

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052323\
 Data File : VN077817.D
 Acq On : 23 May 2023 15:30
 Operator : JC\MD
 Sample : 02884-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 2004

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_N\methods\82N051523W.M
 Title : SW846 8260

Signal : TIC: VN077817.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.089	18	23	31	rVB2	60213	98961	4.50%	0.482%
2	2.306	56	60	68	rVB3	19908	34725	1.58%	0.169%
3	2.489	86	91	95	rBV4	15369	28541	1.30%	0.139%
4	2.671	116	122	129	rBV	22887	38704	1.76%	0.188%
5	2.824	142	148	151	rBV3	18747	33918	1.54%	0.165%
6	3.259	219	222	230	rVB4	11001	22562	1.03%	0.110%
7	4.436	413	422	441	rBV	141941	428183	19.46%	2.084%
8	4.718	463	470	472	rBV	14582	25228	1.15%	0.123%
9	5.530	593	608	623	rBV2	185729	661080	30.05%	3.217%
10	7.241	891	899	907	rBV5	12365	33799	1.54%	0.164%
11	7.494	934	942	951	rBV	12098	27285	1.24%	0.133%
12	8.177	1047	1058	1062	rBV	306134	727379	33.06%	3.540%
13	8.230	1062	1067	1082	rVB	552017	1222275	55.56%	5.949%
14	8.606	1118	1131	1146	rBV2	416047	1449862	65.90%	7.056%
15	8.971	1188	1193	1202	rVB2	13242	29773	1.35%	0.145%
16	9.106	1207	1216	1231	rBV	760191	1599921	72.72%	7.786%
17	9.606	1296	1301	1305	rBV5	13949	24859	1.13%	0.121%
18	10.453	1439	1445	1455	rVB2	37834	71720	3.26%	0.349%
19	10.577	1457	1466	1472	rBV	1161158	2200073	100.00%	10.707%
20	10.635	1472	1476	1490	rVB	409241	782164	35.55%	3.807%
21	10.941	1522	1528	1533	rBV3	13935	29164	1.33%	0.142%
22	11.318	1582	1592	1605	rVB	305862	672801	30.58%	3.274%
23	11.765	1661	1668	1673	rVB5	11617	22465	1.02%	0.109%
24	11.871	1675	1686	1697	rBV	1021656	1880398	85.47%	9.151%
25	11.971	1697	1703	1709	rVV	131307	225135	10.23%	1.096%
26	12.071	1714	1720	1729	rVB	327282	649182	29.51%	3.159%
27	12.212	1740	1744	1750	rVB5	27455	51911	2.36%	0.253%
28	12.406	1768	1777	1790	rBV3	251597	555495	25.25%	2.703%
29	12.500	1790	1793	1798	rVV4	16173	26590	1.21%	0.129%
30	12.647	1810	1818	1822	rVV2	40240	81888	3.72%	0.399%
31	12.700	1822	1827	1835	rVB5	48179	101503	4.61%	0.494%
32	12.853	1845	1853	1861	rBV	817163	1459438	66.34%	7.103%
33	13.041	1880	1885	1891	rBV4	32478	70669	3.21%	0.344%
34	13.106	1891	1896	1899	rVV	94726	161124	7.32%	0.784%
35	13.176	1903	1908	1915	rVV	87528	161033	7.32%	0.784%
36	13.259	1915	1922	1928	rVV7	16161	35509	1.61%	0.173%

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37	13.353	1932	1938	1945	rVB4	81645	171063	7.78%	0.833%
38	13.488	1955	1961	1966	rVV	185986	324336	14.74%	1.578%
39	13.535	1966	1969	1974	rVB2	53550	82968	3.77%	0.404%
40	13.594	1974	1979	1982	rBV2	25153	36529	1.66%	0.178%
41	13.712	1996	1999	2006	rVB5	23665	50929	2.31%	0.248%
42	13.800	2006	2014	2023	rBV2	880233	1690173	76.82%	8.226%
43	13.876	2025	2027	2034	rVB3	29248	42298	1.92%	0.206%
44	14.000	2043	2048	2063	rVB4	46116	142479	6.48%	0.693%
45	14.182	2072	2079	2086	rVB	306036	521058	23.68%	2.536%
46	14.253	2086	2091	2094	rBV6	17367	30517	1.39%	0.149%
47	14.341	2102	2106	2111	rVB3	17521	27644	1.26%	0.135%
48	14.453	2119	2125	2133	rBV3	17614	45127	2.05%	0.220%
49	14.694	2163	2166	2171	rVB	20133	30087	1.37%	0.146%
50	15.041	2219	2225	2233	rBV2	35344	86720	3.94%	0.422%
51	15.123	2233	2239	2244	rVB6	18474	35885	1.63%	0.175%
52	15.217	2247	2255	2263	rVB6	37360	75306	3.42%	0.366%
53	15.317	2267	2272	2278	rBV8	13336	31081	1.41%	0.151%
54	15.500	2298	2303	2310	rVB9	14911	31030	1.41%	0.151%
55	15.647	2320	2328	2339	rVB	705540	1366989	62.13%	6.653%

