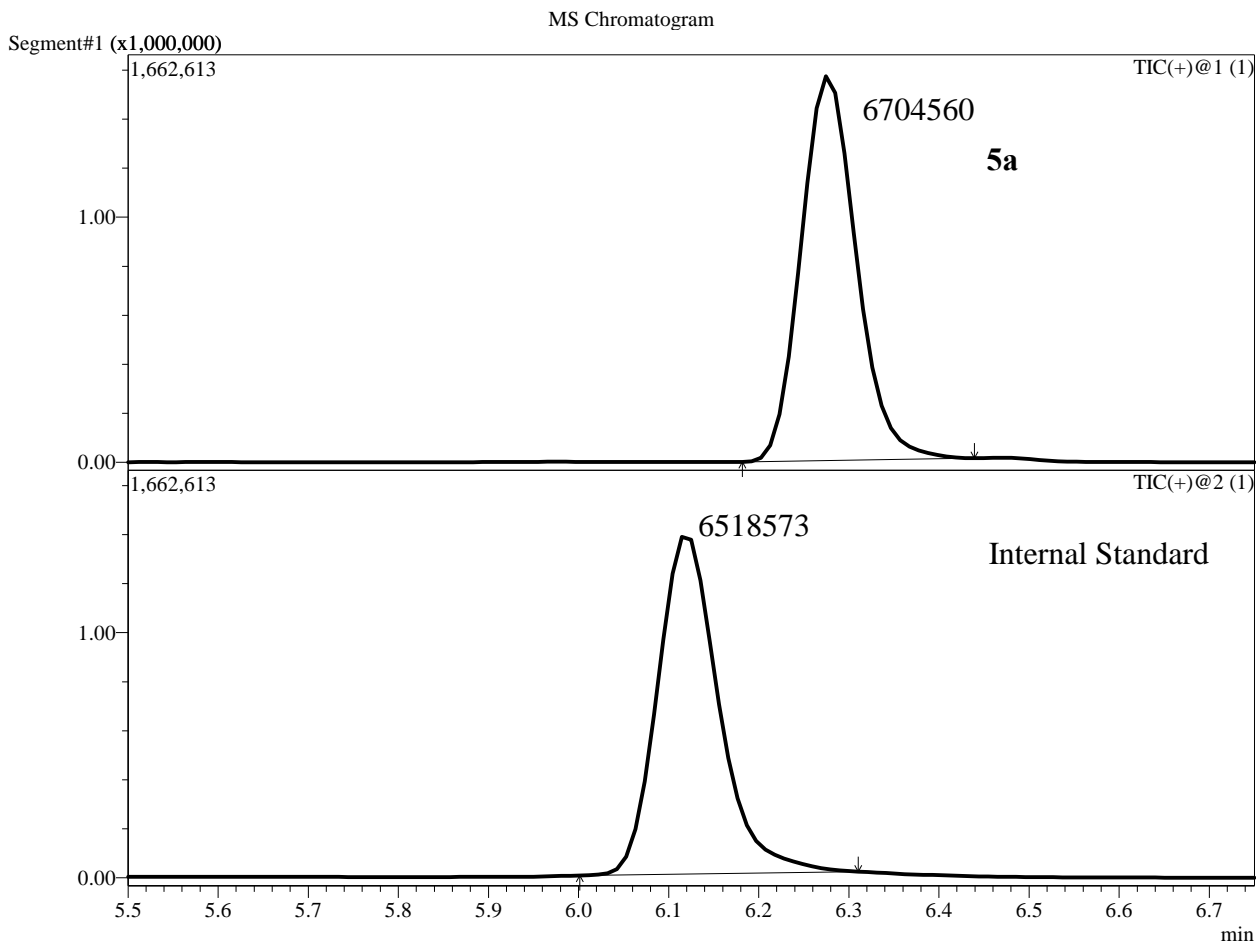
Date Acquired : 3/31/2016 10:02:51 AM
 Sample ID : 1h ipD Plasma
 Injection Volume : 10
 Data File : 28.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.284	TIC	2172793		1-1
2	6.129	TIC	4857855		1-2

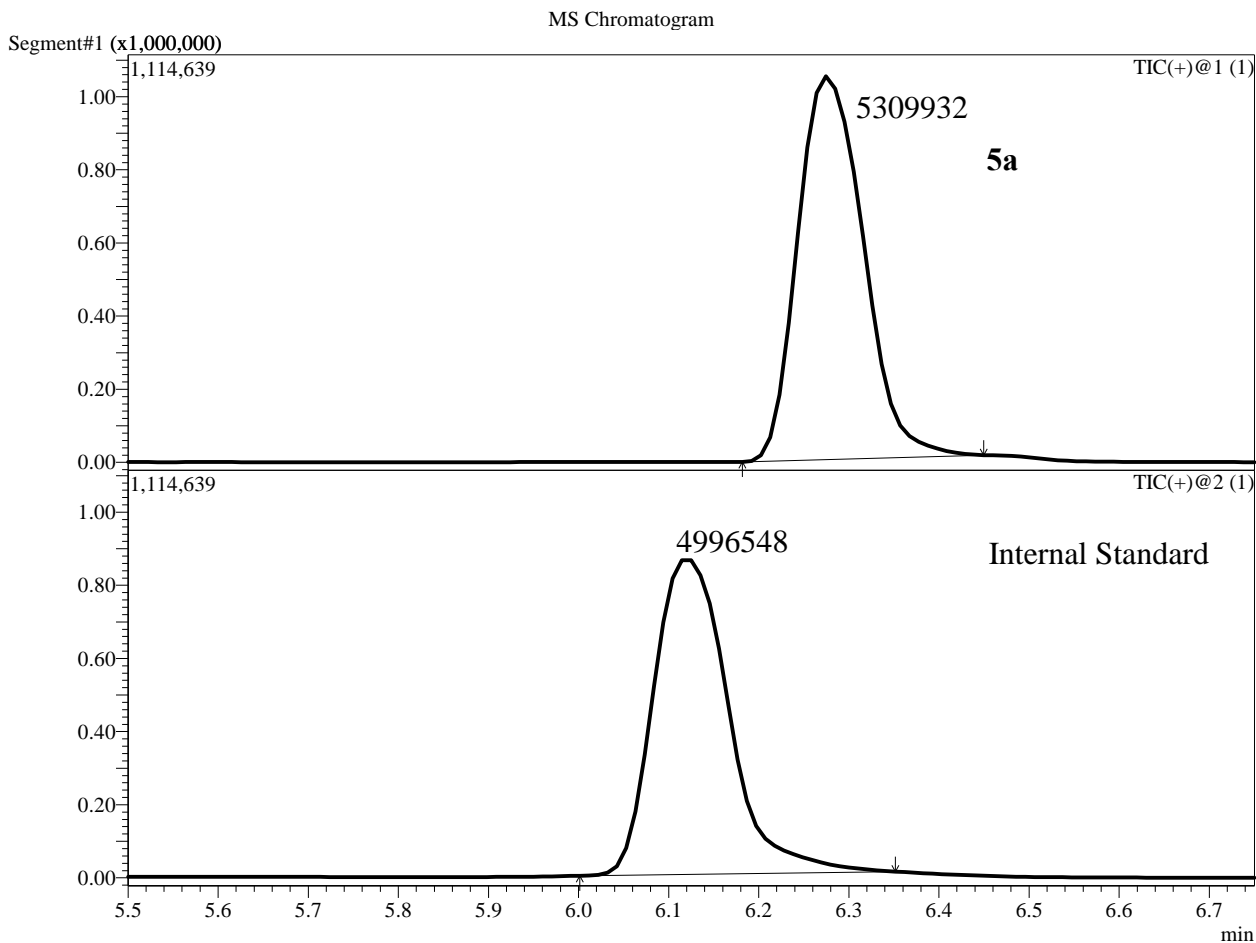
Date Acquired : 3/30/2016 6:04:20 PM
 Sample ID : 2h ipA Brain: 10
 Injection Volume : 5.lcd
 Data File : V1.lcm
 Method File :



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.276	TIC	6704560		1-1
2	6.119	TIC	6518573		1-2

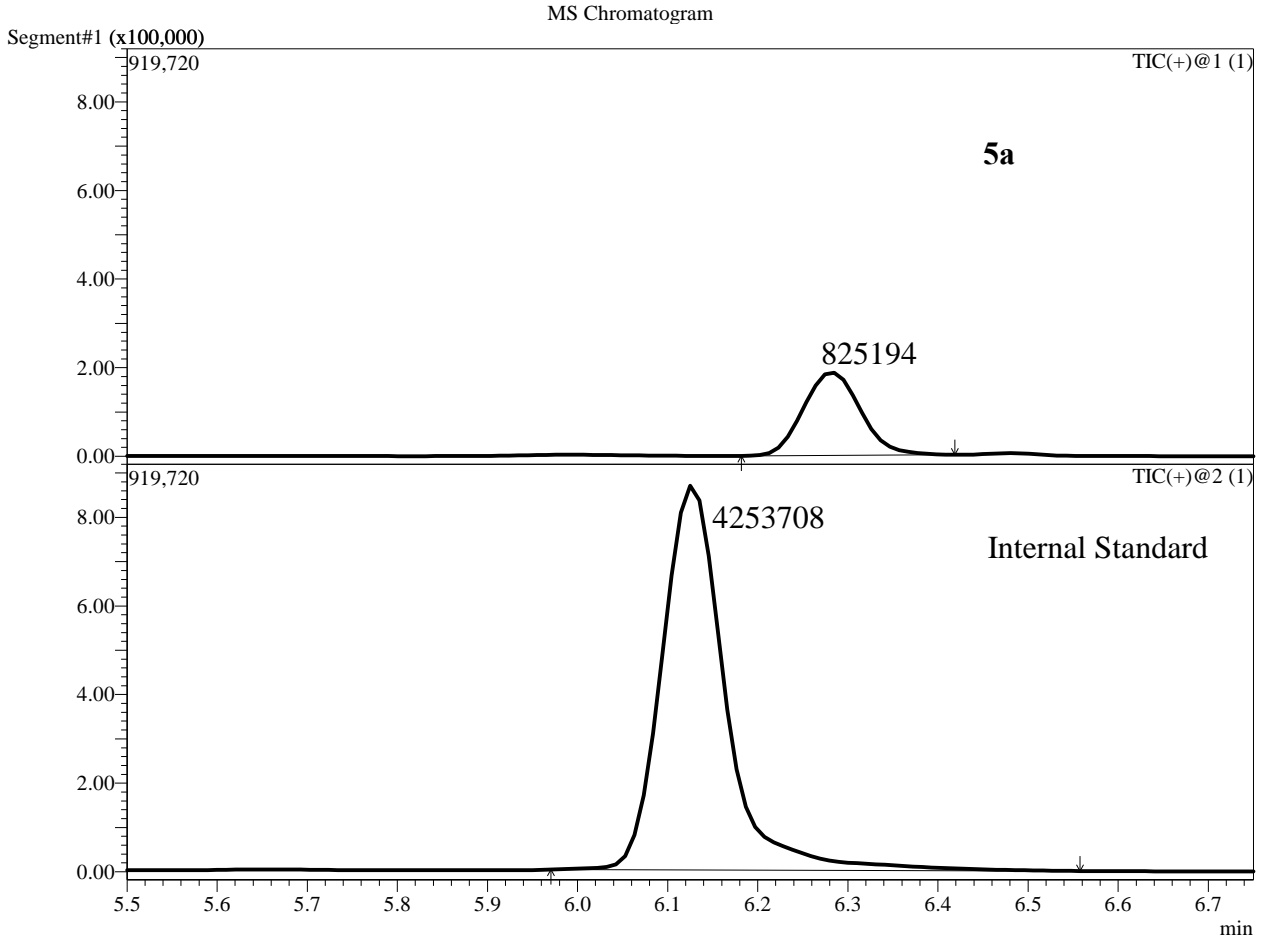
Date Acquired : 3/31/2016 10:13:20 AM :
 Sample ID : 2h ipA Plasma
 Injection Volume : 10
 Data File : 29.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.275	TIC	5309932		1-1
2	6.120	TIC	4996548		1-2

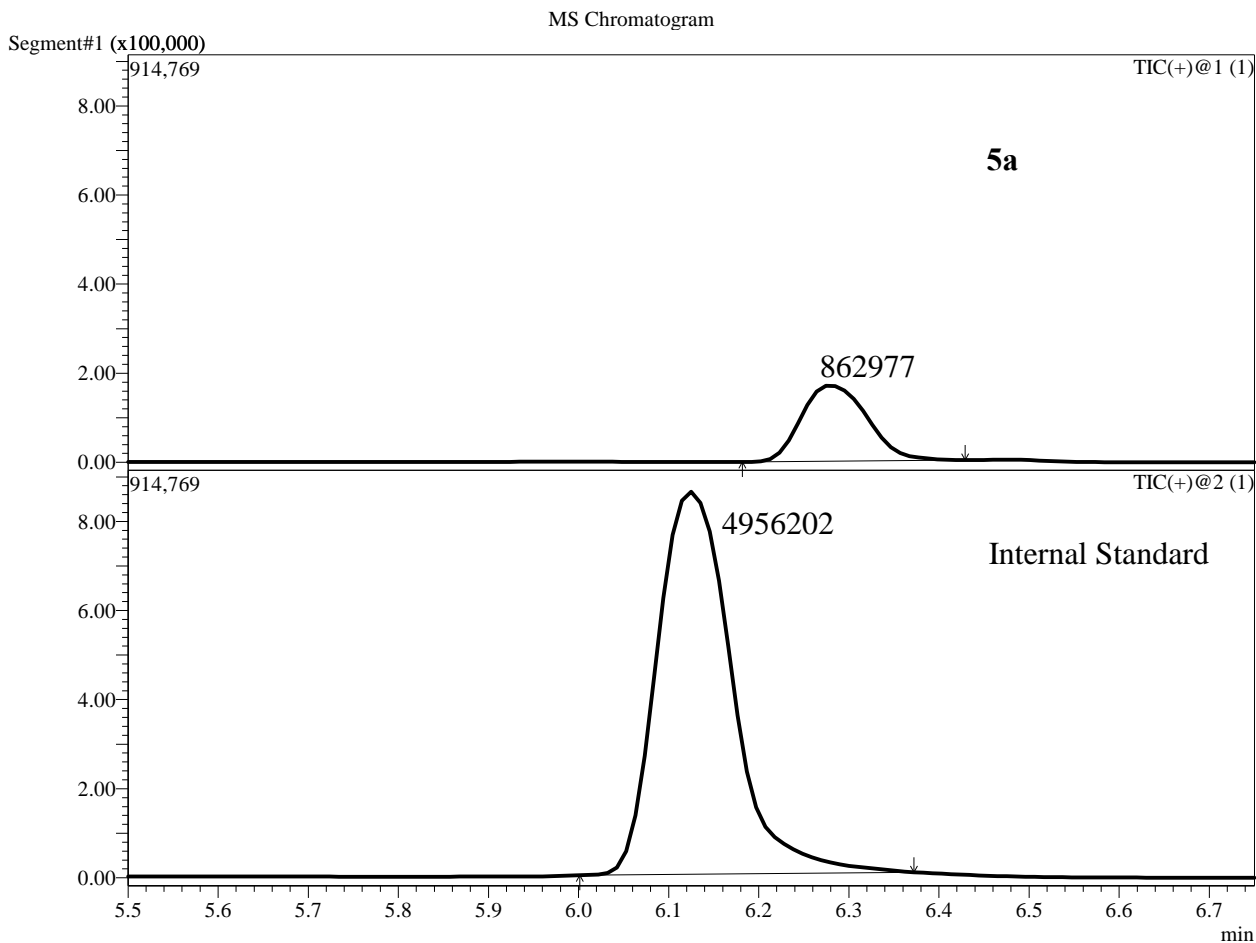
Date Acquired : 3/30/2016 6:14:50 PM
 Sample ID : 2h ipB Brain
 Injection Volume : 10
 Data File : 6.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.282	TIC	825194		1-1
2	6.127	TIC	4253708		1-2

Date Acquired : 3/31/2016 10:23:50 AM
 Sample ID : 2h ipB Plasma
 Injection Volume : 10
 Data File : 30.lcd
 Method File : V1.lcm

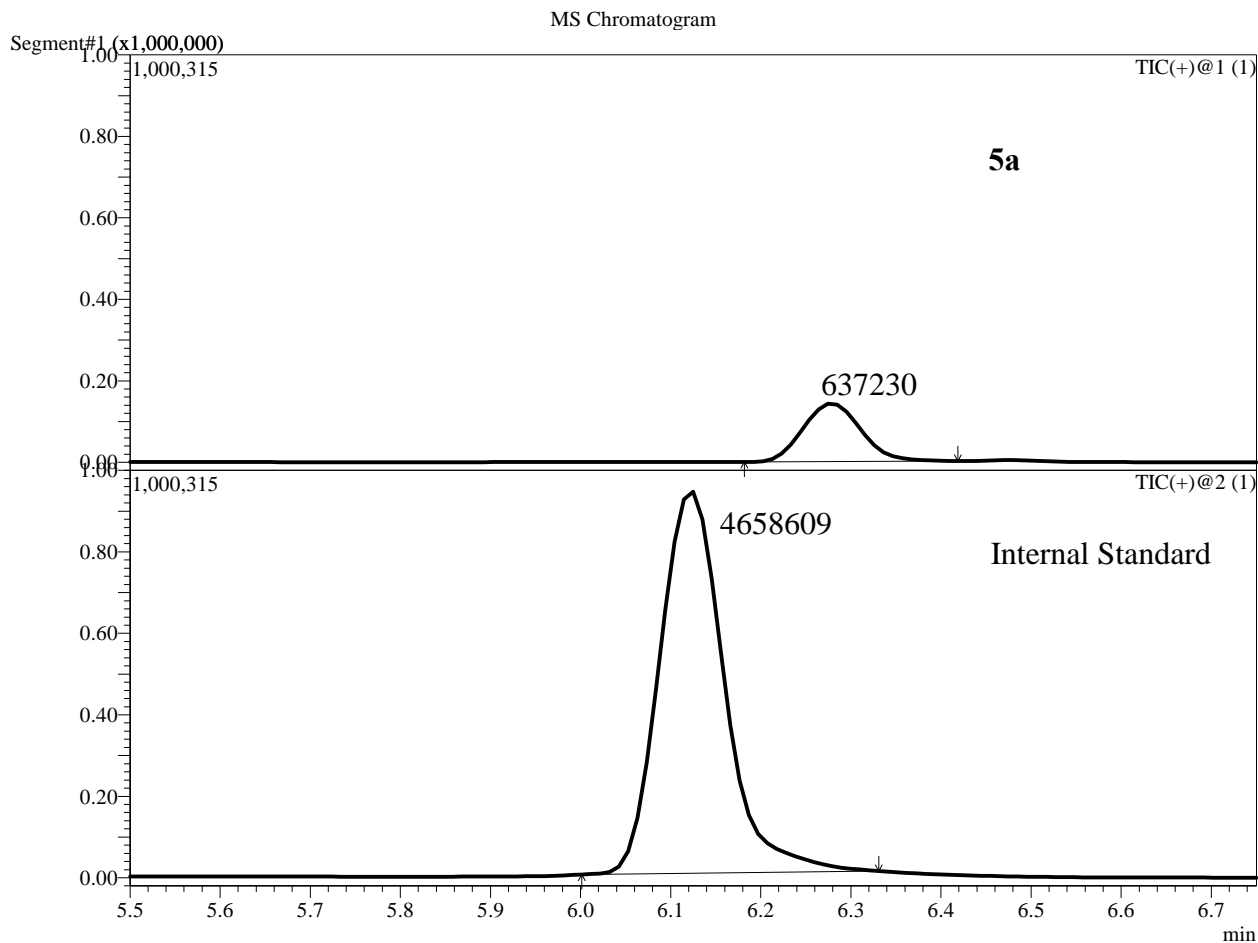


MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.279	TIC	862977		1-1
2	6.125	TIC	4956202		1-2

Sample Information

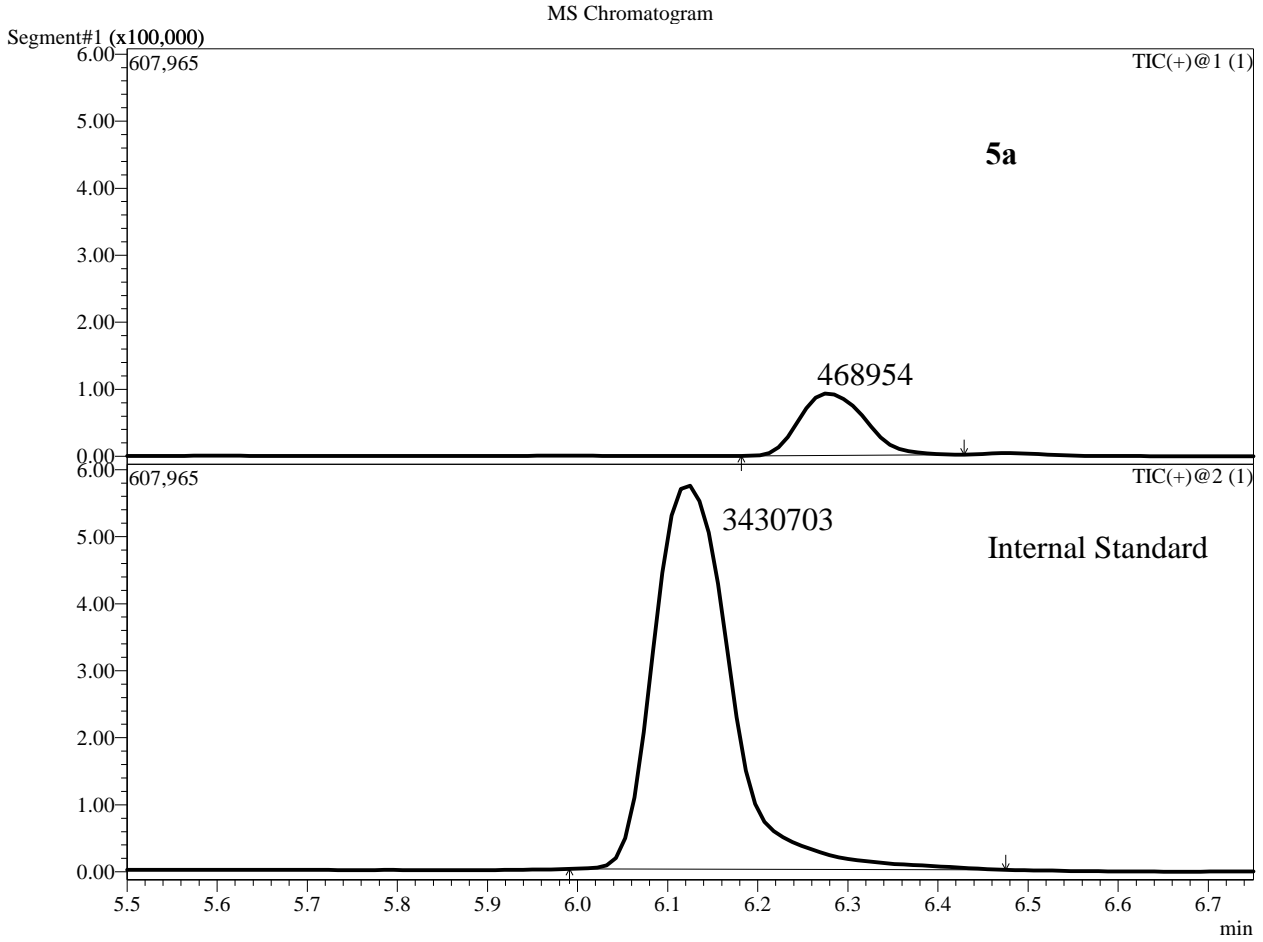
Date Acquired : 3/30/2016 6:25:21 PM
 Sample ID : 2h ipC Brain
 Injection Volume : 10
 Data File : 7.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.278	TIC	637230		1-1
2	6.122	TIC	4658609		1-2

