

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081523\
 Data File : VY015127.D
 Acq On : 16 Aug 2023 01:19
 Operator : SY/MD
 Sample : 03973-01
 Misc : 5.02g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SB-01-14.5-15.0

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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_Y\methods\82Y081423S.M
 Title : SW846 8260

Signal : TIC: VY015127.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.125	43	50	51	rBV2	1193	1941	2.63%	0.820%
2	2.320	79	82	84	rBV3	699	1030	1.40%	0.435%
3	2.668	136	139	146	rVB4	645	1405	1.90%	0.594%
4	7.722	962	968	973	rVB3	913	1750	2.37%	0.739%
5	7.795	973	980	988	rBV2	3884	8680	11.76%	3.668%
6	8.142	1032	1037	1044	rVB5	1871	4593	6.22%	1.941%
7	8.697	1121	1128	1136	rBV	5333	9916	13.43%	4.190%
8	10.185	1365	1372	1377	rBV	8231	14543	19.70%	6.145%
9	10.483	1416	1421	1425	rBV3	427	777	1.05%	0.328%
10	10.800	1470	1473	1475	rBV3	683	939	1.27%	0.397%
11	11.276	1546	1551	1557	rBV6	456	1097	1.49%	0.464%
12	11.416	1572	1574	1577	rVB3	1056	1025	1.39%	0.433%
13	11.453	1577	1580	1582	rBV3	929	1200	1.63%	0.507%
14	11.495	1582	1587	1592	rBV2	7884	13178	17.85%	5.568%
15	11.880	1646	1650	1652	rBV4	536	852	1.15%	0.360%
16	11.983	1663	1667	1669	rVB5	673	819	1.11%	0.346%
17	12.111	1669	1688	1690	rBV8	7090	24234	32.82%	10.240%
18	12.319	1720	1722	1724	rBV3	932	1000	1.35%	0.423%
19	12.422	1738	1739	1742	rBV3	896	1000	1.35%	0.423%
20	12.483	1745	1749	1753	rBV4	6569	10795	14.62%	4.561%
21	12.812	1801	1803	1805	rBV3	1184	1071	1.45%	0.453%
22	12.916	1818	1820	1824	rVB4	1962	2140	2.90%	0.904%
23	12.959	1824	1827	1828	rBV3	1095	1334	1.81%	0.564%
24	12.983	1829	1831	1833	rVV2	1313	946	1.28%	0.400%
25	13.081	1845	1847	1849	rBV3	1048	1236	1.67%	0.522%
26	13.148	1856	1858	1859	rBV2	1151	806	1.09%	0.341%
27	13.190	1860	1865	1866	rBV5	5029	6838	9.26%	2.889%
28	13.361	1891	1893	1894	rBV2	1840	1683	2.28%	0.711%
29	13.422	1894	1903	1918	rVB7	20614	73834	100.00%	31.198%
30	13.629	1927	1937	1938	rBV8	6014	15115	20.47%	6.387%
31	13.763	1952	1959	1964	rBV9	6378	19103	25.87%	8.072%
32	14.532	2083	2085	2086	rBV2	1707	960	1.30%	0.406%
33	14.617	2097	2099	2101	rBV2	1961	1601	2.17%	0.677%
34	14.934	2150	2151	2153	rBV2	2082	2096	2.84%	0.886%
35	15.129	2181	2183	2187	rBV5	2234	2396	3.25%	1.012%
36	15.330	2214	2216	2217	rBV2	2852	2210	2.99%	0.934%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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

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37	16.537	2411	2414	2417	rBV4	1413	1604	2.17%	0.678%
38	16.610	2424	2426	2427	rBV2	1028	912	1.24%	0.385%

