

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120621\
 Data File : VX025562.D
 Acq On : 06 Dec 2021 20:26
 Operator : JC/MD
 Sample : M4940-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-4

Integration Parameters: RTEINT.P

Integrator: RTE

Soothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M

Title : SW846 8260

Signal : TIC: VX025562.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	32	rBV	3915	6238	1.27%	0.143%
2	1.746	103	108	119	rBV	20595	29057	5.91%	0.665%
3	2.209	180	184	193	rVB3	3028	5705	1.16%	0.131%
4	2.386	209	213	220	rVB	4024	6921	1.41%	0.158%
5	2.776	269	277	282	rBV	9177	20671	4.20%	0.473%
6	2.867	288	292	301	rVB2	7366	14602	2.97%	0.334%
7	2.965	301	308	319	rVV	33500	69298	14.08%	1.586%
8	3.117	322	333	346	rVB	24604	61297	12.46%	1.403%
9	3.770	428	440	446	rBV5	2235	8202	1.67%	0.188%
10	3.855	446	454	462	rVV6	2822	6957	1.41%	0.159%
11	4.306	519	528	539	rVB3	7725	21835	4.44%	0.500%
12	4.428	539	548	559	rBV8	1691	5577	1.13%	0.128%
13	5.391	695	706	715	rBV2	57811	167152	33.97%	3.825%
14	5.477	716	720	724	rVV4	5503	13121	2.67%	0.300%
15	5.556	724	733	756	rVB	97862	295929	60.14%	6.771%
16	5.842	771	780	789	rBV6	2615	7686	1.56%	0.176%
17	5.964	789	800	808	rVV	59773	162670	33.06%	3.722%
18	6.044	808	813	827	rVV2	10588	28727	5.84%	0.657%
19	6.245	827	846	857	rVV3	24041	79753	16.21%	1.825%
20	6.361	857	865	874	rVB5	5325	15757	3.20%	0.361%
21	6.769	921	932	943	rBV	148830	367169	74.62%	8.401%
22	6.861	943	947	955	rVB5	4069	10387	2.11%	0.238%
23	7.178	992	999	1007	rVB4	3991	8958	1.82%	0.205%
24	7.367	1022	1030	1040	rVB5	6358	17678	3.59%	0.404%
25	7.885	1105	1115	1122	rBV5	2724	9210	1.87%	0.211%
26	7.988	1122	1132	1142	rVB4	4684	13056	2.65%	0.299%
27	8.110	1144	1152	1155	rBV2	10454	21176	4.30%	0.485%
28	8.147	1155	1158	1163	rVV	9766	14956	3.04%	0.342%
29	8.312	1179	1185	1191	rBV6	2212	5386	1.09%	0.123%
30	8.427	1199	1204	1211	rVB	16470	26234	5.33%	0.600%
31	8.507	1211	1217	1226	rVB	24737	42040	8.54%	0.962%
32	8.653	1229	1241	1249	rBV	316170	492038	100.00%	11.258%
33	8.842	1266	1272	1281	rBV	22488	35592	7.23%	0.814%
34	8.964	1288	1292	1299	rVV4	5587	12814	2.60%	0.293%
35	9.049	1299	1306	1312	rVV5	5262	11359	2.31%	0.260%

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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

