

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD052824\
 Data File : VD079049.D
 Acq On : 28 May 2024 15:00
 Operator : RP/MD
 Sample : P2589-19RE
 Misc : 5.18G/10ml/MSVOA_D/SOIL/B
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 BH6D3RE

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM051724SMA.M
 Title : SFAM01.0

Signal : TIC: VD079049.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.646	7	10	13	rBV2	624	713	0.32%	0.052%
2	1.681	13	16	18	rBV2	1224	1321	0.59%	0.096%
3	1.734	18	25	33	rBV	124569	222611	100.00%	16.208%
4	2.275	111	117	124	rBV	27619	42863	19.25%	3.121%
5	2.799	201	206	213	rVB2	25778	48412	21.75%	3.525%
6	3.587	339	340	343	rVB	682	493	0.22%	0.036%
7	3.764	368	370	371	rVB2	654	406	0.18%	0.030%
8	3.822	377	380	382	rBV2	625	663	0.30%	0.048%
9	3.916	387	396	404	rVB2	15561	38373	17.24%	2.794%
10	4.169	435	439	441	rBV	594	516	0.23%	0.038%
11	4.211	443	446	447	rBV	820	564	0.25%	0.041%
12	4.246	451	452	453	rBV	591	399	0.18%	0.029%
13	4.311	460	463	464	rBV	622	607	0.27%	0.044%
14	4.487	489	493	494	rBV	560	514	0.23%	0.037%
15	4.511	496	497	500	rVV	459	448	0.20%	0.033%
16	4.681	523	526	527	rVB	597	534	0.24%	0.039%
17	4.699	527	529	532	rBV2	522	630	0.28%	0.046%
18	4.799	537	546	556	rBV3	6654	18454	8.29%	1.344%
19	4.905	563	564	566	rBV2	891	645	0.29%	0.047%
20	4.952	569	572	574	rVB2	480	551	0.25%	0.040%
21	4.987	576	578	580	rBV	519	459	0.21%	0.033%
22	5.040	584	587	588	rBV2	384	485	0.22%	0.035%
23	5.122	599	601	605	rVB2	571	645	0.29%	0.047%
24	5.181	610	611	614	rBV	496	426	0.19%	0.031%
25	5.310	631	633	636	rVB	952	595	0.27%	0.043%
26	5.334	636	637	640	rBV	481	437	0.20%	0.032%
27	5.452	655	657	660	rVB2	644	592	0.27%	0.043%
28	5.499	660	665	666	rBV2	668	765	0.34%	0.056%
29	5.540	666	672	674	rVB	655	906	0.41%	0.066%
30	5.822	718	720	723	rBV	587	542	0.24%	0.039%
31	5.863	725	727	731	rVB	608	647	0.29%	0.047%
32	5.899	731	733	735	rBV2	455	429	0.19%	0.031%
33	6.052	758	759	763	rBV2	541	683	0.31%	0.050%
34	6.552	841	844	846	rVB	600	655	0.29%	0.048%
35	6.575	846	848	855	rBV	638	774	0.35%	0.056%
36	6.657	858	862	864	rBV	583	854	0.38%	0.062%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD052824\
 Data File : VD079049.D
 Acq On : 28 May 2024 15:00
 Operator : RP/MD
 Sample : P2589-19RE
 Misc : 5.18G/10ml/MSVOA_D/SOIL/B
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 BH6D3RE

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM051724SMA.M
 Title : SFAM01.0

