

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
 Data File : VX021573.D
 Acq On : 29 Mar 2021 13:42
 Operator : JC/MD
 Sample : M1785-14DL 40X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-3RDL

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_X\Method\82X032421W.M
 Title : SW846 8260

Signal : TIC: VX021573.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.593	79	86	91	rVB7	3086	6440	1.23%	0.163%
2	5.464	730	744	760	rBV2	48951	141454	27.02%	3.587%
3	5.629	760	772	784	rVB	72258	198753	37.97%	5.039%
4	6.029	828	840	852	rBV2	54804	141011	26.94%	3.575%
5	6.829	966	976	987	rBV	121356	288045	55.03%	7.303%
6	8.694	1287	1293	1311	rVB	261662	404802	77.33%	10.264%
7	10.094	1525	1531	1540	rBV	292452	394165	75.30%	9.994%
8	10.165	1540	1543	1549	rVB4	3701	5656	1.08%	0.143%
9	10.235	1549	1555	1560	rBV	10955	15311	2.92%	0.388%
10	10.341	1561	1573	1579	rBV	40913	63034	12.04%	1.598%
11	10.630	1614	1622	1628	rBV6	5656	13835	2.64%	0.351%
12	10.683	1628	1631	1641	rVB3	4185	7659	1.46%	0.194%
13	10.818	1641	1654	1660	rBV3	12313	21035	4.02%	0.533%
14	10.894	1660	1667	1671	rBV3	10848	16977	3.24%	0.430%
15	11.000	1680	1685	1690	rBV	44564	55865	10.67%	1.416%
16	11.118	1700	1705	1711	rBV	242533	319728	61.08%	8.107%
17	11.165	1711	1713	1717	rVB2	5208	6211	1.19%	0.157%
18	11.259	1722	1729	1737	rVV6	6717	11539	2.20%	0.293%
19	11.342	1737	1743	1752	rVV	79231	95849	18.31%	2.430%
20	11.418	1752	1756	1757	rVV	16489	19004	3.63%	0.482%
21	11.436	1757	1759	1763	rVV	19919	23905	4.57%	0.606%
22	11.489	1763	1768	1777	rVB	21583	31536	6.02%	0.800%
23	11.653	1791	1796	1803	rBV4	7854	12716	2.43%	0.322%
24	11.753	1809	1813	1815	rBV	10974	13942	2.66%	0.354%
25	11.789	1815	1819	1830	rVB	435899	523470	100.00%	13.273%
26	11.900	1830	1838	1840	rBV	16598	23379	4.47%	0.593%
27	11.930	1840	1843	1849	rVB	31093	38643	7.38%	0.980%