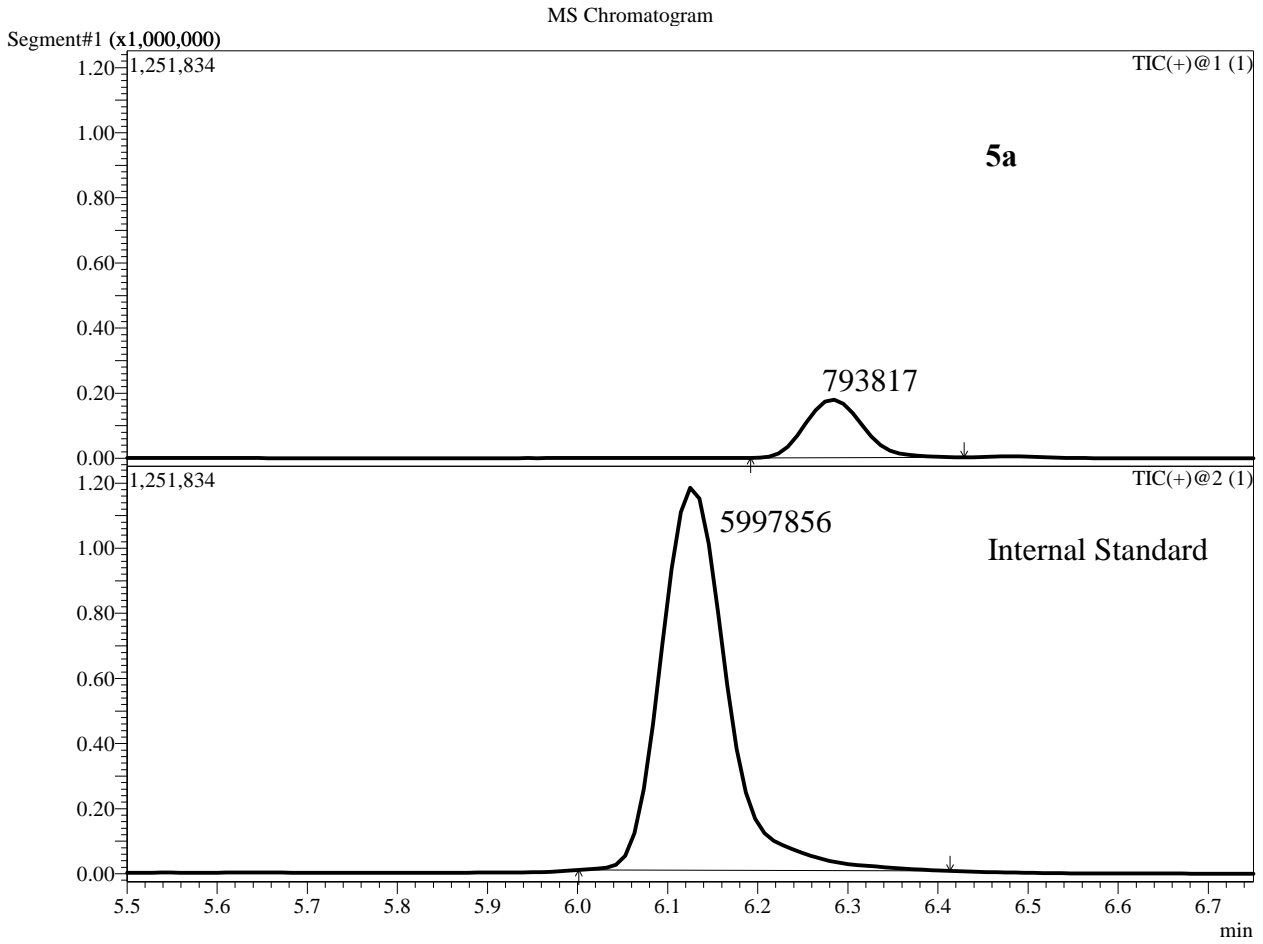
Date Acquired : 3/31/2016 10:34:20 AM
 Sample ID : 2h ipC Plasma
 Injection Volume : 10
 Data File : 31.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.278	TIC	468954		1-1
2	6.122	TIC	3430703		1-2

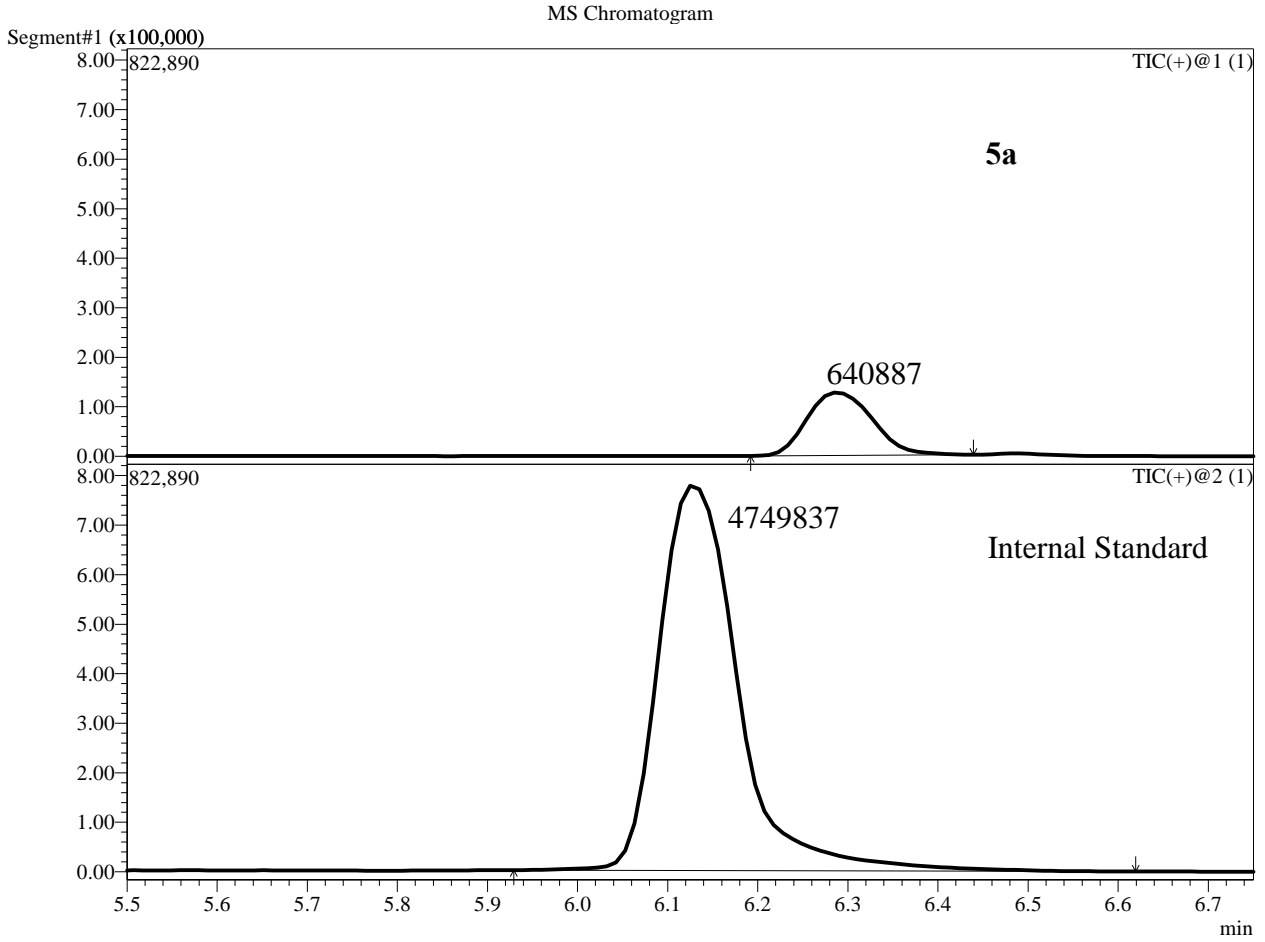
Date Acquired : 3/30/2016 6:35:52 PM
 Sample ID : 2h ipD Brain
 Injection Volume : 10
 Data File : 8.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.283	TIC	793817		1-1
2	6.127	TIC	5997856		1-2

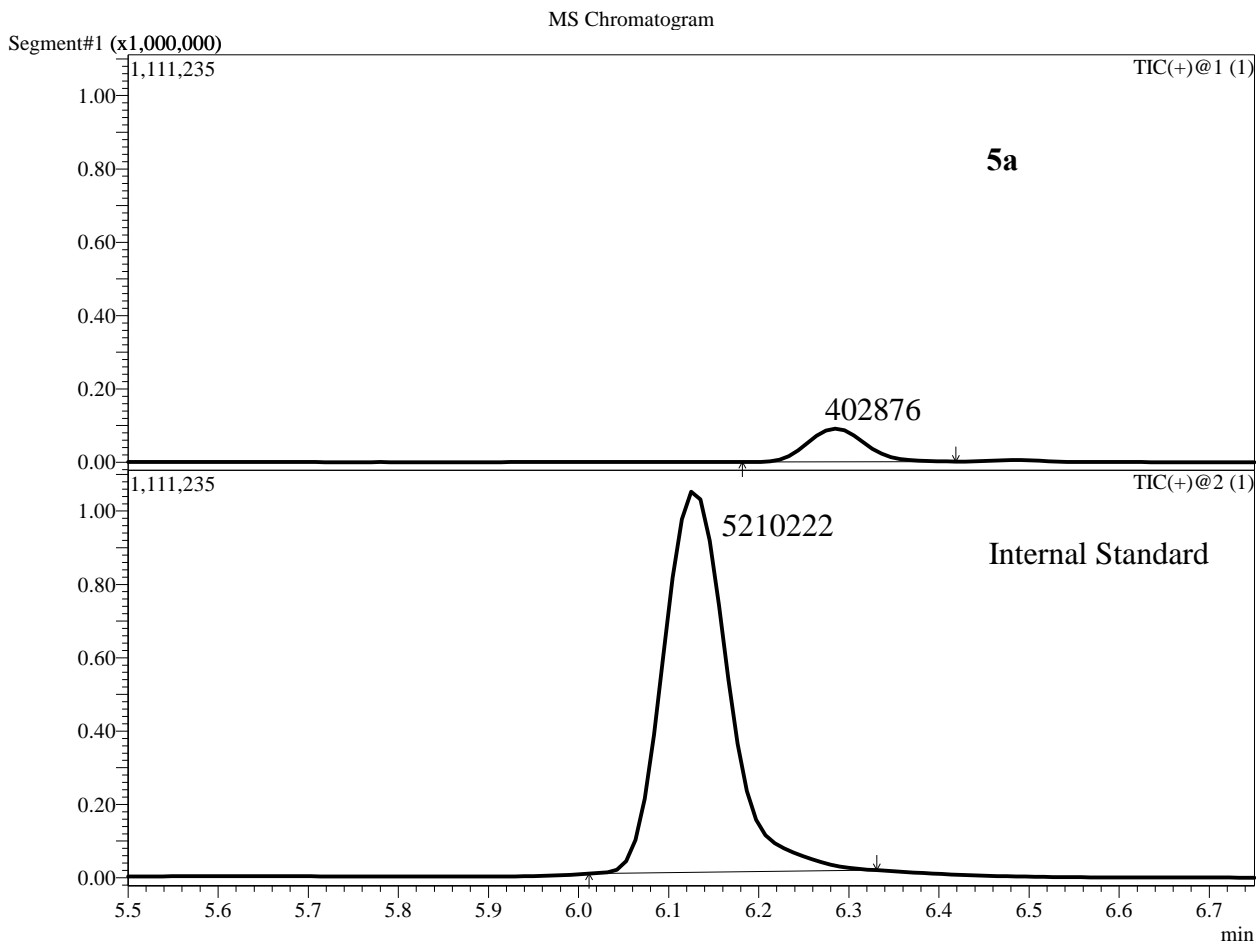
Date Acquired : 3/31/2016 10:44:51 AM
 Sample ID : 2h ipD Plasma
 Injection Volume : 10
 Data File : 32.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.288	TIC	640887		1-1
2	6.129	TIC	4749837		1-2

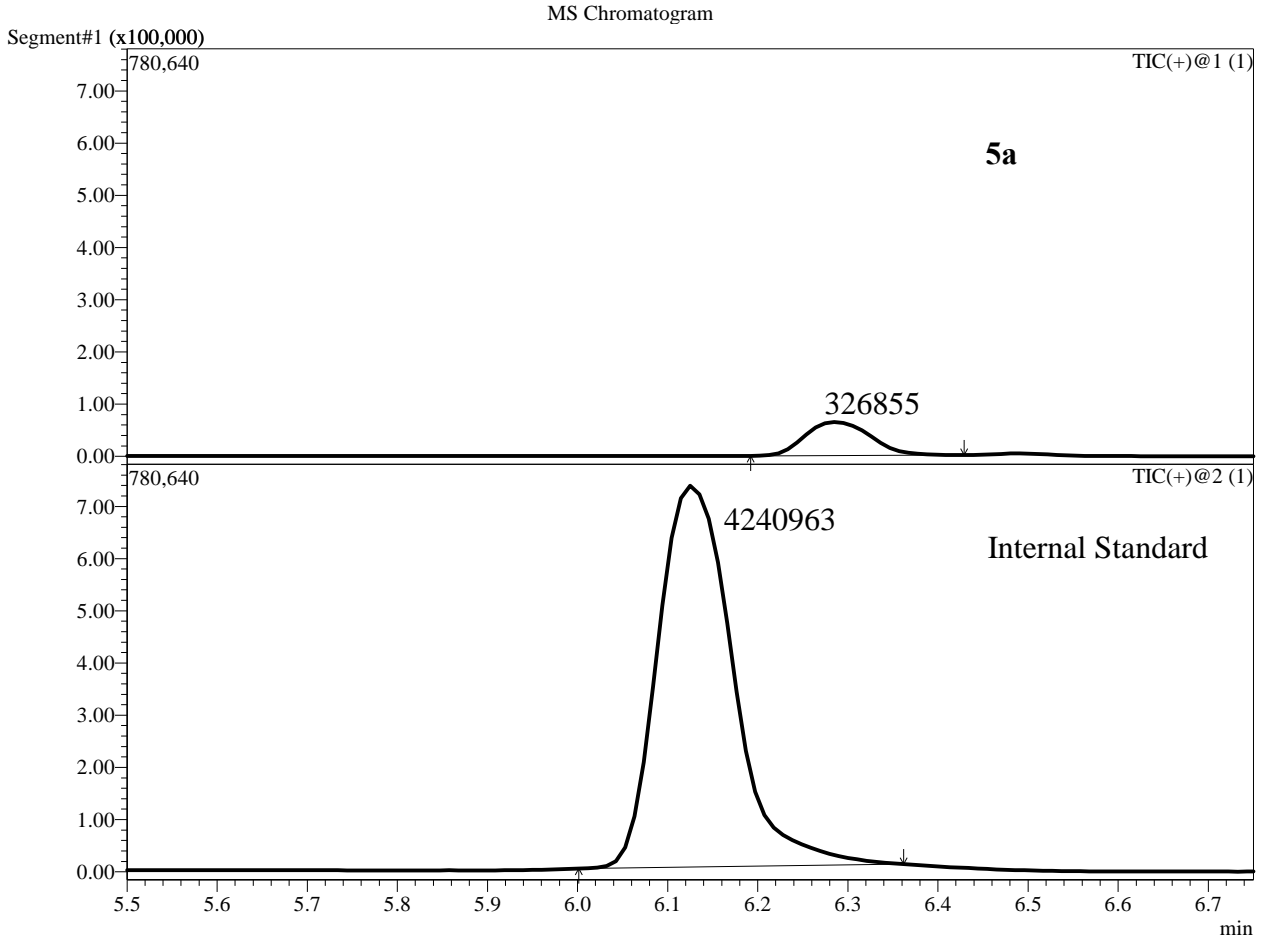
Date Acquired : 3/30/2016 6:46:23 PM
 Sample ID : 12h ipA Brain
 Injection Volume : 10
 Data File : 9.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.285	TIC	402876		1-1
2	6.128	TIC	5210222		1-2

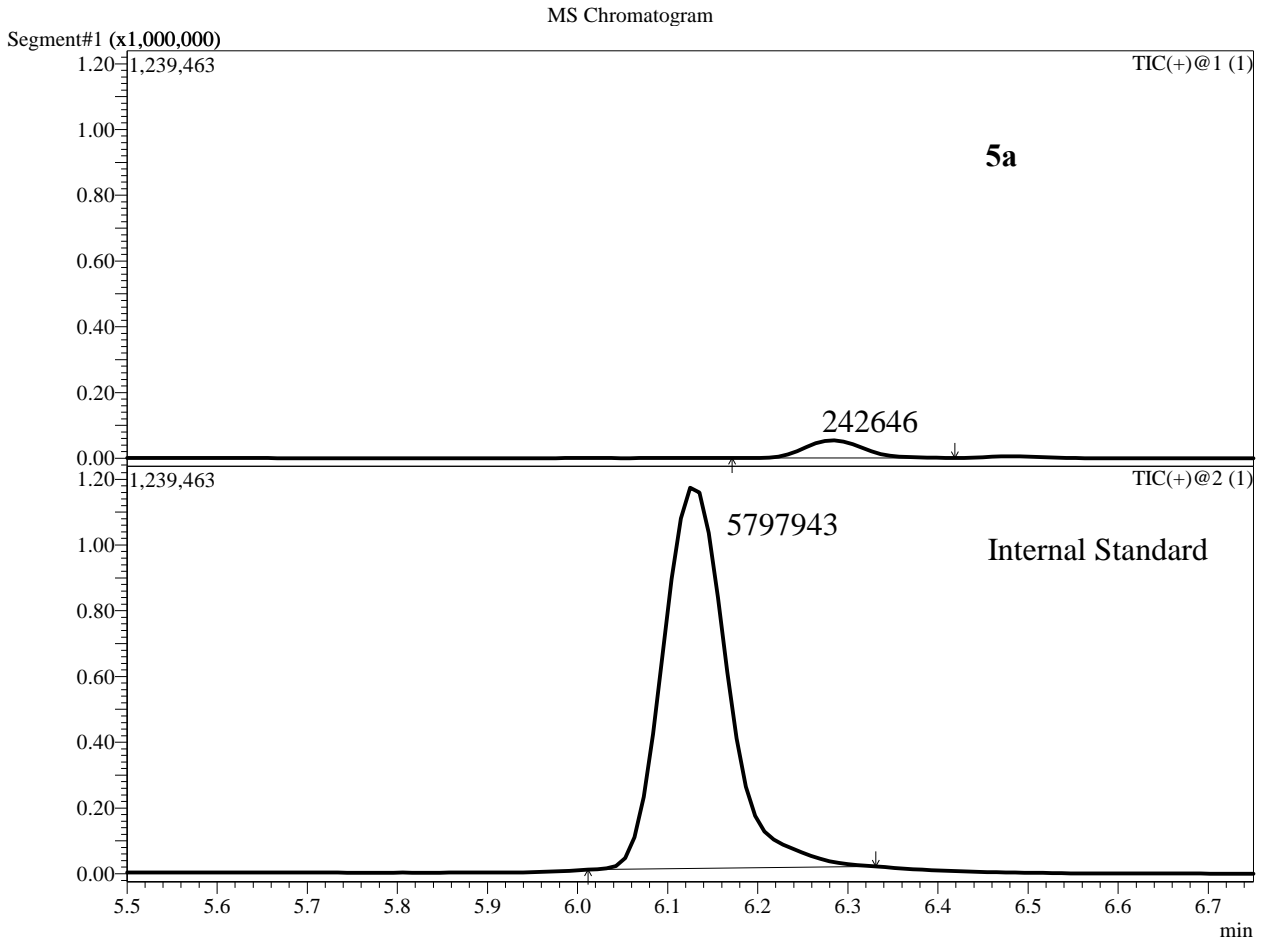
Date Acquired : 3/31/2016 10:55:21 AM
 Sample ID : 12h ipA Plasma
 Injection Volume : 10
 Data File : 33.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.285	TIC	326855		1-1
2	6.126	TIC	4240963		1-2