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 Title : SW846 8260

36	9.104	1312	1315	1320	rVV2	4058	6290	1.28%	0.144%
37	9.165	1320	1325	1334	rVB	15591	24589	5.00%	0.563%
38	9.458	1363	1373	1377	rBV4	13783	30302	6.16%	0.693%
39	9.500	1377	1380	1386	rVB6	4035	7469	1.52%	0.171%
40	9.567	1386	1391	1395	rBV2	9062	13790	2.80%	0.316%
41	9.762	1418	1423	1434	rBV5	4544	8859	1.80%	0.203%
42	10.055	1460	1471	1476	rBV	309435	437159	88.85%	10.003%
43	10.104	1476	1479	1482	rVV3	9725	15027	3.05%	0.344%
44	10.147	1482	1486	1492	rVV3	19877	31021	6.30%	0.710%
45	10.250	1496	1503	1507	rVV2	13514	27664	5.62%	0.633%
46	10.305	1507	1512	1517	rVB	18693	27937	5.68%	0.639%
47	10.415	1525	1530	1534	rBV4	4186	6792	1.38%	0.155%
48	10.793	1584	1592	1598	rBV4	6048	14367	2.92%	0.329%
49	10.848	1598	1601	1606	rVV4	4954	9112	1.85%	0.208%
50	10.903	1606	1610	1613	rVV3	5762	9055	1.84%	0.207%
51	10.963	1617	1620	1625	rVB	11021	14668	2.98%	0.336%
52	11.085	1635	1640	1650	rVV	242650	310794	63.16%	7.111%
53	11.177	1650	1655	1662	rVB2	5411	9527	1.94%	0.218%
54	11.274	1667	1671	1673	rVV2	7735	10153	2.06%	0.232%
55	11.305	1673	1676	1686	rVB	19859	29028	5.90%	0.664%
56	11.396	1686	1691	1695	rBV6	3554	6388	1.30%	0.146%
57	11.439	1695	1698	1700	rVV3	4669	6585	1.34%	0.151%
58	11.463	1700	1702	1710	rVB3	4784	6519	1.32%	0.149%
59	11.616	1721	1727	1731	rBV	6110	8899	1.81%	0.204%
60	11.713	1735	1743	1747	rVB6	3494	7054	1.43%	0.161%
61	11.890	1764	1772	1778	rBV7	5906	12678	2.58%	0.290%
62	12.024	1789	1794	1801	rVB	299377	368616	74.92%	8.434%
63	12.097	1801	1806	1816	rBV7	5069	13936	2.83%	0.319%
64	12.177	1816	1819	1824	rVB	10370	13208	2.68%	0.302%
65	12.244	1824	1830	1835	rBV	141977	180112	36.61%	4.121%
66	12.317	1838	1842	1851	rVV	56719	68616	13.95%	1.570%
67	12.408	1853	1857	1861	rVV	17820	21195	4.31%	0.485%
68	12.616	1886	1891	1894	rBV	12038	13812	2.81%	0.316%
69	12.646	1894	1896	1900	rVV3	5542	6572	1.34%	0.150%
70	12.701	1900	1905	1912	rVV3	33713	61024	12.40%	1.396%
71	12.762	1912	1915	1920	rVB	8015	10291	2.09%	0.235%
72	12.841	1922	1928	1935	rVB	19304	25195	5.12%	0.576%
73	12.927	1935	1942	1947	rBV2	17366	28599	5.81%	0.654%
74	13.036	1954	1960	1965	rVB	17817	22602	4.59%	0.517%
75	13.116	1968	1973	1974	rBV	4633	5551	1.13%	0.127%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

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Max Peaks: 100

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Peak Location: TOP

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76	13.140	1974	1977	1979	rVV2	7261	9562	1.94%	0.219%
77	13.170	1979	1982	1984	rVV	16101	20853	4.24%	0.477%
78	13.195	1984	1986	1991	rVB	22085	24117	4.90%	0.552%
79	13.292	1998	2002	2007	rVB2	25129	31819	6.47%	0.728%
80	13.347	2007	2011	2015	rVB2	6348	8427	1.71%	0.193%
81	13.426	2020	2024	2031	rVB	17919	22083	4.49%	0.505%
82	13.518	2031	2039	2041	rBV4	3245	5740	1.17%	0.131%
83	13.548	2041	2044	2046	rVV3	6777	8516	1.73%	0.195%
84	13.585	2046	2050	2053	rVV4	7895	12015	2.44%	0.275%
85	13.622	2053	2056	2057	rVV2	15034	17384	3.53%	0.398%
86	13.646	2057	2060	2061	rVV	16722	21909	4.45%	0.501%
87	13.664	2061	2063	2068	rVB	20627	24072	4.89%	0.551%
88	13.798	2080	2085	2091	rVB4	4310	9741	1.98%	0.223%
89	13.926	2099	2106	2110	rBV3	6238	9776	1.99%	0.224%
90	14.079	2126	2131	2137	rBV	23621	28751	5.84%	0.658%
91	14.225	2149	2155	2158	rBV2	4059	7628	1.55%	0.175%
92	14.323	2167	2171	2176	rBV2	12936	16442	3.34%	0.376%
93	14.378	2176	2180	2189	rVB2	11797	16815	3.42%	0.385%
94	14.597	2211	2216	2220	rBV	13315	18767	3.81%	0.429%
95	14.786	2243	2247	2252	rBV4	6247	9788	1.99%	0.224%