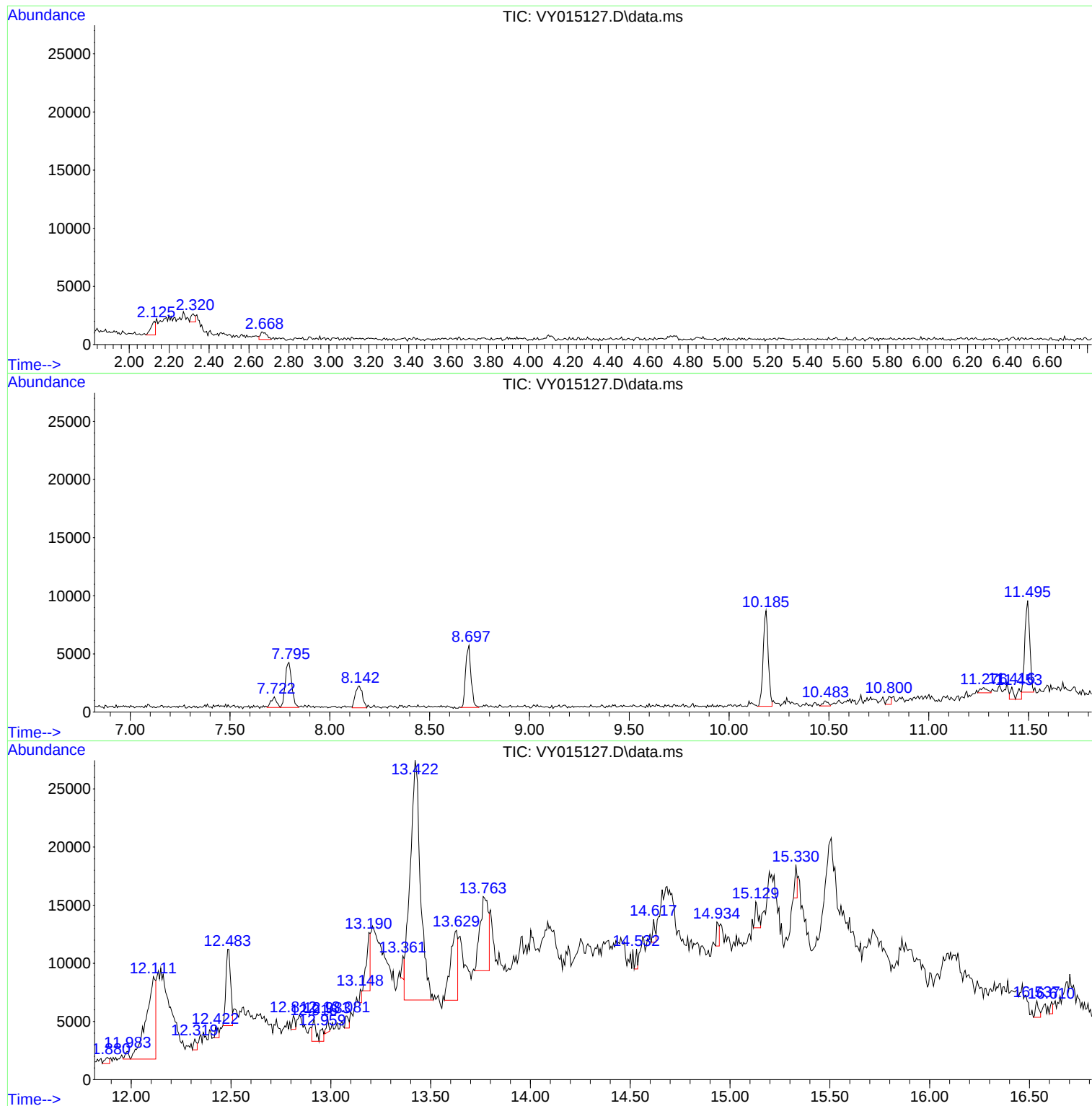
Sum of corrected areas: 236659

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081423S.M
Quant Title : SW846 8260

