

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121422\
 Data File : VN075780.D
 Acq On : 14 Dec 2022 19:15
 Operator : JC\MD
 Sample : N5875-04
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-38D

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\82N121422W.M
 Title : SW846 8260

Signal : TIC: VN075780.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.295	36	41	45	rBV	14166	29769	1.71%	0.219%
2	2.824	123	131	140	rVB5	16213	49175	2.83%	0.361%
3	4.436	393	405	420	rVB6	15035	52988	3.05%	0.389%
4	5.289	534	550	560	rBV4	17530	58140	3.35%	0.427%
5	5.530	578	591	610	rBV2	164728	582879	33.54%	4.284%
6	5.806	623	638	657	rBV	499073	1738037	100.00%	12.775%
7	6.683	776	787	797	rBV3	22687	71621	4.12%	0.526%
8	7.230	870	880	892	rBV4	12901	37006	2.13%	0.272%
9	8.171	1030	1040	1045	rBV	222241	544742	31.34%	4.004%
10	8.230	1045	1050	1061	rVV2	445718	975216	56.11%	7.168%
11	8.330	1061	1067	1078	rVB3	17206	41905	2.41%	0.308%
12	8.583	1102	1110	1119	rBV2	224784	556952	32.04%	4.094%
13	8.659	1119	1123	1133	rVV3	43545	100975	5.81%	0.742%