28	12.006	1853	1856	1860	rVV	14710	17597	3.36%	0.446%
29	12.059	1860	1865	1871	rVV	329775	402795	76.95%	10.213%
30	12.124	1871	1876	1887	rVB	96497	114754	21.92%	2.910%
31	12.218	1887	1892	1897	rVB	12188	15701	3.00%	0.398%
32	12.283	1897	1903	1910	rBV	78735	108440	20.72%	2.750%
33	12.353	1910	1915	1924	rVB4	27542	53283	10.18%	1.351%
34	12.442	1924	1930	1934	rBV	12213	16196	3.09%	0.411%
35	12.571	1946	1952	1954	rBV	22083	32301	6.17%	0.819%
36	12.595	1954	1956	1960	rVV	23569	24706	4.72%	0.626%

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Title : SW846 8260

37	12.648	1960	1965	1969	rVV	47599	61761	11.80%	1.566%
38	12.683	1969	1971	1976	rVV	16865	19305	3.69%	0.489%
39	12.742	1976	1981	1989	rVB3	33373	61178	11.69%	1.551%
40	12.883	1999	2005	2010	rVB2	13461	19538	3.73%	0.495%
41	12.959	2010	2018	2021	rVV	14099	19915	3.80%	0.505%
42	13.001	2021	2025	2032	rVB2	20740	25487	4.87%	0.646%
