

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
 Data File : VX039389.D
 Acq On : 20 Dec 2023 10:09
 Operator : JC/MD
 Sample : 05807-05
 Misc : 3.19g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AX7

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_X\Method\SFAMXML120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039389.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.373	43	47	58	rBV	45222	73891	11.26%	1.637%
2	2.288	191	197	210	rVB	105954	168176	25.63%	3.726%
3	2.404	212	216	223	rVB4	1693	3535	0.54%	0.078%
4	2.715	262	267	274	rBV2	3938	8392	1.28%	0.186%
5	2.775	274	277	281	rVV4	1771	3442	0.52%	0.076%
6	2.849	283	289	298	rVV	36888	74526	11.36%	1.651%
7	2.940	298	304	317	rVB	7987	18959	2.89%	0.420%
8	3.239	352	353	355	rBV	280	193	0.03%	0.004%
9	3.336	367	369	374	rVB2	313	354	0.05%	0.008%
10	3.446	383	387	392	rVB3	248	420	0.06%	0.009%
11	3.501	395	396	400	rVB	368	331	0.05%	0.007%
12	3.544	400	403	404	rBV2	193	257	0.04%	0.006%
13	3.574	406	408	409	rBV	213	197	0.03%	0.004%
14	3.769	438	440	443	rBV	205	189	0.03%	0.004%
15	3.867	454	456	459	rBV	147	218	0.03%	0.005%
16	4.123	496	498	501	rVB	272	236	0.04%	0.005%
17	4.239	515	517	520	rBV2	185	198	0.03%	0.004%
18	4.482	547	557	587	rBV2	40031	184214	28.08%	4.082%
19	4.915	626	628	630	rVB	367	277	0.04%	0.006%
20	4.964	633	636	639	rVB	302	307	0.05%	0.007%
21	5.056	639	651	668	rBV	76502	262886	40.07%	5.825%
22	5.232	677	680	682	rVB2	203	207	0.03%	0.005%
23	5.342	696	698	701	rBV2	189	234	0.04%	0.005%
24	5.385	702	705	706	rBV	320	272	0.04%	0.006%
25	5.543	729	731	732	rBV2	296	269	0.04%	0.006%
26	5.964	789	800	815	rBV2	221935	656141	100.00%	14.539%
27	6.159	830	832	838	rVB2	302	358	0.05%	0.008%
28	6.263	845	849	852	rVB2	176	224	0.03%	0.005%
29	6.409	870	873	874	rVB	263	244	0.04%	0.005%
30	6.458	876	881	882	rBV2	347	363	0.06%	0.008%
31	6.622	906	908	911	rVB2	233	199	0.03%	0.004%
32	6.756	920	930	945	rBV	126125	322306	49.12%	7.142%
33	7.006	969	971	973	rBV	233	213	0.03%	0.005%
34	7.031	973	975	977	rBV	207	183	0.03%	0.004%
35	7.110	984	988	999	rVB5	1142	2431	0.37%	0.054%
36	7.305	1011	1020	1037	rBV	134364	309233	47.13%	6.852%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
 Data File : VX039389.D
 Acq On : 20 Dec 2023 10:09
 Operator : JC/MD
 Sample : 05807-05
 Misc : 3.19g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AX7

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_X\Method\SFAMXML120523WMA.M
 Title : VOC Analysis