14	8.765	1133	1141	1152	rVB3	36417	93184	5.36%	0.685%
15	9.106	1189	1199	1216	rBV	582200	1195075	68.76%	8.784%
16	10.018	1346	1354	1362	rVB2	25451	53248	3.06%	0.391%
17	10.147	1362	1376	1389	rBV2	47071	105972	6.10%	0.779%
18	10.318	1397	1405	1408	rBV3	25723	56047	3.22%	0.412%
19	10.571	1440	1448	1458	rBV	872500	1615427	92.95%	11.874%
20	10.659	1458	1463	1470	rVB3	17064	34539	1.99%	0.254%
21	10.765	1472	1481	1487	rVB5	19502	38633	2.22%	0.284%
22	10.835	1487	1493	1500	rVB3	19234	34170	1.97%	0.251%
23	10.912	1500	1506	1513	rBV4	8447	20407	1.17%	0.150%
24	10.988	1513	1519	1526	rVV5	12038	30527	1.76%	0.224%
25	11.194	1544	1554	1558	rBV5	10430	20942	1.20%	0.154%
26	11.247	1558	1563	1570	rVB	43870	75633	4.35%	0.556%
27	11.712	1632	1642	1647	rBV7	8761	22362	1.29%	0.164%
28	11.865	1660	1668	1677	rBV	769528	1403768	80.77%	10.318%
29	11.971	1682	1686	1691	rVB4	12747	22793	1.31%	0.168%
30	12.071	1696	1703	1707	rBV2	12190	25773	1.48%	0.189%
31	12.582	1782	1790	1798	rBV7	5528	18668	1.07%	0.137%