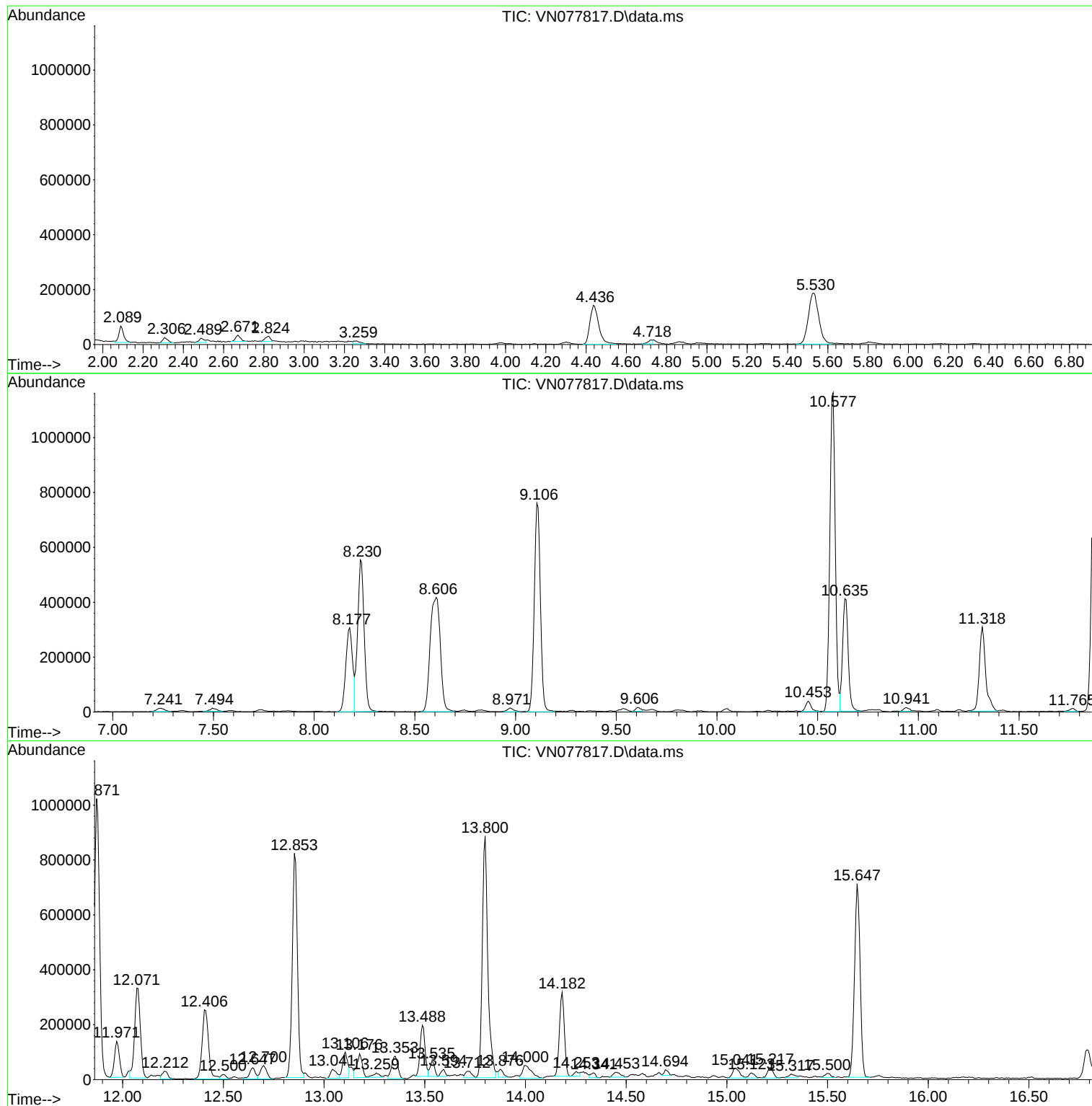
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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