37	6.740	874	876	879	rBV2	459	683	0.31%	0.050%
38	6.852	893	895	897	rBV	413	430	0.19%	0.031%
39	6.922	905	907	908	rBV	604	452	0.20%	0.033%
40	6.987	908	918	926	rVV3	6209	20155	9.05%	1.467%
41	7.063	927	931	941	rVB3	4664	12798	5.75%	0.932%
42	7.157	945	947	948	rBV	545	539	0.24%	0.039%
43	7.334	975	977	979	rBV	393	396	0.18%	0.029%
44	7.404	986	989	991	rBV	570	629	0.28%	0.046%
45	7.452	995	997	1003	rBV2	335	644	0.29%	0.047%
46	7.563	1008	1016	1030	rVB2	24972	67648	30.39%	4.925%
47	7.710	1039	1041	1043	rVB	896	586	0.26%	0.043%
48	7.734	1043	1045	1046	rBV	570	430	0.19%	0.031%
49	8.004	1089	1091	1093	rBV	639	622	0.28%	0.045%
50	8.210	1114	1126	1138	rBV3	44112	146632	65.87%	10.676%
51	8.457	1165	1168	1171	rVB	438	598	0.27%	0.044%
52	8.493	1171	1174	1176	rBV2	343	403	0.18%	0.029%
53	8.775	1215	1222	1232	rBV2	48941	92421	41.52%	6.729%
54	9.210	1287	1296	1305	rBV2	33712	72326	32.49%	5.266%
55	9.322	1313	1315	1316	rVB	724	400	0.18%	0.029%
56	9.357	1319	1321	1324	rBV2	592	719	0.32%	0.052%
57	9.404	1326	1329	1331	rBV2	809	909	0.41%	0.066%
58	9.434	1331	1334	1337	rVB2	538	711	0.32%	0.052%
59	9.498	1343	1345	1347	rVB	1013	719	0.32%	0.052%
60	9.528	1347	1350	1351	rBV	495	632	0.28%	0.046%
61	9.598	1360	1362	1363	rBV	632	475	0.21%	0.035%
62	9.616	1363	1365	1367	rVV	459	426	0.19%	0.031%
63	9.634	1367	1368	1372	rVV	349	428	0.19%	0.031%
64	9.793	1392	1395	1396	rBV	631	450	0.20%	0.033%
65	9.975	1420	1426	1434	rBV	16172	30463	13.68%	2.218%
66	10.122	1448	1451	1454	rBV	584	552	0.25%	0.040%
67	10.269	1470	1476	1485	rVB	49562	87820	39.45%	6.394%
68	10.528	1513	1520	1528	rVB3	12251	20819	9.35%	1.516%
69	10.663	1541	1543	1548	rVB2	2968	3588	1.61%	0.261%
70	10.728	1553	1554	1557	rBV2	577	601	0.27%	0.044%
71	10.875	1573	1579	1588	rBV2	20163	36174	16.25%	2.634%
72	11.028	1602	1605	1611	rBV2	2397	3957	1.78%	0.288%
73	11.104	1616	1618	1621	rVV2	456	492	0.22%	0.036%
74	11.287	1646	1649	1650	rBV	661	650	0.29%	0.047%
75	11.404	1668	1669	1671	rBV2	586	524	0.24%	0.038%
76	11.581	1693	1699	1708	rBV	72878	119049	53.48%	8.668%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD052824\
 Data File : VD079049.D
 Acq On : 28 May 2024 15:00
 Operator : RP/MD
 Sample : P2589-19RE
 Misc : 5.18G/10ml/MSVOA_D/SOIL/B
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 BH6D3RE

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM051724SMA.M
 Title : SFAM01.0

77	11.887	1748	1751	1754	rVB	820	822	0.37%	0.060%
78	11.916	1754	1756	1758	rBV	626	615	0.28%	0.045%
79	12.028	1773	1775	1778	rBV2	459	527	0.24%	0.038%
80	12.122	1790	1791	1794	rBV2	655	427	0.19%	0.031%
81	12.263	1813	1815	1818	rVB	523	442	0.20%	0.032%
82	12.516	1855	1858	1860	rBV2	405	564	0.25%	0.041%
83	12.651	1875	1881	1890	rBV	49717	83958	37.72%	6.113%
84	12.898	1921	1923	1925	rVB2	621	424	0.19%	0.031%
85	13.010	1941	1942	1944	rBV	756	419	0.19%	0.031%
86	13.175	1968	1970	1972	rBV2	541	422	0.19%	0.031%
87	13.434	2011	2014	2015	rBV2	690	759	0.34%	0.055%
88	13.516	2022	2028	2034	rBV	56837	89000	39.98%	6.480%
89	13.745	2064	2067	2070	rBV	884	728	0.33%	0.053%
90	13.816	2072	2079	2085	rBV	41158	68681	30.85%	5.001%
91	13.881	2088	2090	2091	rBV2	717	597	0.27%	0.043%
92	14.310	2161	2163	2165	rVB2	749	516	0.23%	0.038%
93	14.334	2165	2167	2170	rVB2	689	708	0.32%	0.052%
94	14.369	2171	2173	2178	rBV2	582	686	0.31%	0.050%
95	14.445	2184	2186	2188	rBV2	617	542	0.24%	0.039%
96	14.492	2190	2194	2197	rVB2	668	815	0.37%	0.059%
97	14.916	2264	2266	2267	rBV2	854	565	0.25%	0.041%
98	15.210	2314	2316	2317	rBV2	582	485	0.22%	0.035%
99	15.328	2334	2336	2338	rBV2	744	784	0.35%	0.057%
100	15.875	2427	2429	2432	rBV	1437	1397	0.63%	0.102%