32	12.700	1805	1810	1814	rBV2	19998	30848	1.77%	0.227%
33	12.753	1814	1819	1825	rVV2	22065	41186	2.37%	0.303%
34	12.853	1828	1836	1846	rVB	617363	1061965	61.10%	7.806%
35	13.441	1928	1936	1939	rBV	15261	25884	1.49%	0.190%
36	13.618	1959	1966	1971	rVB2	14656	26910	1.55%	0.198%

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	13.794	1989	1996	2006	rBV	747947	1278077	73.54%	9.394%
38	13.888	2006	2012	2017	rVV	31948	51353	2.95%	0.377%
39	13.953	2017	2023	2027	rVV	203875	319049	18.36%	2.345%
40	13.994	2027	2030	2035	rVV	138122	237892	13.69%	1.749%
41	14.035	2035	2037	2045	rVB2	37427	53284	3.07%	0.392%
42	14.118	2045	2051	2056	rBV3	16945	29658	1.71%	0.218%
43	14.276	2067	2078	2083	rBV2	24755	50764	2.92%	0.373%
44	14.400	2094	2099	2102	rVV	35976	63992	3.68%	0.470%
45	14.447	2102	2107	2114	rVB	100621	171177	9.85%	1.258%
46	14.512	2114	2118	2125	rBV6	14153	30855	1.78%	0.227%
47	14.582	2125	2130	2135	rVV	35943	59958	3.45%	0.441%
48	14.776	2159	2163	2168	rVB2	22360	32292	1.86%	0.237%
49	14.941	2185	2191	2197	rVV3	29540	58350	3.36%	0.429%