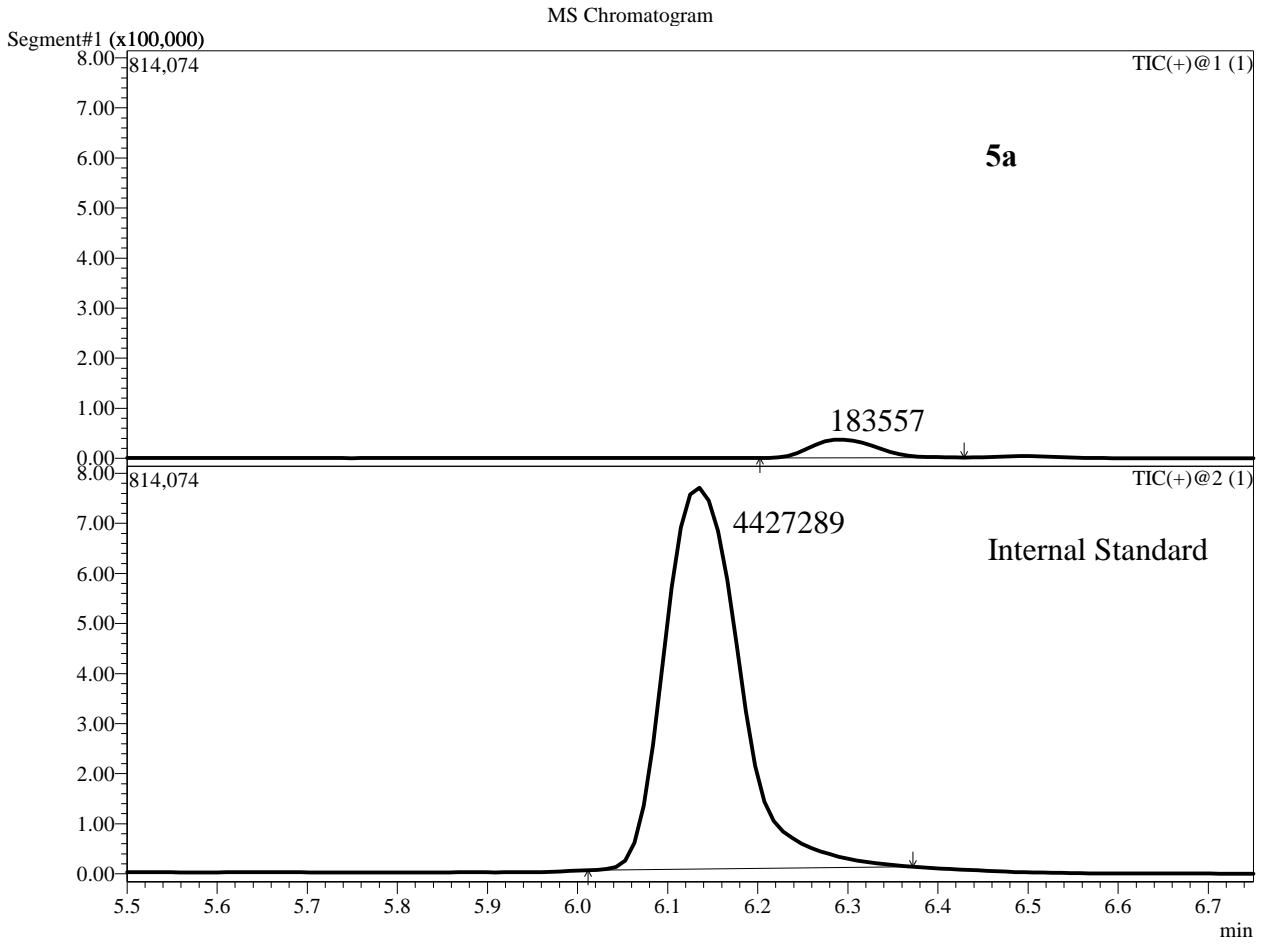
Date Acquired : 3/30/2016 6:56:53 PM
 Sample ID : 12h ipB Brain
 Injection Volume : 10
 Data File : 10.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.283	TIC	242646		1-1
2	6.129	TIC	5797943		1-2

Date Acquired : 3/31/2016 11:05:51 AM
 Sample ID : 12h ipB Plasma
 Injection Volume : 10
 Data File : 34.lcd
 Method File : V1.lcm

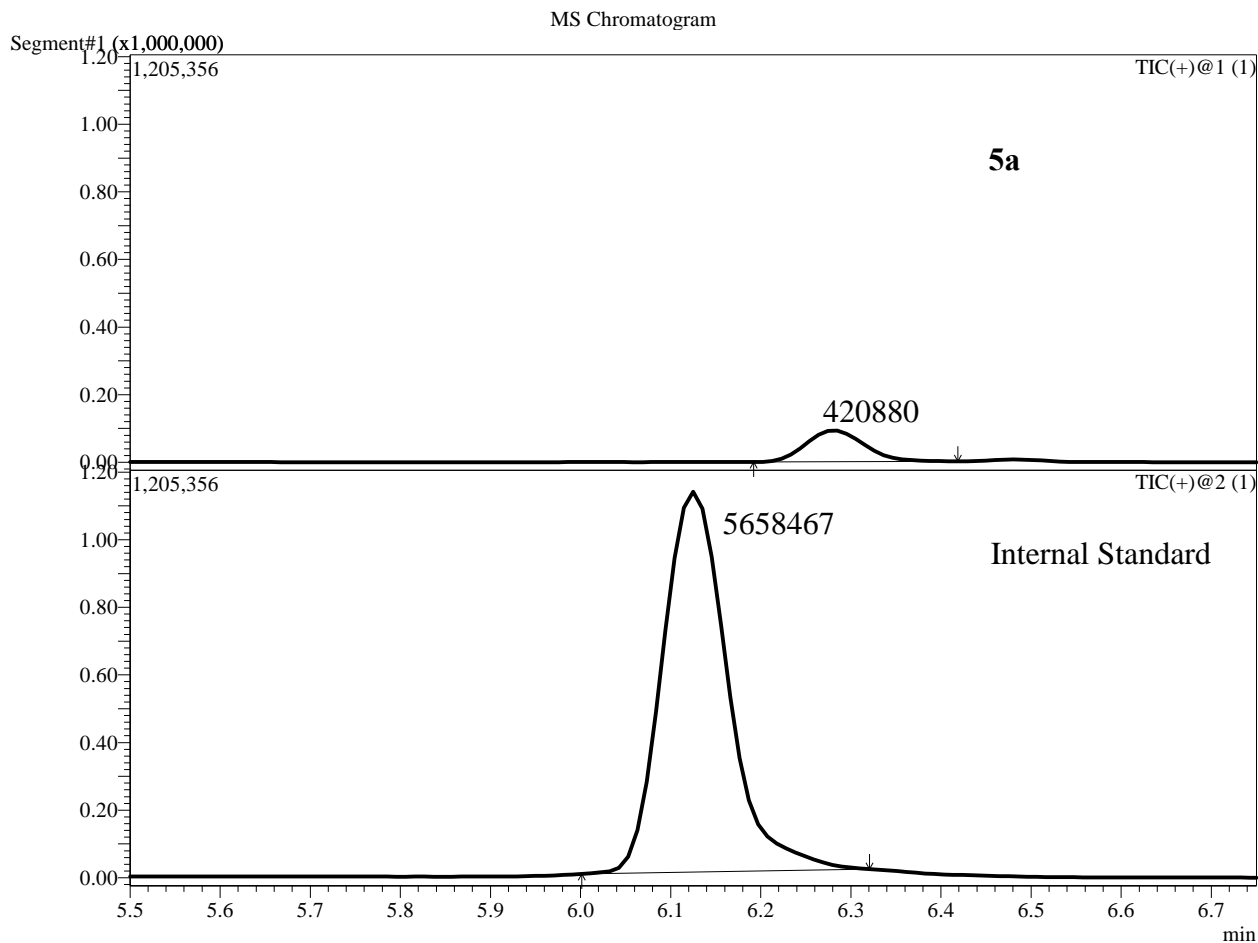


MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.291	TIC	183557		1-1
2	6.134	TIC	4427289		1-2

Sample Information

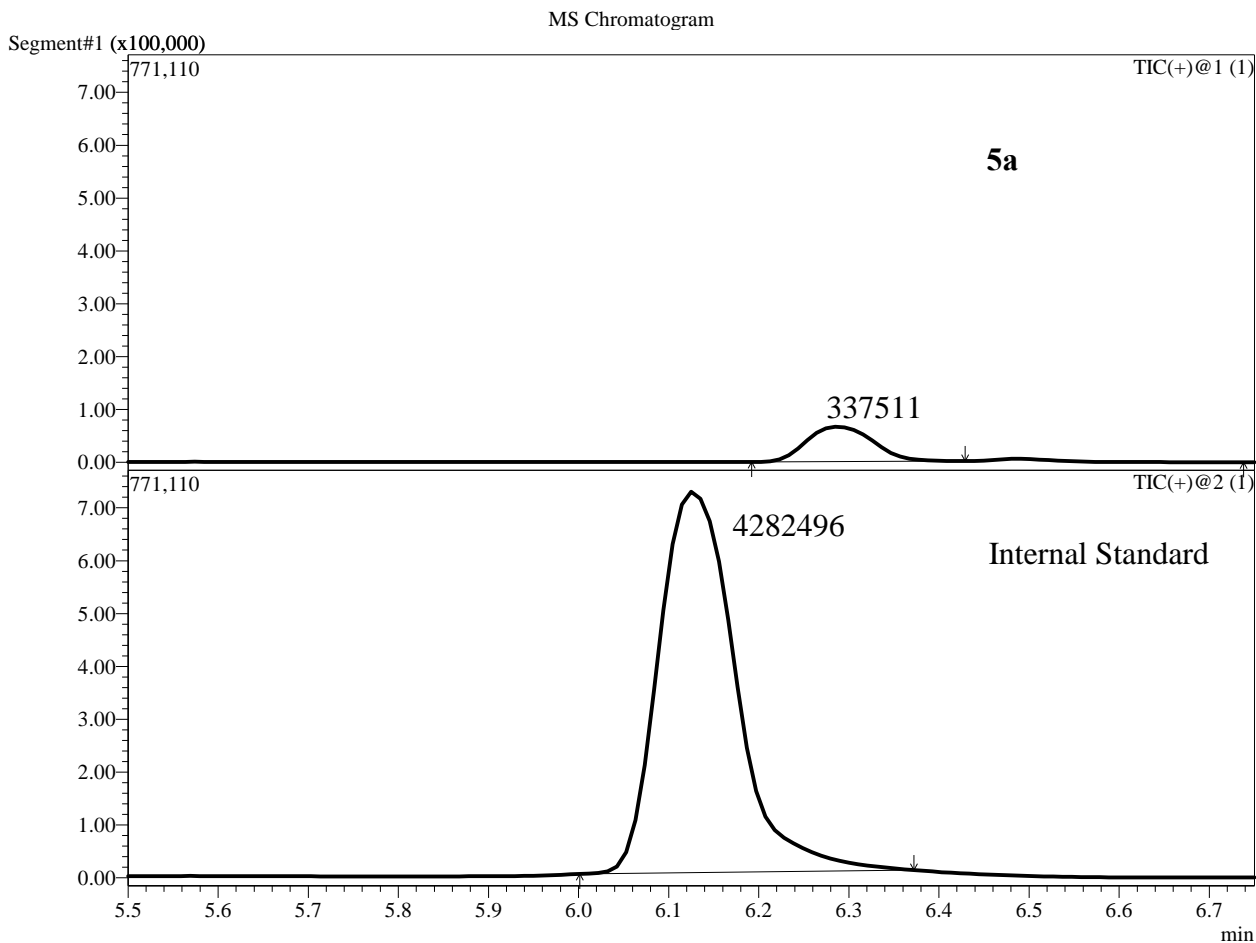
Date Acquired : 3/30/2016 7:07:24 PM
 Sample ID : 12h ipC Brain
 Injection Volume : 10
 Data File : 11.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.281	TIC	420880		1-1
2	6.125	TIC	5658467		1-2

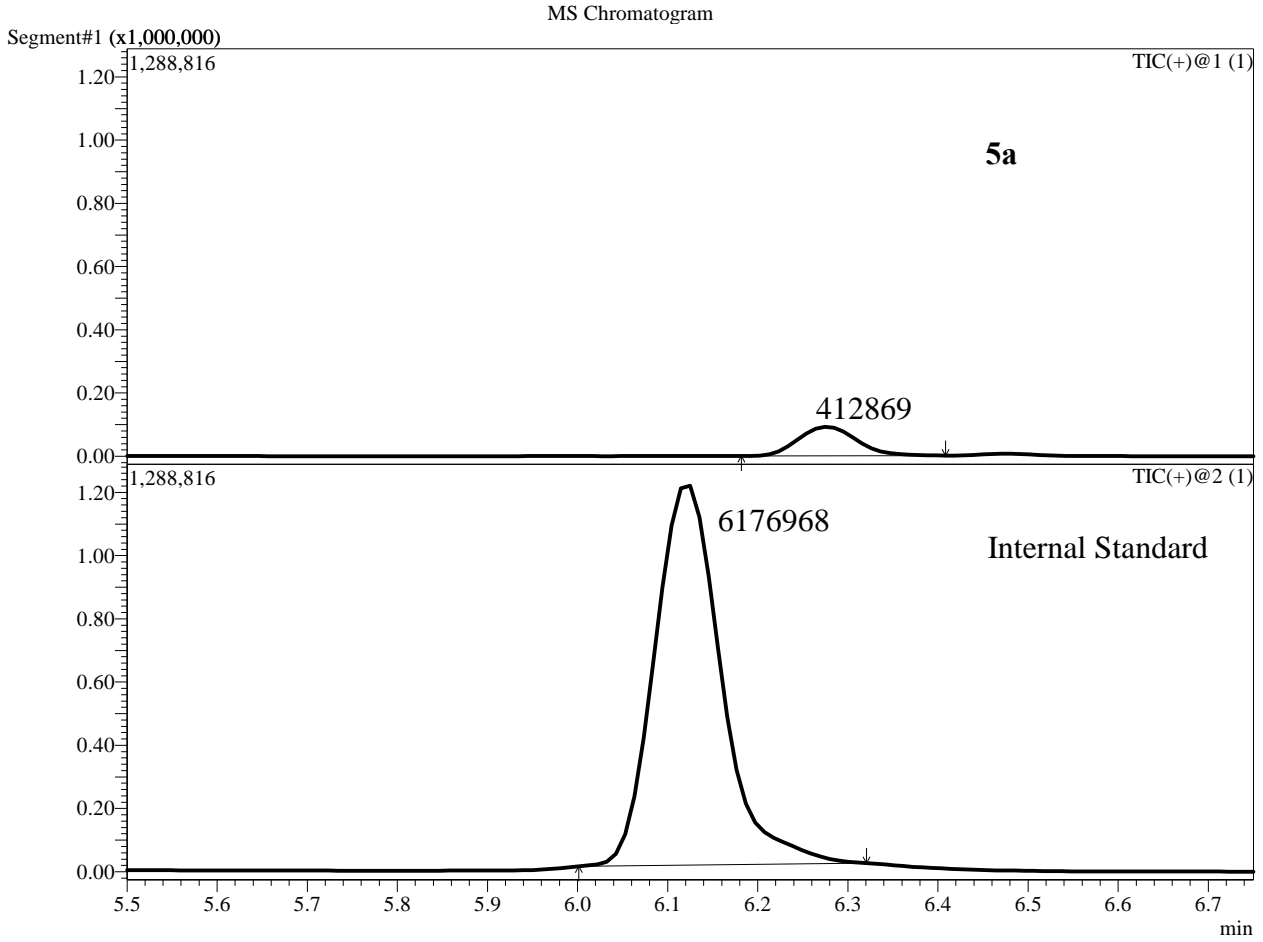
Date Acquired : 3/31/2016 11:16:21 AM
 Sample ID : 12h ipC Plasma
 Injection Volume : 10
 Data File : 35.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.286	TIC	337511		1-1
2	6.127	TIC	4282496		1-2

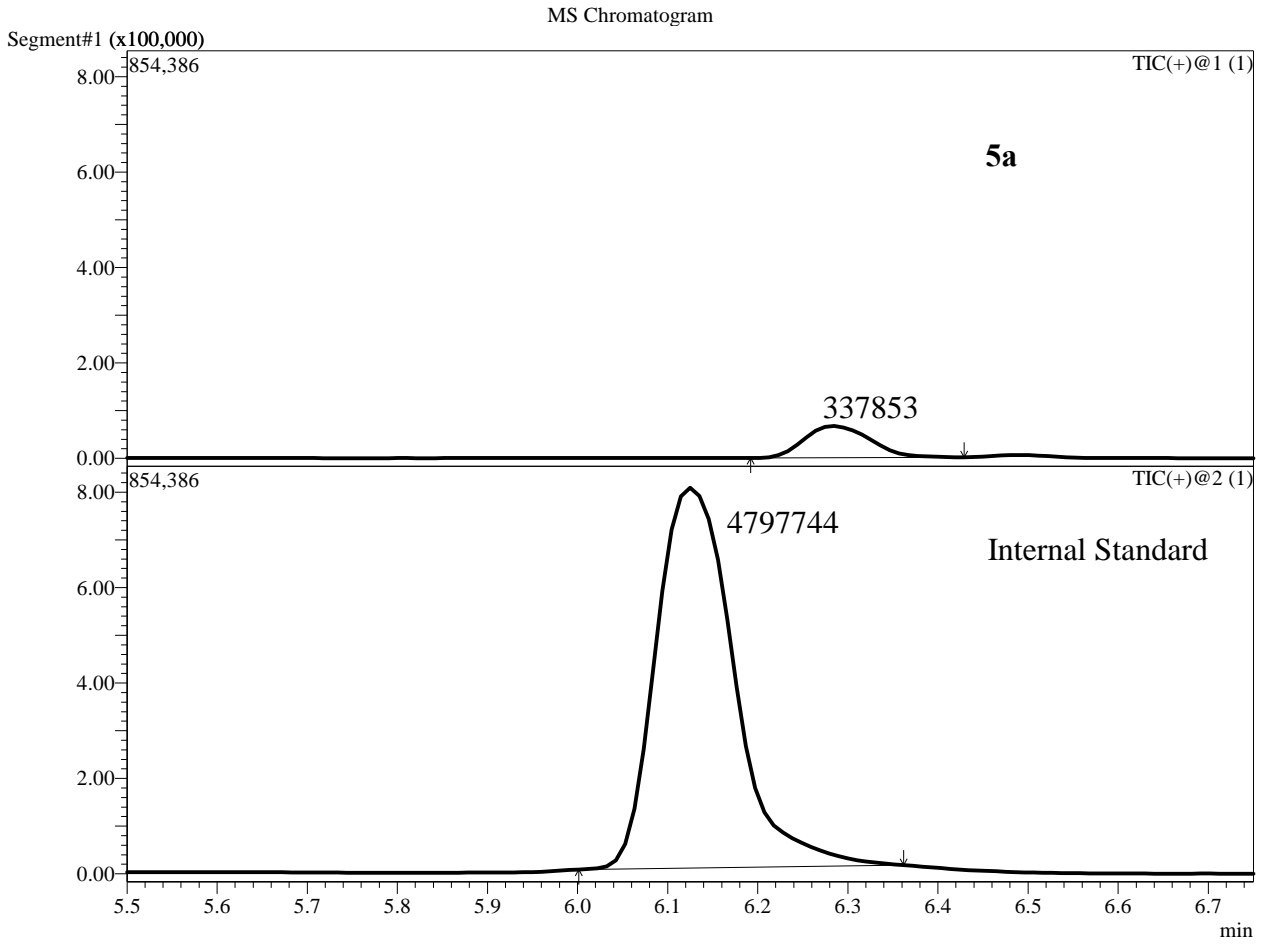
Sample Information
 Date Acquired : 3/30/2016 7:17:55 PM
 Sample ID : 12h ipD Brain
 Injection Volume : 10
 Data File : 12.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.276	TIC	412869		1-1
2	6.121	TIC	6176968		1-2

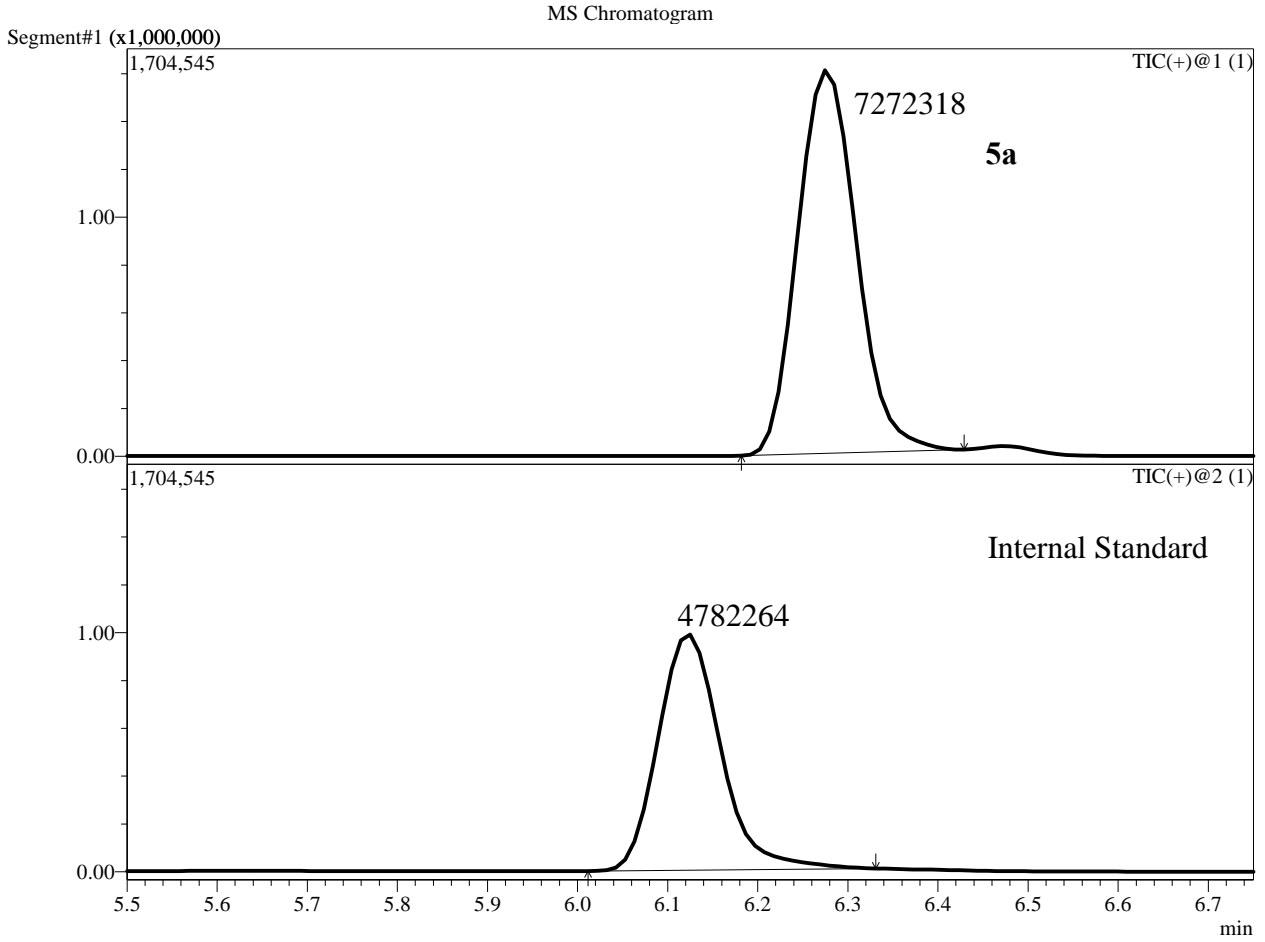
Date Acquired : 3/31/2016 11:26:53 AM
 Sample ID : 12h ipD Plasma
 Injection Volume : 10
 Data File : 36.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.283	TIC	337853		1-1
2	6.125	TIC	4797744		1-2