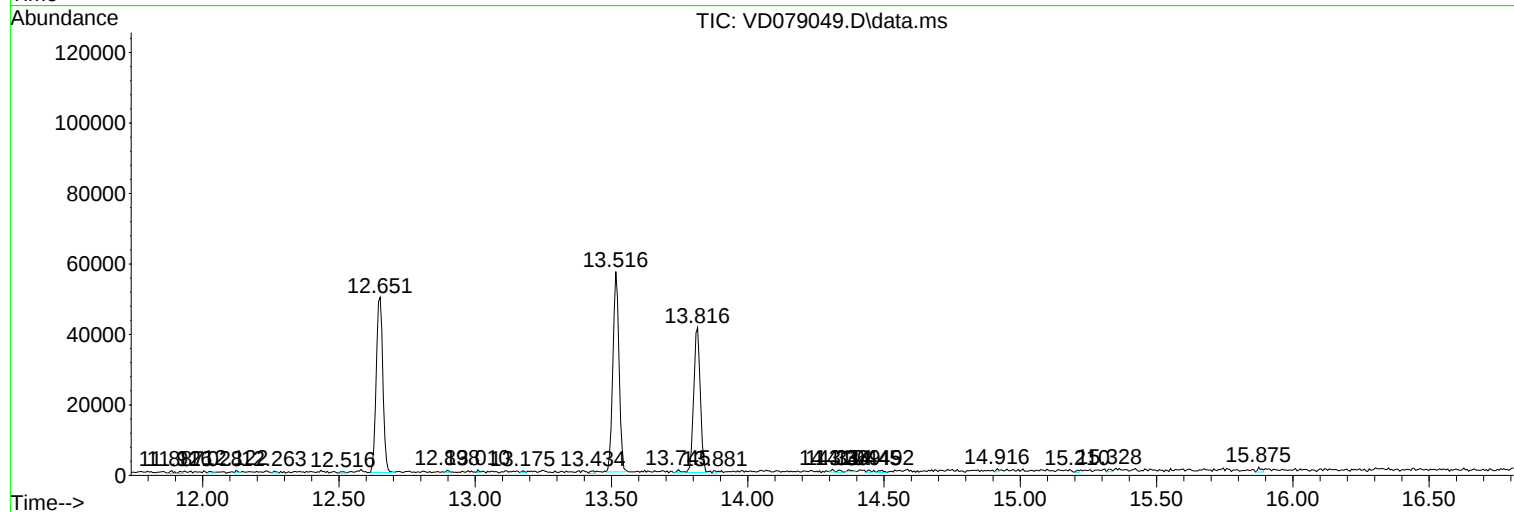
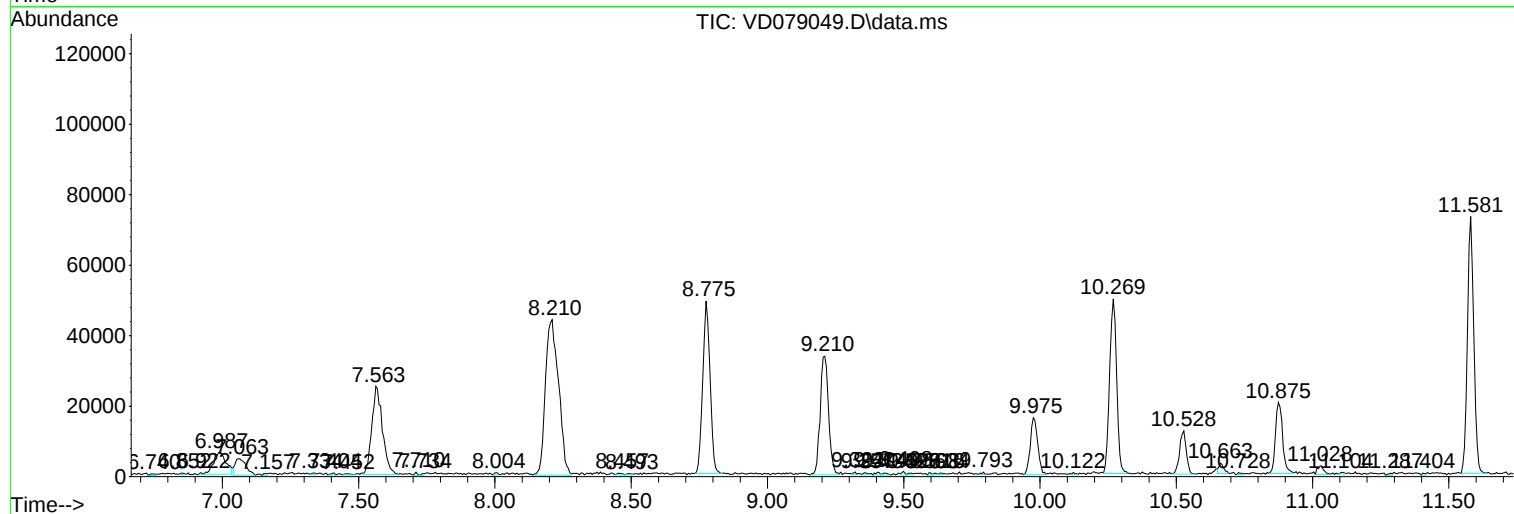