50	15.053	2201	2210	2217	rVB4	21227	48536	2.79%	0.357%
51	15.123	2217	2222	2228	rBV5	14445	23509	1.35%	0.173%
52	15.318	2248	2255	2260	rBV4	14012	26492	1.52%	0.195%
53	15.435	2266	2275	2284	rVB3	51017	141173	8.12%	1.038%
54	15.782	2325	2334	2344	rVB7	11617	34818	2.00%	0.256%

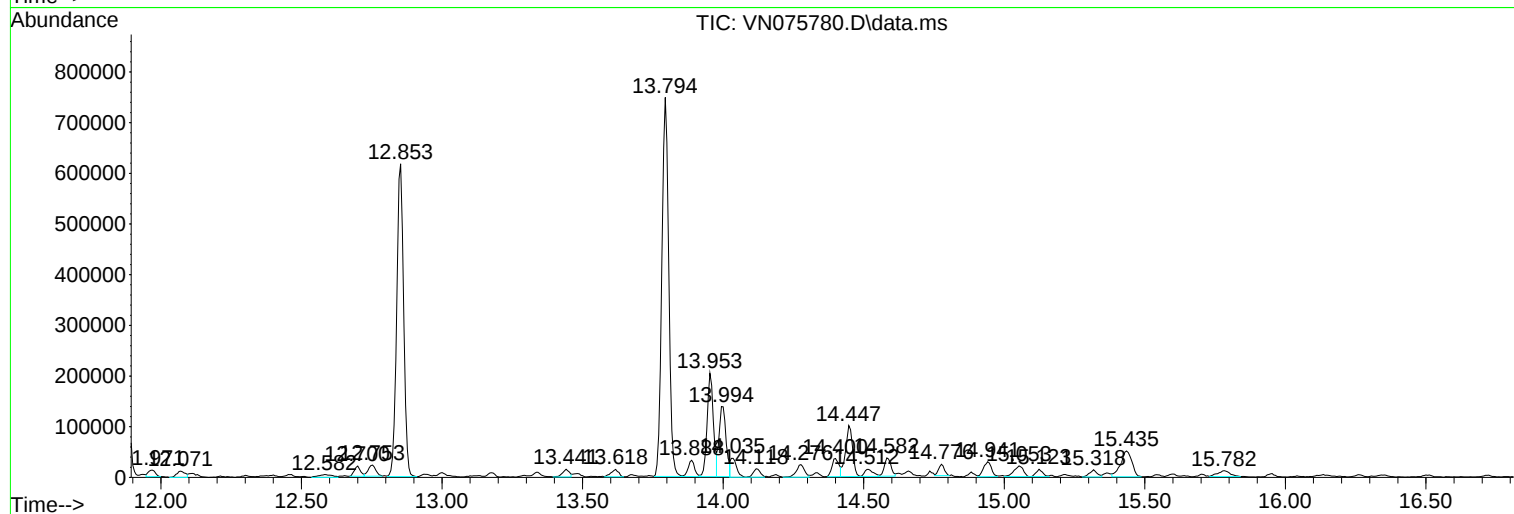
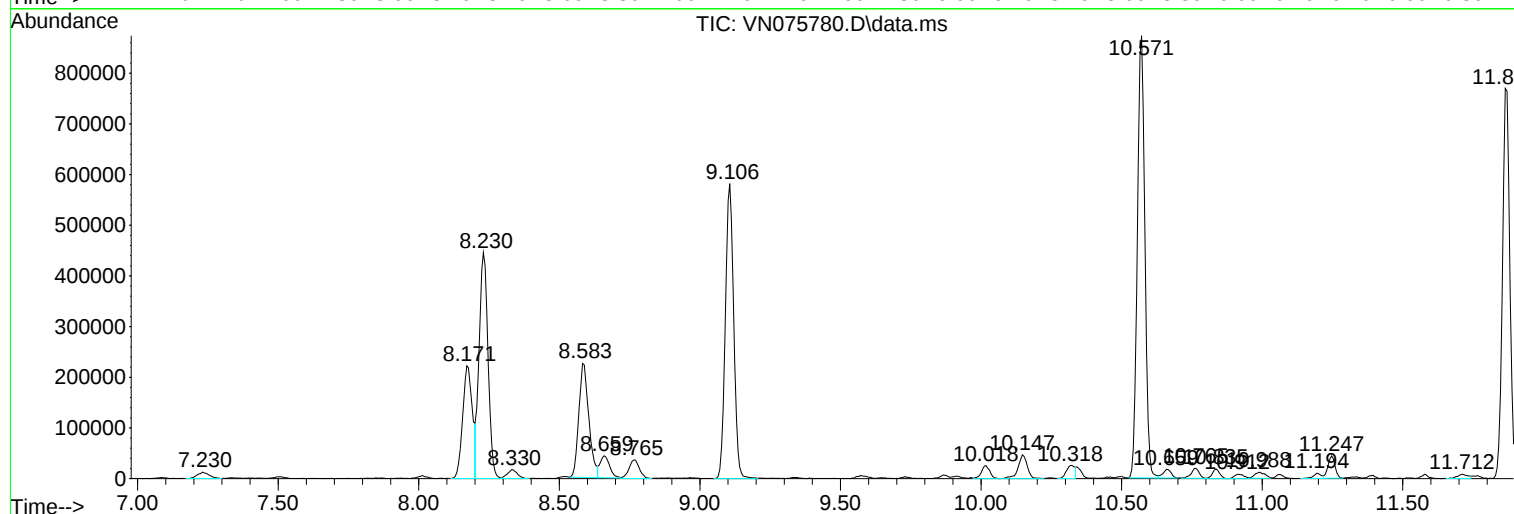
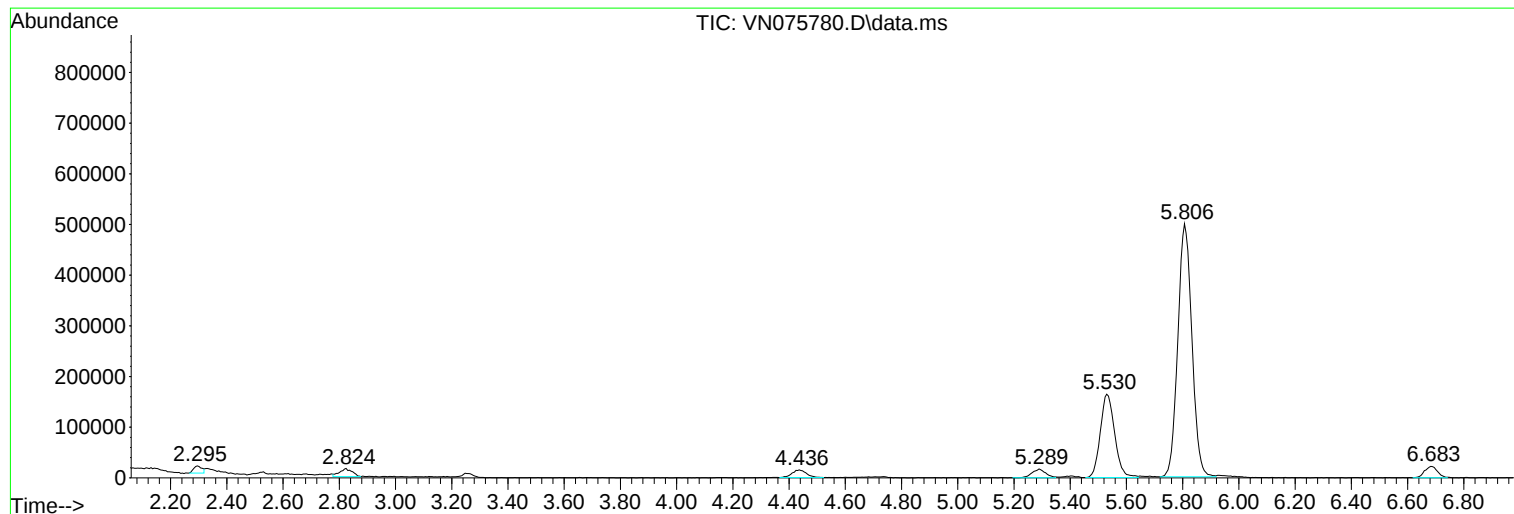
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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ClientSampleId :
MW-38D

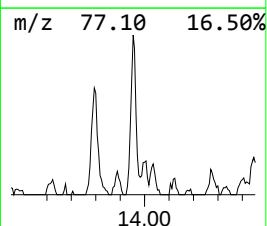
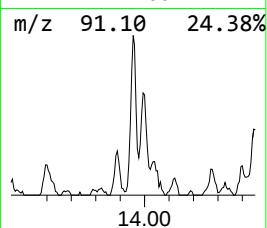
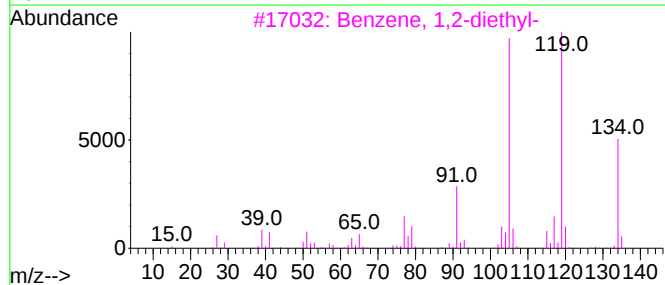
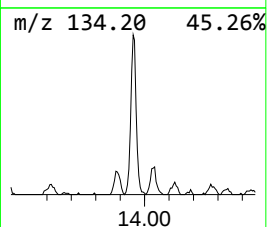
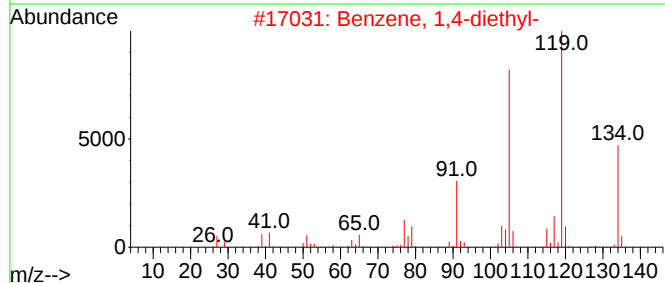
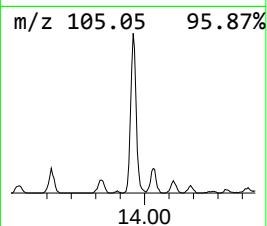
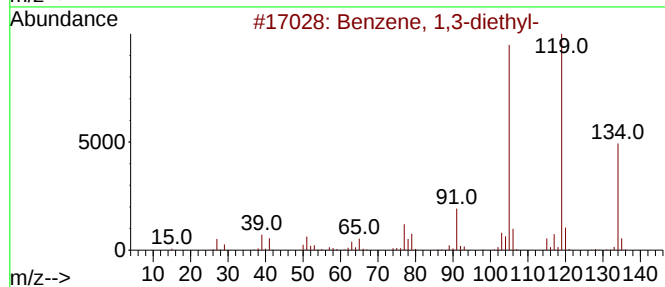
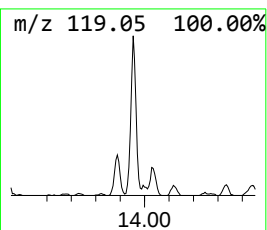
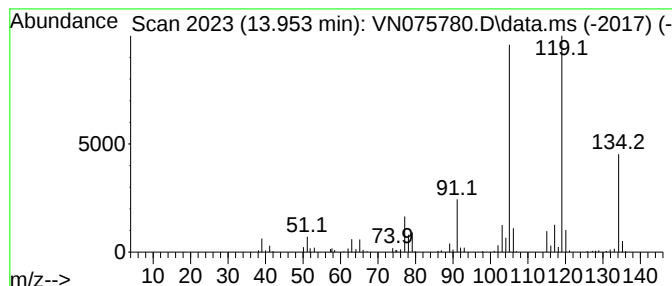
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1,3-diethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.953	12.48 ug/l	319049	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	97