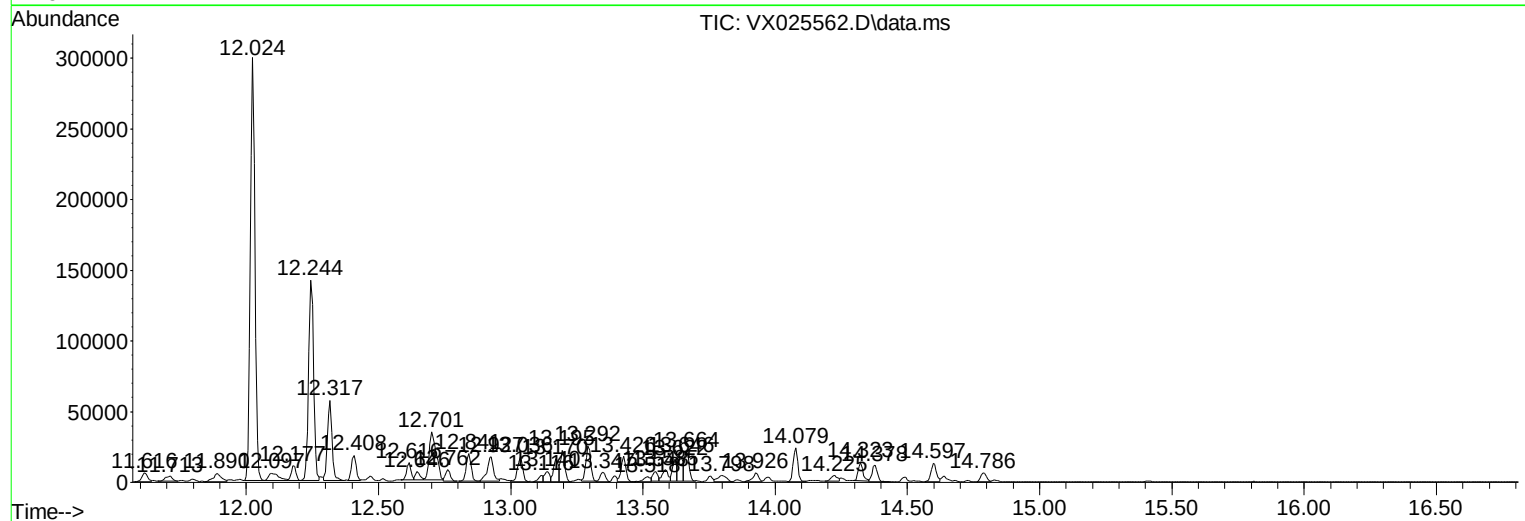
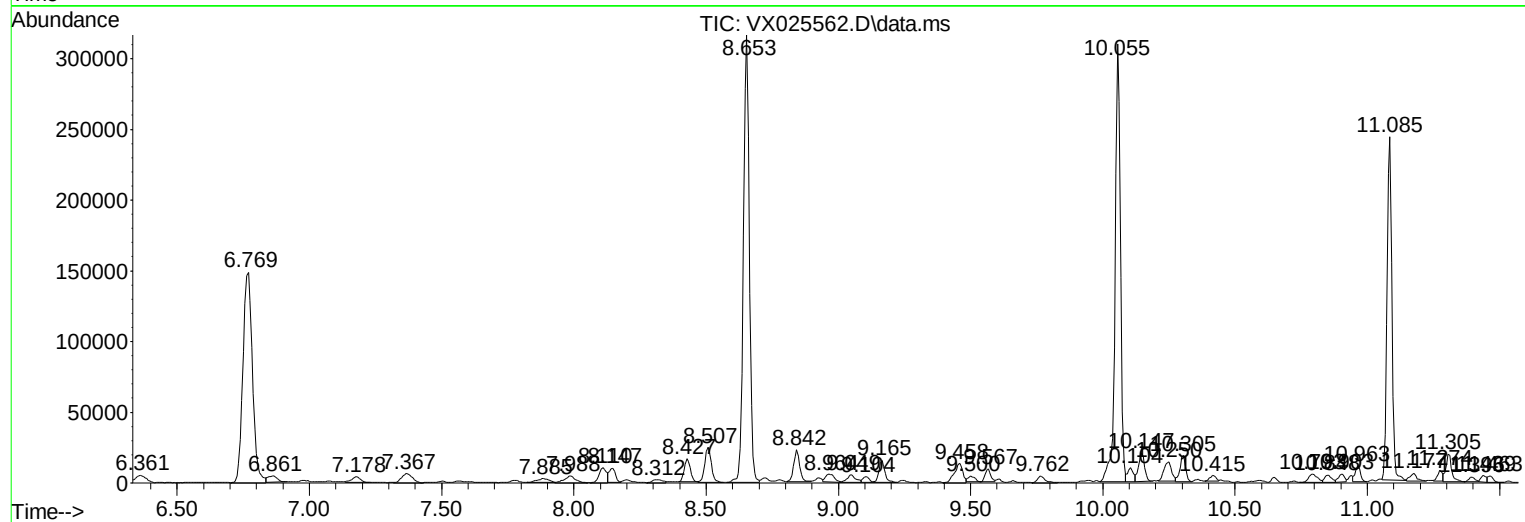
