

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082323\
 Data File : VY015292.D
 Acq On : 23 Aug 2023 19:43
 Operator : SY/MD
 Sample : 04119-03
 Misc : 5.05g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 RB21153

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: VY015292.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.991	26	28	31	rBV2	416	404	1.46%	0.292%
2	2.040	34	36	38	rBV	383	359	1.29%	0.259%
3	2.113	43	48	51	rBV4	1141	2410	8.68%	1.740%
4	2.211	62	64	66	rBV2	795	871	3.14%	0.629%
5	2.662	134	138	139	rBV2	627	628	2.26%	0.453%
6	3.509	275	277	281	rBV2	253	390	1.40%	0.282%
7	4.704	468	473	476	rBV5	776	1422	5.12%	1.027%
8	4.979	516	518	522	rBV2	272	289	1.04%	0.209%
9	5.162	545	548	552	rVB2	276	506	1.82%	0.365%
10	5.753	638	645	651	rVB4	750	1796	6.47%	1.297%
11	6.960	835	843	856	rBV2	2149	7144	25.73%	5.157%
12	7.173	876	878	882	rVB	280	321	1.16%	0.232%
13	7.692	961	963	964	rBV	436	363	1.31%	0.262%
14	7.783	972	978	982	rBV5	1476	3247	11.70%	2.344%
15	7.874	991	993	997	rVB2	229	318	1.15%	0.230%
16	7.917	997	1000	1003	rBV	276	490	1.76%	0.354%
17	8.143	1026	1037	1045	rBV4	1596	3919	14.12%	2.829%
18	8.691	1120	1127	1135	rBV2	2660	4835	17.42%	3.490%