2			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	97
3			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91
5			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	87



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ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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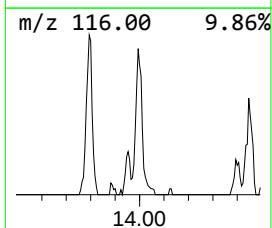
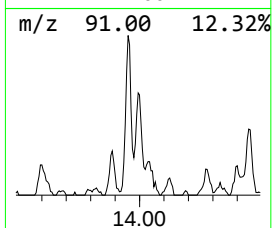
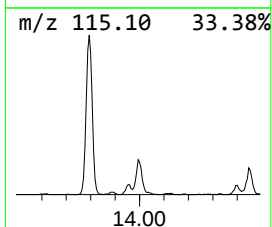
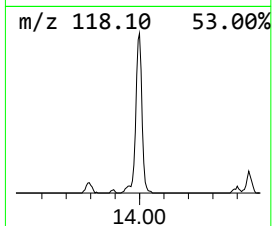
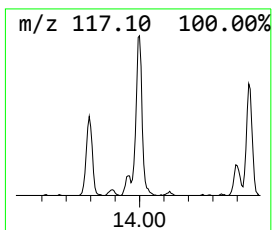
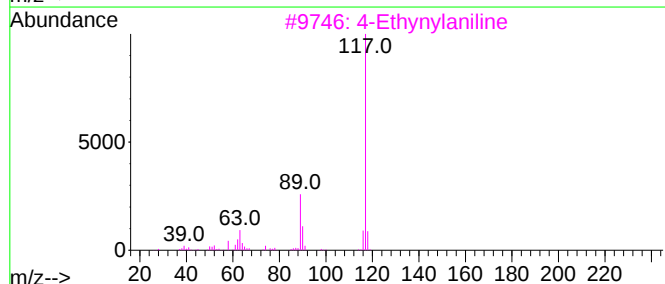
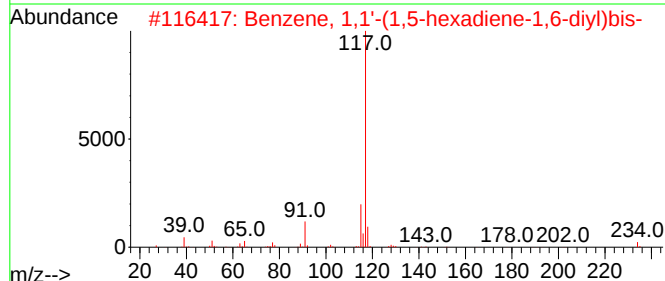
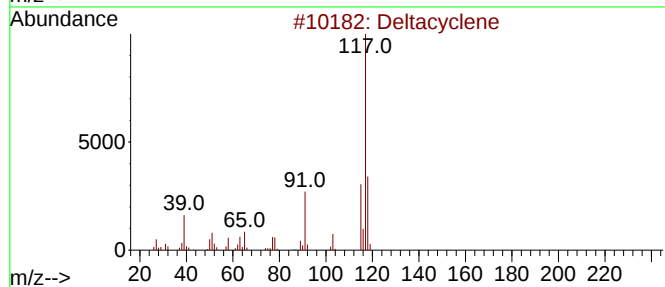
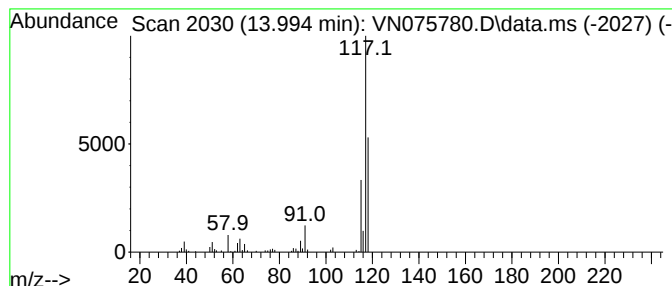
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	9.31 ug/l	237892	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Deltacyclene	118	C9H10	007785-10-6	64
2			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
3			4-Ethynylaniline	117	C8H7N	014235-81-5	47