43	13.065	2032	2036	2042	rBV4	3895	5670	1.08%	0.144%
44	13.330	2076	2081	2087	rVB2	23864	35284	6.74%	0.895%
45	13.459	2099	2103	2110	rVB	13147	16102	3.08%	0.408%

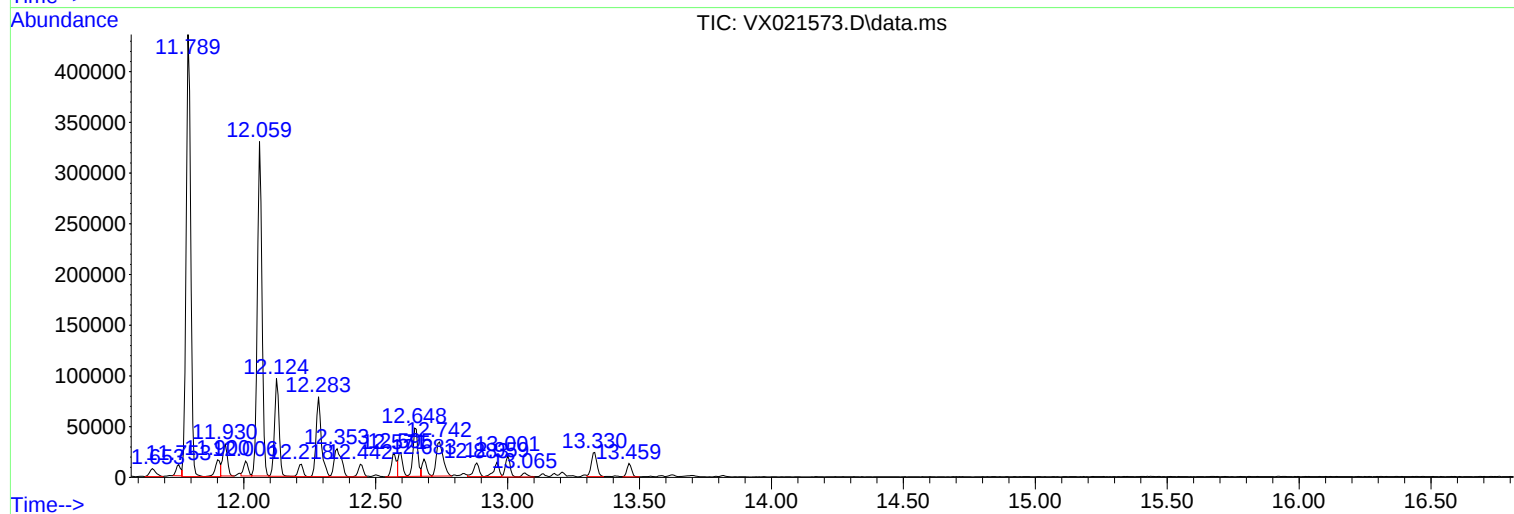
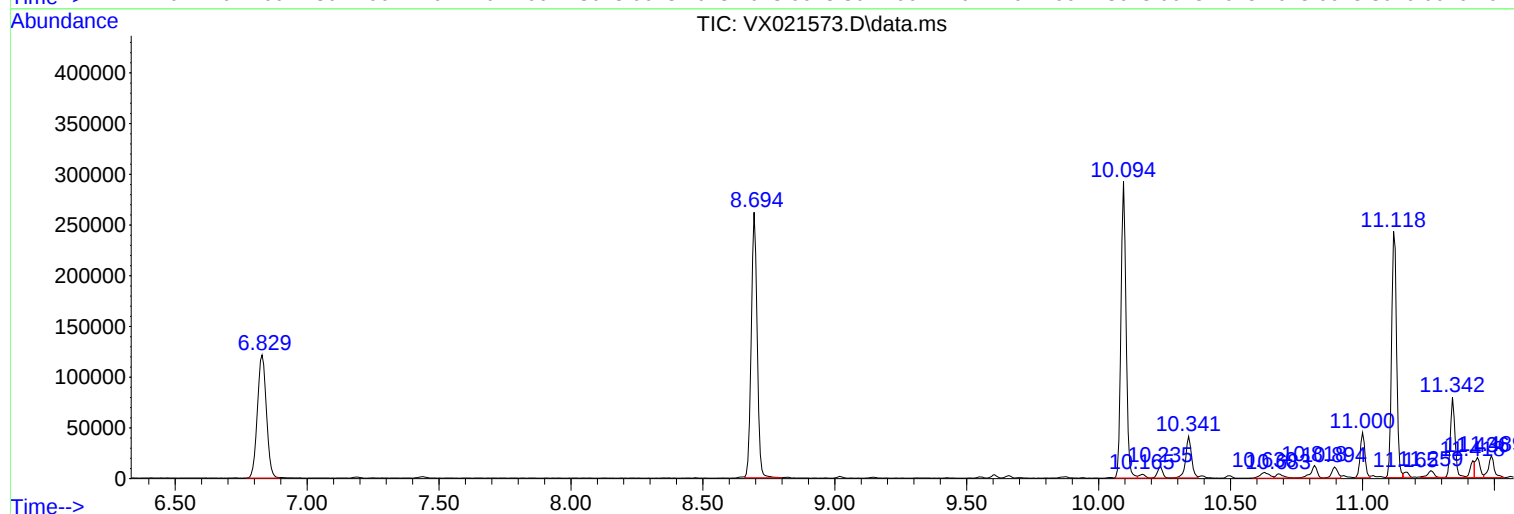
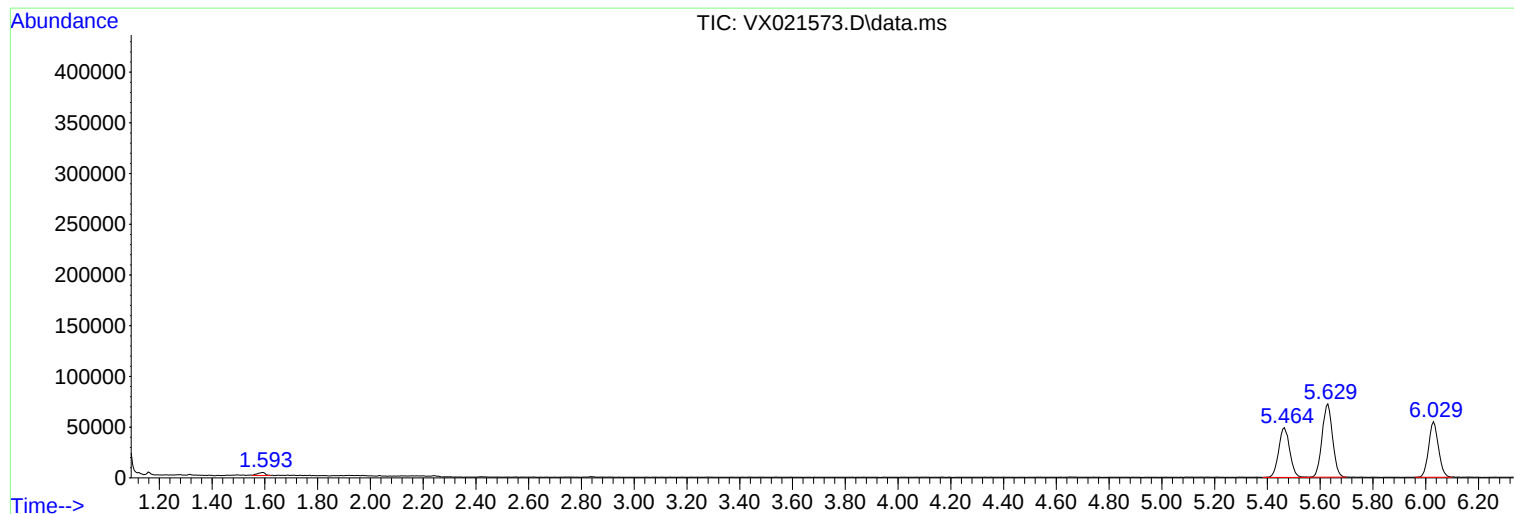
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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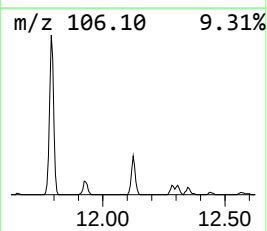
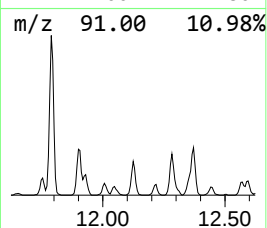
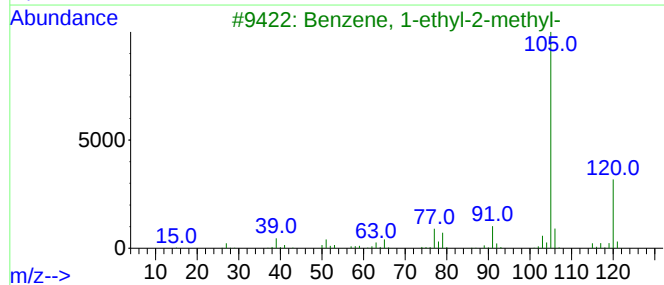
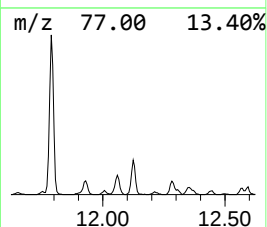
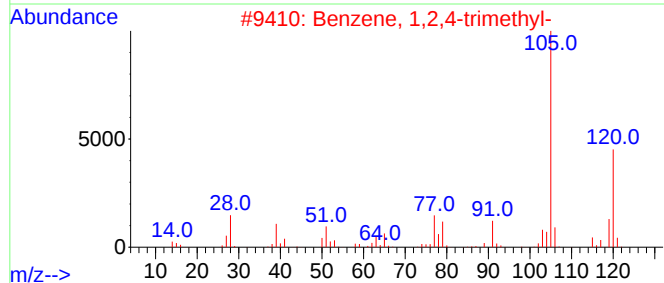
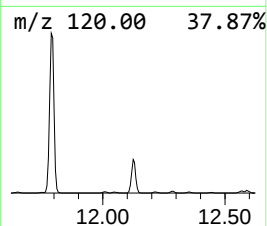
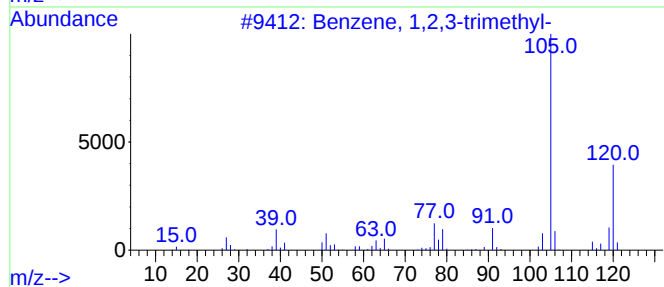
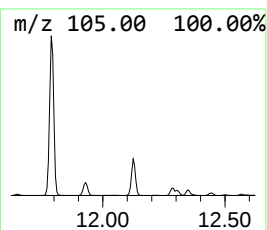
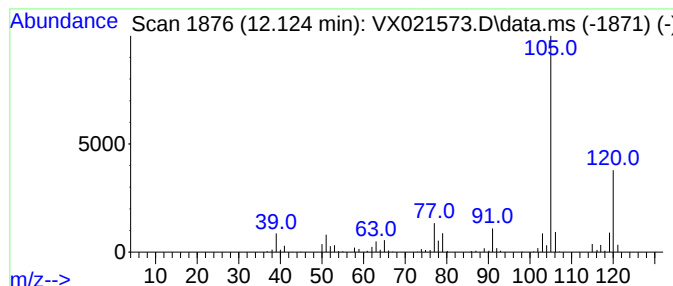
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Benzene, 1,2,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.124	14.24 ug/l	114754	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
