

Supplementary Information
**Synthesis, Molecular Modelling Study and
Quantum Chemical Based Investigations of
Isoindoline-1,3-diones as Anti-mycobacterial
Agents**

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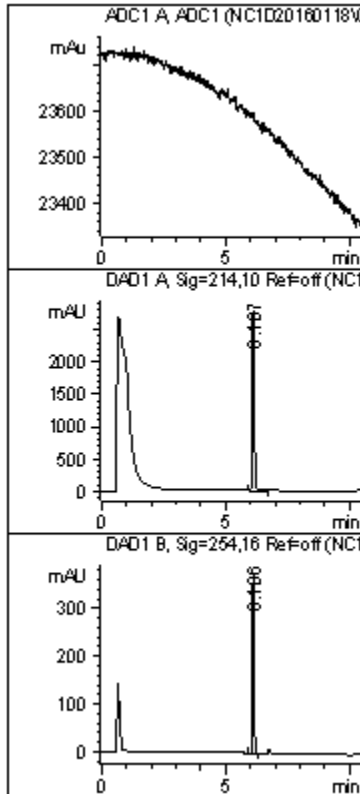
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LCMS of Compound 2



Signal 1: ADC1 A, ADC1

Signal 2: DAD1 A, Sig=214,10 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.107	VV	0.0948	1.65349e4	2803.53711	100.0000

Totals : 1.65349e4 2803.53711

Signal 3: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.106	VB	0.0631	1585.15942	376.94125	100.0000

Totals : 1585.15942 376.94125

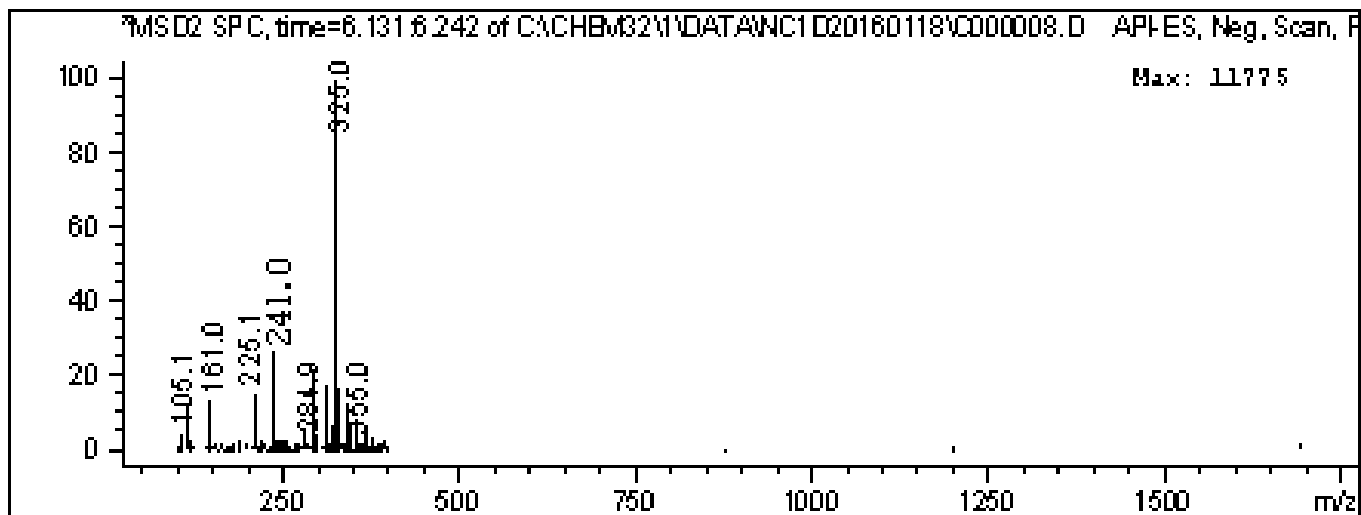
Signal 4: MSD2 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	6.174	BV	0.2440	1.97362e6	1.09253e5	100.0000

Totals : 1.97362e6 1.09253e5

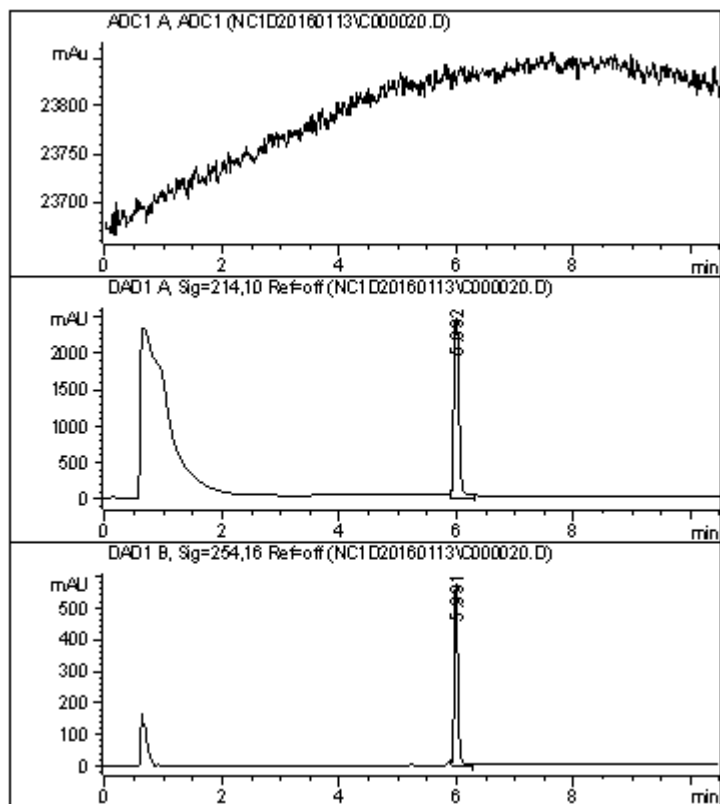
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*** End of Report ***

Retention Time (MS)	MS Area	Mol. Weight or Ion
6.174	1973623	241.00 I



*** End of Report ***

LCMS of Compound 3



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 Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: ADC1 A, ADC1

Signal 2: DAD1 A, Sig=214,10 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.992	VV	0.1003	1.58720e4	2493.75610	100.0000
Totals :				1.58720e4	2493.75610	

Signal 3: DAD1 B, Sig=254,16 Ref=off

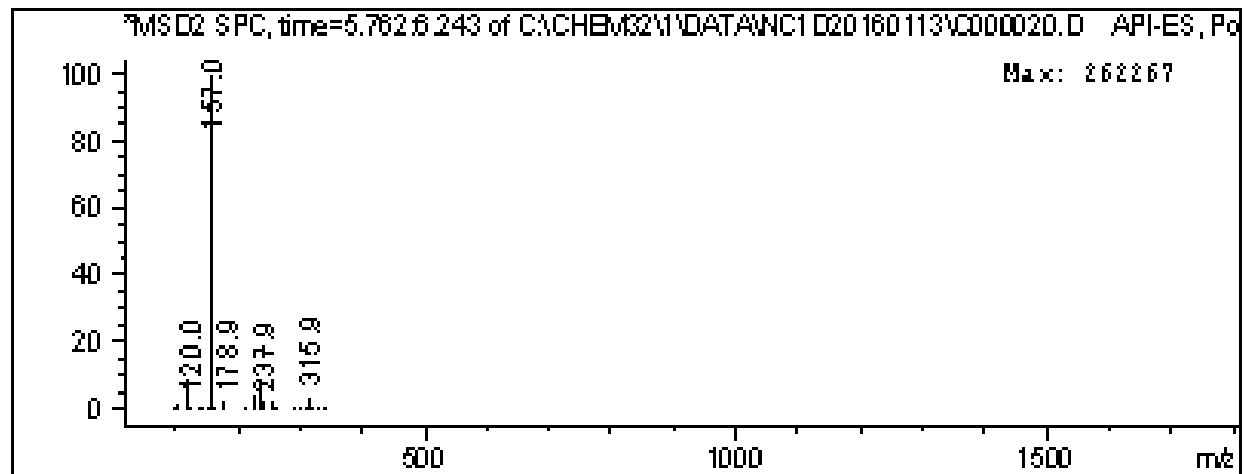
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.991	VB	0.0652	2436.36963	578.12140	100.0000
Totals :				2436.36963	578.12140	

Signal 4: MSD2 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	6.050	VV	0.4081	1.85501e7	5.77425e5	100.0000
Totals :				1.85501e7	5.77425e5	

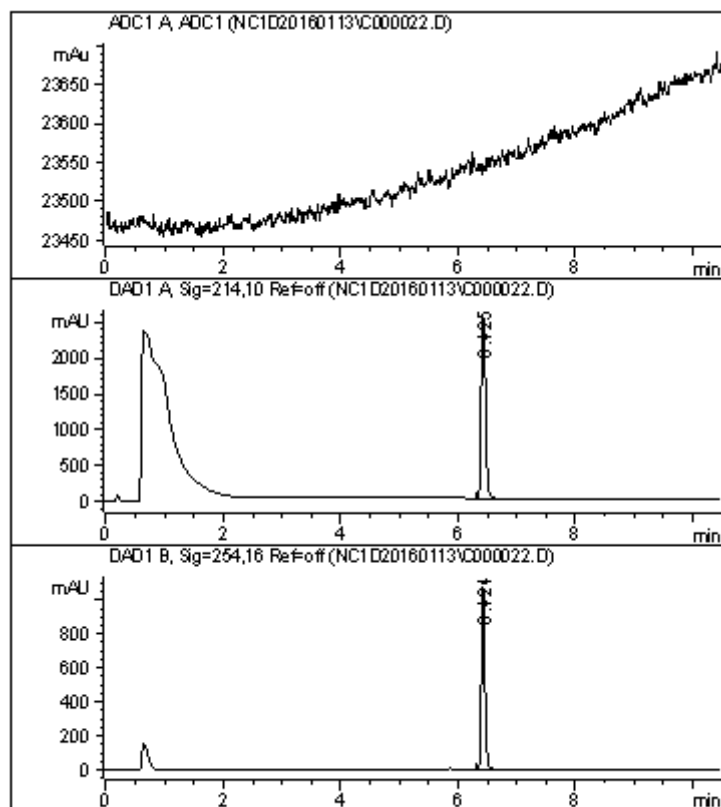
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 *** End of Report ***