4			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45
5			Benzyl nitrile	117	C8H7N	000140-29-4	37



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-38D

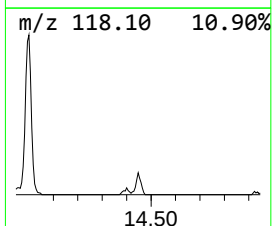
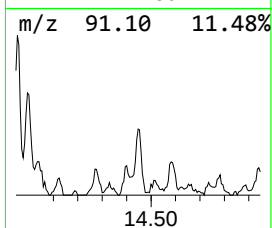
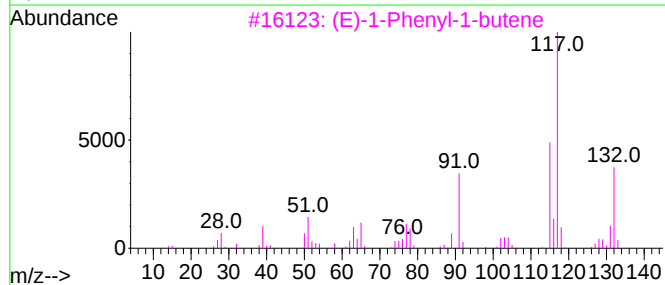
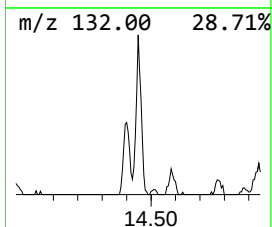
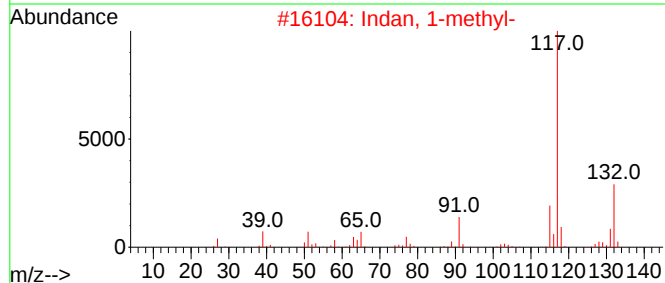
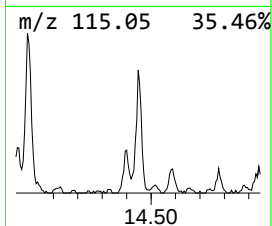
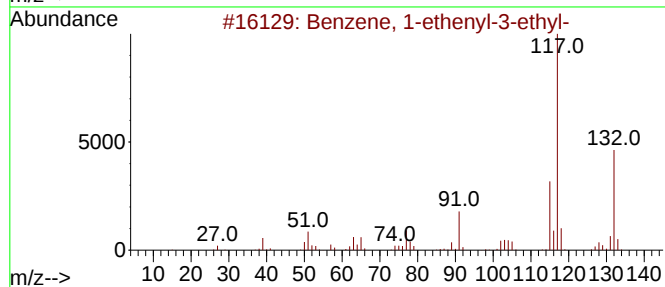
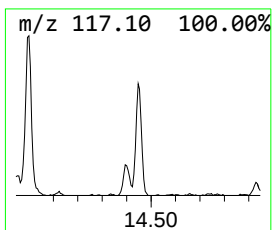
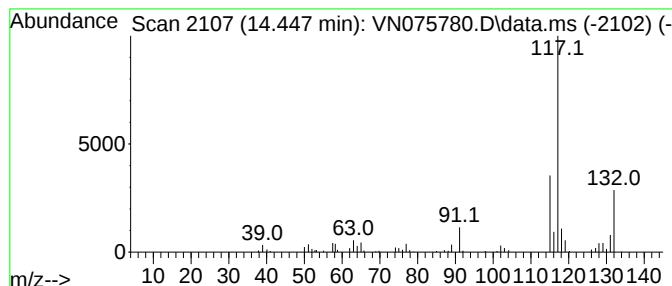
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	6.70 ug/l	171177	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	86
2			Indan, 1-methyl-	132	C10H12	000767-58-8	83
3			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	83
4			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	80
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	80



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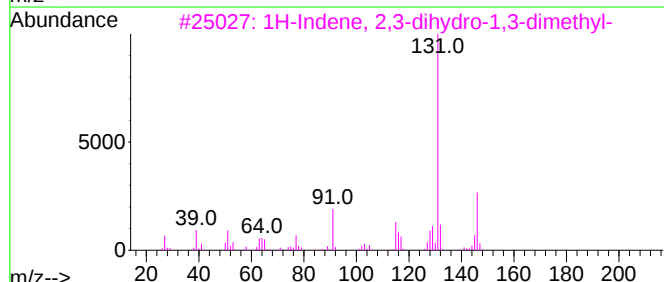
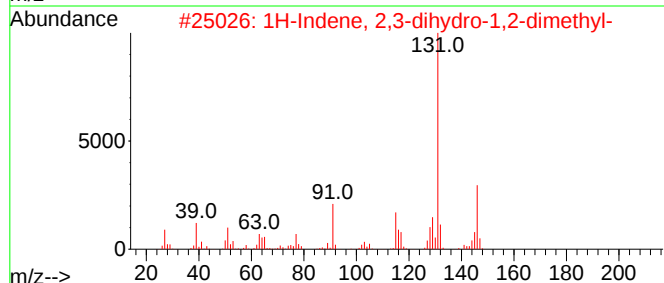