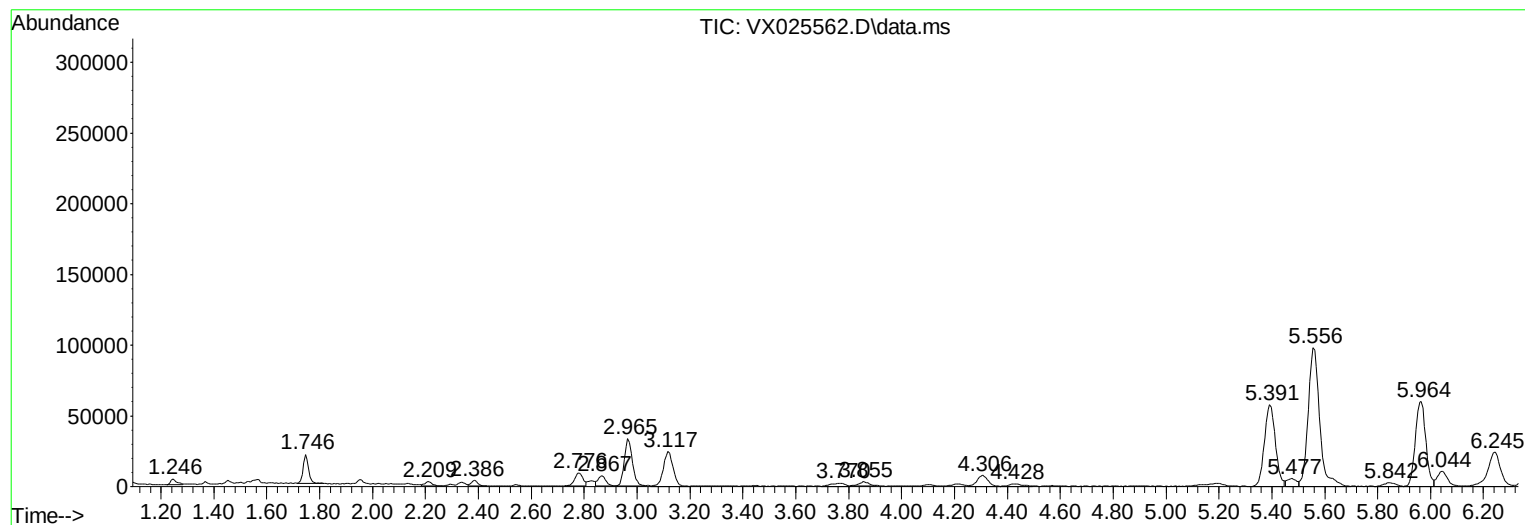
Sum of corrected areas: 4370468