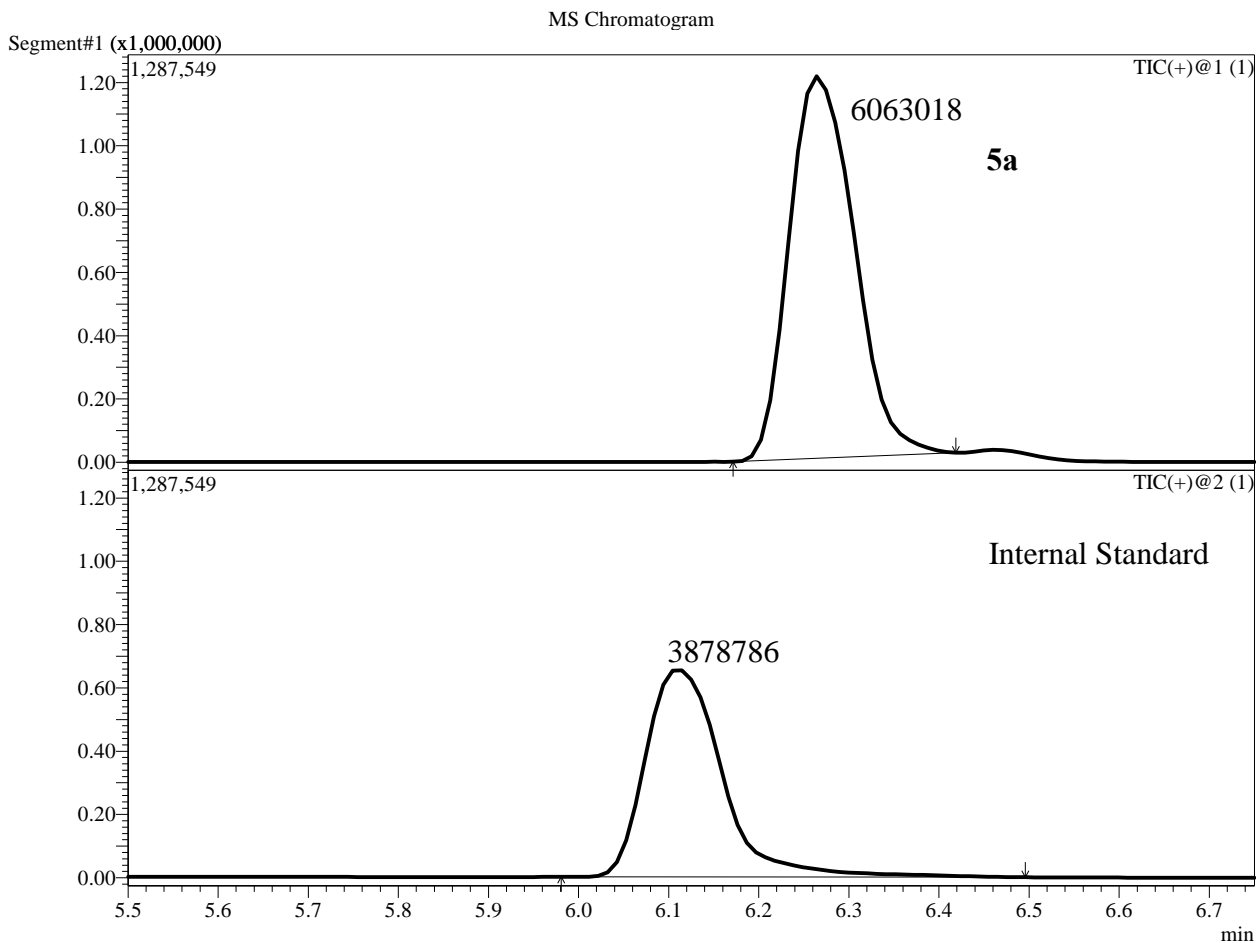
Sample Information
 Date Acquired : 3/30/2016 7:28:26 PM
 Sample ID : 1h poA Brain
 Injection Volume : 10
 Data File : 13.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.276	TIC	7272318		1-1
2	6.122	TIC	4782264		1-2

Date Acquired : 3/31/2016 11:37:24 AM
 Sample ID : 1h poA Plasma
 Injection Volume : 10
 Data File : 37.lcd
 Method File : V1.lcm

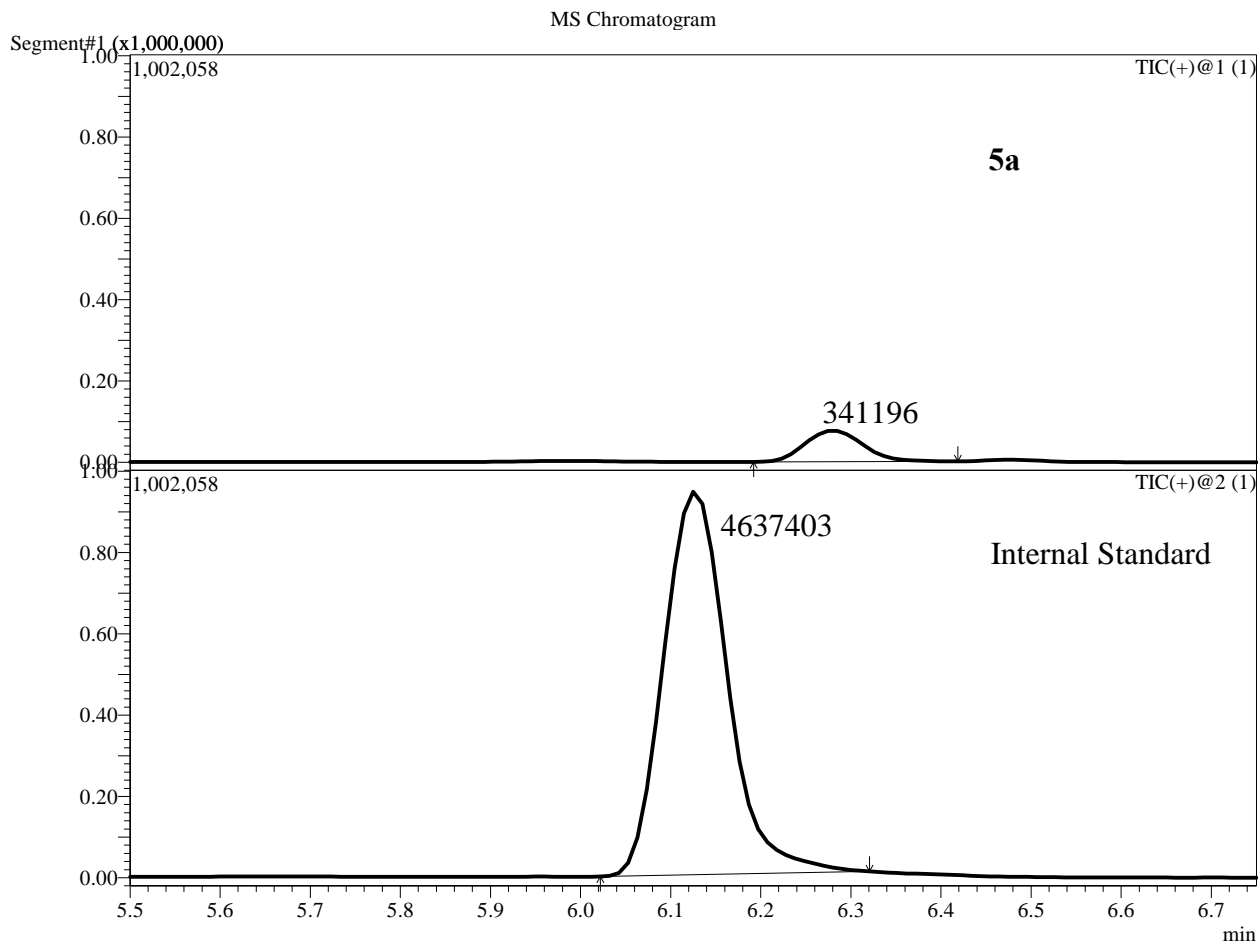


MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.265	TIC	6063018		1-1
2	6.110	TIC	3878786		1-2

Sample Information

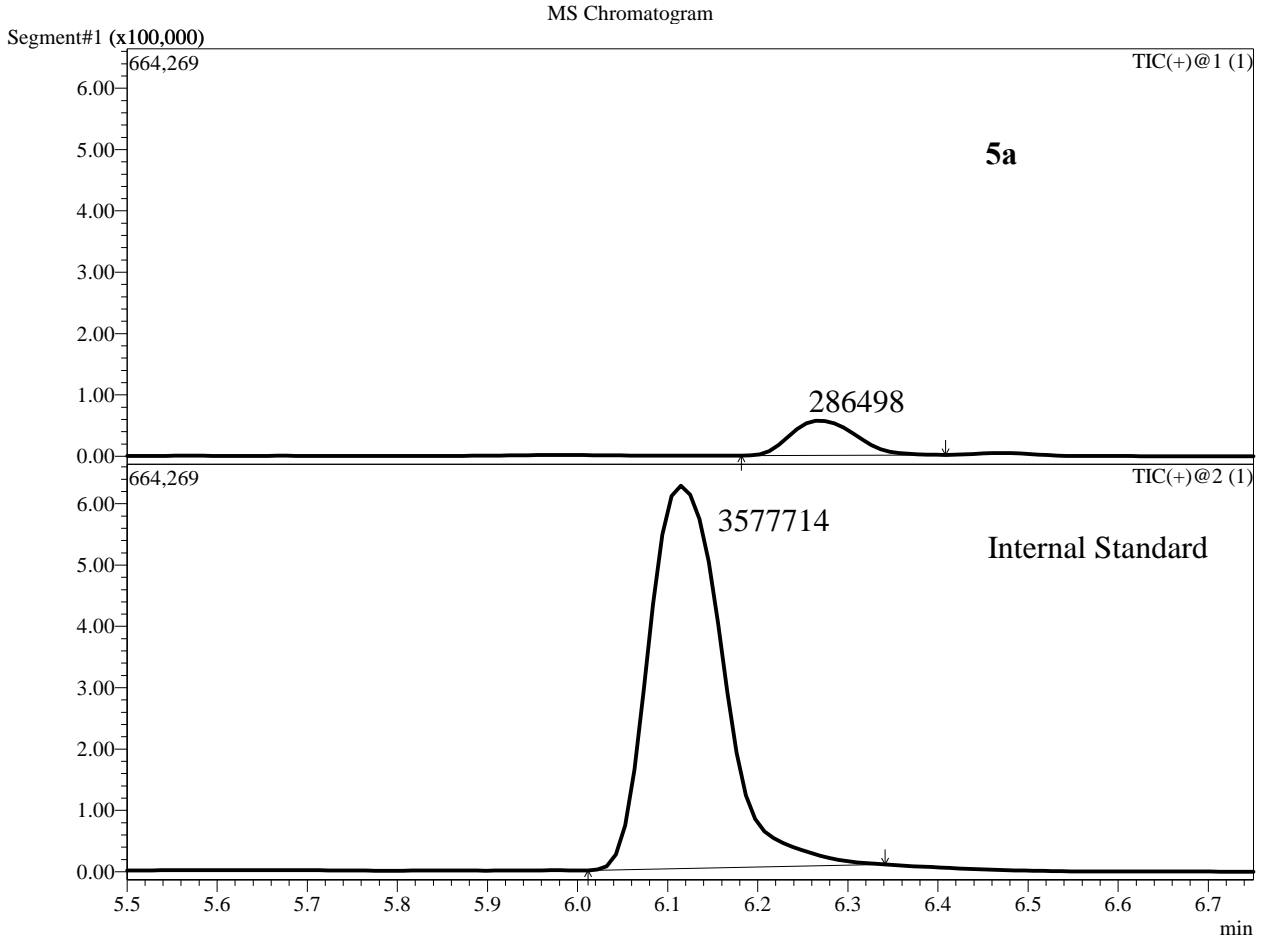
Date Acquired : 3/30/2016 7:38:57 PM
 Sample ID : 1h poB Brain
 Injection Volume : 10
 Data File : 14.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.280	TIC	341196		1-1
2	6.127	TIC	4637403		1-2

Sample Information
 Date Acquired : 3/31/2016 11:47:55AM
 Sample ID : 1h poB Plasma
 Injection Volume : 10
 Data File : 38.lcd
 Method File : V1.lcm

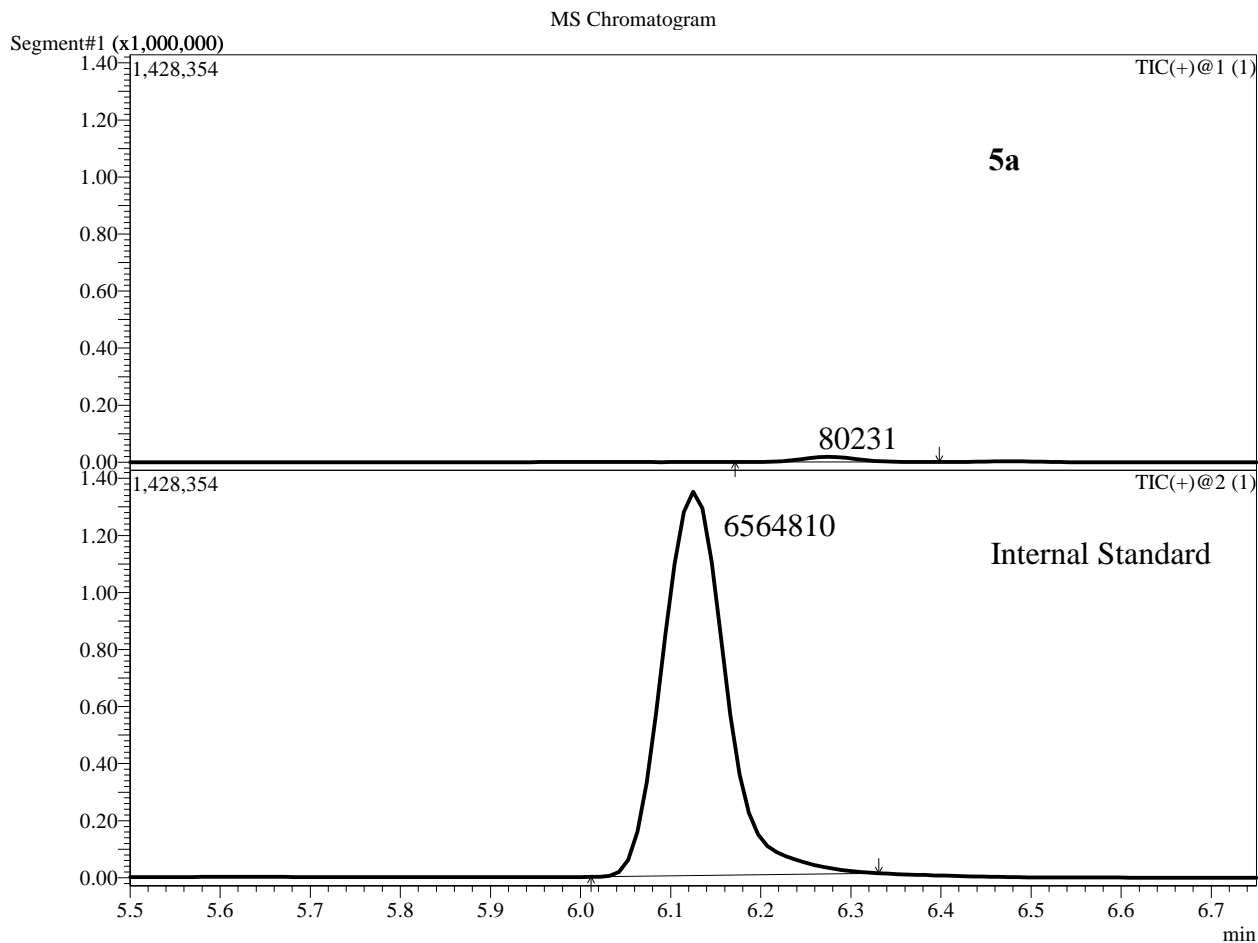


MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.268	TIC	286498		1-1
2	6.115	TIC	3577714		1-2

Sample Information

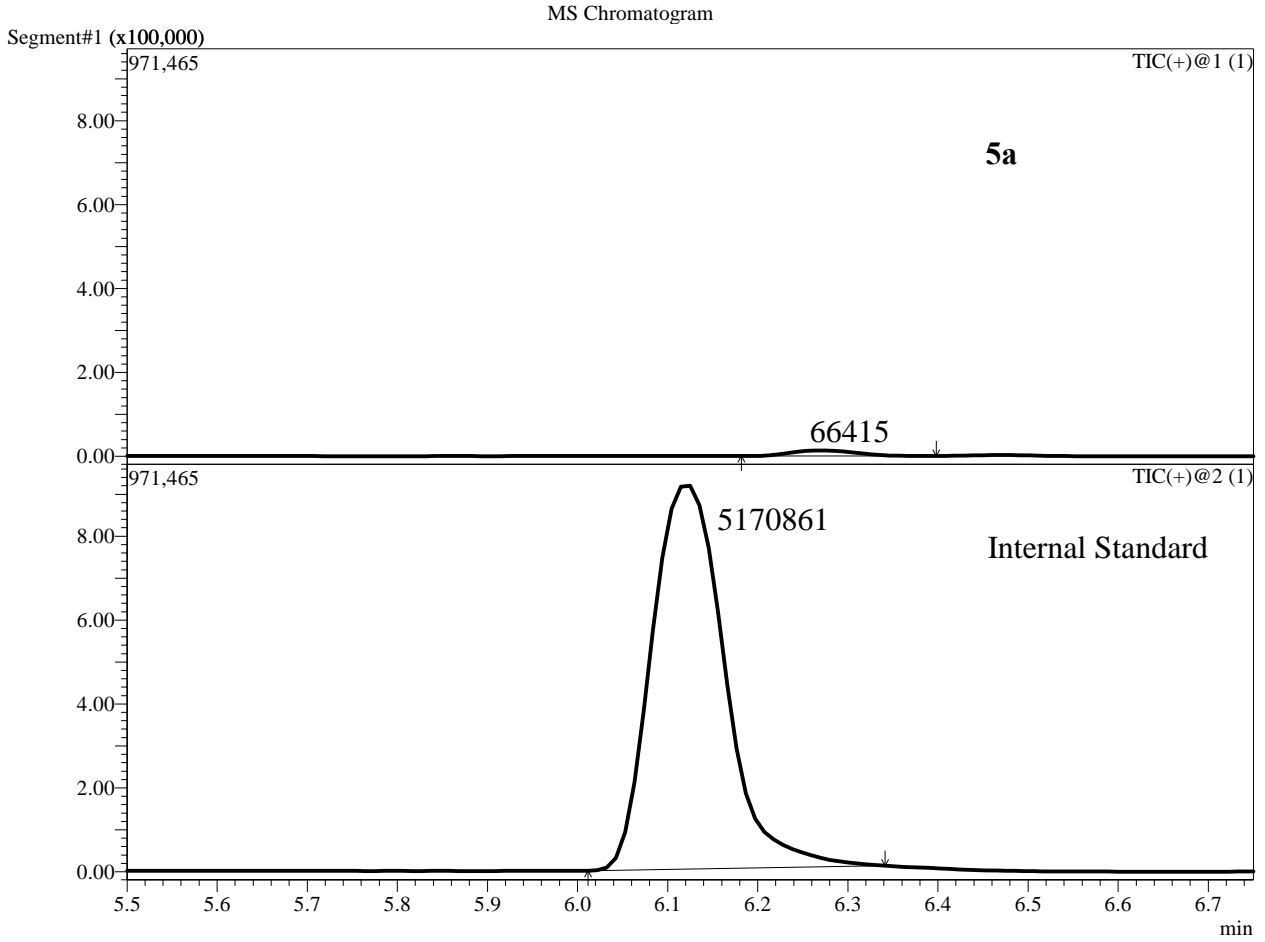
Date Acquired : 3/30/2016 7:49:29 PM
 Sample ID : 1h poC Brain
 Injection Volume : 10
 Data File : 15.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.275	TIC	80231		1-1
2	6.126	TIC	6564810		1-2

Sample Information
 Date Acquired : 3/31/2016 11:58:27 AM
 Sample ID : 1h poC Plasma
 Injection Volume : 10
 Data File : 39.lcd
 Method File : V1.lcm