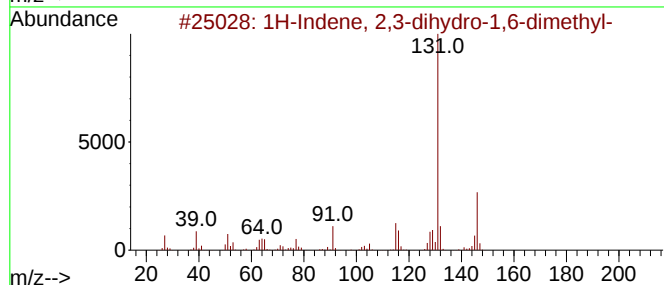
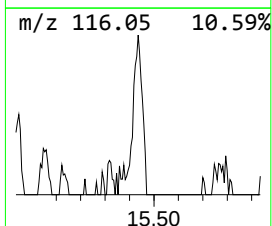
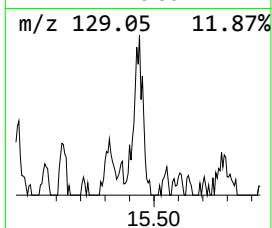
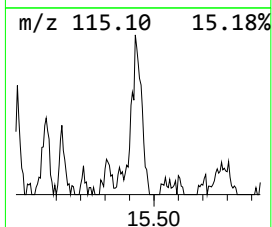
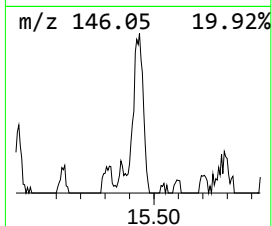
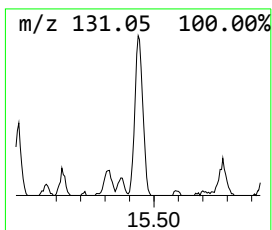
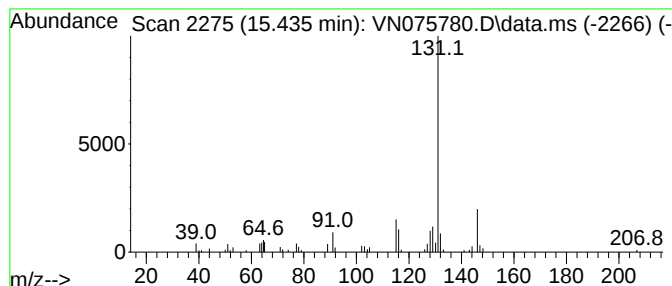
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 4 1H-Indene, 2,3-dihydro-1,6-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.435	5.52 ug/l	141173	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	91
2			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	91
3			1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	91
4			Benzene, 1-methyl-2-(1-methyl-2-...	146	C11H14	097664-19-2	90
5			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	90



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1,3-di...	13.953	12.5	ug/l	319049	4	13.794	1278080	50.0
Benzene, 1,1'-(...	13.994	9.3	ug/l	237892	4	13.794	1278080	50.0
Benzene, 1-ethe...	14.447	6.7	ug/l	171177	4	13.794	1278080	50.0
1H-Indene, 2,3-...	15.435	5.5	ug/l	141173	4	13.794	1278080	50.0