37	8.323	1181	1187	1201	rVV	78401	139399	21.25%	3.089%
38	8.439	1204	1206	1208	rVV2	412	352	0.05%	0.008%
39	8.500	1211	1216	1219	rBV2	313	625	0.10%	0.014%
40	8.585	1227	1230	1231	rBV2	276	268	0.04%	0.006%
41	8.646	1231	1240	1254	rBV	249902	409680	62.44%	9.078%
42	8.854	1271	1274	1276	rBV3	202	221	0.03%	0.005%
43	8.909	1280	1283	1285	rBV2	291	294	0.04%	0.007%
44	8.951	1285	1290	1306	rBV	53525	92883	14.16%	2.058%
45	9.085	1311	1312	1314	rBV2	255	183	0.03%	0.004%
46	9.201	1327	1331	1332	rVB2	252	291	0.04%	0.006%
47	9.274	1338	1343	1347	rVB3	1254	1736	0.26%	0.038%
48	9.402	1357	1364	1377	rBV	210236	417289	63.60%	9.246%
49	9.658	1404	1406	1407	rVB2	327	190	0.03%	0.004%
50	9.713	1411	1415	1420	rVB3	2051	3494	0.53%	0.077%
51	9.793	1426	1428	1431	rVB2	285	198	0.03%	0.004%
52	9.890	1441	1444	1447	rBV2	250	342	0.05%	0.008%
53	10.055	1465	1471	1473	rBV	246417	356569	54.34%	7.901%
54	10.396	1524	1527	1530	rBV2	180	256	0.04%	0.006%
55	10.518	1545	1547	1551	rVB	204	189	0.03%	0.004%
56	10.640	1565	1567	1568	rBV	341	263	0.04%	0.006%
57	10.658	1568	1570	1574	rVV2	397	383	0.06%	0.008%
58	10.719	1576	1580	1582	rBV	185	188	0.03%	0.004%
59	10.762	1585	1587	1590	rVB2	204	201	0.03%	0.004%
60	11.091	1638	1641	1646	rVB2	321	495	0.08%	0.011%
61	11.195	1652	1658	1668	rVV	248602	330508	50.37%	7.323%
62	11.311	1673	1677	1682	rVB2	759	1116	0.17%	0.025%
63	11.439	1696	1698	1699	rBV	252	189	0.03%	0.004%
64	11.481	1702	1705	1708	rVB2	525	549	0.08%	0.012%
65	11.609	1722	1726	1727	rBV2	178	182	0.03%	0.004%
66	11.762	1747	1751	1755	rVB2	414	658	0.10%	0.015%
67	11.884	1767	1771	1772	rBV	190	199	0.03%	0.004%
68	11.945	1778	1781	1783	rBV2	226	194	0.03%	0.004%
69	11.975	1783	1786	1789	rBV4	879	1226	0.19%	0.027%
70	12.024	1789	1794	1803	rBV	243787	308280	46.98%	6.831%
71	12.176	1816	1819	1823	rVB2	255	348	0.05%	0.008%
72	12.323	1837	1843	1856	rBV	254336	330717	50.40%	7.328%
73	12.444	1862	1863	1866	rBV2	246	245	0.04%	0.005%
74	12.761	1909	1915	1921	rBV3	2468	3573	0.54%	0.079%
75	12.883	1933	1935	1937	rBV2	389	361	0.06%	0.008%
76	13.115	1970	1973	1976	rBV3	448	548	0.08%	0.012%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
 Data File : VX039389.D
 Acq On : 20 Dec 2023 10:09
 Operator : JC/MD
 Sample : 05807-05
 Misc : 3.19g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AX7

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_X\Method\SFAMXLM120523WMA.M
 Title : VOC Analysis

77	13.536	2040	2042	2045	rVB2	229	227	0.03%	0.005%
78	13.591	2048	2051	2056	rBV3	978	1049	0.16%	0.023%
79	13.731	2070	2074	2077	rBV2	156	251	0.04%	0.006%
80	13.786	2079	2083	2089	rVB3	445	827	0.13%	0.018%
81	13.865	2095	2096	2099	rVB2	335	218	0.03%	0.005%
82	13.962	2110	2112	2115	rVB	610	512	0.08%	0.011%
83	14.127	2134	2139	2144	rBV	3051	4247	0.65%	0.094%
84	14.505	2198	2201	2203	rBV3	341	416	0.06%	0.009%
85	14.603	2215	2217	2219	rVV2	214	188	0.03%	0.004%
86	14.779	2242	2246	2249	rVV	222	270	0.04%	0.006%
87	14.883	2262	2263	2265	rBV	419	243	0.04%	0.005%
88	15.151	2305	2307	2308	rBV2	283	208	0.03%	0.005%
89	15.304	2330	2332	2335	rVB2	332	391	0.06%	0.009%
90	15.383	2342	2345	2350	rVB3	1297	2026	0.31%	0.045%
91	15.493	2361	2363	2364	rBV	289	180	0.03%	0.004%
92	15.578	2375	2377	2380	rBV2	275	263	0.04%	0.006%
93	15.657	2387	2390	2392	rBV3	295	373	0.06%	0.008%
94	15.718	2398	2400	2403	rBV2	224	199	0.03%	0.004%
95	15.804	2410	2414	2417	rBV	262	359	0.05%	0.008%
96	16.200	2478	2479	2481	rBV2	283	229	0.03%	0.005%
97	16.249	2486	2487	2490	rBV2	310	303	0.05%	0.007%
98	16.395	2509	2511	2514	rBV3	327	442	0.07%	0.010%
99	16.566	2537	2539	2540	rBV	369	284	0.04%	0.006%
100	16.694	2558	2560	2563	rBV3	336	458	0.07%	0.010%