5			Mesitylene	120	C9H12	000108-67-8	91



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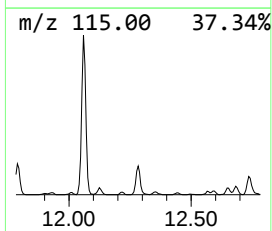
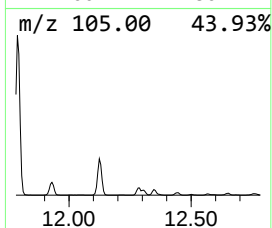
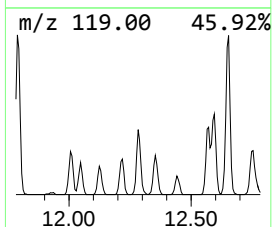
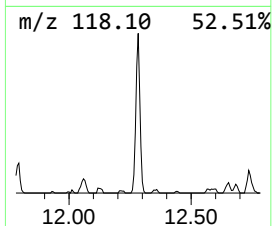
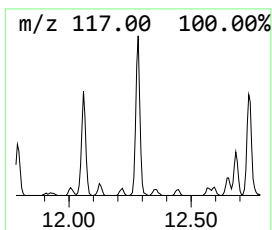
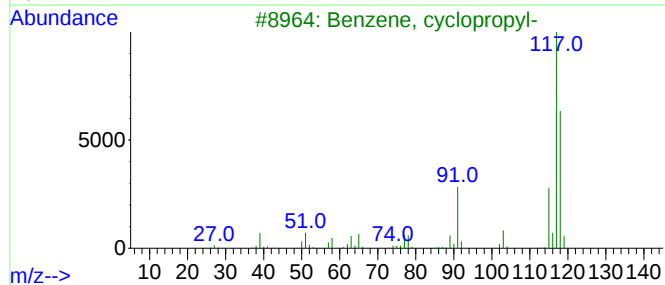
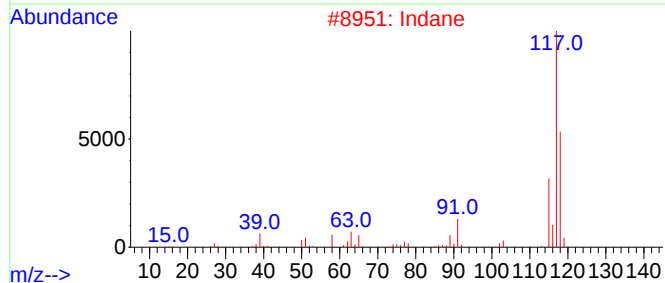
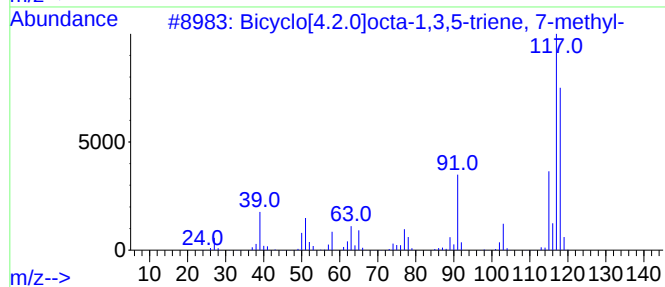
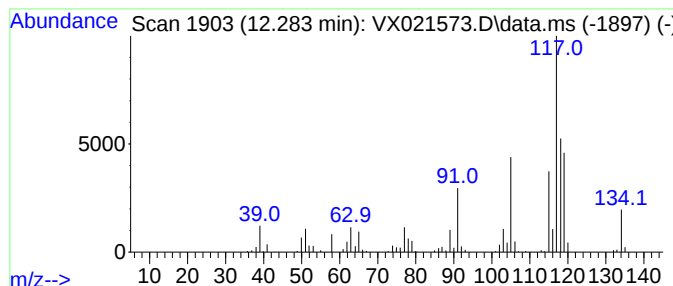
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Bicyclo[4.2.0]octa-1,3,5-tr... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.283	13.46 ug/l	108440	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	78
2			Indane	118	C9H10	000496-11-7	78
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	64
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	60



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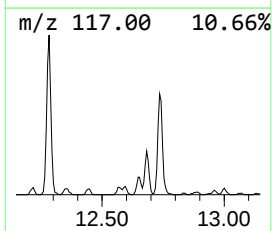