Retention Time (MS)	MS Area	Mol. Weight or Ion
6.050	18550132	237.9 I



*** End of Report ***

LCMS of Compound 4



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 Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: ADC1 A, ADC1

Signal 2: DAD1 A, Sig=214,10 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.425	VV	0.0868	1.34865e4	2505.05908	100.0000
Totals :				1.34865e4	2505.05908	

Signal 3: DAD1 B, Sig=254,16 Ref=off

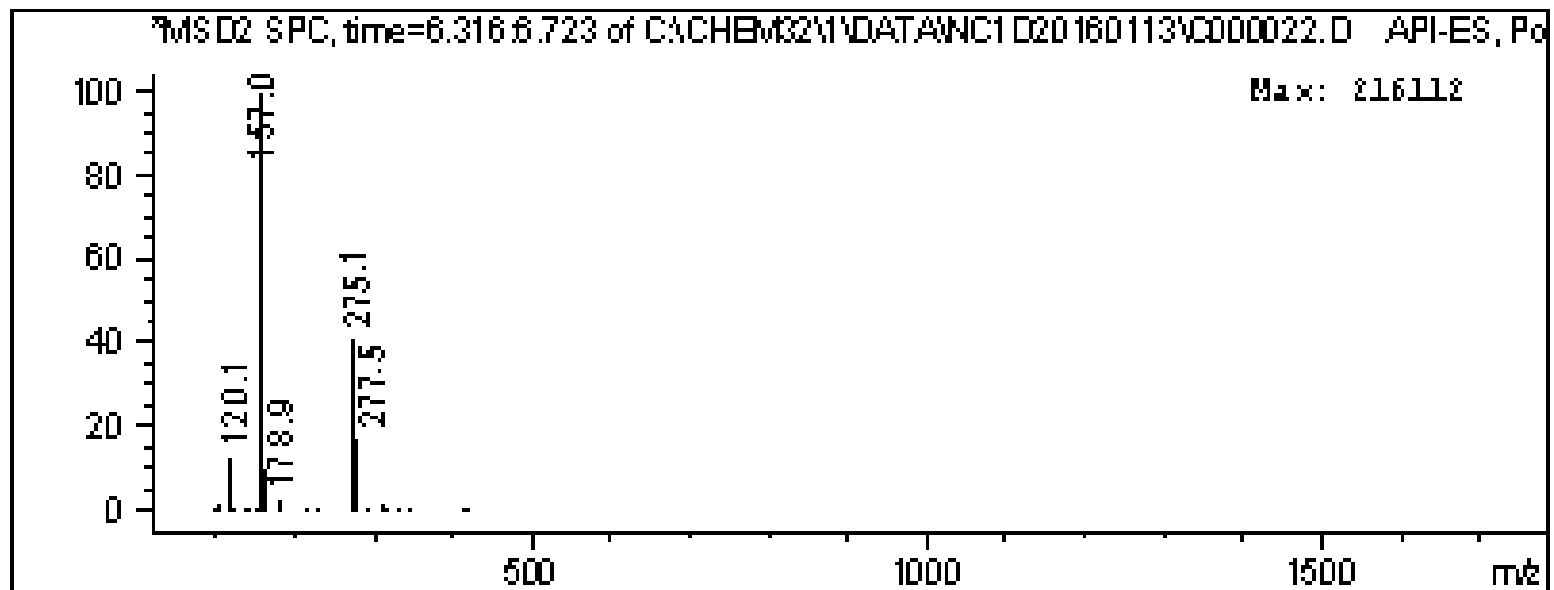
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.424	BV	0.0644	4491.55518	1083.52832	100.0000
Totals :				4491.55518	1083.52832	

Signal 4: MSD2 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	6.500	VV	0.2533	6.90508e6	3.66076e5	100.0000
Totals :				6.90508e6	3.66076e5	

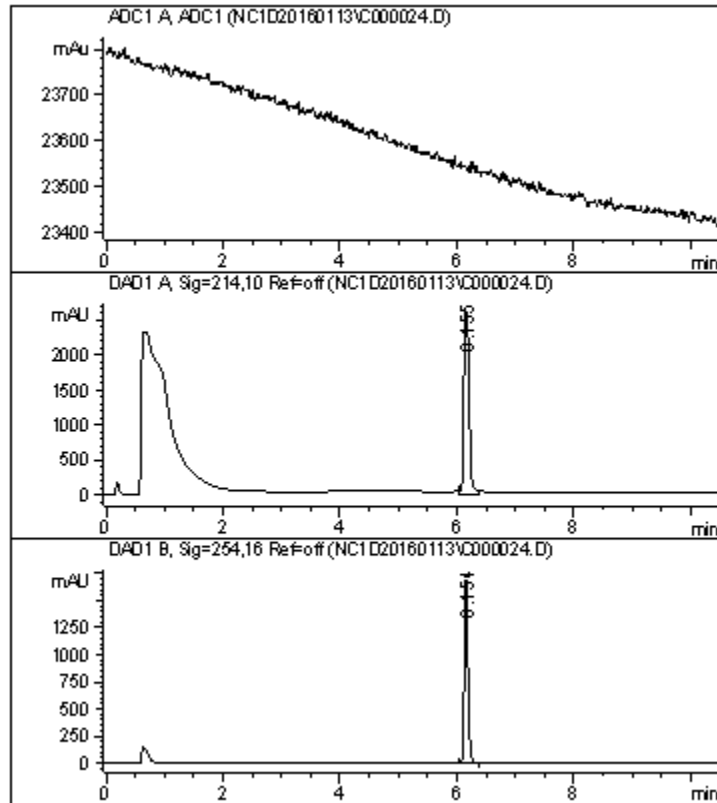
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 *** End of Report ***

Retention Time (MS)	MS Area	Mol. Weight or Ion
6.500	6905077	275.1



*** End of Report ***

LCMS of Compound 5



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 Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: ADC1 A, ADC1

Signal 2: DAD1 A, Sig=214,10 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.155	VV	0.1031	1.67024e4	2596.01855	100.0000
Totals :				1.67024e4	2596.01855	

Signal 3: DAD1 B, Sig=254,16 Ref=off

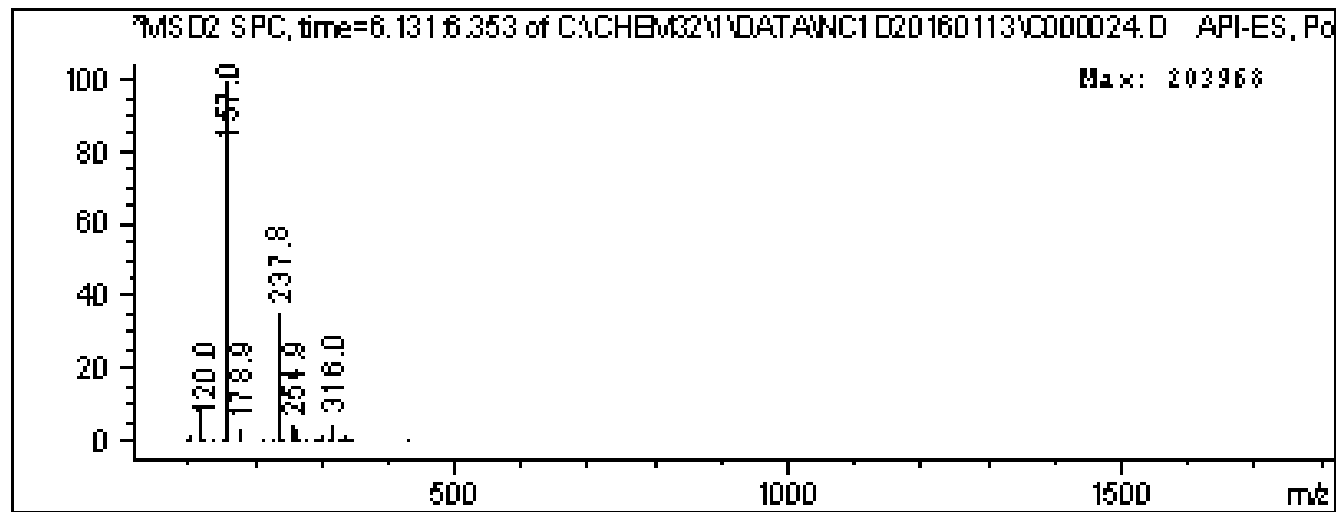
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.154	VV	0.0659	7280.68262	1701.35840	100.0000
Totals :				7280.68262	1701.35840	

Signal 4: MSD2 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	6.218	VV	0.2806	1.23543e7	5.82721e5	100.0000
Totals :				1.23543e7	5.82721e5	

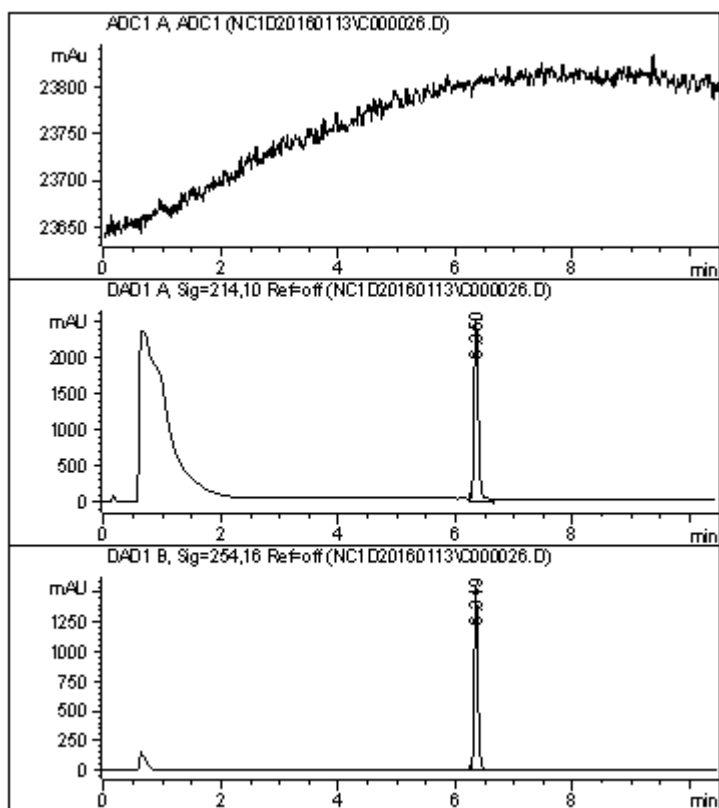
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 *** End of Report ***
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Retention Time (MS)	MS Area	Mol. Weight or Ion
6.218	12354342	237.8 I