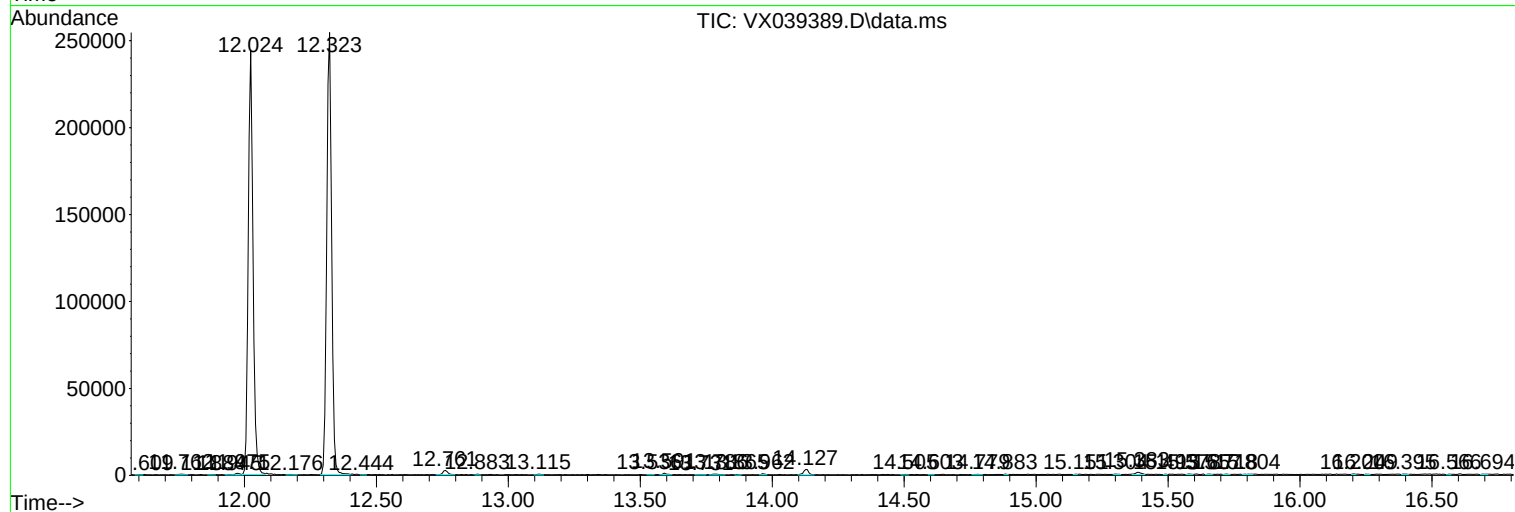
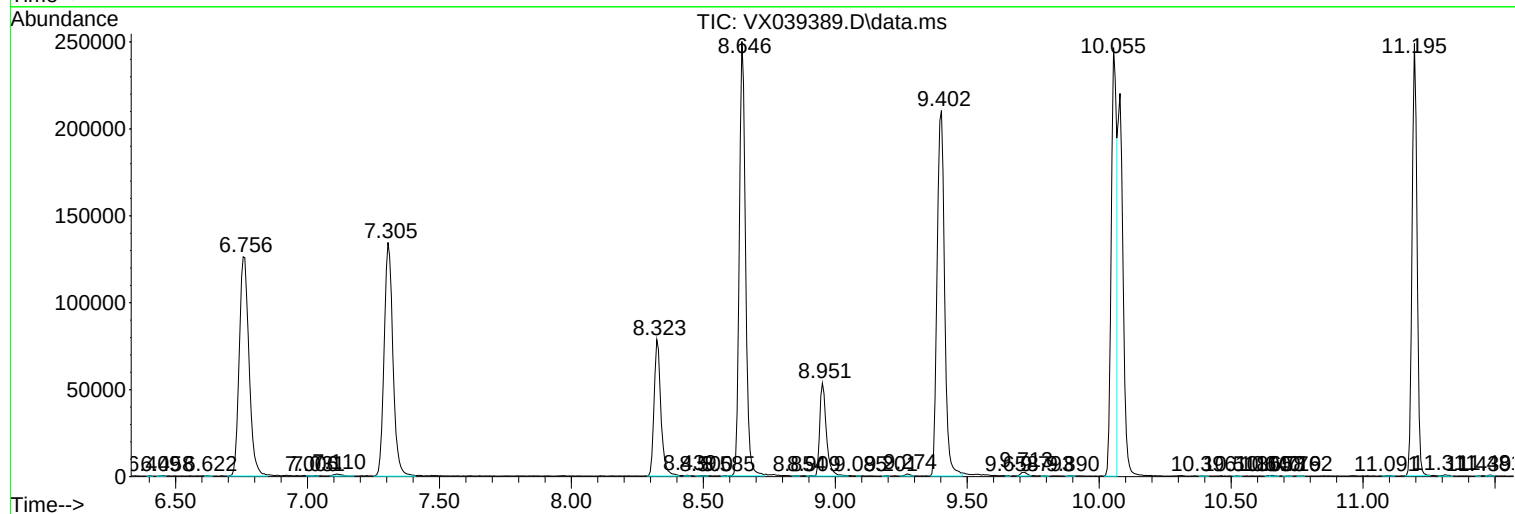