19	9.472	1252	1255	1260	rVB	245	328	1.18%	0.237%
20	9.831	1311	1314	1315	rBV	304	313	1.13%	0.226%
21	9.917	1326	1328	1330	rVB2	370	304	1.09%	0.219%
22	9.966	1332	1336	1337	rBV2	372	432	1.56%	0.312%
23	10.075	1349	1354	1357	rBV3	435	714	2.57%	0.515%
24	10.179	1366	1371	1378	rVB2	5401	9080	32.71%	6.555%
25	10.234	1378	1380	1381	rBV2	440	419	1.51%	0.302%
26	10.380	1402	1404	1405	rBV2	598	343	1.24%	0.248%
27	10.398	1405	1407	1409	rVV3	475	358	1.29%	0.258%
28	10.429	1410	1412	1417	rVB3	481	454	1.64%	0.328%
29	10.508	1423	1425	1427	rBV	601	426	1.53%	0.308%
30	10.526	1427	1428	1430	rBV	528	408	1.47%	0.295%
31	10.557	1430	1433	1436	rVV4	376	575	2.07%	0.415%
32	10.612	1439	1442	1443	rBV	519	545	1.96%	0.393%
33	10.685	1453	1454	1456	rBV	379	320	1.15%	0.231%
34	10.856	1480	1482	1484	rBV2	522	655	2.36%	0.473%
35	10.880	1484	1486	1488	rVB	610	392	1.41%	0.283%
36	10.965	1498	1500	1504	rVB3	406	431	1.55%	0.311%

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37	11.002	1504	1506	1508	rVB3	431	293	1.06%	0.212%
38	11.026	1508	1510	1513	rBV2	720	859	3.09%	0.620%
39	11.167	1531	1533	1538	rVB4	620	958	3.45%	0.692%
40	11.209	1538	1540	1541	rBV2	614	478	1.72%	0.345%
41	11.270	1548	1550	1551	rBV2	657	444	1.60%	0.321%