*** End of Report ***

LCMS of Compound 6



Area Percent Report

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Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
    
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Signal 1: ADC1 A, ADC1

Signal 2: DAD1 A, Sig=214,10 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.350	VV	0.0826	1.30179e4	2507.36230	100.0000
Totals :				1.30179e4	2507.36230	

Signal 3: DAD1 B, Sig=254,16 Ref=off

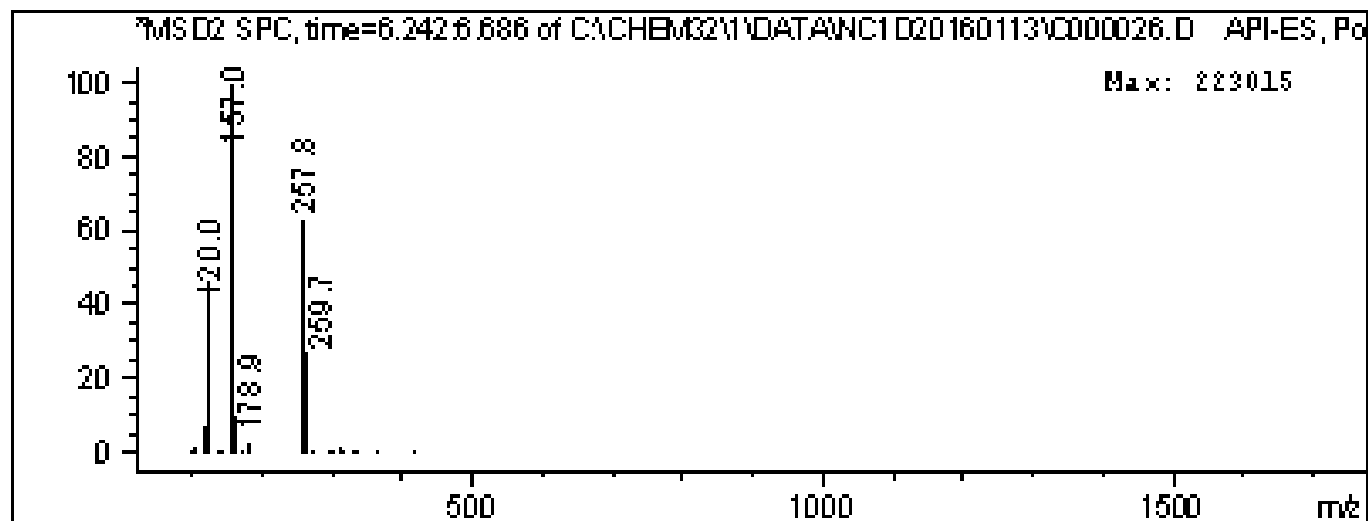
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.349	VV	0.0652	6547.25830	1553.14368	100.0000
Totals :				6547.25830	1553.14368	

Signal 4: MSD2 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	6.421	VV	0.2740	8.12757e6	3.93910e5	100.0000
Totals :				8.12757e6	3.93910e5	

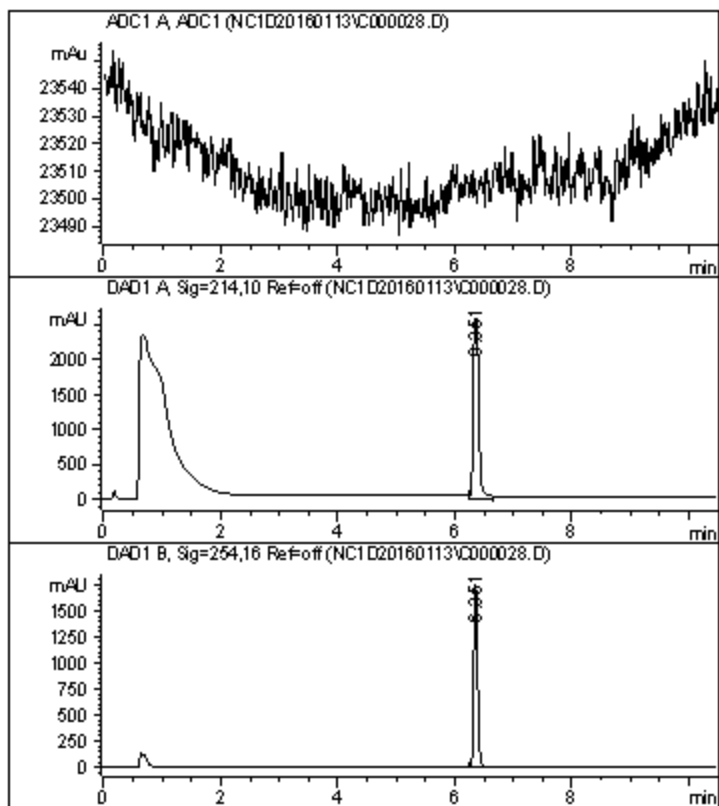
*** End of Report ***

Retention Time (MS)	MS Area	Mol. Weight or Ion
6.421	8127571	257.8



*** End of Report ***

LCMS of Compound 7



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 Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: ADC1 A, ADC1

Signal 2: DAD1 A, Sig=214,10 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.351	VV	0.1061	1.73579e4	2591.47925	100.0000

Totals : 1.73579e4 2591.47925

Signal 3: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.351	VV	0.0675	7801.28760	1768.18237	100.0000

Totals : 7801.28760 1768.18237

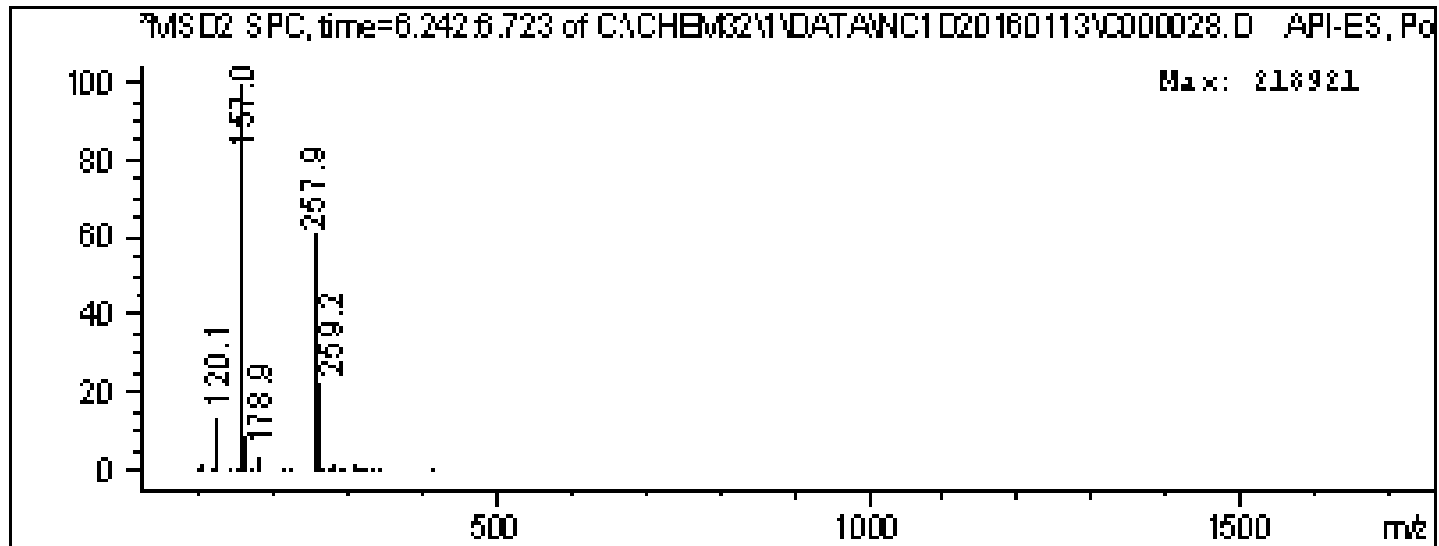
Signal 4: MSD2 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	6.419	VV	0.2881	8.79154e6	4.20797e5	100.0000

Totals : 8.79154e6 4.20797e5

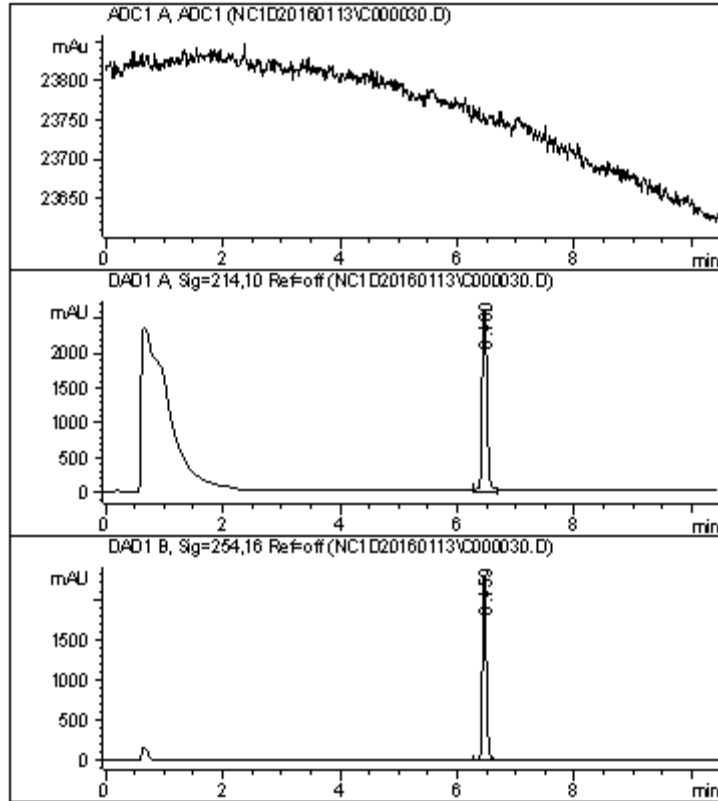
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 *** End of Report ***