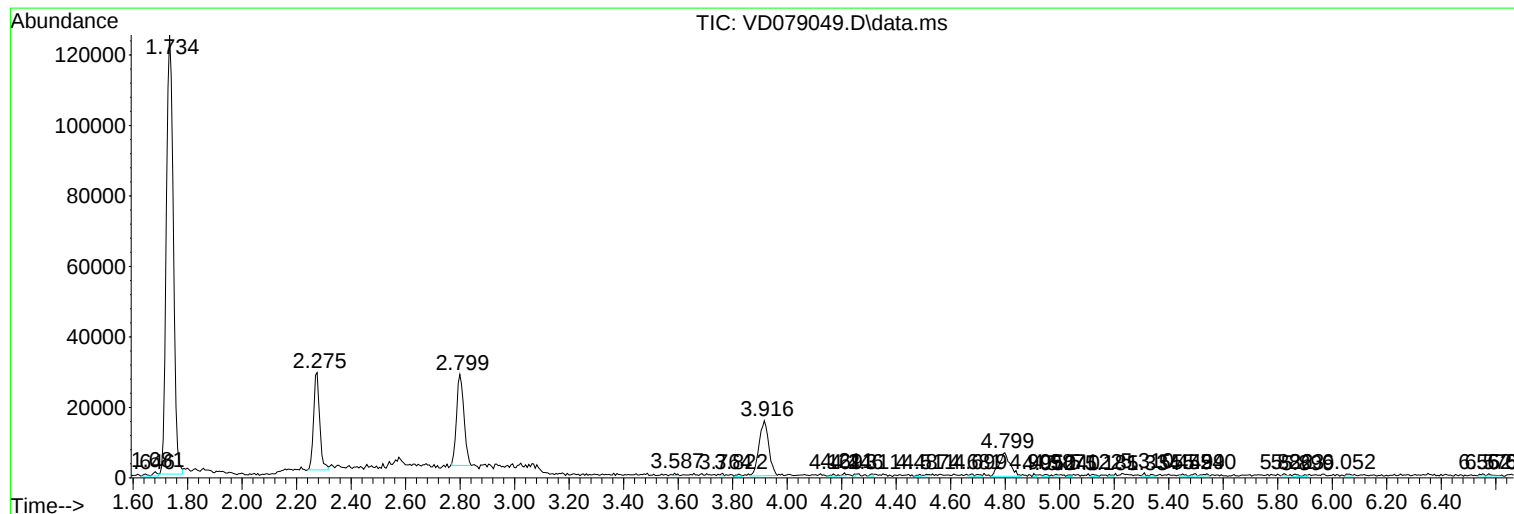
Sum of corrected areas: 1373444