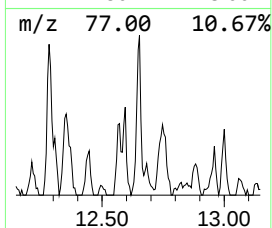
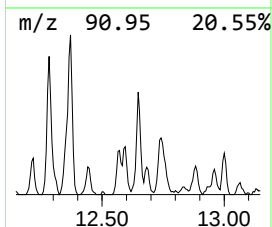
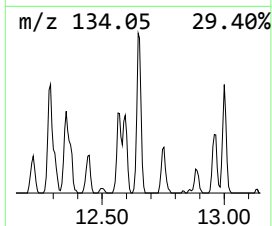
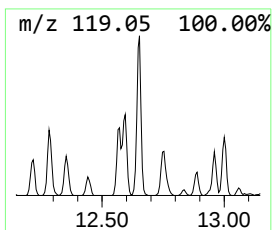
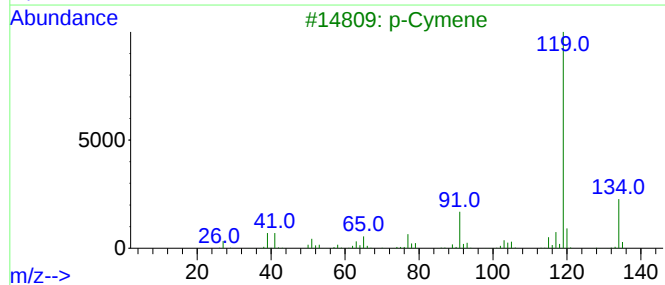
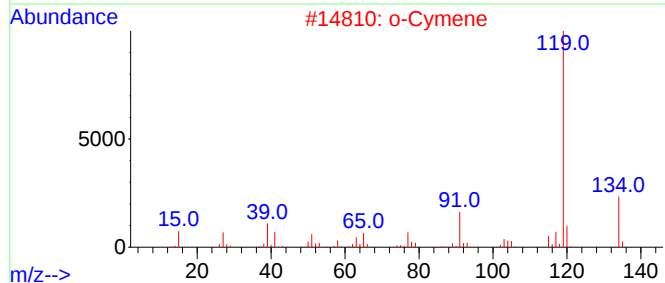
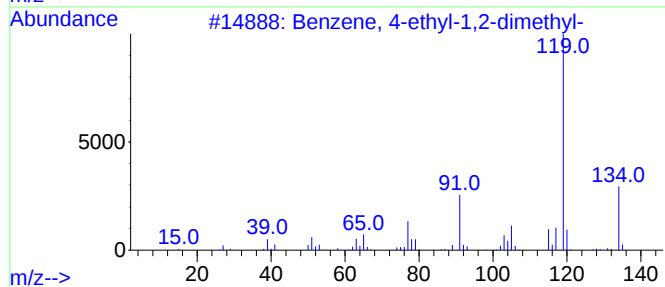
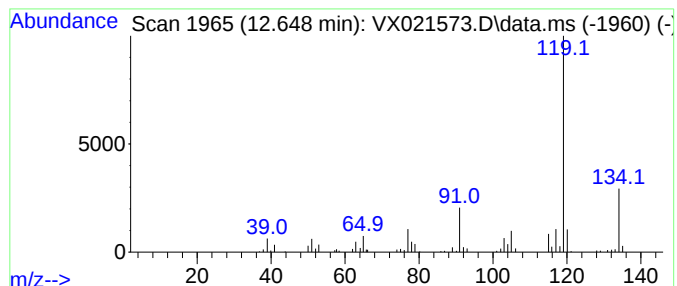
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.648	7.67 ug/l	61761	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2			o-Cymene	134	C10H14	000527-84-4	95
3			p-Cymene	134	C10H14	000099-87-6	95
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95



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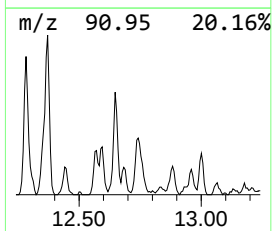
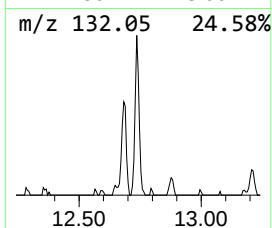
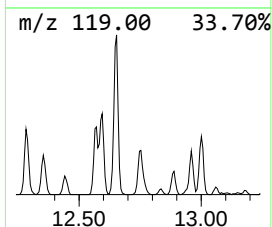
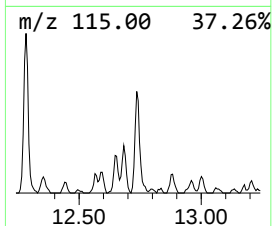
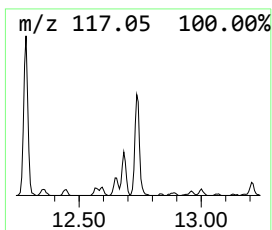