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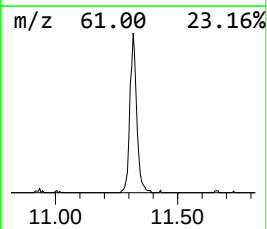
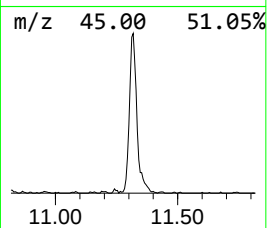
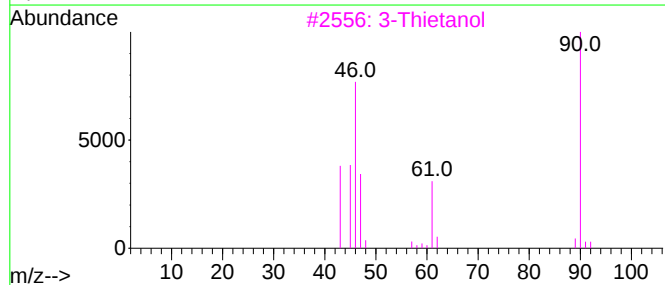
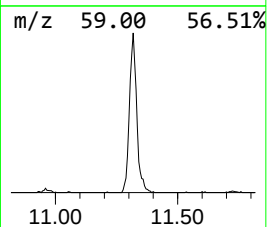
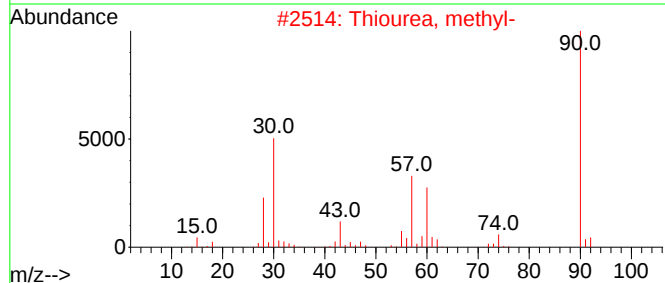
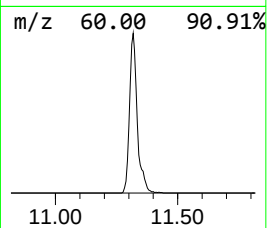
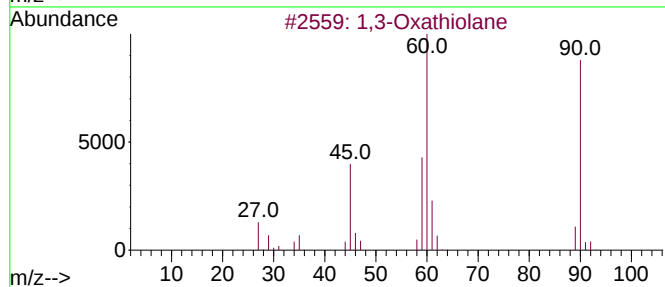
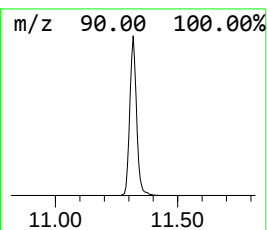
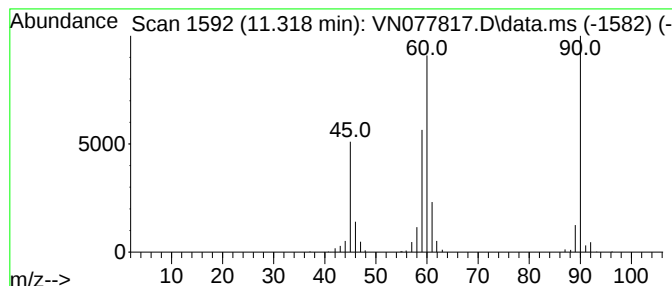
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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

Peak Number 1 1,3-Oxathiolane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.318	17.89 ug/l	672801	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Oxathiolane	90	C3H6OS	002094-97-5	91
2			Thiourea, methyl-	90	C2H6N2S	000598-52-7	50
3			3-Thietanol	90	C3H6OS	010304-16-2	42
4			Hydrazinecarboxylic acid, methyl...	90	C2H6N2O2	006294-89-9	38
5			(S)-Methyl 2,3-dihydroxypropanoate	120	C4H8O4	010303-88-5	33