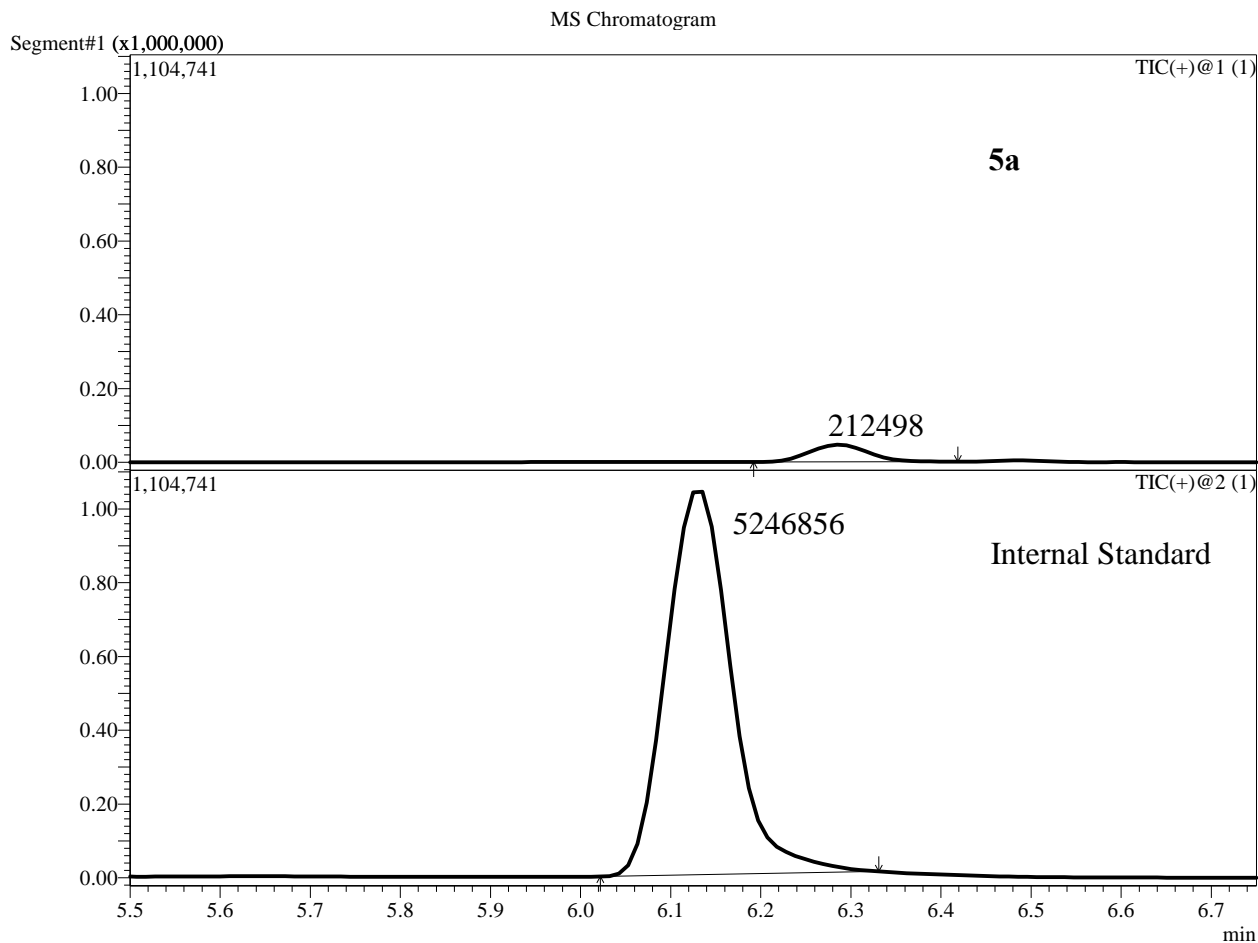


MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.269	TIC	66415		1-1
2	6.121	TIC	5170861		1-2

Sample Information

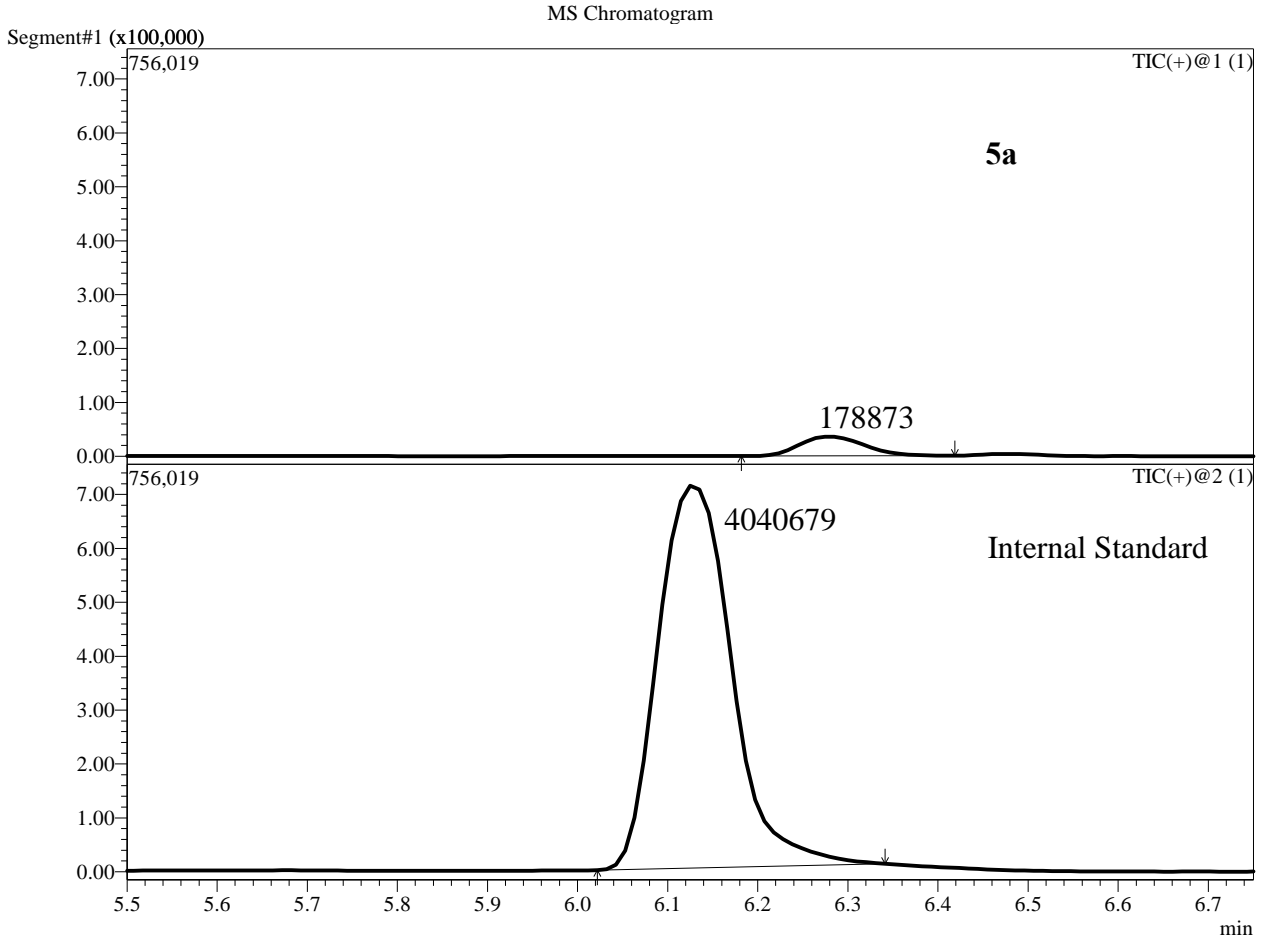
Date Acquired : 3/30/2016 8:00:00 PM
 Sample ID : 1h poD Brain
 Injection Volume : 10
 Data File : 16.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.286	TIC	212498		1-1
2	6.130	TIC	5246856		1-2

Sample Information
 Date Acquired : 3/31/2016 12:08:57 PM
 Sample ID : 1h poD Plasma
 Injection Volume : 10
 Data File : 40.lcd
 Method File : V1.lcm

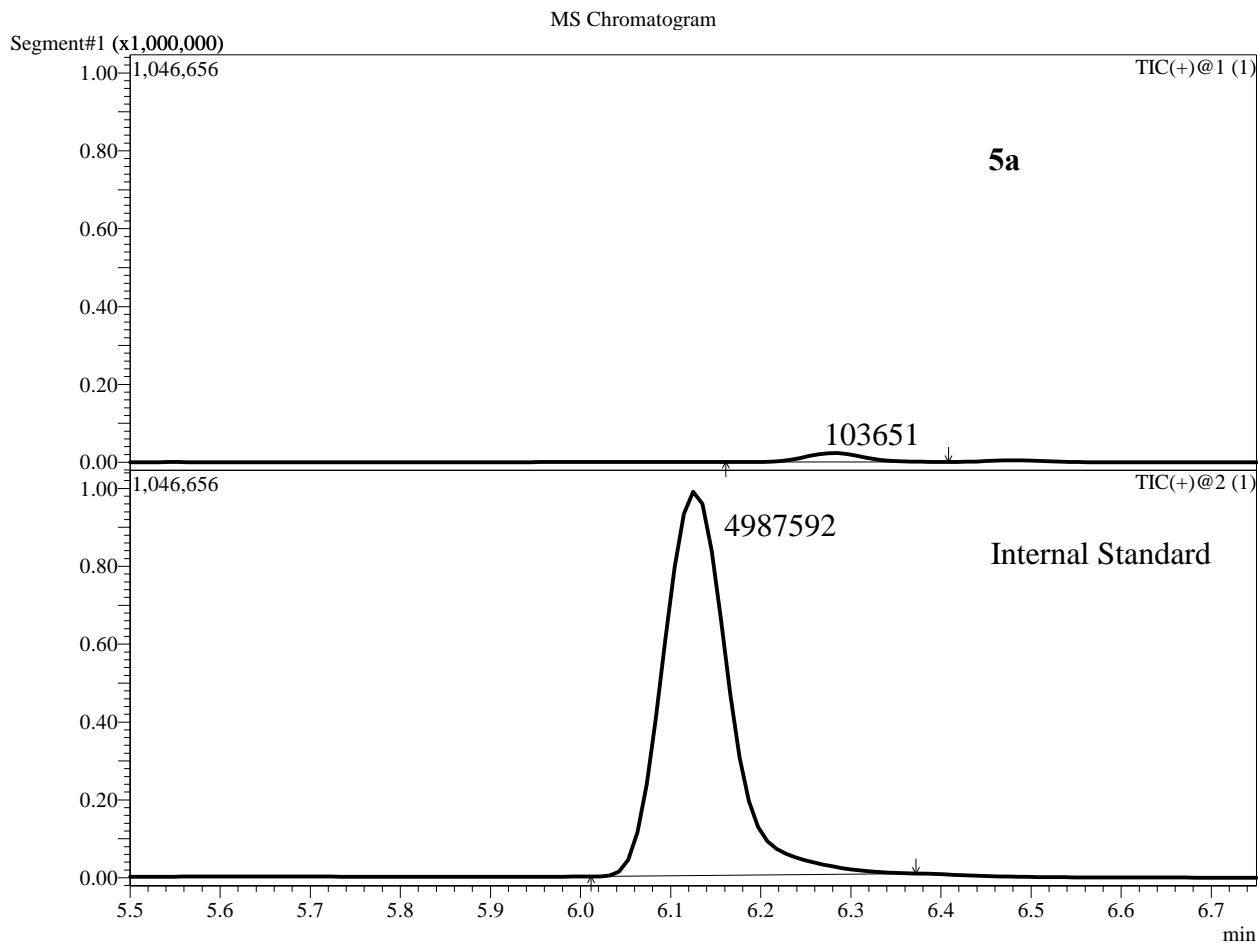


MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.279	TIC	178873		1-1
2	6.128	TIC	4040679		1-2

Sample Information

Date Acquired : 3/30/2016 8:10:30 PM
 Sample ID : 2h poA Brain
 Injection Volume : 10
 Data File : 17.lcd
 Method File : V1.lcm

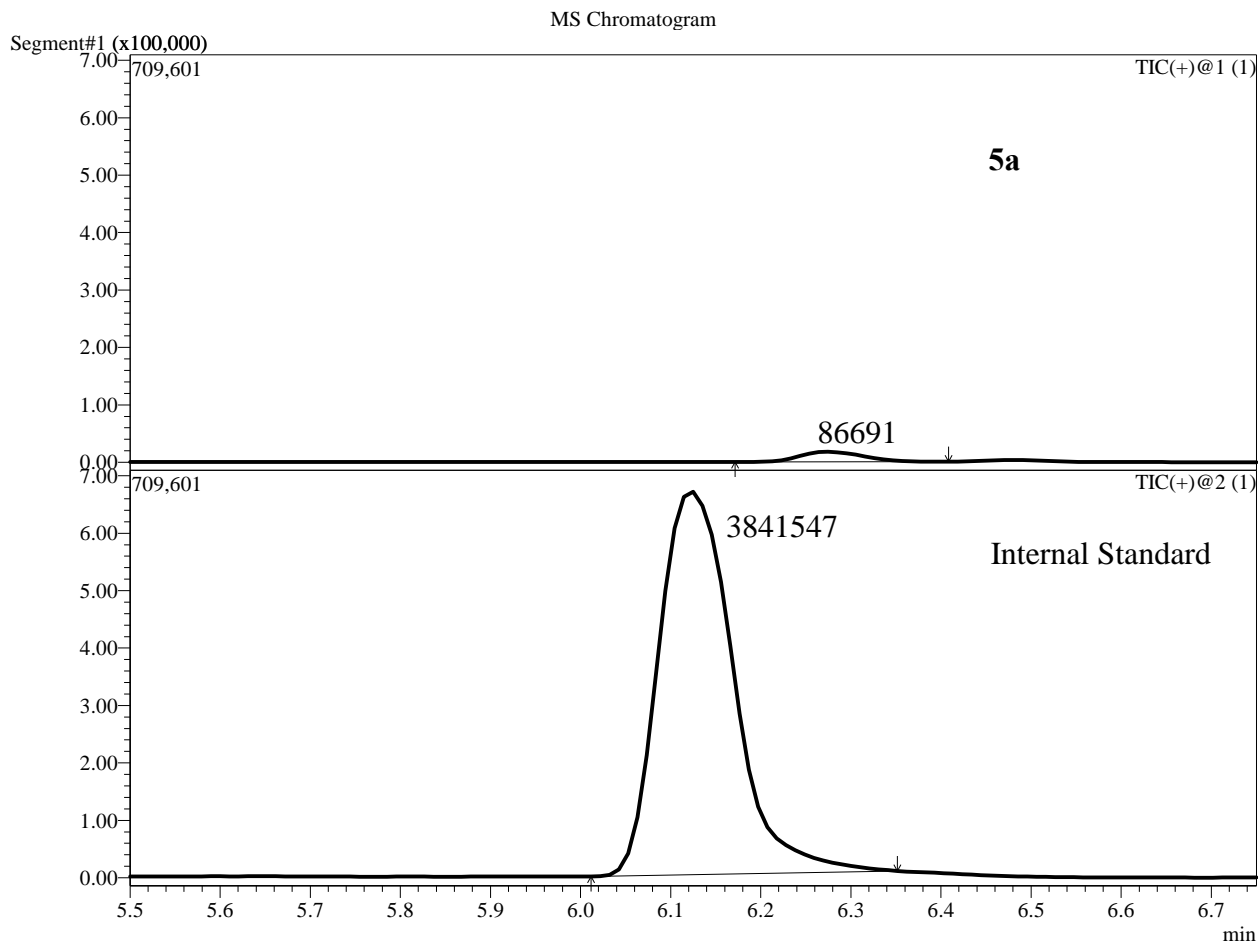


MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.282	TIC	103651		1-1
2	6.127	TIC	4987592		1-2

Sample Information

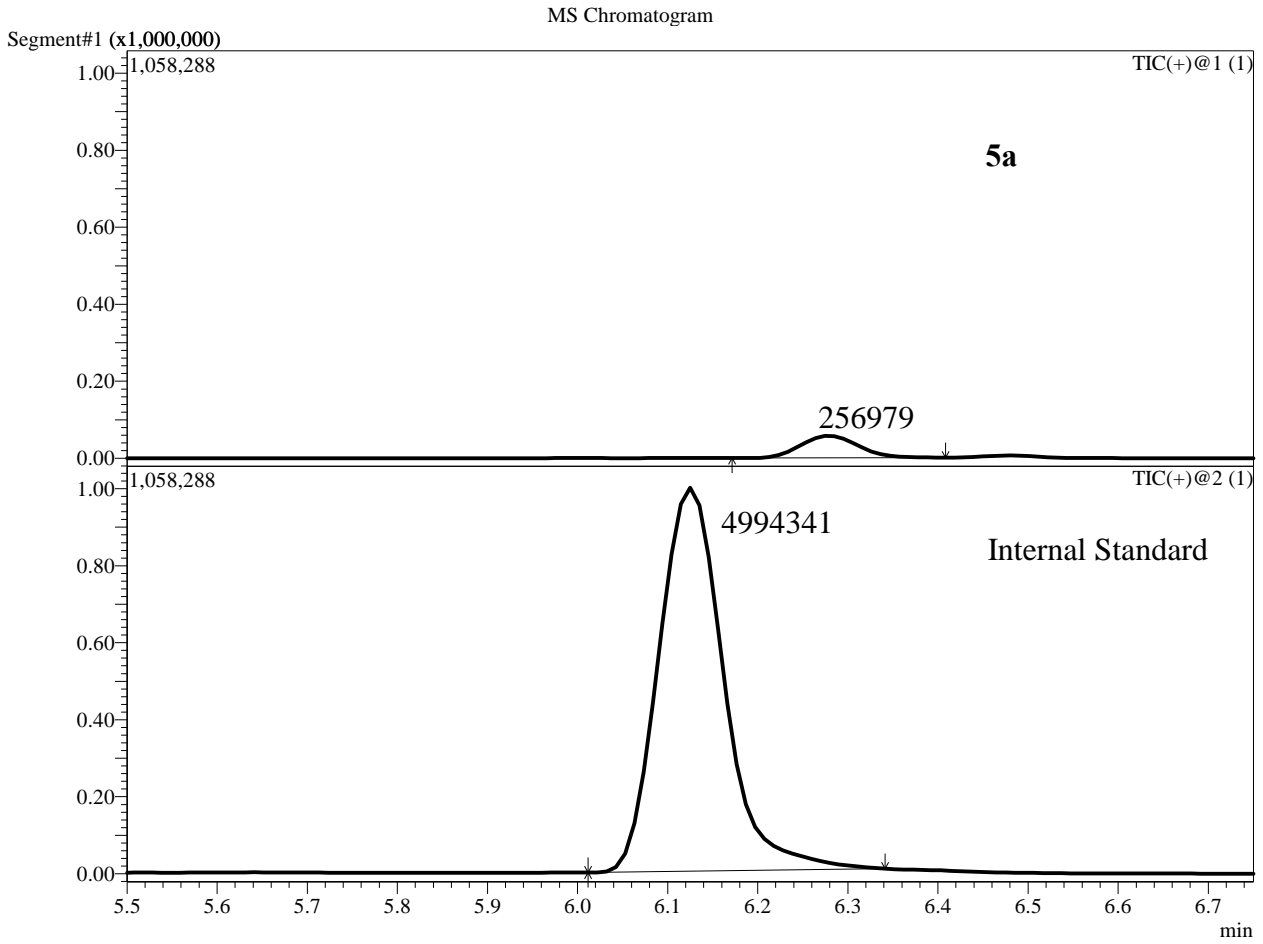
Date Acquired : 3/31/2016 12:19:29 PM
 Sample ID : 2h poA Plasma
 Injection Volume : 10
 Data File : 41.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.274	TIC	86691		1-1
2	6.123	TIC	3841547		1-2

Date Acquired : 3/30/2016 8:21:00 PM
 Sample ID : 2h poB Brain
 Injection Volume : 10
 Data File : 18.lcd
 Method File : V1.lcm

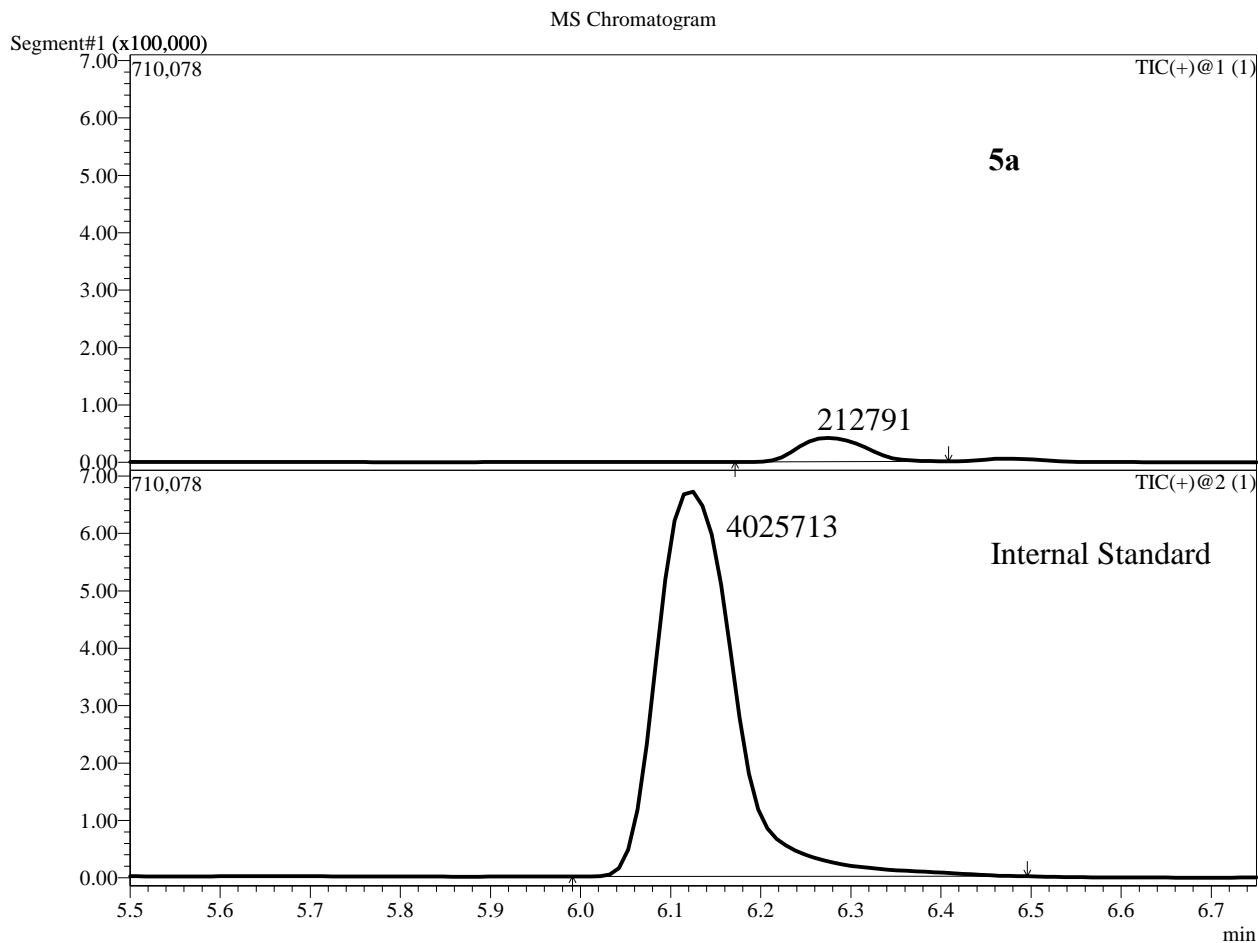


MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.279	TIC	256979		1-1
2	6.125	TIC	4994341		1-2