42	11.282	1551	1552	1554	rVB2	799	621	2.24%	0.448%
43	11.392	1569	1570	1571	rBV	821	475	1.71%	0.343%
44	11.496	1581	1587	1592	rBV	5701	9531	34.33%	6.880%
45	11.605	1602	1605	1609	rBV5	618	1038	3.74%	0.749%
46	11.782	1632	1634	1637	rBV3	569	706	2.54%	0.510%
47	11.855	1645	1646	1648	rBV3	916	613	2.21%	0.443%
48	11.874	1648	1649	1651	rVB2	615	349	1.26%	0.252%
49	11.965	1662	1664	1668	rVB5	447	379	1.37%	0.274%
50	12.014	1668	1672	1673	rBV4	670	836	3.01%	0.603%
51	12.118	1681	1689	1690	rBV5	2911	6118	22.04%	4.416%
52	12.483	1745	1749	1753	rBV4	5421	7978	28.74%	5.759%
53	12.746	1791	1792	1794	rBV2	673	575	2.07%	0.415%
54	12.855	1808	1810	1813	rBV4	512	656	2.36%	0.474%
55	12.886	1813	1815	1818	rVV3	571	504	1.82%	0.364%
56	13.130	1853	1855	1856	rBV2	845	785	2.83%	0.567%
57	13.428	1894	1904	1916	rVB8	10118	27763	100.00%	20.042%
58	13.745	1953	1956	1963	rBV6	2911	7031	25.33%	5.076%
59	13.873	1975	1977	1978	rVB2	758	336	1.21%	0.243%
60	13.898	1978	1981	1982	rBV2	747	734	2.64%	0.530%
61	13.910	1982	1983	1984	rVV	1080	505	1.82%	0.365%
62	13.947	1987	1989	1990	rBV2	527	358	1.29%	0.258%
63	14.075	2008	2010	2011	rVB2	925	562	2.02%	0.406%
64	14.136	2018	2020	2025	rVB4	629	1008	3.63%	0.728%