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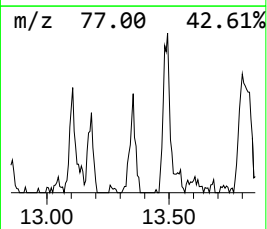
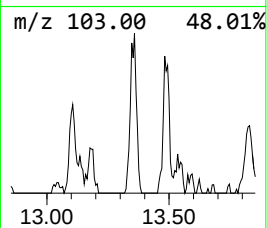
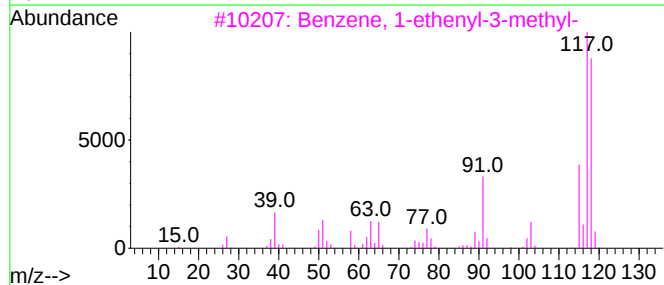
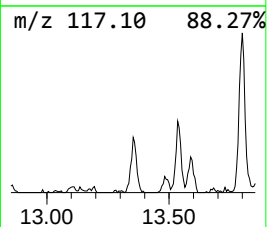
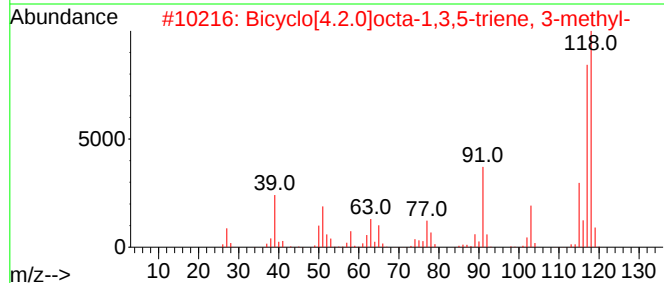
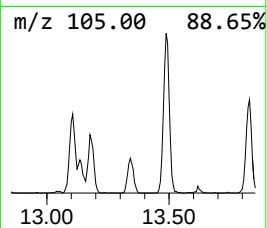
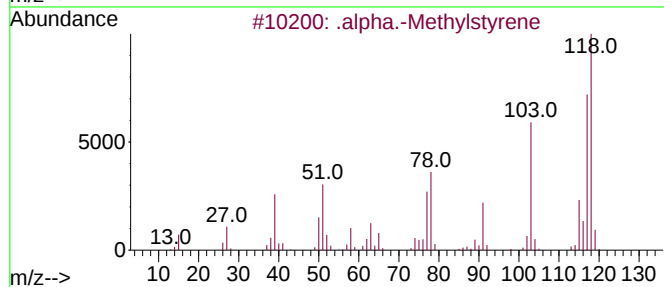
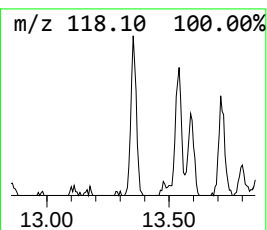
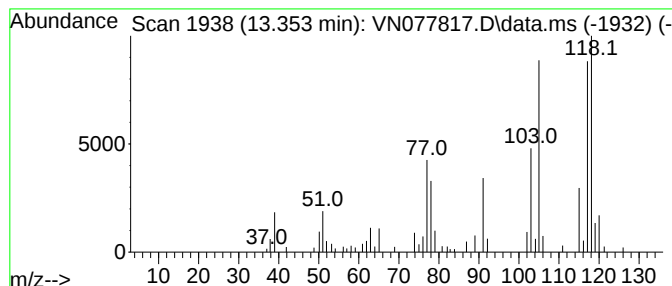
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Quant Title : SW846 8260

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

Peak Number 2 .alpha.-Methylstyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.353	5.06 ug/l	171063	1,4-Dichlorobenzene-d4	13.800

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.alpha.-Methylstyrene	118	C9H10	000098-83-9	76
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	022250-74-4	60
3		Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	55
4		Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	55
5		Benzene, 2-propenyl-	118	C9H10	000300-57-2	46