Sample Information

Date Acquired : 3/31/2016 12:30:00 PM
 Sample ID : 2h poB Plasma
 Injection Volume : 10
 Data File : 42.lcd
 Method File : V1.lcm

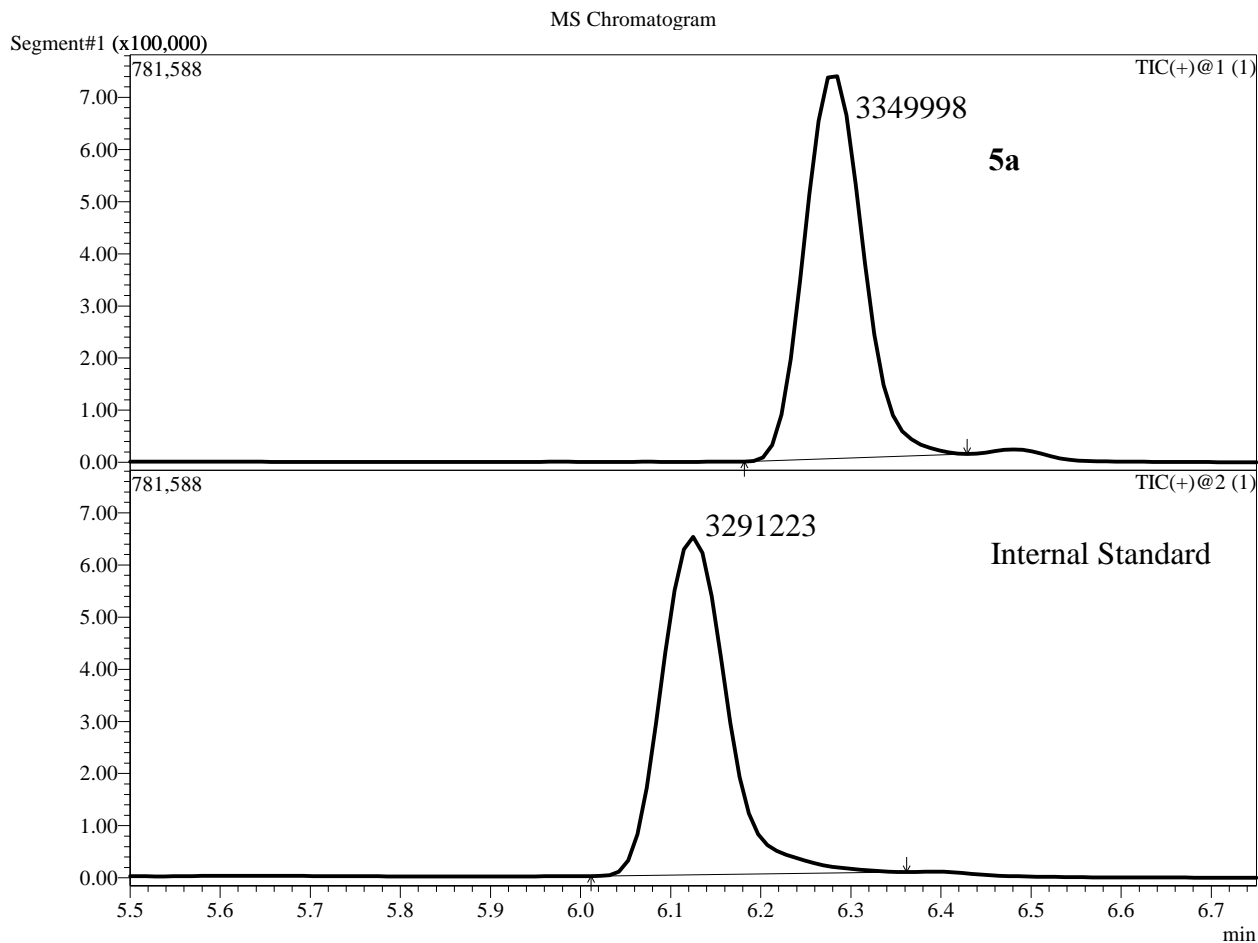


MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.274	TIC	212791		1-1
2	6.122	TIC	4025713		1-2

Sample Information

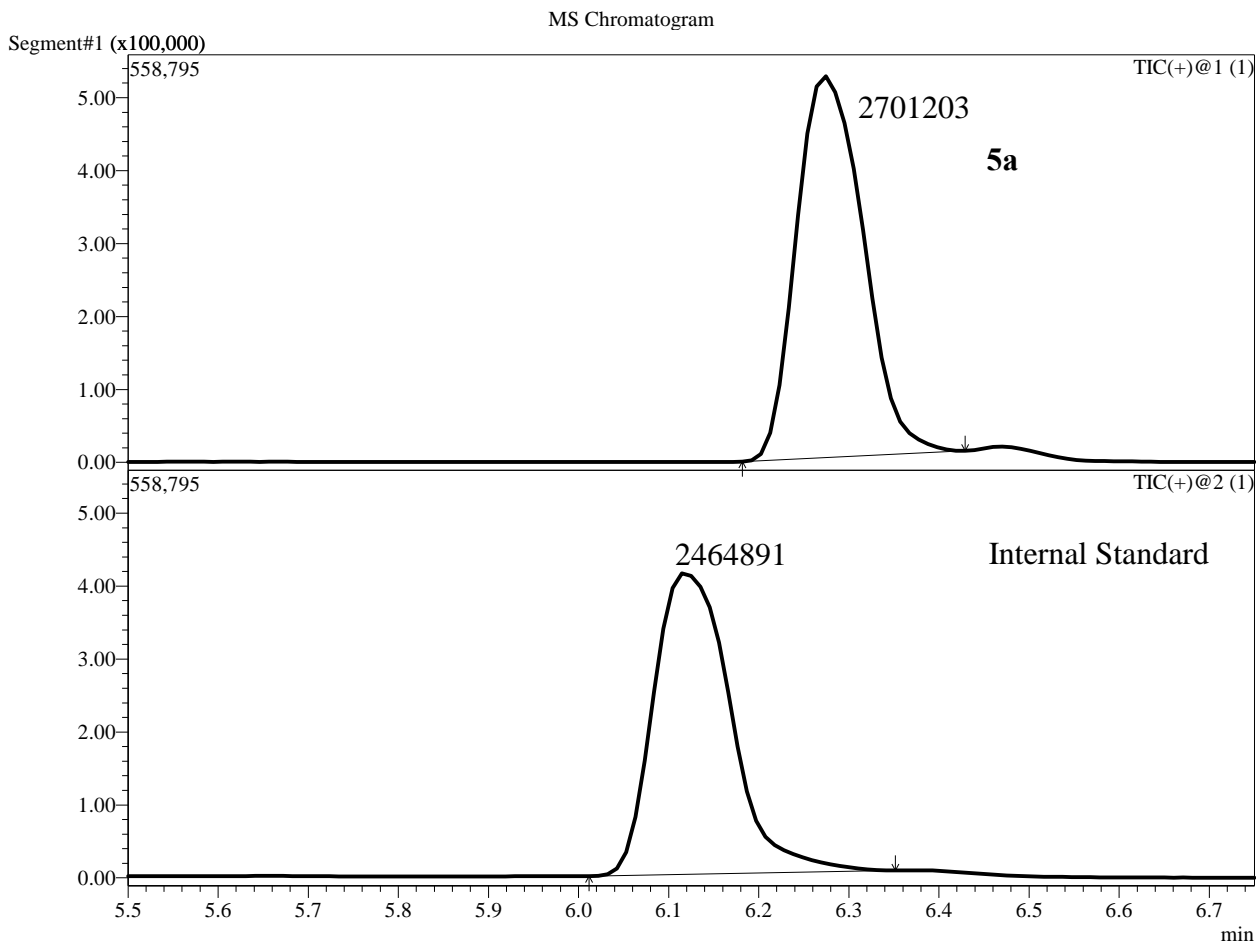
Date Acquired : 3/30/2016 8:31:29 PM
 Sample ID : 2h poC Brain
 Injection Volume : 10
 Data File : 19.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.280	TIC	3349998		1-1
2	6.125	TIC	3291223		1-2

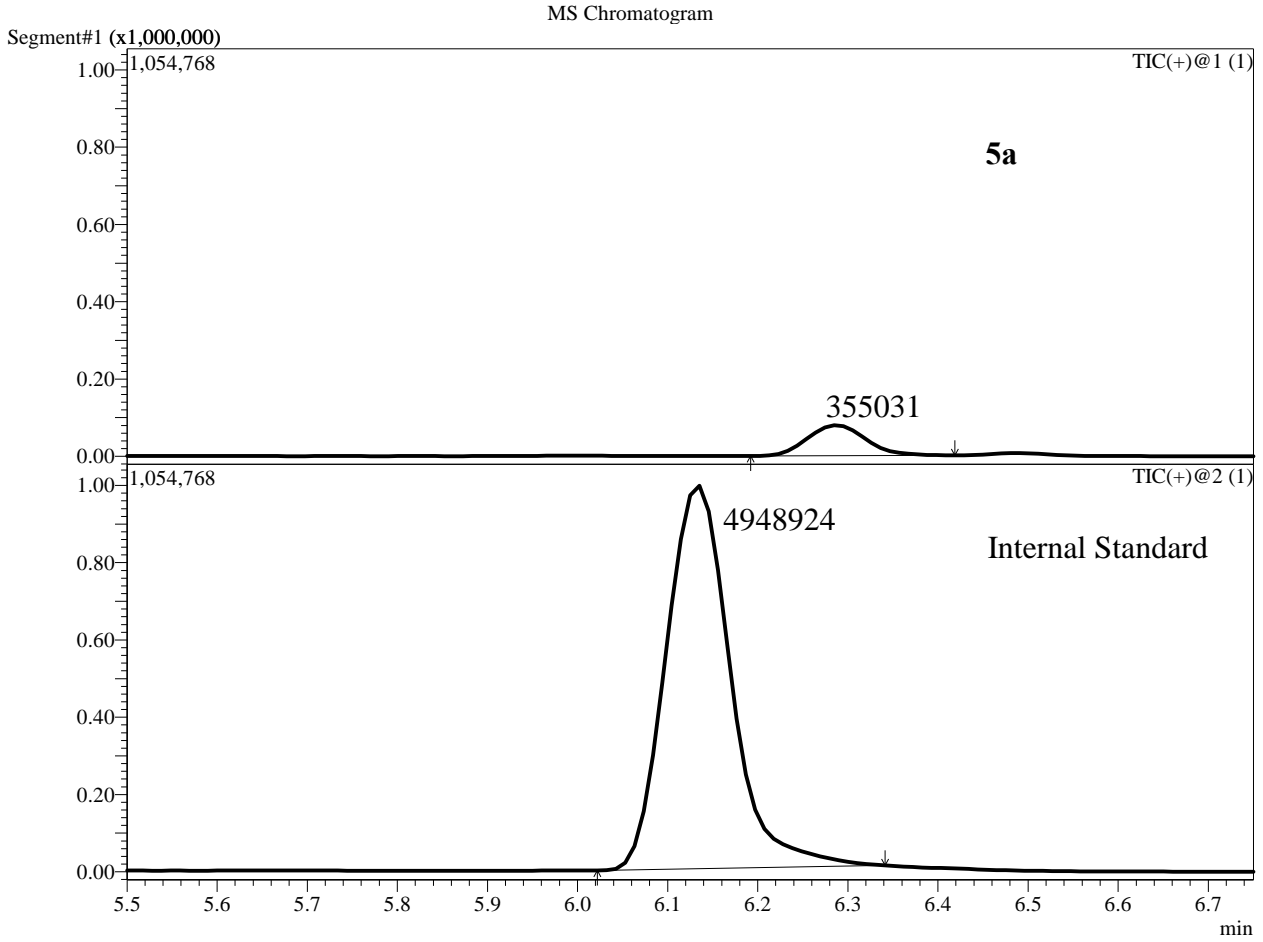
Date Acquired : 3/31/2016 12:40:31 PM
 Sample ID : 2h poC Plasma
 Injection Volume : 10
 Data File : 43.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.273	TIC	2701203		1-1
2	6.119	TIC	2464891		1-2

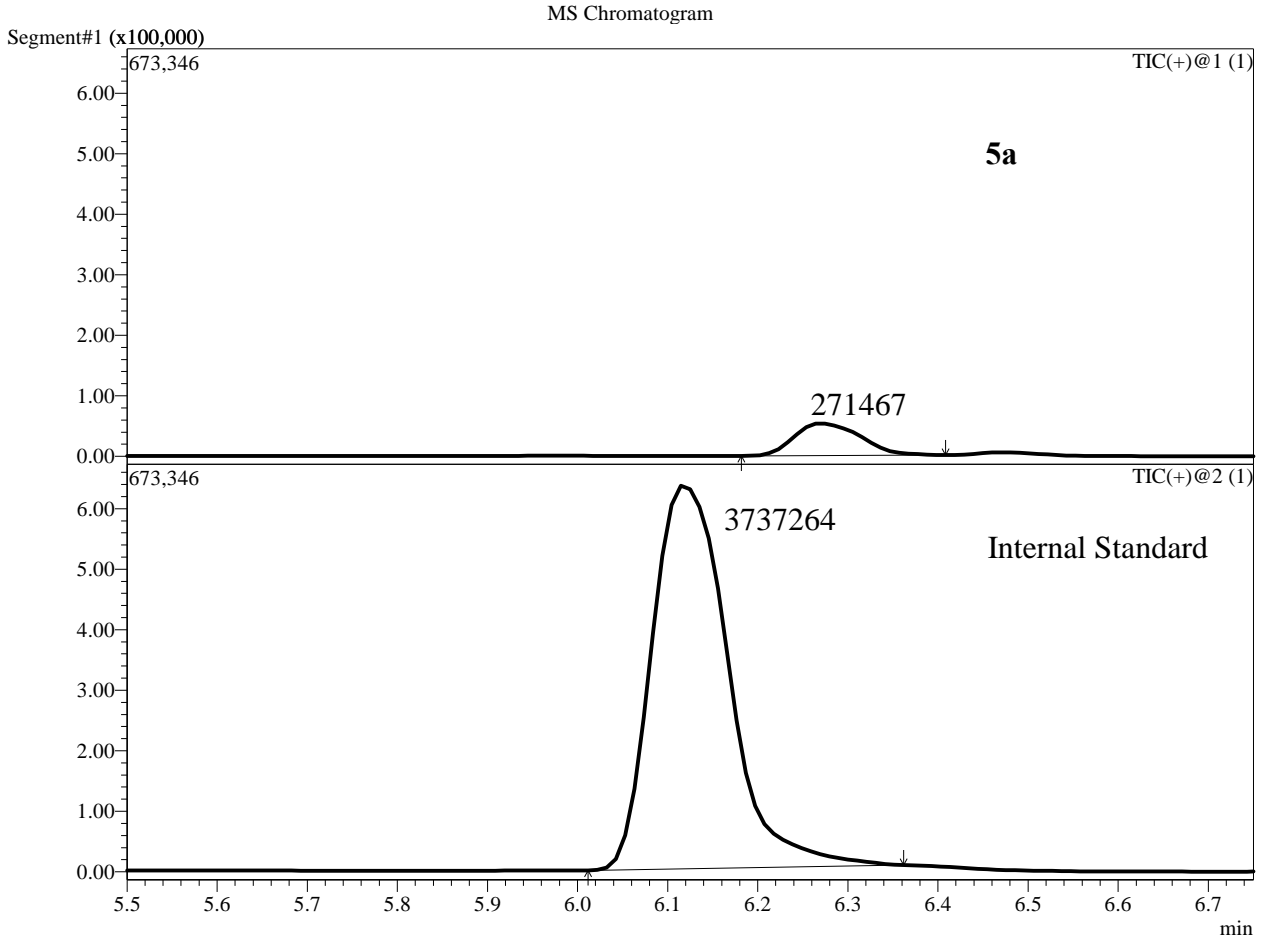
Sample Information
 Date Acquired : 3/30/2016 8:41:59 PM
 Sample ID : 2h poD Brain
 Injection Volume : 10
 Data File : 20.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.287	TIC	355031		1-1
2	6.133	TIC	4948924		1-2

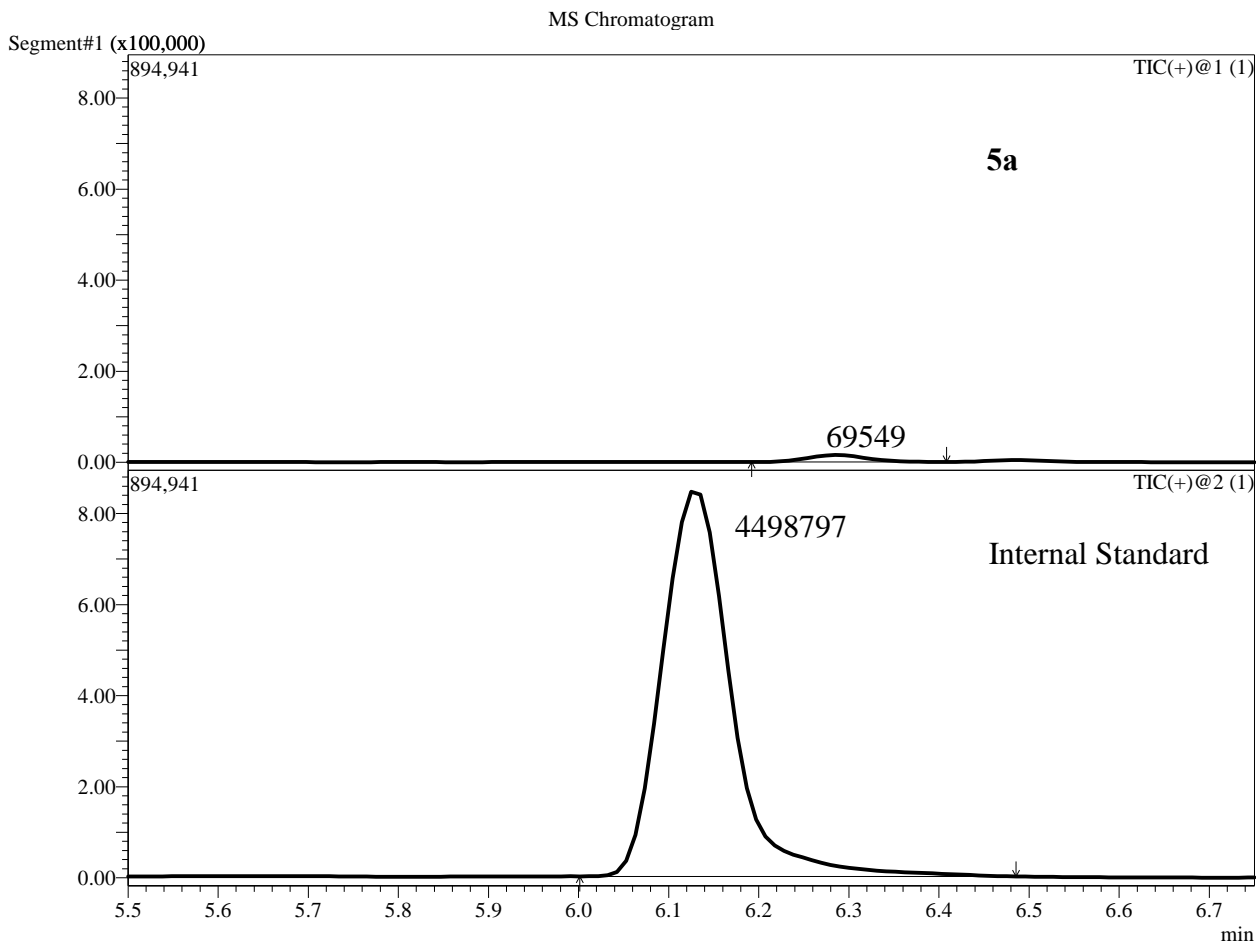
Sample Information
 Date Acquired : 3/31/2016 12:51:01 PM
 Sample ID : 2h poD Plasma
 Injection Volume : 10
 Data File : 44.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.270	TIC	271467		1-1
2	6.118	TIC	3737264		1-2