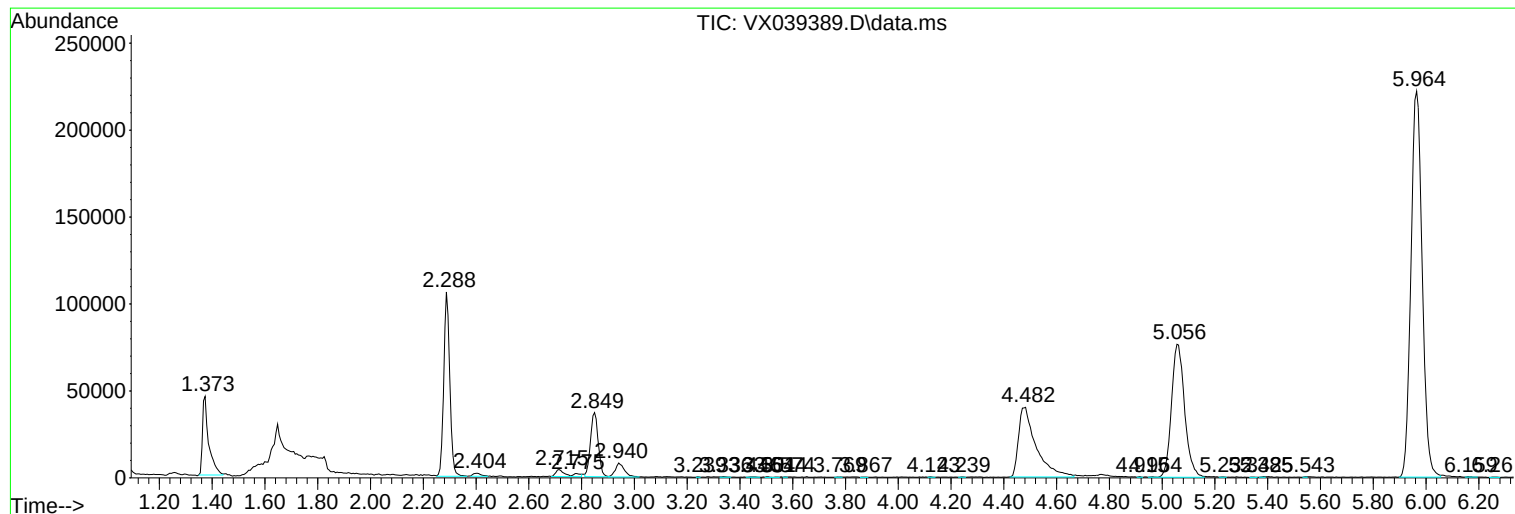
Sum of corrected areas: 4513120