Retention Time (MS)	MS Area	Mol. Weight or Ion
6.419	8791537	257.9



*** End of Report ***

LCMS of Compound 8



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 Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: ADC1 A, ADC1

Signal 2: DAD1 A, Sig=214,10 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.460	VV	0.0951	1.54873e4	2612.95581	100.0000
Totals :				1.54873e4	2612.95581	

Signal 3: DAD1 B, Sig=254,16 Ref=off

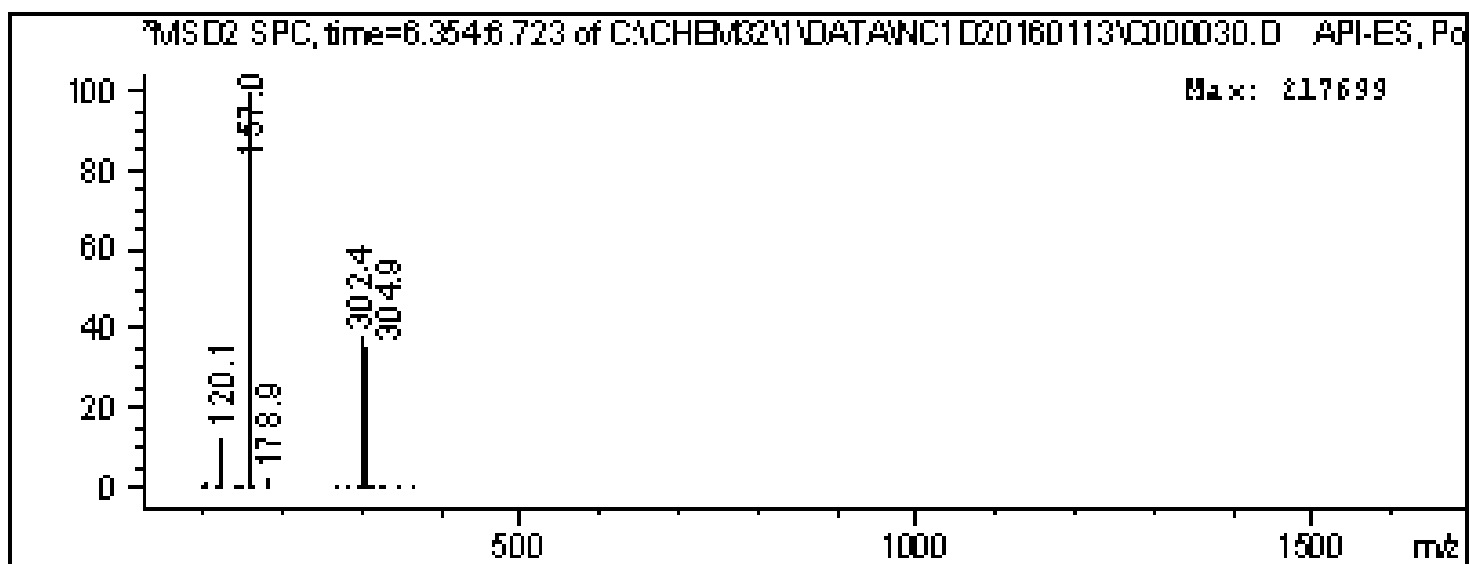
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.459	BV	0.0731	1.03985e4	2283.74463	100.0000
Totals :				1.03985e4	2283.74463	

Signal 4: MSD2 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	6.525	VV	0.2676	8.04251e6	4.20272e5	100.0000
Totals :				8.04251e6	4.20272e5	

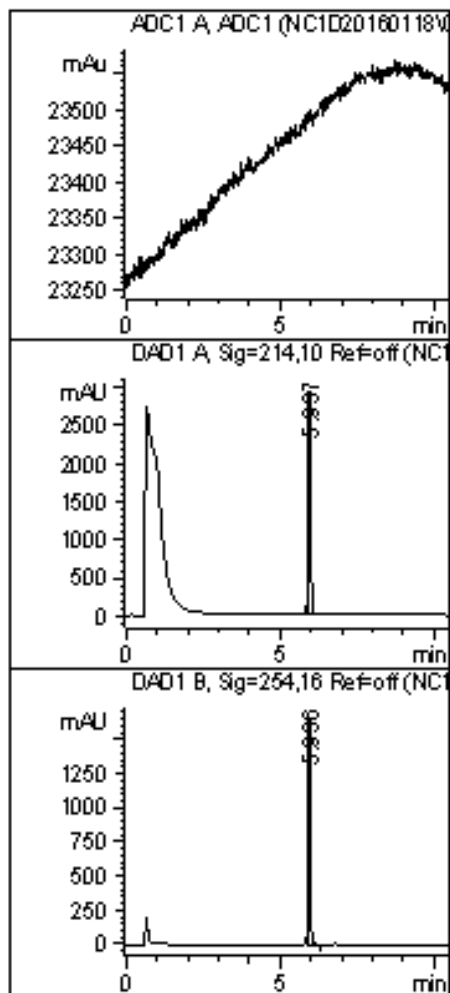
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 *** End of Report ***

Retention Time (MS)	MS Area	Mol. Weight or Ion
6.525	8042512	302.4 I



*** End of Report ***

LCMS of Compound 9



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Signal 1: ADC1 A, ADC1

Signal 2: DAD1 A, Sig=214,10 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.937	VV	0.0948	1.74424e4	2956.19556	100.0000

Totals : 1.74424e4 2956.19556

Signal 3: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.936	VB	0.0660	7113.25879	1659.08154	100.0000

Totals : 7113.25879 1659.08154

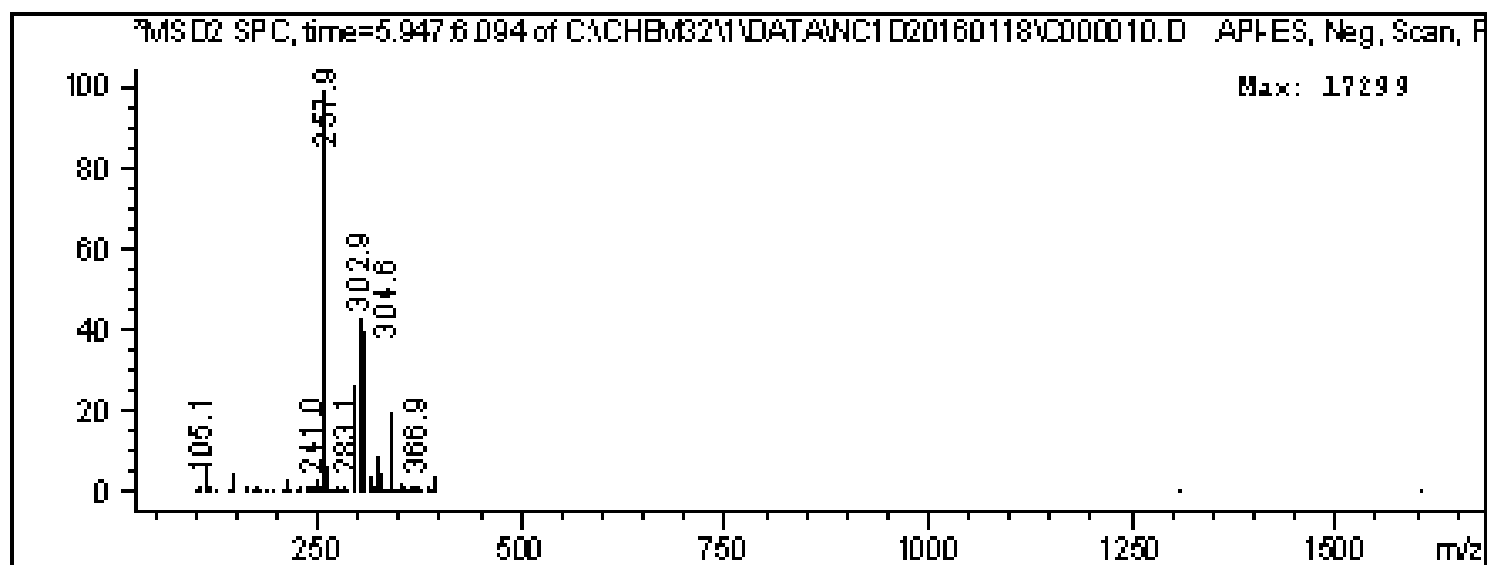
Signal 4: MSD2 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	6.013	VV	0.2600	2.25189e6	1.21848e5	100.0000

Totals : 2.25189e6 1.21848e5

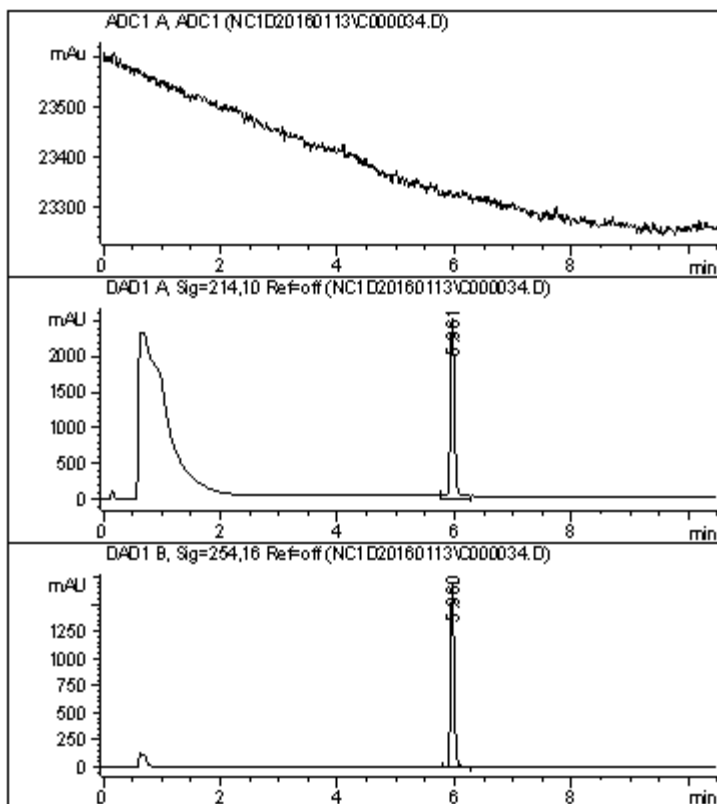
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*** End of Report ***