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



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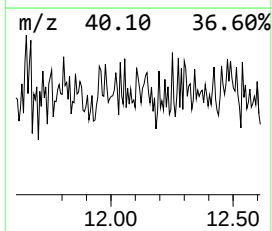
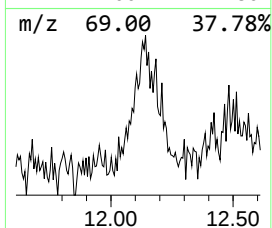
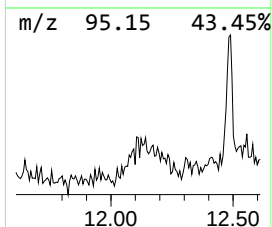
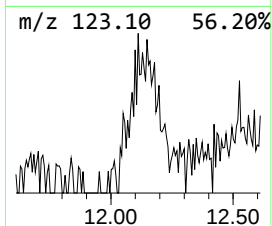
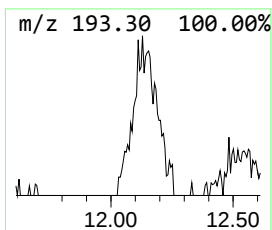
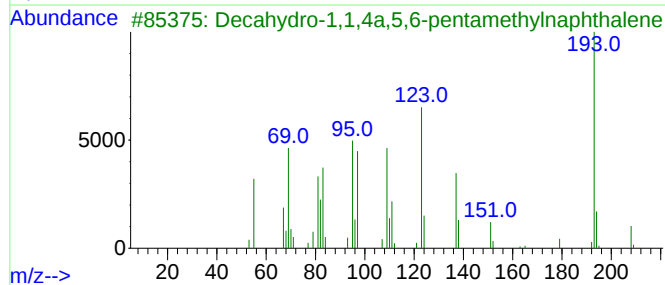
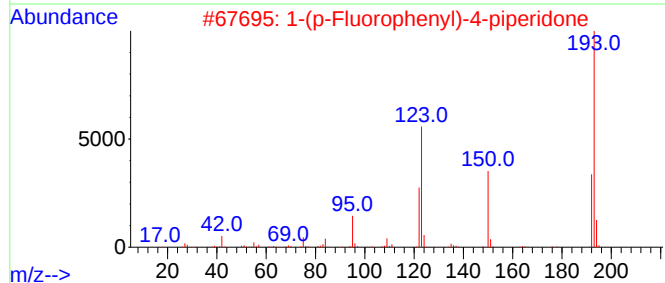
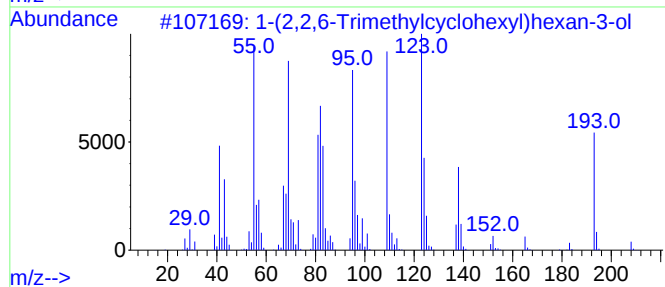
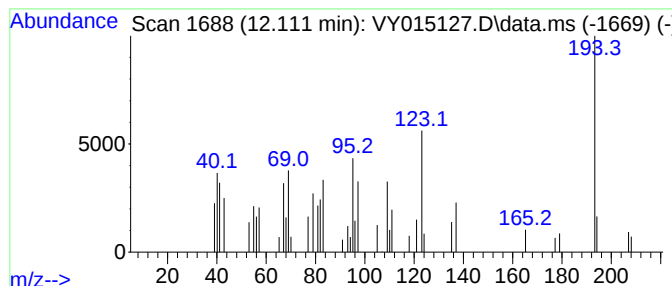
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Peak Number 4 unknown12.111 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.111	91.95 ug/l	24234	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(2,2,6-Trimethylcyclohexyl)hex...	226	C15H30O	070788-30-6	53
2			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	49
3			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	49
4			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	40
5			4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	35