65	14.227	2033	2035	2037	rBV2	656	777	2.80%	0.561%
66	14.318	2047	2050	2053	rBV5	1015	1598	5.76%	1.154%
67	14.611	2095	2098	2102	rVB3	2315	2600	9.36%	1.877%
68	14.678	2107	2109	2114	rVB5	1689	2531	9.12%	1.827%
69	14.721	2114	2116	2117	rBV2	619	362	1.30%	0.261%
70	14.824	2131	2133	2134	rBV2	579	522	1.88%	0.377%
71	14.873	2139	2141	2145	rVB4	903	930	3.35%	0.671%
72	14.989	2158	2160	2161	rBV	577	344	1.24%	0.248%
73	15.215	2192	2197	2199	rBV6	760	1255	4.52%	0.906%
74	15.276	2204	2207	2209	rVB4	617	723	2.60%	0.522%
75	15.300	2209	2211	2212	rBV2	518	284	1.02%	0.205%
76	15.349	2218	2219	2221	rVB2	1163	593	2.14%	0.428%

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77	15.519	2245	2247	2250	rVB3	843	870	3.13%	0.628%
78	15.550	2250	2252	2257	rBV4	630	747	2.69%	0.539%
79	15.586	2257	2258	2261	rBV3	656	567	2.04%	0.409%
80	15.733	2278	2282	2286	rVV5	1176	1768	6.37%	1.276%
81	15.763	2286	2287	2289	rVB2	631	390	1.40%	0.282%
82	15.983	2321	2323	2327	rBV4	354	566	2.04%	0.409%
83	16.019	2327	2329	2330	rBV	766	549	1.98%	0.396%
84	16.160	2350	2352	2354	rVB3	744	595	2.14%	0.430%
85	16.361	2383	2385	2388	rVB3	435	447	1.61%	0.323%
86	16.385	2388	2389	2392	rVB2	500	297	1.07%	0.214%