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
Data File : VX039389.D
Acq On : 20 Dec 2023 10:09
Operator : JC/MD
Sample : 05807-05
Misc : 3.19g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AX7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
Data File : VX039389.D
Acq On : 20 Dec 2023 10:09
Operator : JC/MD
Sample : 05807-05
Misc : 3.19g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

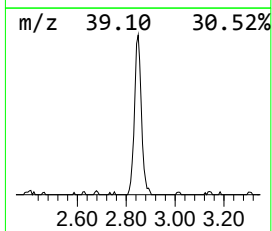
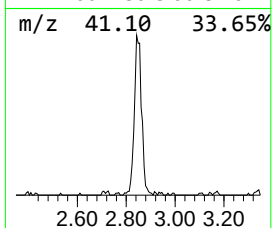
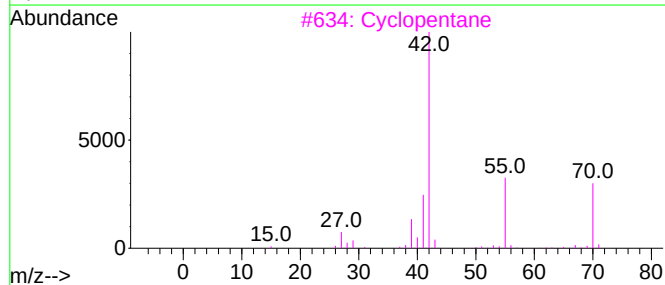
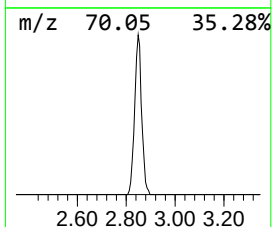
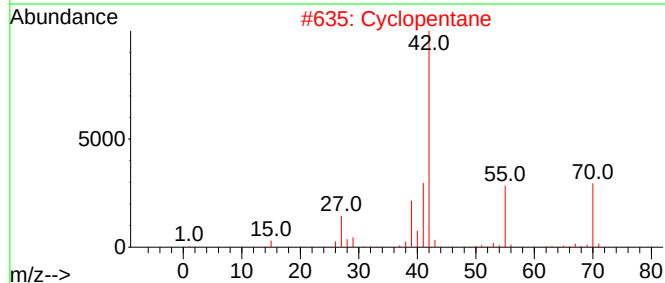
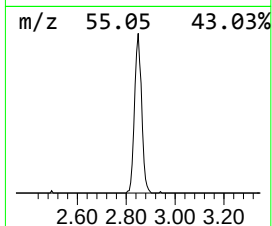
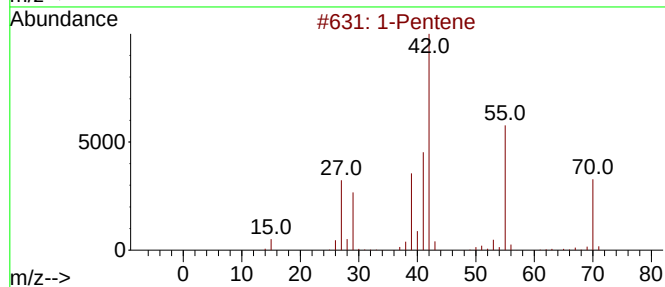
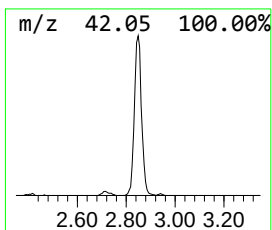
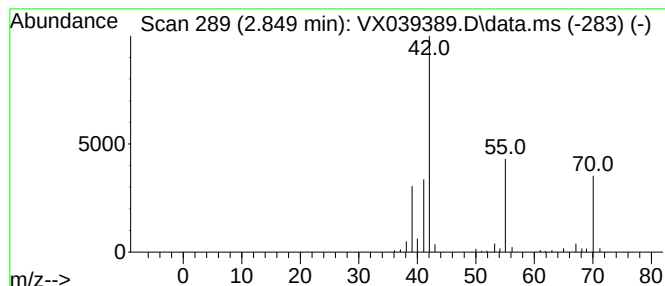
Instrument :
MSVOA_X
ClientSampleId :
C0AX7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.849	11.56 ug/L	74526	1,4-Difluorobenzene	6.763	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	91
2	Cyclopentane	70	C5H10	000287-92-3	90
3	Cyclopentane	70	C5H10	000287-92-3	78
4	Cyclopentane	70	C5H10	000287-92-3	72
5	1-Pentene	70	C5H10	000109-67-1	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
Data File : VX039389.D
Acq On : 20 Dec 2023 10:09
Operator : JC/MD
Sample : 05807-05
Misc : 3.19g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AX7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	2.849	11.6	ug/L	74526	1	6.763	322306	50.0