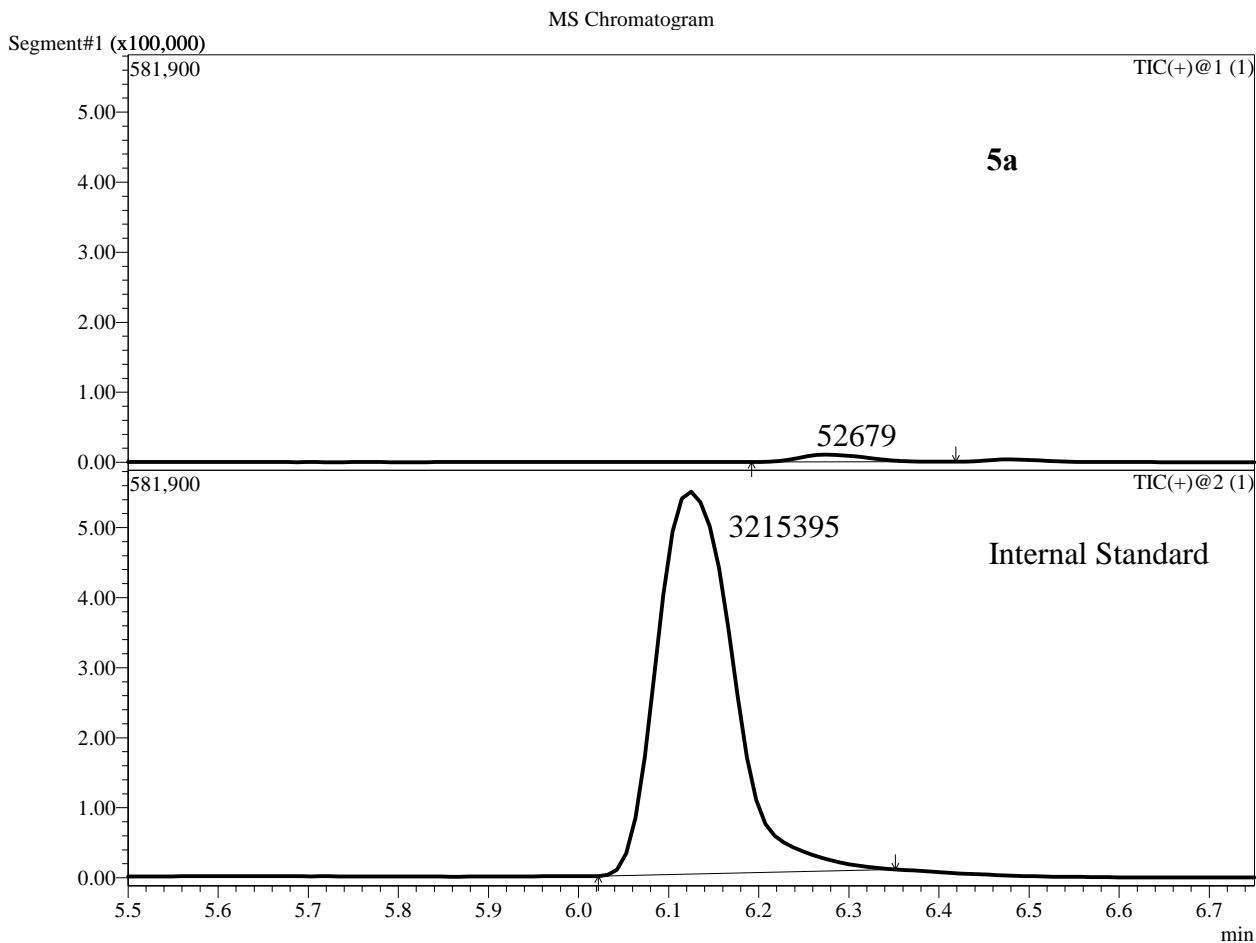
Date Acquired : 3/30/2016 8:52:30 PM
 Sample ID : 12h poA Brain
 Injection Volume : 10
 Data File : 21.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.286	TIC	69549		1-1
2	6.129	TIC	4498797		1-2

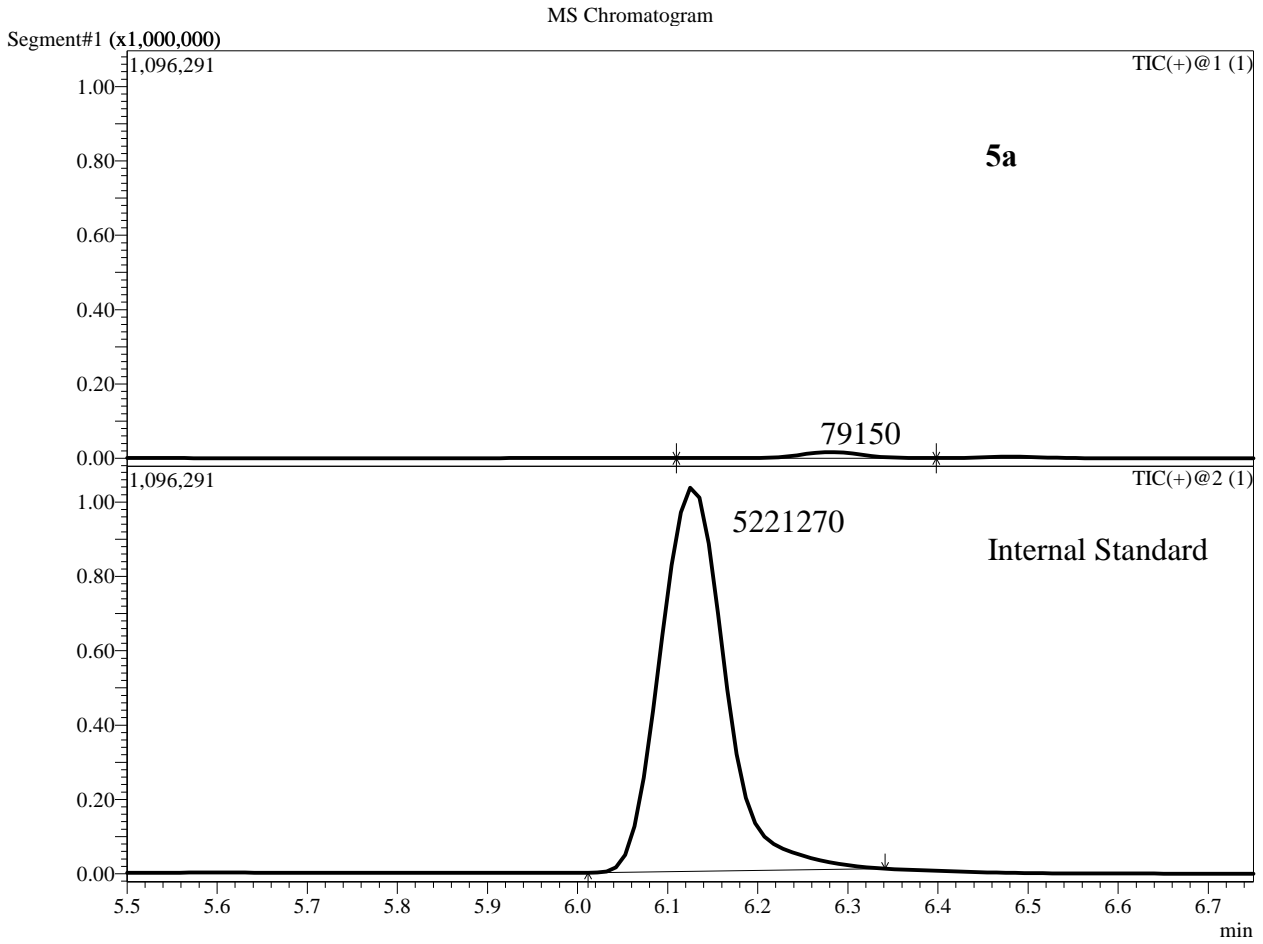
Date Acquired : 3/31/2016 1:01:31 PM
 Sample ID : 12h poA Plasma
 Injection Volume : 10
 Data File : 45.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.276	TIC	52679		1-1
2	6.124	TIC	3215395		1-2

Date Acquired : 3/30/2016 9:03:00 PM
 Sample ID : 12h poB Brain
 Injection Volume : 10
 Data File : 22.lcd
 Method File : V1.lcm

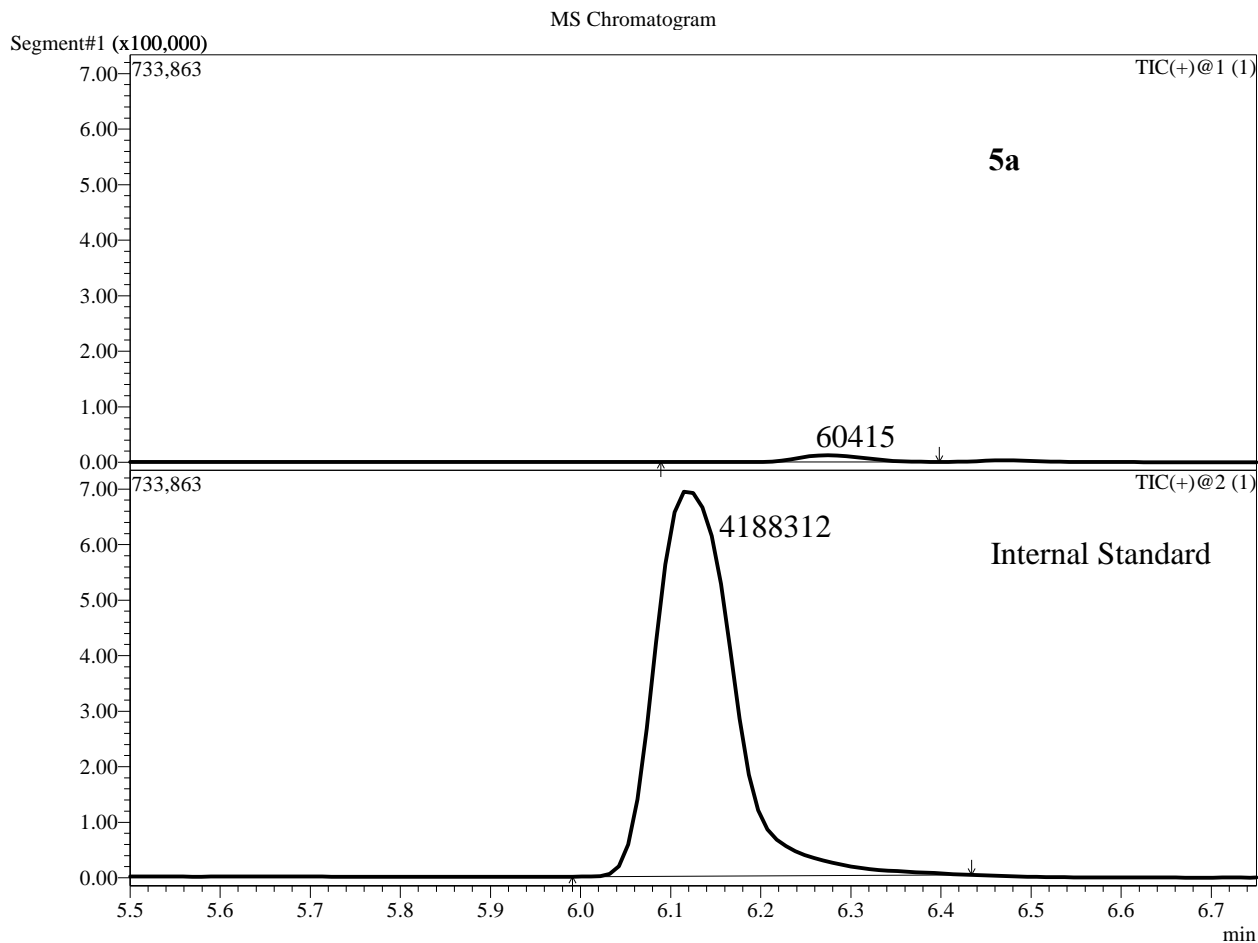


MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.270	TIC	79150		1-1
2	6.127	TIC	5221270		1-2

Sample Information

Date Acquired : 3/31/2016 1:12:01 PM
 Sample ID : 12h poB Plasma
 Injection Volume : 10
 Data File : 46.lcd
 Method File : V1.lcm

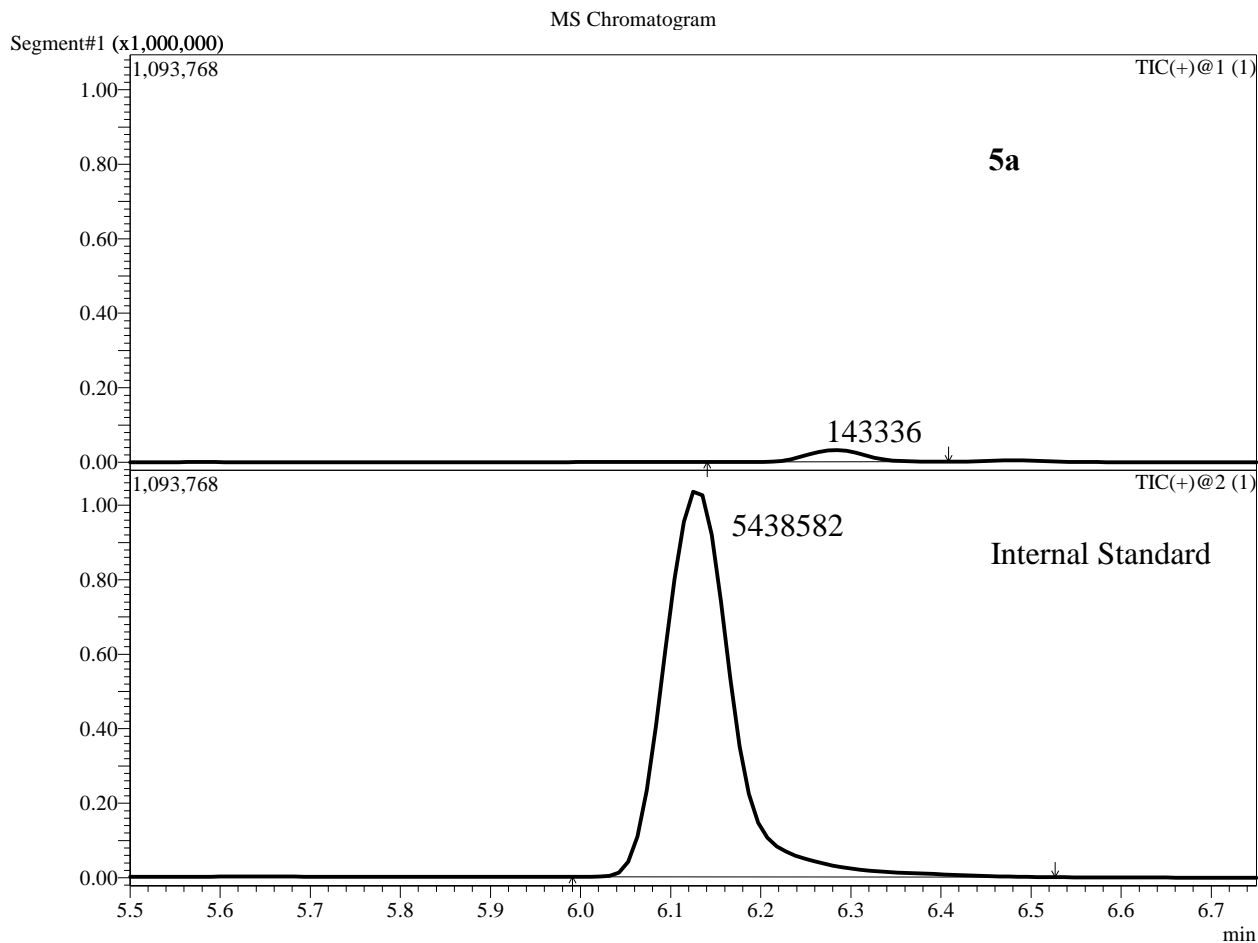


MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.272	TIC	60415		1-1
2	6.119	TIC	4188312		1-2

Sample Information

Date Acquired : 3/30/2016 9:13:30 PM
 Sample ID : 12h poC Brain
 Injection Volume : 10
 Data File : 23.lcd
 Method File : V1.lcm

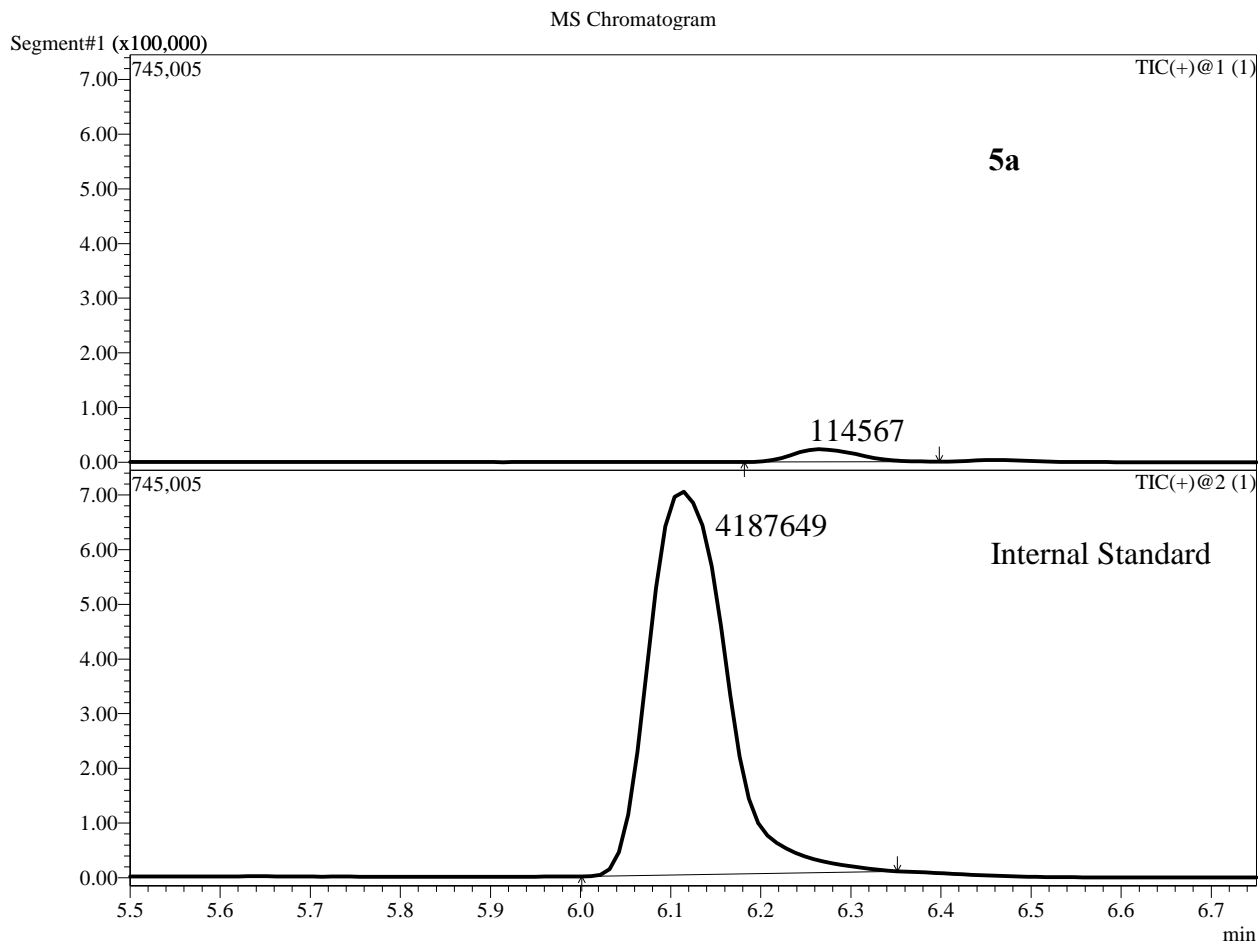


MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.283	TIC	143336		1-1
2	6.129	TIC	5438582		1-2

Sample Information

Date Acquired : 3/31/2016 1:22:32 PM
 Sample ID : 12h poC Plasma
 Injection Volume : 10
 Data File : 47.lcd
 Method File : V1.lcm

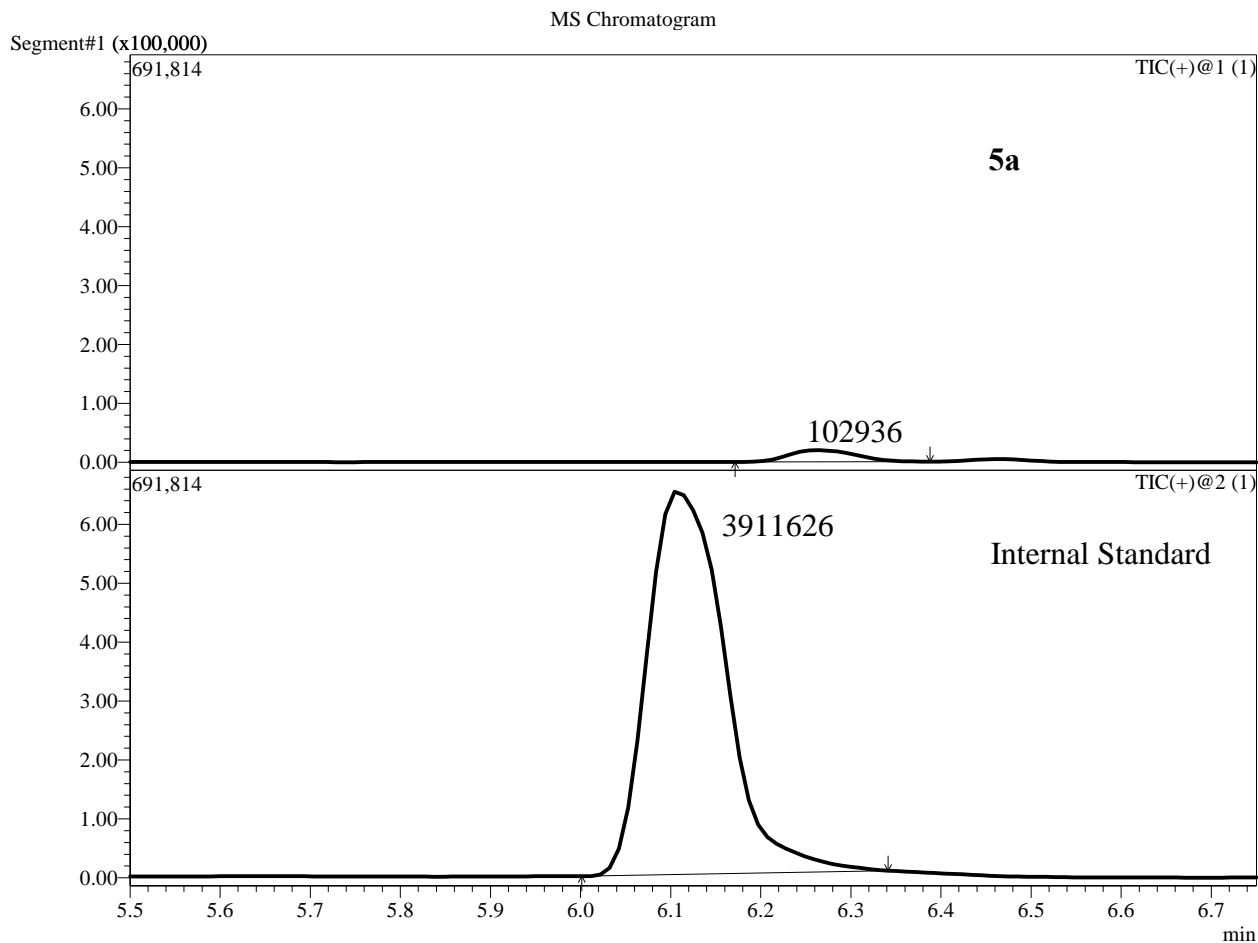


MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.265	TIC	114567		1-1
2	6.113	TIC	4187649		1-2