Retention Time (MS)	MS Area	Mol. Weight or Ion
6.013	2251889	302.9



*** End of Report ***

LCMS of Compound 10



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 Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: ADC1 A, ADC1

Signal 2: DAD1 A, Sig=214,10 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.961	VV	0.0792	1.28939e4	2540.30762	100.0000

Totals : 1.28939e4 2540.30762

Signal 3: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.960	BV	0.0652	7118.76807	1689.70288	100.0000

Totals : 7118.76807 1689.70288

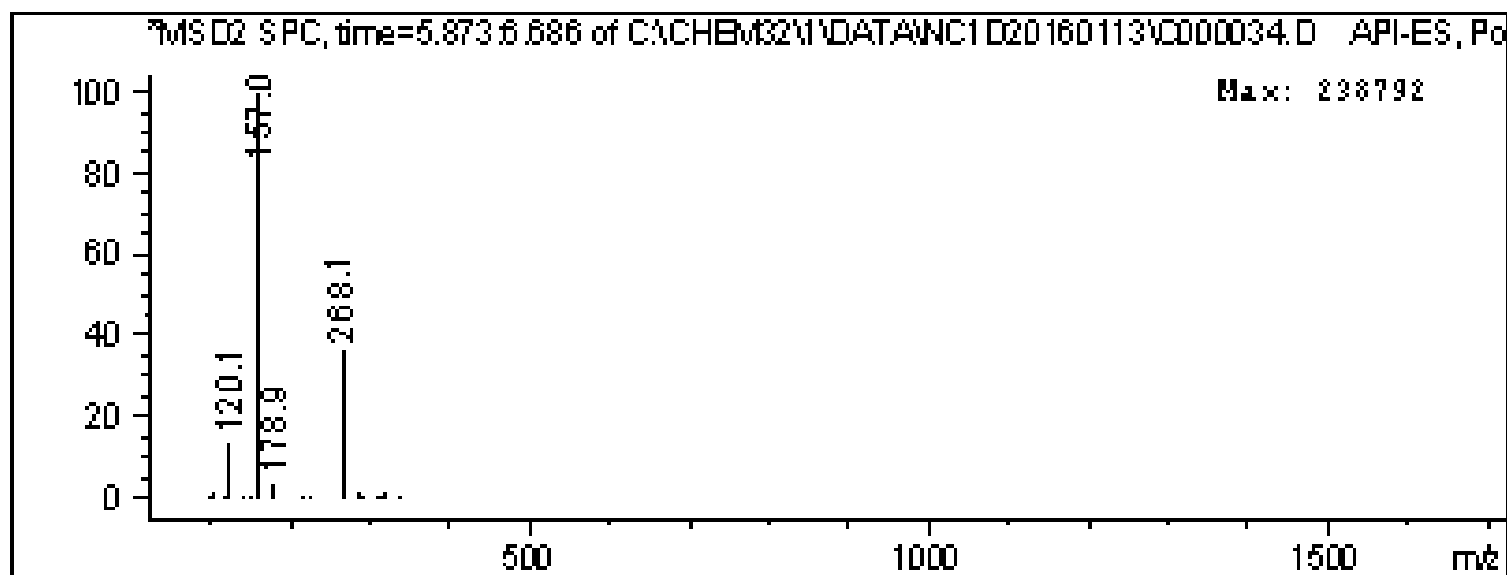
Signal 4: MSD2 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	6.034	VV	0.4727	1.55015e7	4.22216e5	100.0000

Totals : 1.55015e7 4.22216e5

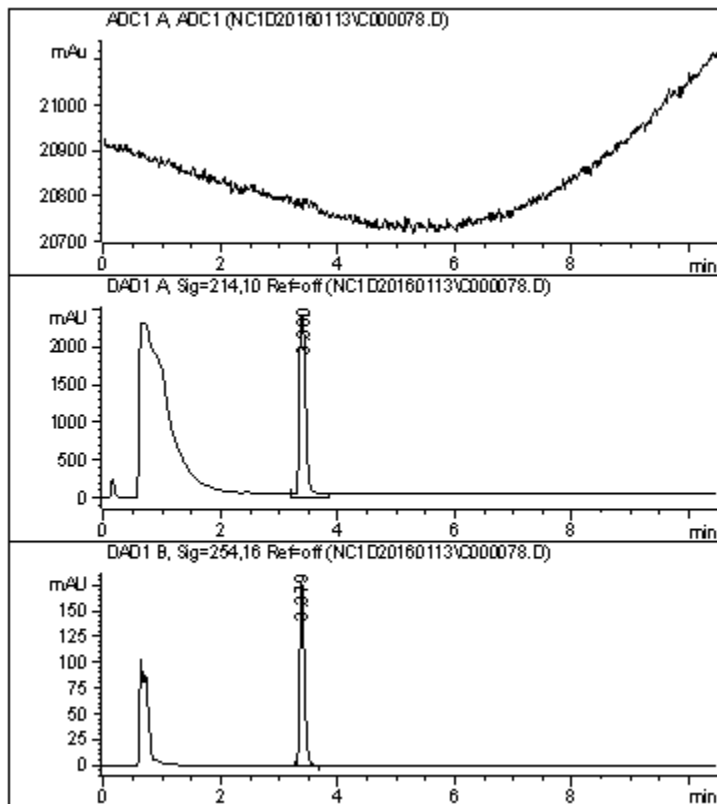
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 *** End of Report ***

Retention Time (MS)	MS Area	Mol. Weight or Ion
6.034	15501548	268.1



*** End of Report ***

LCMS of Compound 11



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 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: ADC1 A, ADC1

Signal 2: DAD1 A, Sig=214,10 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.380	VV	0.1291	1.95934e4	2404.72925	100.0000

Totals : 1.95934e4 2404.72925

Signal 3: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.379	BB	0.0843	985.55957	178.78323	100.0000

Totals : 985.55957 178.78323

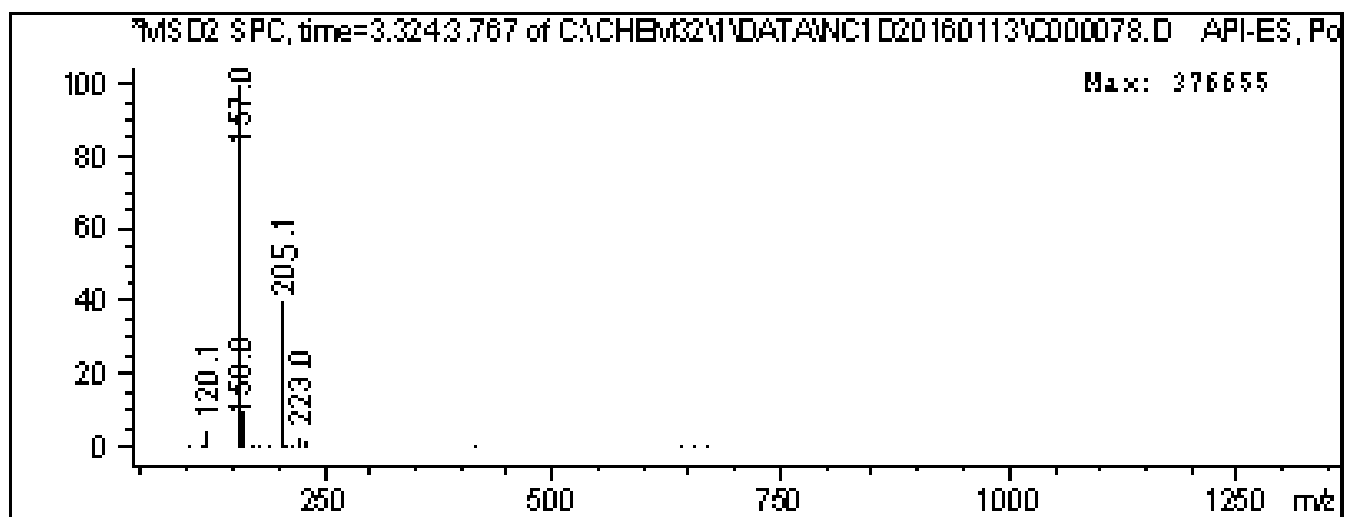
Signal 4: MSD2 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	3.452	VV	0.3159	1.35053e7	5.80174e5	100.0000

Totals : 1.35053e7 5.80174e5

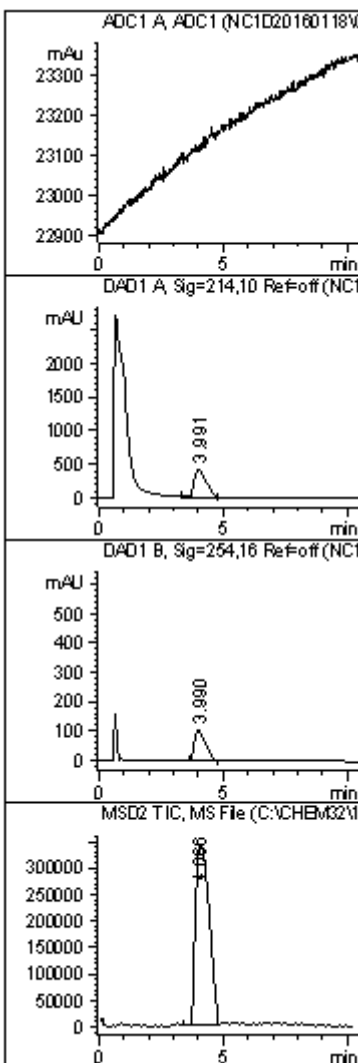
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 *** End of Report ***

Retention Time (MS)	MS Area	Mol. Weight or Ion
3.452	13505338	205.1



*** End of Report ***

LCMS of Compound 14



Signal 1: ADC1 A, ADC1

Signal 2: DAD1 A, Sig=214,10 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.991	WV	0.4863	1.49376e4	439.70038	100.0000

Totals : 1.49376e4 439.70038

Signal 3: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.990	BV	0.4900	3252.58398	105.40896	100.0000