87	16.513	2407	2410	2411	rBV	445	509	1.83%	0.367%

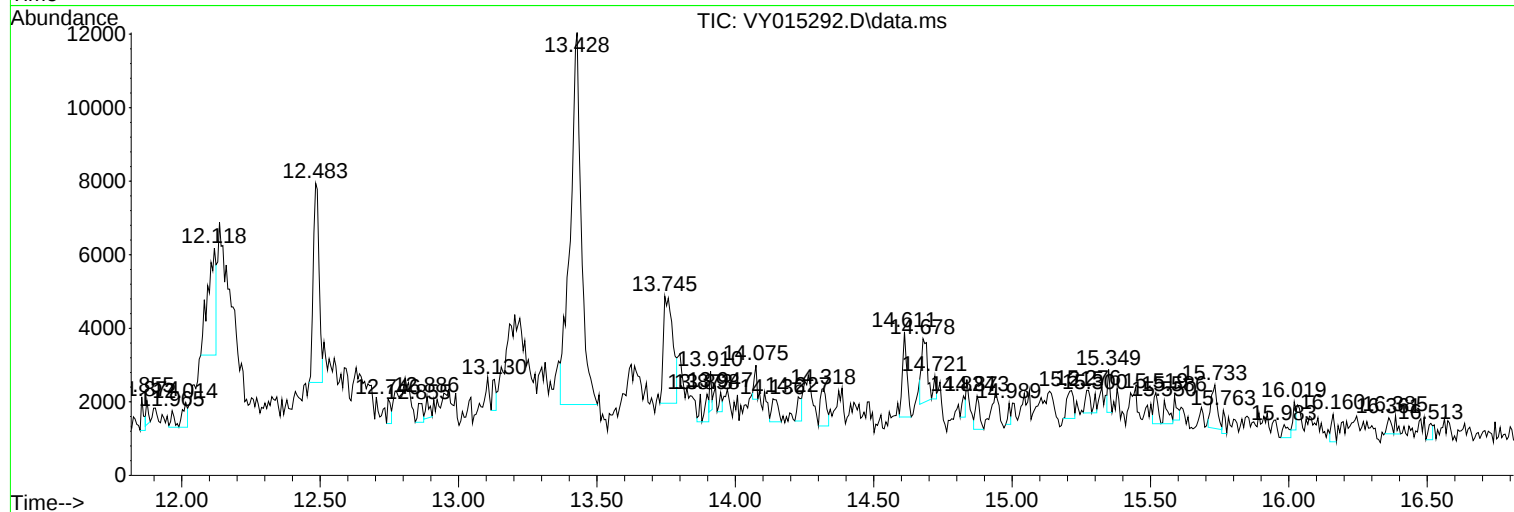
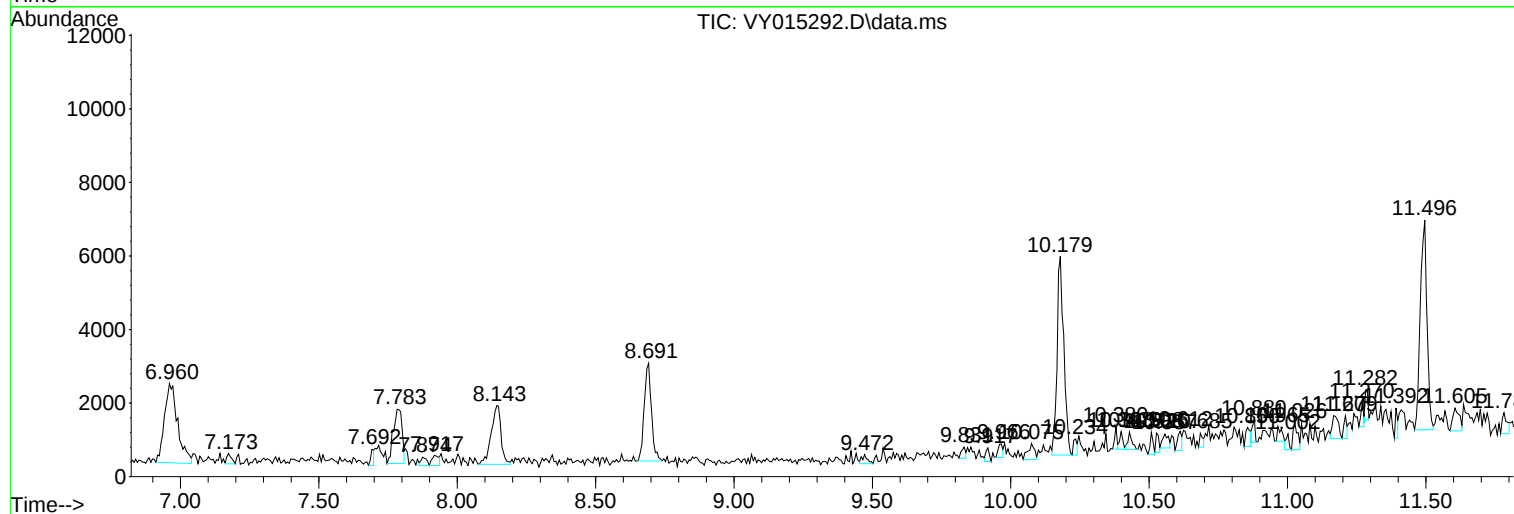
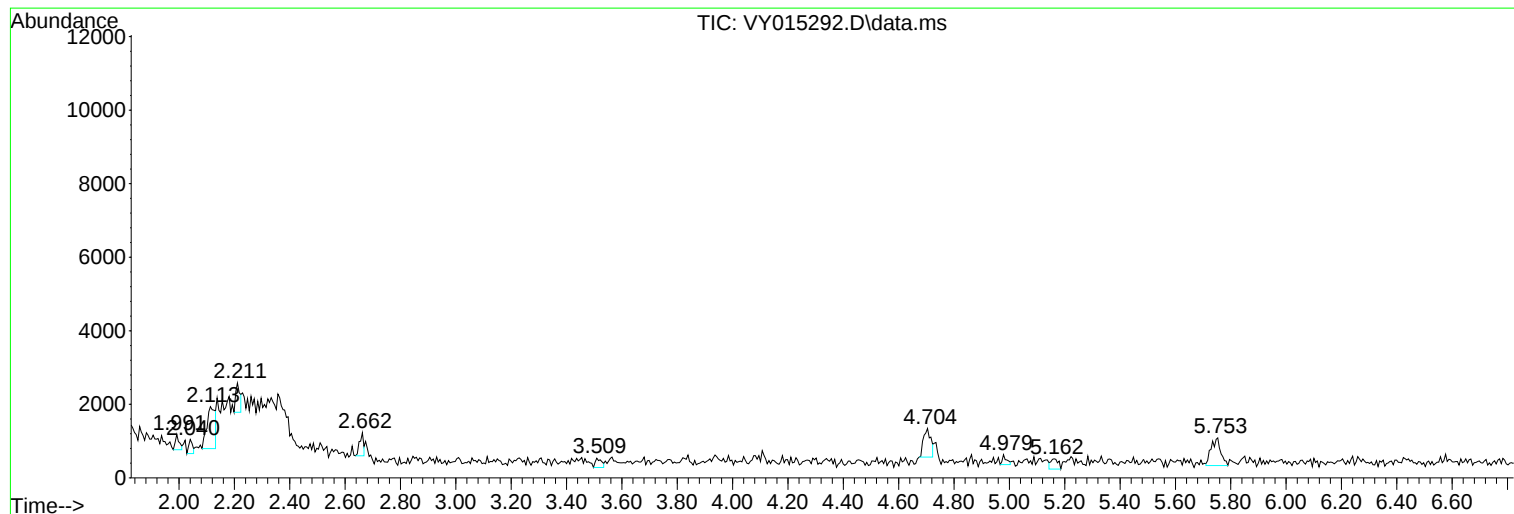
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081423S.M
Quant Title : SW846 8260

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



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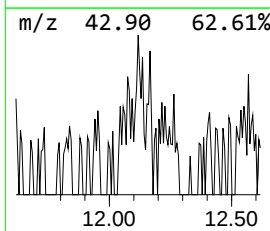
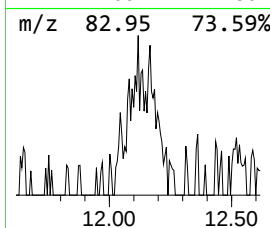
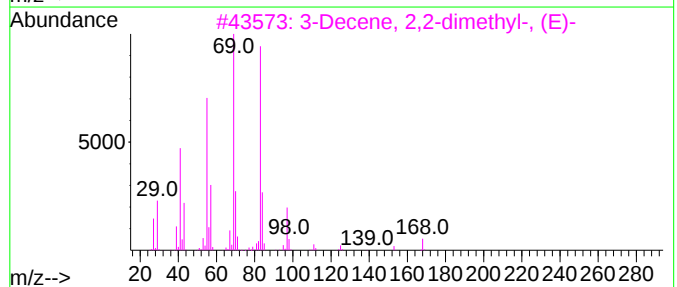
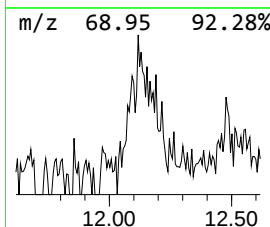
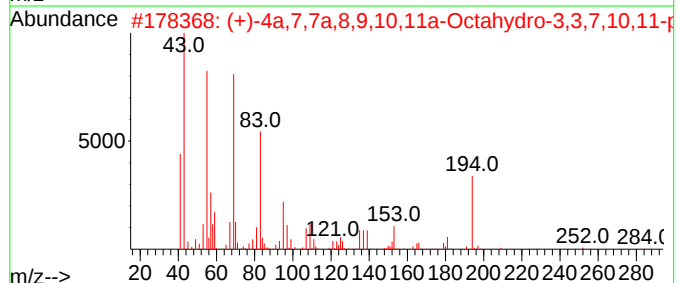
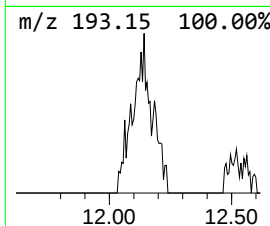
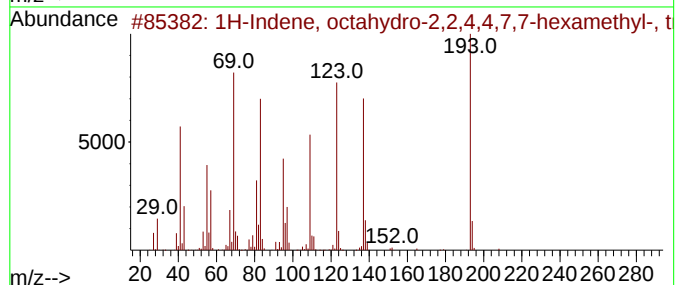
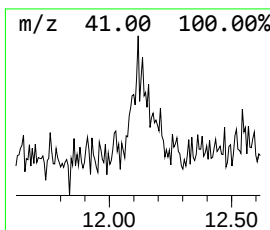
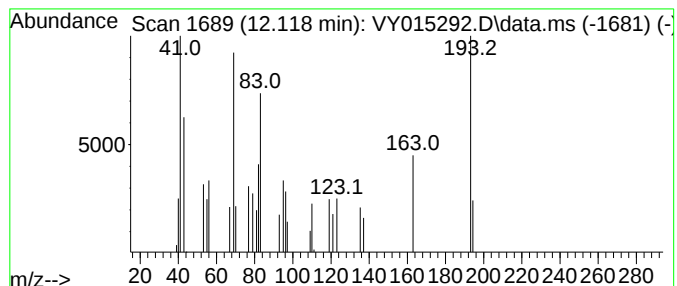
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081423S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown12.118 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.118	32.10 ug/l	6118	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, octahydro-2,2,4,7,7...	208	C15H28	054832-83-6	42
2			(+)-4a,7,7a,8,9,10,11a-Octahydro...	284	C15H24O5	1000211-94-1	25
3			3-Decene, 2,2-dimethyl-, (E)-	168	C12H24	055499-02-0	16