Sample Information

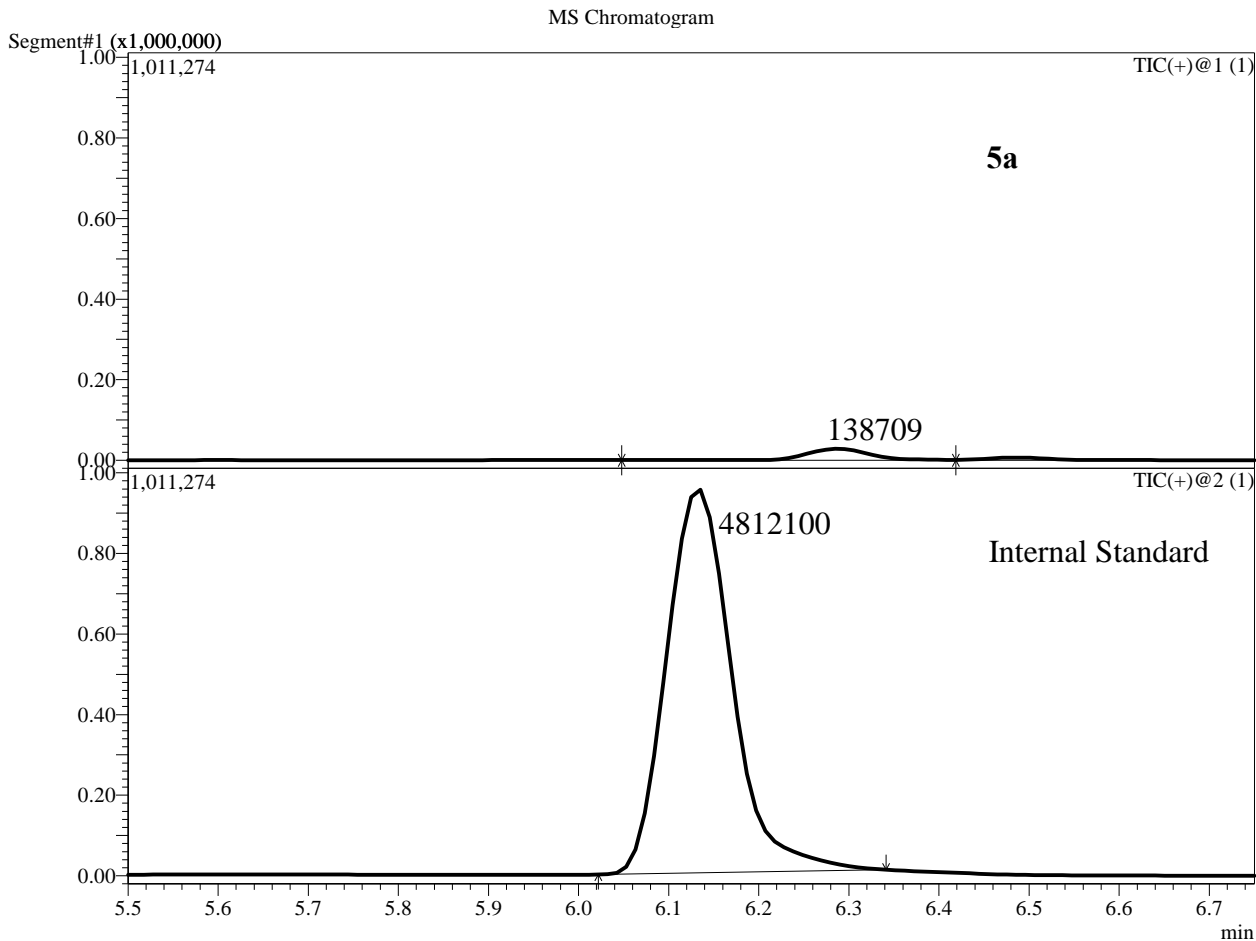
Date Acquired : 3/31/2016 1:33:04 PM
 Sample ID : 12h poD Brain
 Injection Volume : 10
 Data File : 48.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.262	TIC	102936		1-1
2	6.108	TIC	3911626		1-2

Date Acquired : 3/30/2016 9:24:00 PM
 Sample ID : 12h poD Plasma
 Injection Volume : 10
 Data File : 24.lcd
 Method File : V1.lcm



MASS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Compound Name	Event#
1	6.287	TIC	138709		1-1
2	6.132	TIC	4812100		1-2

Supplemental Crystallographic Data

Furoxans (oxadiazole-4N-oxides) with Attenuated Reactivity are Neuroprotective, Cross the Blood Brain Barrier, and Improve Passive Avoidance Memory

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Aparna Raghavan[†], Jatin Tulsulkar[†], Qasim Alhadidi[†], Nathan Wamer[†], Bryn Langenderfer[†],
Kalee Royster[†], Maxwell Ducharme[†], Katelyn Hagood[†], Megan Post[†], Zahoor A. Shah[†], Isaac T.
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Crystal Structure Report for 5a (IS141_3)

A clear colorless irregular prism-like specimen of $C_{15}H_{18}FN_3O_2$, approximate dimensions 0.058 mm x 0.156 mm x 0.270 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The integration of the data using a monoclinic unit cell yielded a total of 26380 reflections to a maximum θ angle of 33.11° (0.65 Å resolution), of which 5531 were independent (average redundancy 4.769, completeness = 95.1%, $R_{\text{int}} = 4.72\%$, $R_{\text{sig}} = 4.02\%$) and 4041 (73.06%) were greater than $2\sigma(F^2)$. The final cell constants of $a = 11.3374(14)$ Å, $b = 7.2234(9)$ Å, $c = 18.825(2)$ Å, $\beta = 97.601(2)^\circ$, volume = $1528.1(3)$ Å³, are based upon the refinement of the XYZ-centroids of reflections above $20\sigma(I)$.

The final anisotropic full-matrix least-squares refinement on F^2 with 255 variables converged at $R1 = 5.17\%$, for the observed data and $wR2 = 14.18\%$ for all data. The methyl group (C15) is disordered. The occupancy of the C15 atoms was refined to be 50% and then fixed. They are refined with isotropic atomic displacement parameters; the bonded hydrogen atoms were calculated on idealized hydrogens and refined as riding atoms. The goodness-of-fit was 1.012. The largest peak in the final difference electron density synthesis was $0.487 e^-/\text{Å}^3$ and the largest hole was $-0.540 e^-/\text{Å}^3$ with an RMS deviation of $0.058 e^-/\text{Å}^3$. On the basis of the final model, the calculated density was 1.266 g/cm^3 and $F(000)$, 616 e^- .

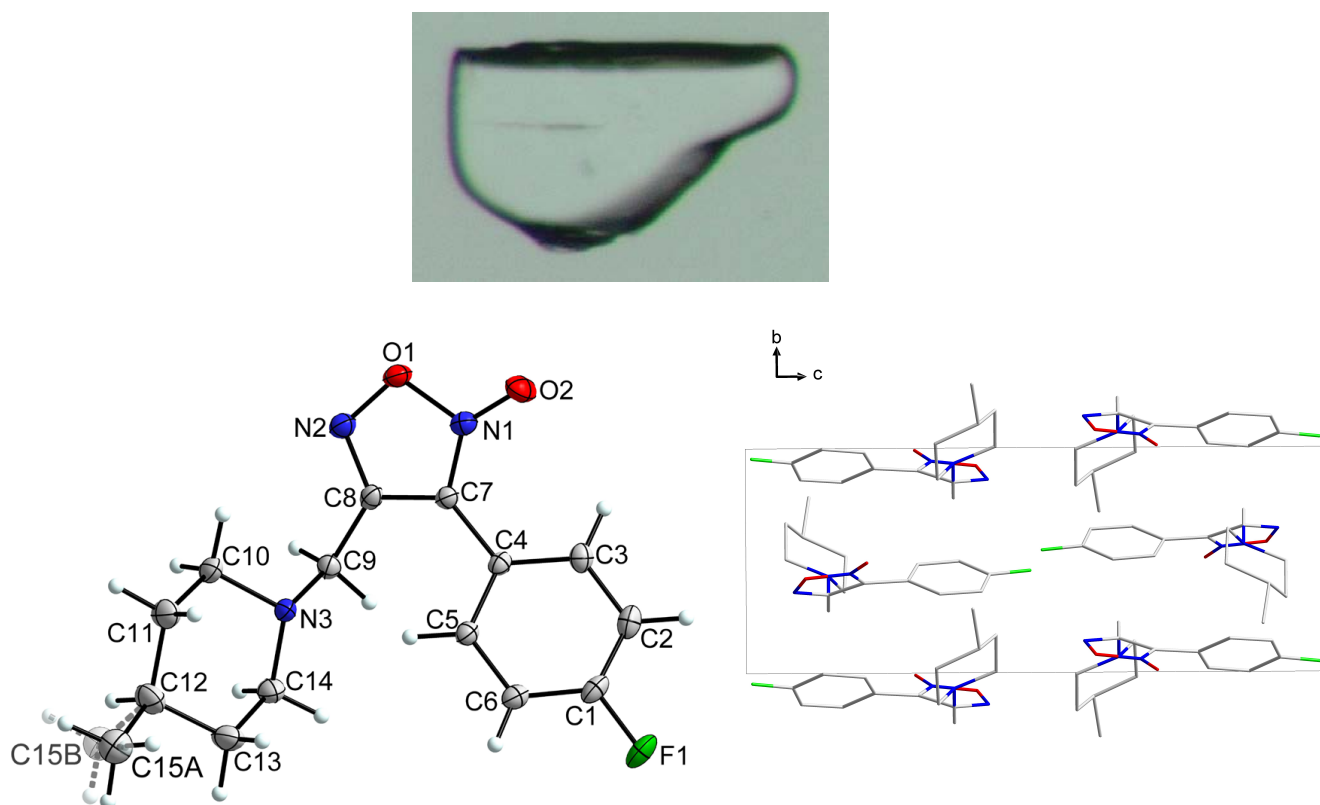


Table 1. Sample and crystal data for IS141_3.

Chemical formula	C ₁₅ H ₁₈ FN ₃ O ₂	
Formula weight	291.32 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.058 x 0.156 x 0.270 mm	
Crystal habit	clear colorless irregular prism	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 11.3374(14) Å	α = 90°
	b = 7.2234(9) Å	β = 97.601(2)°
	c = 18.825(2) Å	γ = 90°
Volume	1528.1(3) Å ³	
Z	4	
Density (calculated)	1.266 g/cm ³	
Absorption coefficient	0.094 mm ⁻¹	
F(000)	616	

Table 2. Data collection and structure refinement for IS141_3.

Theta range for data collection	2.18 to 33.11°	
Index ranges	-16<=h<=16, -10<=k<=10, -28<=l<=28	
Reflections collected	26380	
Independent reflections	5531 [R(int) = 0.0472]	
Refinement method	Full-matrix least-squares on F ²	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	Σ w(F _o ² - F _c ²) ²	
Data / restraints / parameters	5531 / 0 / 255	
Goodness-of-fit on F²	1.012	
Final R indices	4041 data; I>2σ(I)	R1 = 0.0517, wR2 = 0.1252
	all data	R1 = 0.0794, wR2 = 0.1418
Weighting scheme	w=1/[σ ² (F _o ²)+(0.0662P) ² +0.6040P] where P=(F _o ² +2F _c ²)/3	
Largest diff. peak and hole	0.487 and -0.540 eÅ ⁻³	
R.M.S. deviation from mean	0.058 eÅ ⁻³	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (\AA^2) for IS141_3.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
F1	0.31894(8)	0.54560(13)	0.51068(4)	0.0328(2)
O1	0.64913(8)	0.57881(13)	0.89702(5)	0.02322(19)
O2	0.72029(8)	0.50985(14)	0.79156(5)	0.0279(2)
N1	0.63260(9)	0.55790(15)	0.81989(6)	0.0200(2)
N2	0.54205(10)	0.63937(16)	0.91653(6)	0.0222(2)
N3	0.25619(9)	0.56969(15)	0.85780(5)	0.0187(2)
C1	0.36877(12)	0.56305(18)	0.58001(6)	0.0224(2)
C2	0.48134(12)	0.63739(18)	0.59438(7)	0.0233(2)
C3	0.53301(11)	0.64905(17)	0.66571(6)	0.0202(2)
C4	0.46964(10)	0.58888(16)	0.72049(6)	0.0165(2)
C5	0.35444(10)	0.51745(16)	0.70360(6)	0.0177(2)
C6	0.30356(11)	0.50271(17)	0.63257(6)	0.0204(2)
C7	0.52028(10)	0.59930(16)	0.79628(6)	0.0166(2)
C8	0.46649(10)	0.65105(16)	0.85770(6)	0.0179(2)
C9	0.34215(11)	0.72097(17)	0.85802(6)	0.0195(2)
C10	0.25910(12)	0.4930(2)	0.93044(7)	0.0241(3)
C11	0.17264(13)	0.3330(2)	0.93051(8)	0.0300(3)
C12	0.04613(13)	0.3927(2)	0.90175(9)	0.0335(3)
C13	0.04648(13)	0.4804(2)	0.82762(8)	0.0331(3)
C14	0.13635(11)	0.6371(2)	0.83078(7)	0.0256(3)
C15A	0.9623(4)	0.2173(6)	0.8909(2)	0.0348(8)
C15B	0.9542(3)	0.2489(5)	0.9067(2)	0.0344(8)

Table 4. Bond lengths (Å) for IS141_3.

F1-C1	1.3577(14)	O1-N2	1.3849(14)
O1-N1	1.4470(13)	O2-N1	1.2384(13)
N1-C7	1.3263(15)	N2-C8	1.3102(15)
N3-C9	1.4639(16)	N3-C14	1.4692(16)
N3-C10	1.4716(15)	C1-C2	1.3780(19)
C1-C6	1.3817(18)	C2-C3	1.3947(17)
C2-H2	0.976(19)	C3-C4	1.4016(16)
C3-H3	0.993(16)	C4-C5	1.4011(16)
C4-C7	1.4676(15)	C5-C6	1.3885(16)
C5-H5	0.985(17)	C6-H6	0.947(18)
C7-C8	1.4266(16)	C8-C9	1.4981(17)
C9-H9A	0.934(17)	C9-H9B	0.991(15)
C10-C11	1.5158(19)	C10-H10A	1.027(18)
C10-H10B	1.010(18)	C11-C12	1.527(2)
C11-H11A	0.991(19)	C11-H11B	0.959(16)
C12-C15B	1.482(4)	C12-C13	1.533(2)
C12-C15A	1.581(4)	C12-H12	1.06(2)
C13-C14	1.519(2)	C13-H13A	1.01(2)
C13-H13B	1.015(18)	C14-H14A	0.979(17)
C14-H14B	1.014(19)	C15A-H15A	0.98
C15A-H15B	0.98	C15A-H15C	0.98
C15B-H15D	0.98	C15B-H15E	0.98
C15B-H15F	0.98		

Table 5. Bond angles (°) for IS141_3.

N2-O1-N1	107.30(8)	O2-N1-C7	135.13(11)
O2-N1-O1	117.17(9)	C7-N1-O1	107.69(9)
C8-N2-O1	107.11(10)	C9-N3-C14	109.79(10)
C9-N3-C10	110.19(9)	C14-N3-C10	110.63(10)
F1-C1-C2	118.80(11)	F1-C1-C6	117.71(12)
C2-C1-C6	123.49(11)	C1-C2-C3	118.21(11)
C1-C2-H2	121.9(11)	C3-C2-H2	119.8(11)
C2-C3-C4	119.91(12)	C2-C3-H3	120.4(9)
C4-C3-H3	119.6(9)	C5-C4-C3	120.03(10)
C5-C4-C7	118.20(10)	C3-C4-C7	121.77(11)
C6-C5-C4	120.19(11)	C6-C5-H5	120.3(10)
C4-C5-H5	119.5(10)	C1-C6-C5	118.16(12)
C1-C6-H6	119.3(11)	C5-C6-H6	122.5(11)
N1-C7-C8	106.37(10)	N1-C7-C4	123.31(10)
C8-C7-C4	130.32(10)	N2-C8-C7	111.50(11)
N2-C8-C9	121.92(11)	C7-C8-C9	126.50(10)
N3-C9-C8	112.01(10)	N3-C9-H9A	111.3(10)
C8-C9-H9A	107.9(10)	N3-C9-H9B	108.0(9)
C8-C9-H9B	107.7(9)	H9A-C9-H9B	109.9(13)
N3-C10-C11	110.66(11)	N3-C10-H10A	110.2(10)
C11-C10-H10A	110.2(10)	N3-C10-H10B	108.5(10)
C11-C10-H10B	111.7(10)	H10A-C10-H10B	105.4(14)
C10-C11-C12	111.21(12)	C10-C11-H11A	109.0(11)
C12-C11-H11A	110.4(11)	C10-C11-H11B	111.2(9)
C12-C11-H11B	108.5(9)	H11A-C11-H11B	106.5(15)
C15B-C12-C11	114.53(19)	C15B-C12-C13	115.7(2)
C11-C12-C13	108.91(12)	C11-C12-C15A	109.90(19)
C13-C12-C15A	106.69(19)	C15B-C12-H12	98.2(11)
C11-C12-H12	110.5(11)	C13-C12-H12	108.4(11)
C15A-C12-H12	112.3(11)	C14-C13-C12	110.79(12)
C14-C13-H13A	109.4(12)	C12-C13-H13A	111.1(12)
C14-C13-H13B	108.9(10)	C12-C13-H13B	108.5(10)
H13A-C13-H13B	108.0(15)	N3-C14-C13	110.59(12)
N3-C14-H14A	109.0(10)	C13-C14-H14A	109.6(10)
N3-C14-H14B	111.3(10)	C13-C14-H14B	109.8(10)
H14A-C14-H14B	106.5(15)	C12-C15A-H15A	109.5
C12-C15A-H15B	109.5	H15A-C15A-H15B	109.5
C12-C15A-H15C	109.5	H15A-C15A-H15C	109.5
H15B-C15A-H15C	109.5	C12-C15B-H15D	109.5
C12-C15B-H15E	109.5	H15D-C15B-H15E	109.5
C12-C15B-H15F	109.5	H15D-C15B-H15F	109.5
H15E-C15B-H15F	109.5		

Table 6. Anisotropic atomic displacement parameters (\AA^2) for IS141_3.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F1	0.0453(5)	0.0384(5)	0.0132(3)	0.0006(3)	-0.0022(3)	0.0002(4)
O1	0.0209(4)	0.0274(4)	0.0196(4)	0.0009(3)	-0.0038(3)	-0.0004(3)
O2	0.0188(4)	0.0335(5)	0.0312(5)	-0.0035(4)	0.0030(4)	0.0045(4)
N1	0.0189(5)	0.0206(5)	0.0197(5)	-0.0002(4)	-0.0006(4)	-0.0007(4)
N2	0.0225(5)	0.0246(5)	0.0185(5)	0.0007(4)	-0.0008(4)	-0.0027(4)
N3	0.0164(4)	0.0236(5)	0.0157(4)	0.0041(4)	0.0009(3)	-0.0020(4)
C1	0.0314(6)	0.0220(5)	0.0131(5)	-0.0004(4)	0.0000(4)	0.0047(5)
C2	0.0323(6)	0.0204(5)	0.0185(5)	0.0007(4)	0.0086(5)	0.0014(5)
C3	0.0235(6)	0.0179(5)	0.0202(5)	-0.0012(4)	0.0061(4)	-0.0001(4)
C4	0.0189(5)	0.0163(5)	0.0143(5)	-0.0001(4)	0.0021(4)	0.0025(4)
C5	0.0187(5)	0.0186(5)	0.0155(5)	0.0005(4)	0.0014(4)	0.0021(4)
C6	0.0216(5)	0.0211(5)	0.0175(5)	-0.0010(4)	-0.0008(4)	0.0031(4)
C7	0.0167(5)	0.0169(5)	0.0156(5)	0.0008(4)	0.0001(4)	-0.0009(4)
C8	0.0205(5)	0.0182(5)	0.0147(5)	0.0005(4)	0.0010(4)	-0.0042(4)
C9	0.0210(5)	0.0206(5)	0.0172(5)	0.0001(4)	0.0032(4)	-0.0010(4)
C10	0.0223(6)	0.0315(6)	0.0178(5)	0.0072(5)	0.0005(4)	-0.0039(5)
C11	0.0259(6)	0.0326(7)	0.0308(7)	0.0110(6)	0.0012(5)	-0.0068(5)
C12	0.0231(6)	0.0394(8)	0.0381(8)	0.0093(6)	0.0043(6)	-0.0077(6)
C13	0.0203(6)	0.0418(8)	0.0350(7)	0.0078(6)	-0.0037(5)	-0.0055(6)
C14	0.0197(6)	0.0319(7)	0.0247(6)	0.0078(5)	0.0004(4)	0.0014(5)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters (\AA^2) for IS141_3.

	x/a	y/b	z/c	U(eq)
H2	0.5259(16)	0.678(3)	0.5563(10)	0.039(5)
H3	0.6140(14)	0.702(2)	0.6781(8)	0.023(4)
H5	0.3103(15)	0.476(2)	0.7425(9)	0.024(4)
H6	0.2270(16)	0.451(2)	0.6191(9)	0.028(4)
H9A	0.3416(14)	0.797(2)	0.8982(9)	0.025(4)
H9B	0.3207(13)	0.795(2)	0.8137(8)	0.019(4)
H10A	0.2391(15)	0.594(2)	0.9652(9)	0.027(4)
H10B	0.3434(15)	0.454(2)	0.9483(9)	0.028(4)
H12	0.0148(17)	0.492(3)	0.9360(11)	0.041(5)
H11A	0.1759(16)	0.285(3)	0.9800(10)	0.041(5)
H11B	0.1947(14)	0.232(2)	0.9018(8)	0.020(4)
H13A	-0.0351(18)	0.529(3)	0.8082(11)	0.040(5)
H13B	0.0690(15)	0.382(2)	0.7935(9)	0.028(4)
H14A	0.1371(15)	0.689(2)	0.7828(9)	0.030(4)
H14B	0.1114(16)	0.741(3)	0.8616(10)	0.034(5)
H15A	-0.1179	0.2559	0.8704	0.052
H15B	-0.0411	0.1571	0.9372	0.052
H15C	-0.0062	0.1300	0.8582	0.052
H15D	-0.1245	0.2999	0.8896	0.052
H15E	-0.0434	0.2095	0.9567	0.052
H15F	-0.0302	0.1424	0.8771	0.052