Totals : 3252.58398 105.40896

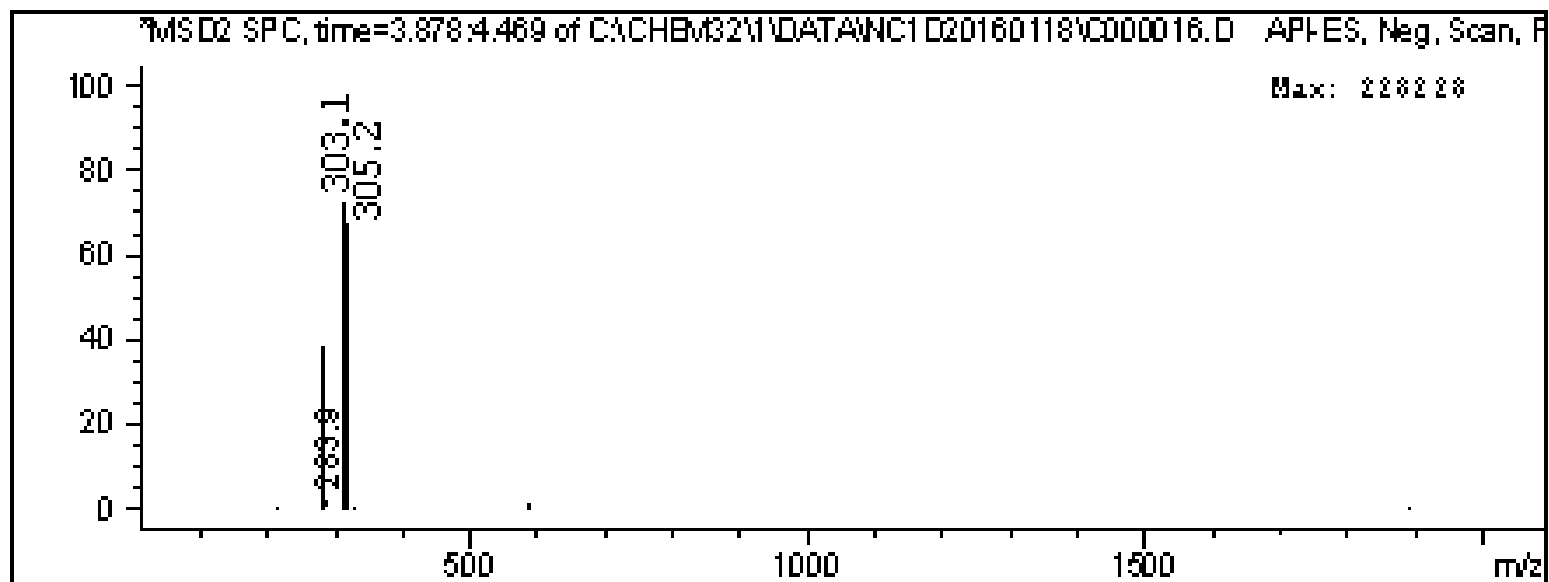
Signal 4: MSD2 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	4.066	WV	0.5335	1.30286e7	3.41681e5	100.0000

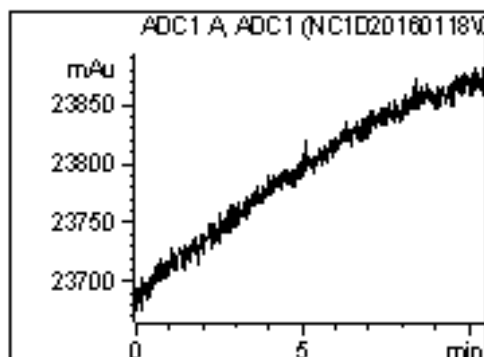
Totals : 1.30286e7 3.41681e5

*** End of Report ***

Retention Time (MS)	MS Area	Mol. Weight or Ion
4.066	13028626	303.10 I



LCMS of Compound 15

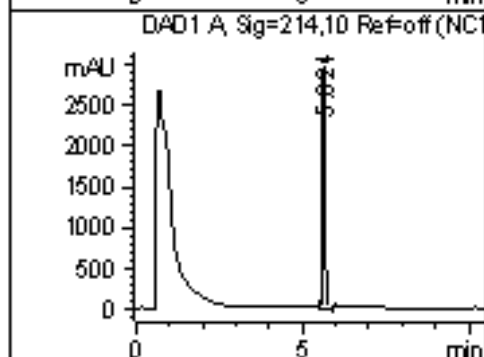


Signal 1: ADC1 A, ADC1

Signal 2: DAD1 A, Sig=214,10 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.624	UV	0.0866	1.60866e4	2996.74463	100.0000

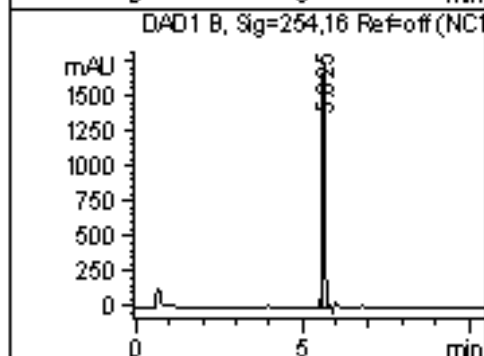
Totals : 1.60866e4 2996.74463



Signal 3: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.625	BV	0.0704	7792.25195	1733.70581	100.0000

Totals : 7792.25195 1733.70581



Signal 4: MSD2 TIC, MS File

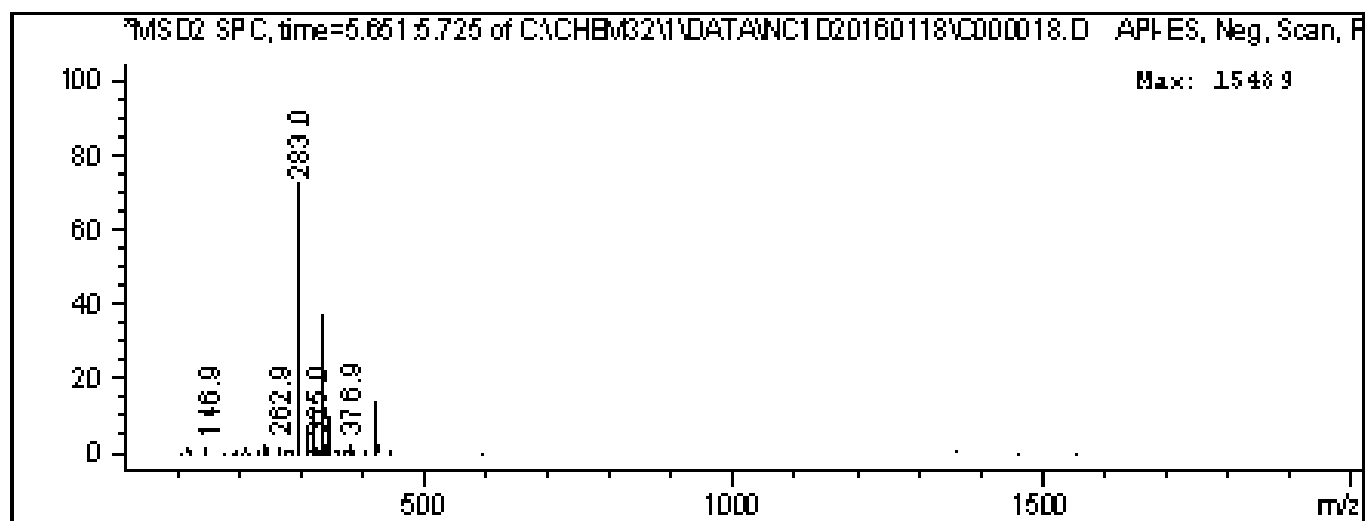
Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	5.691	BV	0.1693	8.15201e5	6.98976e4	100.0000

Totals : 8.15201e5 6.98976e4

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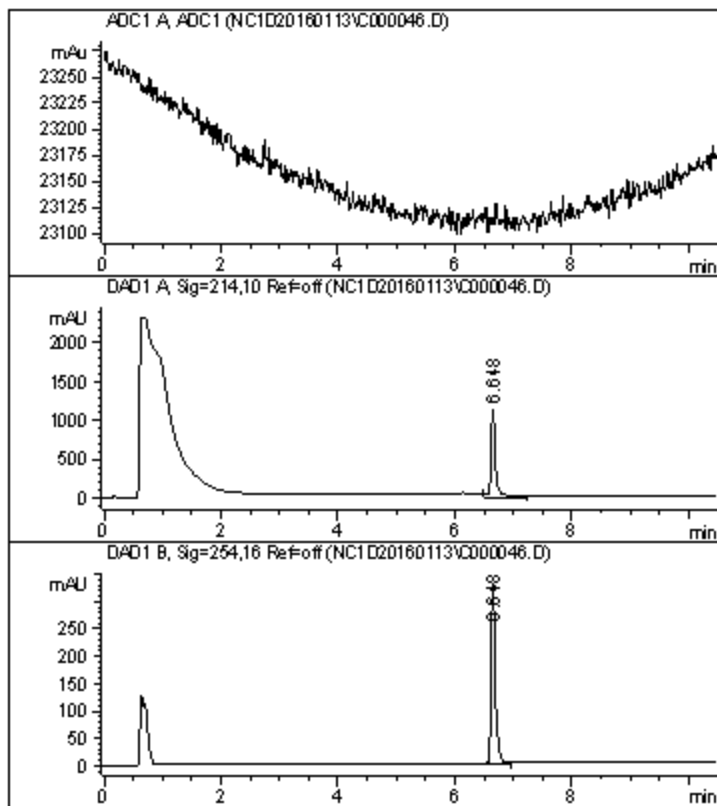
*** End of Report ***

Retention Time (MS)	MS Area	Mol. Weight or Ion
5.691	815201	283.0



*** End of Report ***

LCMS of Compound 21



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: ADC1 A, ADC1

Signal 2: DAD1 A, Sig=214,10 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.648	VV	0.0840	6593.68359	1130.68005	100.0000

Totals : 6593.68359 1130.68005

Signal 3: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.648	VB	0.0729	1618.78113	332.18597	100.0000