4			Cyclopentane, (2-methylpropyl)-	126	C9H18	003788-32-7	16
5			2-Hexenal, (E)-	98	C6H10O	006728-26-3	16



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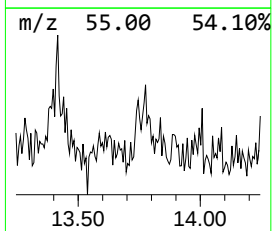
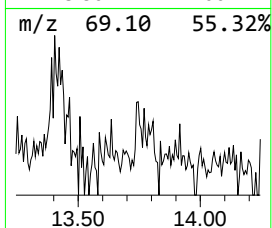
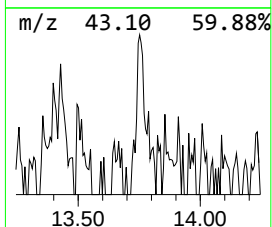
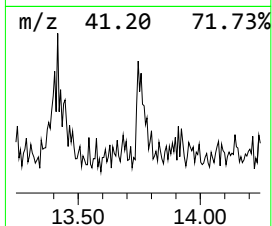
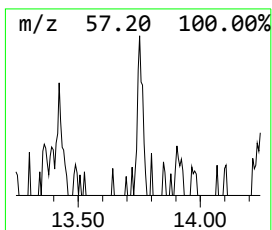
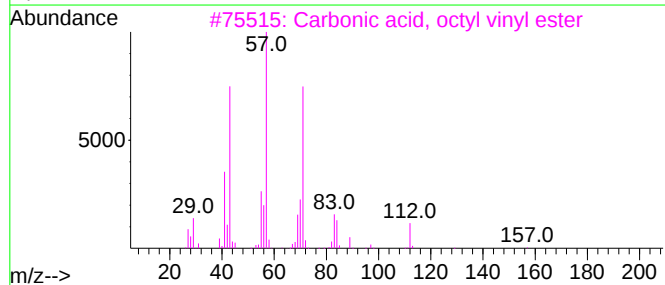
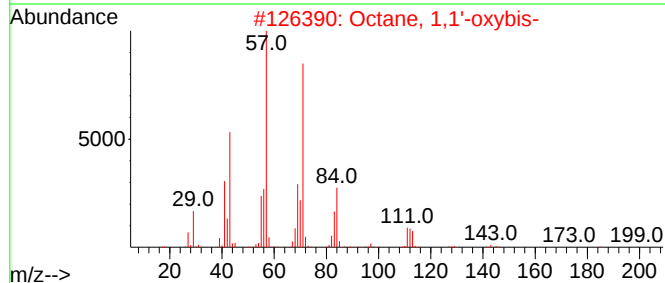
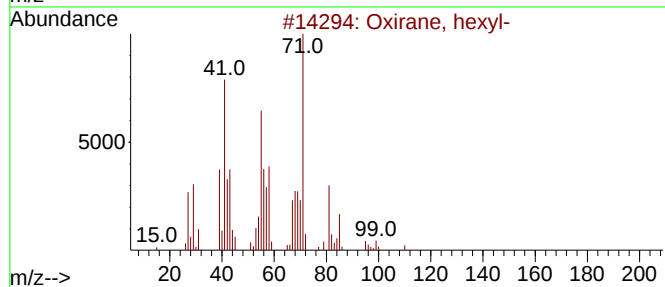
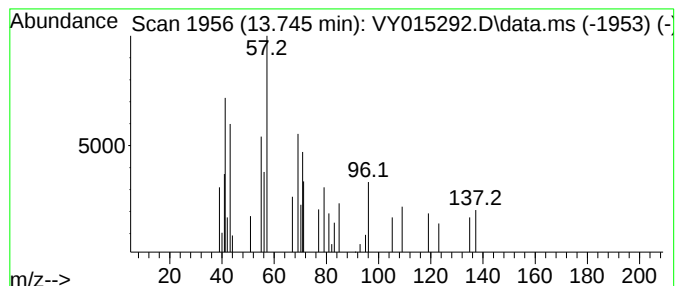
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TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown13.745 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.745	12.66 ug/l	7031	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexyl-	128	C8H16O	002984-50-1	27
2			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	22
3			Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	22
4			Isooctyl mercaptoacetate	204	C10H20O2S	025103-09-7	22
5			Oxirane, pentyl-	114	C7H14O	005063-65-0	17



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown12.118	12.118	32.1	ug/l	6118	3	11.496	9531	50.0
unknown13.745	13.745	12.7	ug/l	7031	4	13.428	27763	50.0