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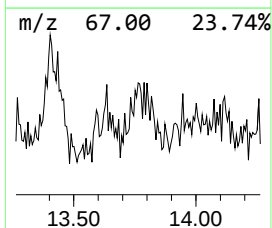
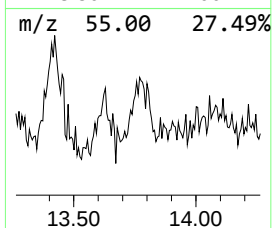
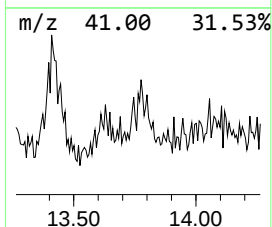
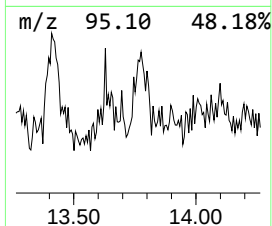
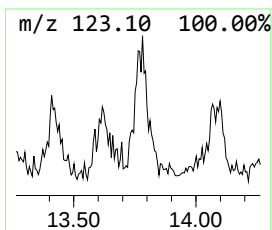
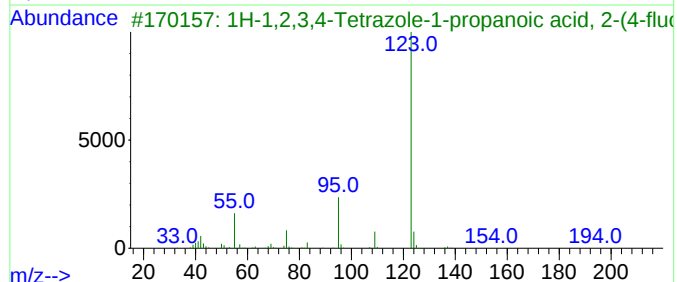
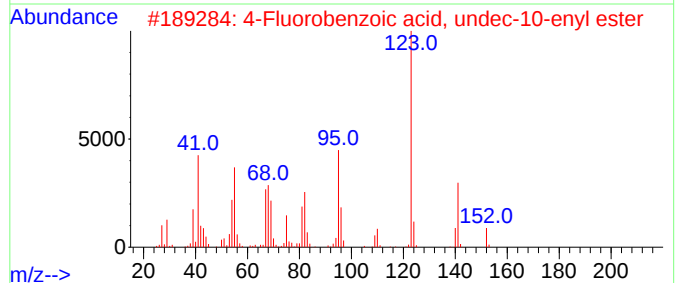
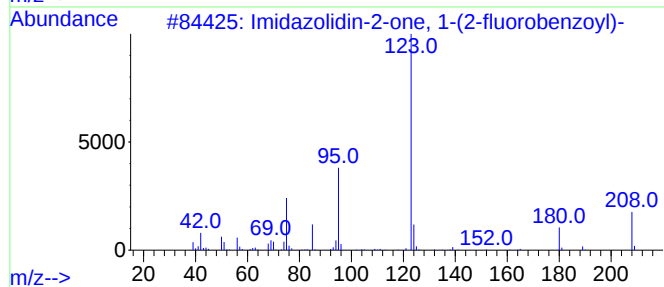
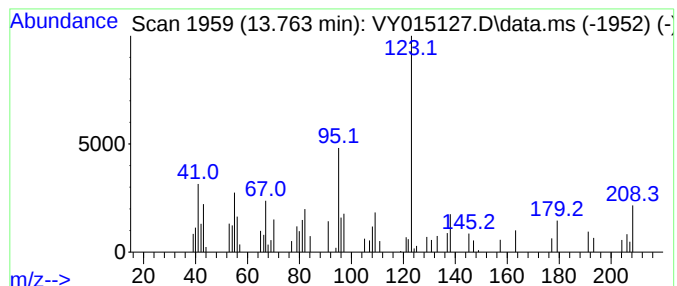
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Peak Number 6 Imidazolidin-2-one, 1-(2-fl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.763	12.94 ug/l	19103	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Imidazolidin-2-one, 1-(2-fluorob...	208	C10H9FN2O2	1010310-62-2	50
2			4-Fluorobenzoic acid, undec-10-e...	292	C18H25FO2	1000279-02-8	47
3			1H-1,2,3,4-Tetrazole-1-propanoic...	278	C12H11FN4O3	1010350-19-5	47
4			Ethanone, 1-(4-fluorophenyl)-	138	C8H7FO	000403-42-9	47
5			1,4-Hexadiene, 2,3,4,5-tetramethyl-	138	C10H18	051504-54-2	46



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown12.111	12.111	92.0	ug/l	24234	3	11.496	13178	50.0
Imidazolidin-2-...	13.763	12.9	ug/l	19103	4	13.434	73834	50.0