Totals : 1618.78113 332.18597

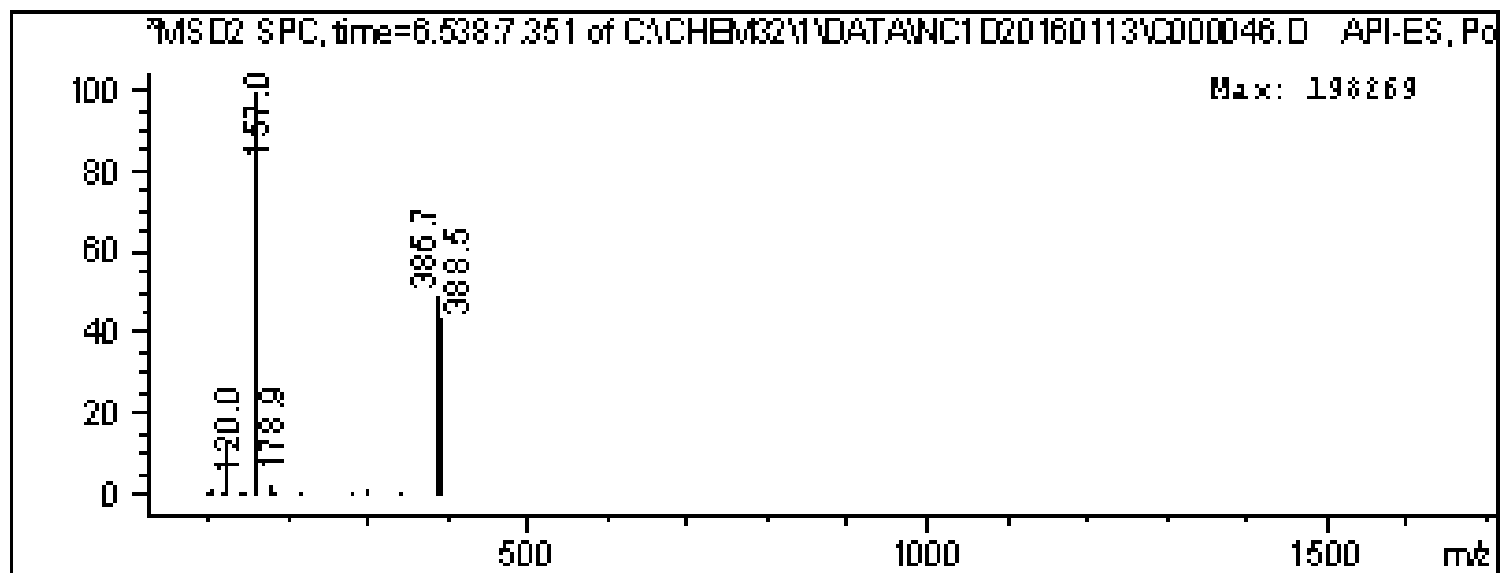
Signal 4: MSD2 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	6.739	VV	0.4942	1.46084e7	3.98464e5	100.0000

Totals : 1.46084e7 3.98464e5

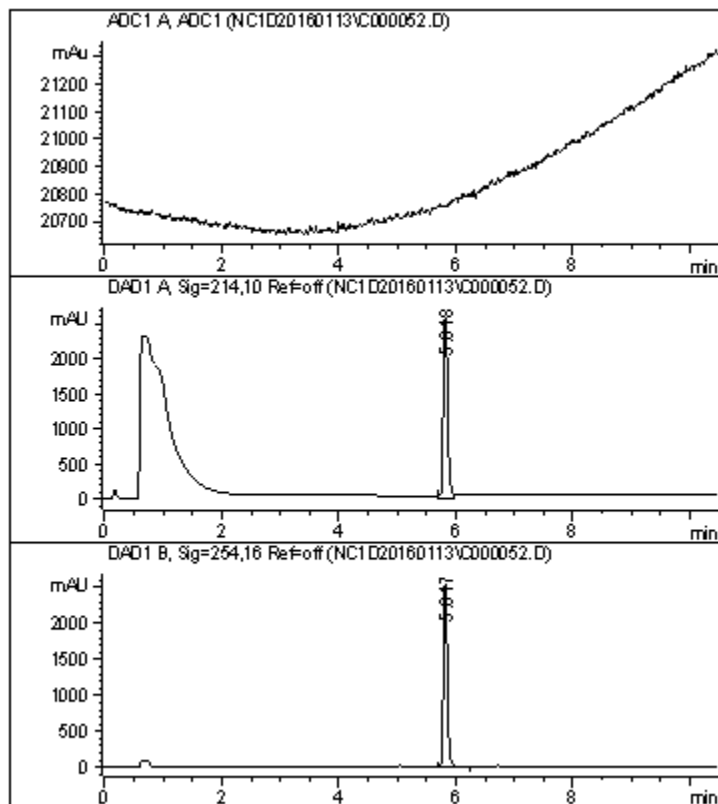
*** End of Report ***

Retention Time (MS)	MS Area	Mol. Weight or Ion
6.739	14608362	386.7 I



*** End of Report ***

LCMS of Compound 24



Area Percent Report

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Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
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Signal 1: ADC1 A, ADC1

Signal 2: DAD1 A, Sig=214,10 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.818	VV	0.0861	1.38652e4	2604.76611	100.0000

Totals : 1.38652e4 2604.76611

Signal 3: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.817	BV	0.0738	1.18322e4	2568.20996	100.0000

Totals : 1.18322e4 2568.20996

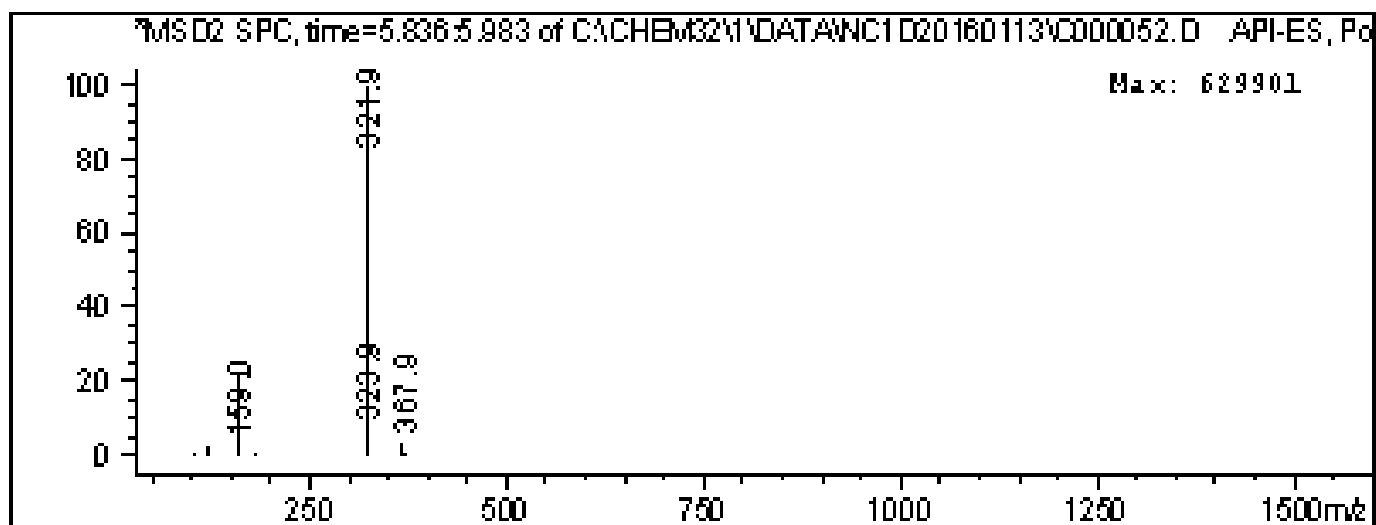
Signal 4: MSD2 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	5.888	VV	0.2254	2.23091e7	1.43776e6	100.0000

Totals : 2.23091e7 1.43776e6

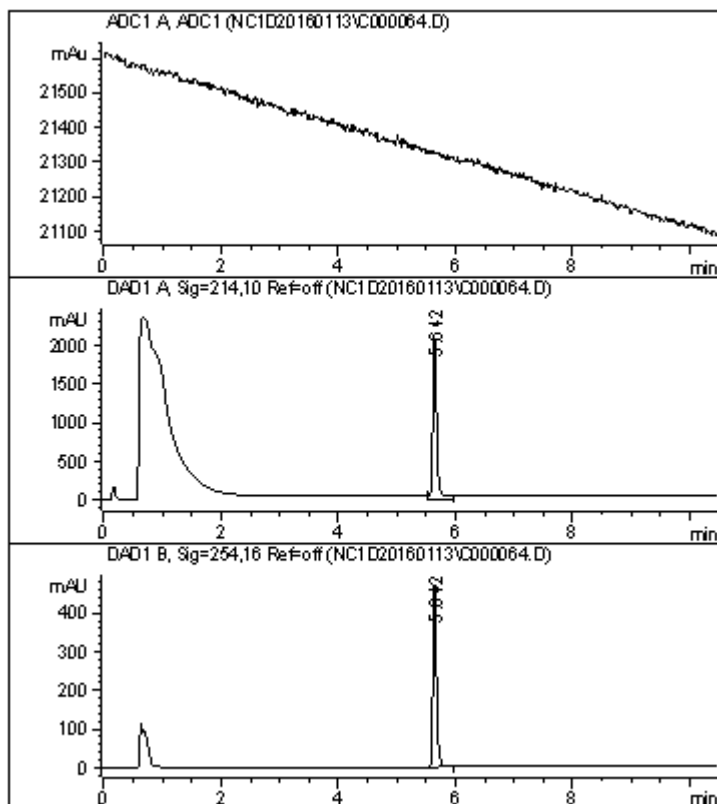
*** End of Report ***

Retention Time (MS)	MS Area	Mol. Weight or Ion
5.888	22309054	321.90 I



*** End of Report ***

LCMS of Compound 30



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 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: ADC1 A, ADC1

Signal 2: DAD1 A, Sig=214,10 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.642	VV	0.0746	1.01365e4	2087.83521	100.0000
Totals :				1.01365e4	2087.83521	