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD052824\
Data File : VD079049.D
Acq On : 28 May 2024 15:00
Operator : RP/MD
Sample : P2589-19RE
Misc : 5.18G/10ml/MSVOA_D/SOIL/B
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
BH6D3RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM051724SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD052824\
Data File : VD079049.D
Acq On : 28 May 2024 15:00
Operator : RP/MD
Sample : P2589-19RE
Misc : 5.18G/10ml/MSVOA_D/SOIL/B
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
BH6D3RE

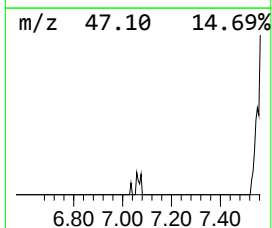
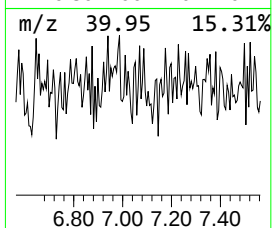
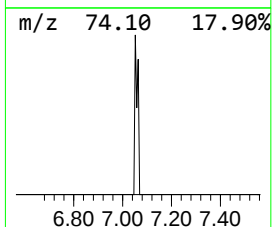
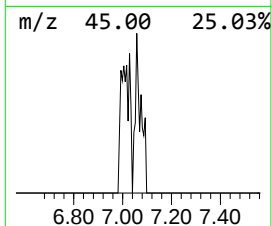
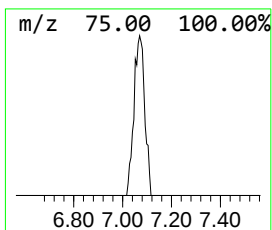
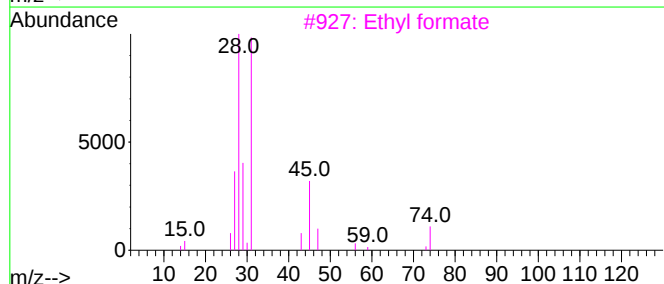
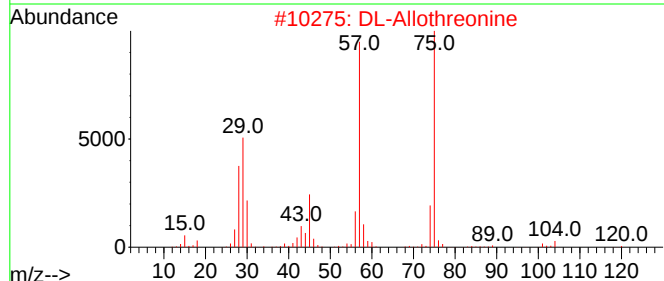
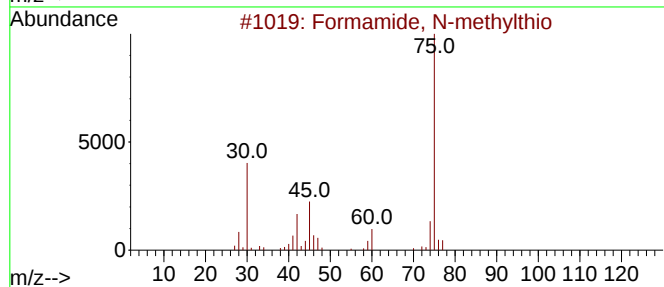
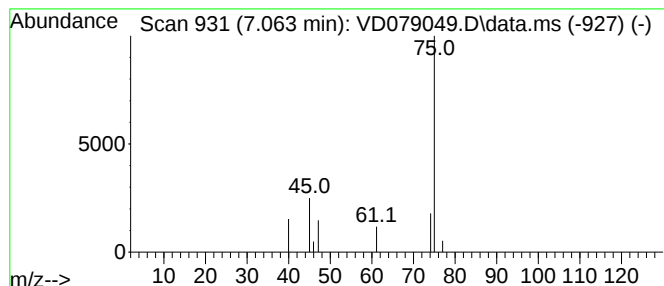
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM051724SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.063	3.46 ug/L	12798	1,4-Difluorobenzene	8.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formamide, N-methylthio	75	C2H5NS	018952-41-5	9
2			DL-Allothreonine	119	C4H9NO3	000144-98-9	9
3			Ethyl formate	74	C3H6O2	000109-94-4	5
4			Ethanethioamide	75	C2H5NS	000062-55-5	5
5			Mercaptamine	77	C2H7NS	000060-23-1	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD052824\
Data File : VD079049.D
Acq On : 28 May 2024 15:00
Operator : RP/MD
Sample : P2589-19RE
Misc : 5.18G/10ml/MSVOA_D/SOIL/B
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
BH6D3RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM051724SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	7.063	3.5	ug/L	12798	1	8.775	92421	25.0