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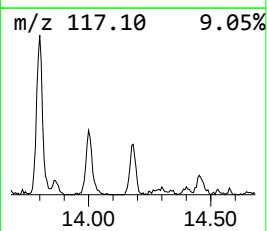
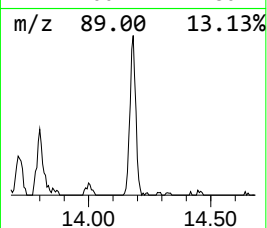
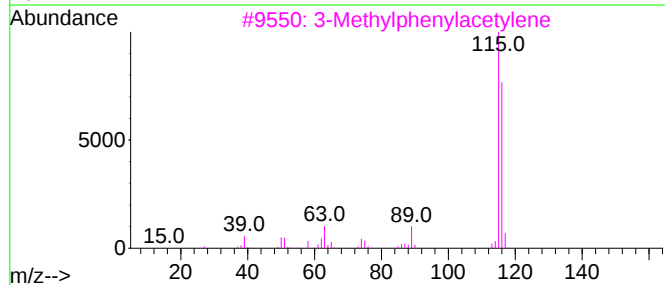
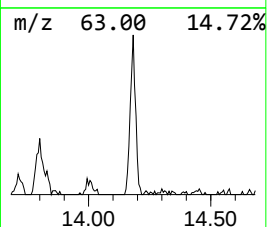
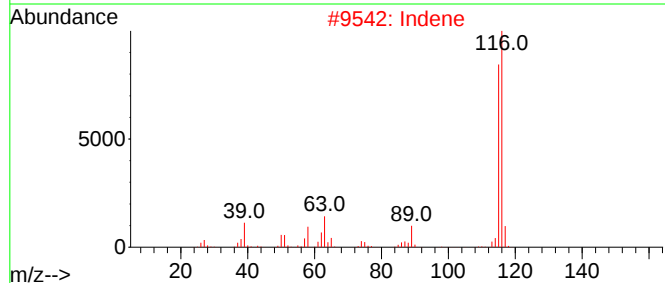
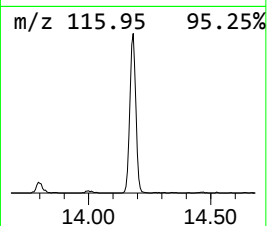
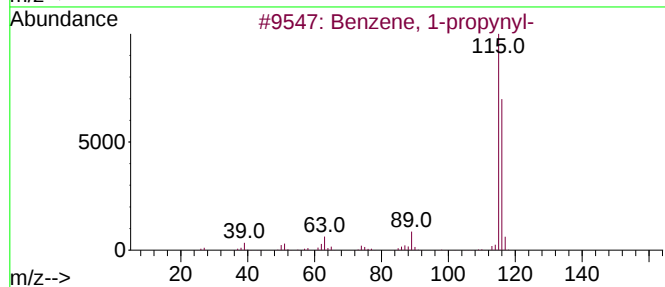
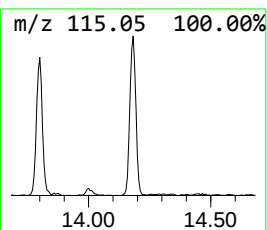
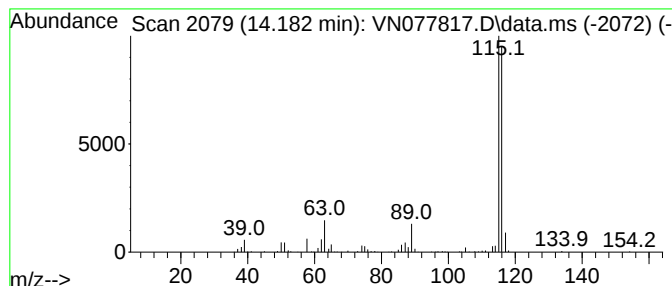
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzene, 1-propynyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.182	15.41 ug/l	521058	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
2			Indene	116	C9H8	000095-13-6	94
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	90
5			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	87



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,3-Oxathiolane	11.318	17.9	ug/l	672801	3	11.871	1880400	50.0
.alpha.-Methyls...	13.353	5.1	ug/l	171063	4	13.800	1690170	50.0
Benzene, 1-prop...	14.182	15.4	ug/l	521058	4	13.800	1690170	50.0