Signal 3: DAD1 B, Sig=254,16 Ref=off

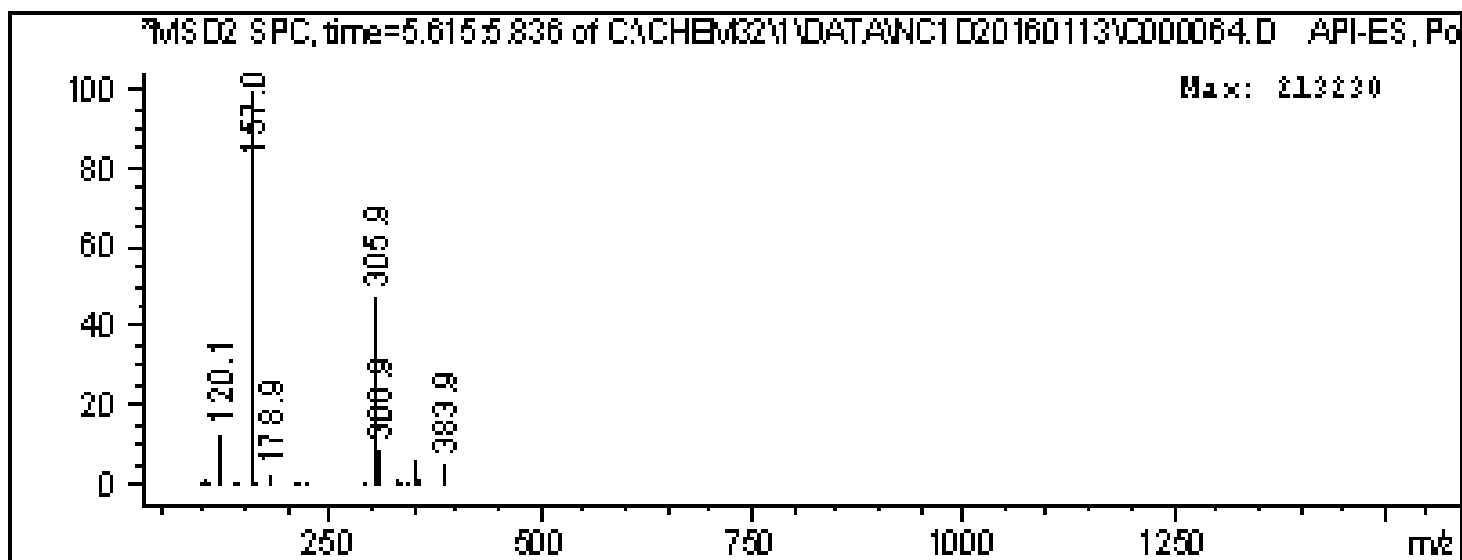
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.642	BV	0.0640	2025.57593	472.49197	100.0000
Totals :				2025.57593	472.49197	

Signal 4: MSD2 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	5.719	VV	0.2478	1.33714e7	7.66846e5	100.0000
Totals :				1.33714e7	7.66846e5	

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 *** End of Report ***

Retention Time (MS)	MS Area	Mol. Weight or Ion
5.719	13371382	305.9 I



*** End of Report ***

Table 1S. Per residue binding free energy during 100 ns time

Amino Acid	Per residue binding free energy	Amino Acid	Per residue binding free energy	Amino Acid	Per residue binding free energy	Amino Acid	Per residue binding free energy
THR_2	32.42	GLU_69	-54.48	PRO_136	0.89	VAL_203	-15.26
GLY_3	-24.61	HIS_70	-36.36	ILE_137	-9.23	GLY_204	-29.95
LEU_4	-15.51	LEU_71	-17.77	MET_138	-29.05	GLY_205	-25.34
LEU_5	-24.55	ALA_72	-22.16	ASN_139	-37.17	ALA_206	-22.5
ASP_6	-56.06	SER_73	-21.55	PRO_140	1.66	LEU_207	-23.88
GLY_7	-31.38	LEU_74	-23.85	GLY_141	-25.07	GLY_208	-27.6
LYS_8	-36.48	ALA_75	-36.85	GLY_142	-33.82	GLU_209	-49.84
ARG_9	-58.98	GLY_76	-30.26	SER_143	-22.39	GLU_210	-53.81
ILE_10	-19.35	ARG_77	-55.86	ILE_144	-16.31	ALA_211	-31.2
LEU_11	-23.05	VAL_78	-24.75	VAL_145	-21.39	GLY_212	-29.6
VAL_12	-23.95	THR_79	-11.46	GLY_146	-30.91	ALA_213	-25.31
SER_13	-25.25	GLU_80	-43.14	MET_147	-17.96	GLN_214	-60.17
GLY_14	-23.5	ALA_81	-27.11	ASP_148	-52.46	ILE_215	-15.85
ILE_15	-13.14	ILE_82	-13.74	PHE_149	-9.63	GLN_216	-56.38
ILE_16	-14.08	GLY_83	-21.46	ASP_150	-49.04	LEU_217	-16.6
THR_17	-5.77	ALA_84	-20.88	PRO_151	-4.36	LEU_218	-24.31
ASP_18	-62.39	GLY_85	-25.94	SER_152	-14.53	GLU_219	-50.7
SER_19	-21.52	ASN_86	-56.03	ARG_153	-41.38	GLU_220	-48.09
SER_20	-23.23	LYS_87	-29.01	ALA_154	-21.32	GLY_221	-27.01
ILE_21	-7.78	LEU_88	-25.6	MET_155	-15.65	TRP_222	-35.48
ALA_22	-29.55	ASP_89	-68.67	PRO_156	6.94	ASP_223	-60.31
PHE_23	-20.83	GLY_90	-32.49	ALA_157	-24.74	GLN_224	-56.97
HIS_24	-34.56	VAL_91	-22.92	TYR_158	-33.6	ARG_225	-54.53
ILE_25	-21.73	VAL_92	-22.71	ASN_159	-57.4	ALA_226	-18.55
ALA_26	-32.04	HIS_93	-41.79	TRP_160	-28.71	PRO_227	3.15

Amino Acid	Per residue binding free energy	Amino Acid	Per residue binding free energy	Amino Acid	Per residue binding free energy	Amino Acid	Per residue binding free energy
ARG_27	-49.74	SER_94	-19.3	MET_161	-28.92	ILE_228	-9.7
VAL_28	-18.68	ILE_95	-18.49	THR_162	-13.95	GLY_229	-24.94
ALA_29	-32.8	GLY_96	-23.53	VAL_163	-11.57	TRP_230	-23.54
GLN_30	-65.89	PHE_97	2.23	ALA_164	-26	ASN_231	-45.21
GLU_31	-46.25	MET_98	-10.9	LYS_165	-31.04	MET_232	-23.98
GLN_32	-65.74	PRO_99	-0.4	SER_166	-26.33	LYS_233	-19.05
GLY_33	-31.43	GLN_100	-58.88	ALA_167	-25.53	ASP_234	-61.61
ALA_34	-28.43	THR_101	-14.4	LEU_168	-26.2	ALA_235	-32.97
GLN_35	-54.46	GLY_102	-21.25	GLU_169	-58.98	THR_236	-2.03
LEU_36	-18.9	MET_103	-29.62	SER_170	-20.55	PRO_237	-2.47
VAL_37	-22.91	GLY_104	-31.87	VAL_171	-23.66	VAL_238	-19.25
LEU_38	-24.26	ILE_105	-1.98	ASN_172	-63.65	ALA_239	-31.06
THR_39	-19.48	ASN_106	-42.76	ARG_173	-53.87	LYS_240	-31.34
GLY_40	-22.26	PRO_107	3.18	PHE_174	-10.44	THR_241	-19.75
PHE_41	-6.29	PHE_108	-9.3	VAL_175	-22.82	VAL_242	-17.77
ASP_42	-56.43	PHE_109	-11.27	ALA_176	-27.74	CYS_243	-23.86
ARG_43	-47.71	ASP_110	-58.25	ARG_177	-47.49	ALA_244	-31.54
LEU_44	-20.87	ALA_111	-10.68	GLU_178	-54	LEU_245	-27.63
ARG_45	-44.2	PRO_112	7.16	ALA_179	-33.02	LEU_246	-24.97
LEU_46	-16.01	TYR_113	-21.38	GLY_180	-26.38	SER_247	-24.21
ILE_47	-19.01	ALA_114	-25.21	LYS_181	-30.61	ASP_248	-55.06
GLN_48	-54.64	ASP_115	-65.72	TYR_182	-22.44	TRP_249	-20.92
ARG_49	-42.9	VAL_116	-23.14	GLY_183	-28.04	LEU_250	-0.3
ILE_50	-16.05	SER_117	-18.11	VAL_184	-25.72	PRO_251	8.27
THR_51	-15.39	LYS_118	-29.63	ARG_185	-50.55	ALA_252	-24.79
ASP_52	-53.6	GLY_119	-35.11	SER_186	-24.67	THR_253	-14.68
ARG_53	-52.06	ILE_120	-19.81	ASN_187	-66.8	THR_254	-10.99

Amino Acid	Per residue binding free energy	Amino Acid	Per residue binding free energy	Amino Acid	Per residue binding free energy	Amino Acid	Per residue binding free energy
LEU_54	-7.59	HIS_121	-34.8	LEU_188	-29.7	GLY_255	-24.79
PRO_55	1.67	ILE_122	-19.14	VAL_189	-26.77	ASP_256	-60.83
ALA_56	-20.72	SER_123	-24.48	ALA_190	-27.85	ILE_257	-13.9
LYS_57	-21.15	ALA_124	-29.79	ALA_191	-30.8	ILE_258	-15.58
ALA_58	-9.67	TYR_125	-26.05	GLY_192	-20.57	TYR_259	-20.35
PRO_59	3.79	SER_126	-30.85	PRO_193	-7.02	ALA_260	-16.73
LEU_60	-23.45	TYR_127	-33.1	ILE_194	-15.71	ASP_261	-70.85
LEU_61	-17.42	ALA_128	-28.24	ARG_195	-48.13	GLY_262	-35.01
GLU_62	-47.96	SER_129	-26.08	THR_196	-8.89	GLY_263	-29.24
LEU_63	-16.01	MET_130	-26.02	LEU_197	-6.69	ALA_264	-32.87
ASP_64	-57.74	ALA_131	-29.34	ALA_198	-25.96	HIS_265	-34.28
VAL_65	-20.17	LYS_132	-31.55	MET_199	-32.32	THR_266	-12.3
GLN_66	-55.15	ALA_133	-27.48	SER_200	-16.29	GLN_267	-56.33
ASN_67	-56.63	LEU_134	-23.88	ALA_201	-26.85	LEU_268	-6.36
GLU_68	-53.07	LEU_135	-12.3	ILE_202	-14.77	LEU_269	8.92