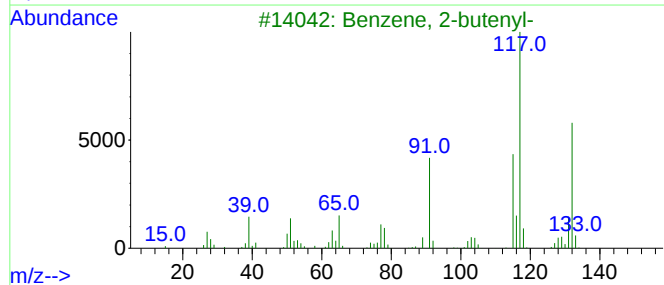
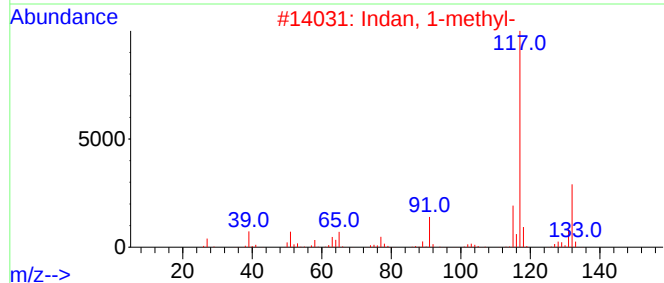
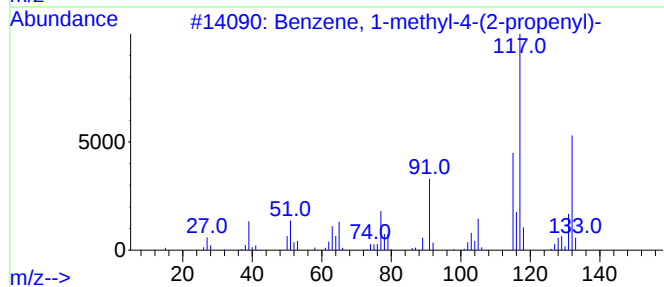
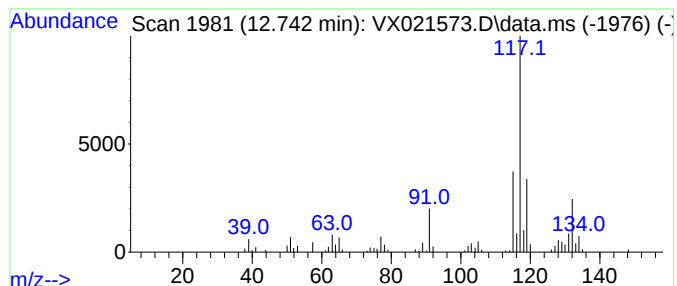
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-methyl-4-(2-prop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.742	7.59 ug/l	61178	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	81
2			Indan, 1-methyl-	132	C10H12	000767-58-8	81
3			Benzene, 2-butenyl-	132	C10H12	001560-06-1	74
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	74
5			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	72



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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1,2,3-...	12.124	14.2	ug/l	114754	4	12.059	402795	50.0
Bicyclo[4.2.0]o...	12.283	13.5	ug/l	108440	4	12.059	402795	50.0
Benzene, 4-ethy...	12.648	7.7	ug/l	61761	4	12.059	402795	50.0
Benzene, 1-meth...	12.742	7.6	ug/l	61178	4	12.059	402795	50.0