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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



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Instrument :
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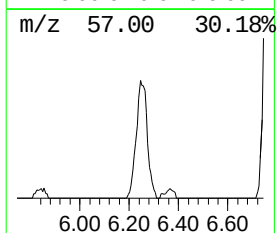
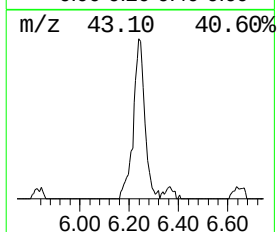
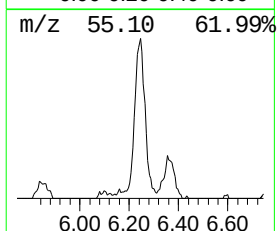
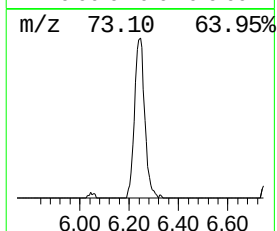
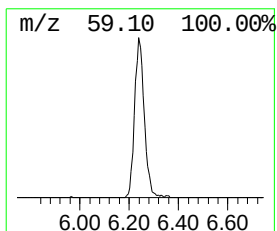
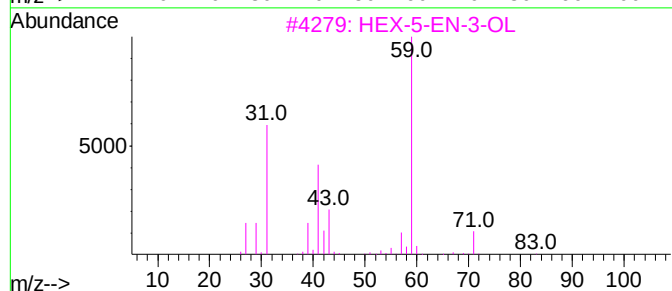
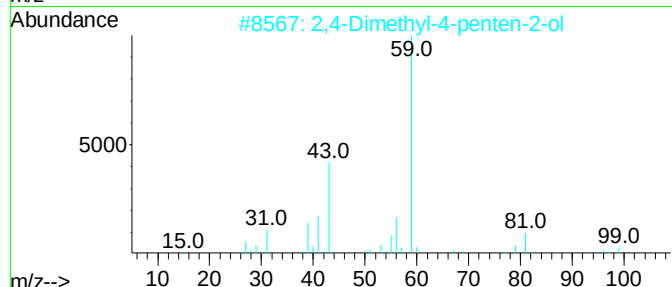
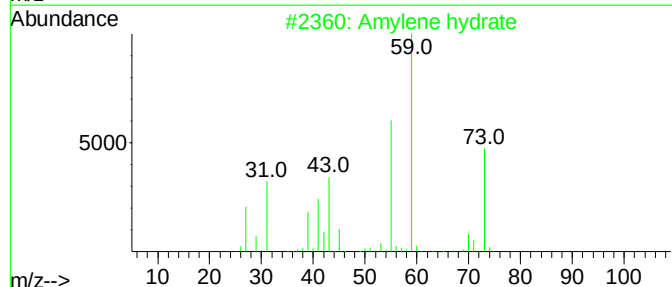
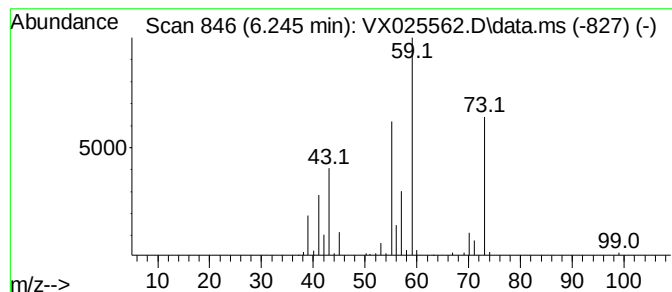
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 1 Amylene hydrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.245	10.86 ug/l	79753	1,4-Difluorobenzene	6.769

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Amylene hydrate	88	C5H12O	000075-85-4	78
2		2,4-Dimethyl-4-penten-2-ol	114	C7H14O	019781-53-4	50
3		HEX-5-EN-3-OL	100	C6H12O	000688-99-3	50
4		2,3-Butanediol, 2,3-dimethyl-	118	C6H14O2	000076-09-5	40
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	38



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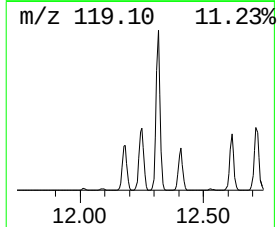
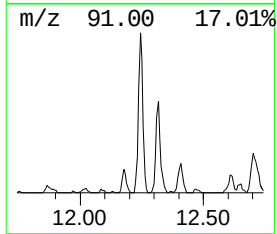
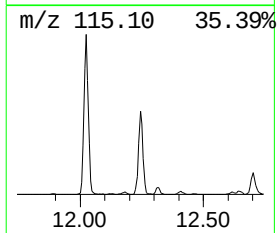
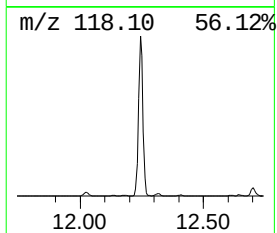
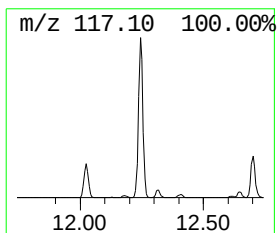
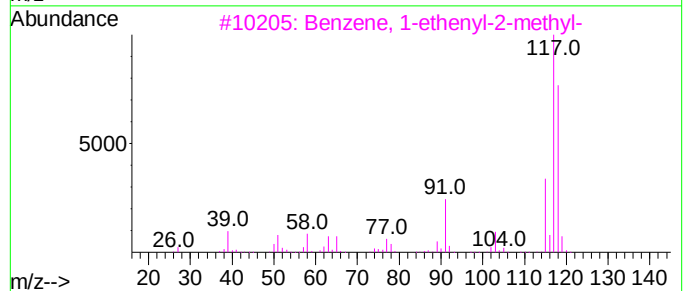
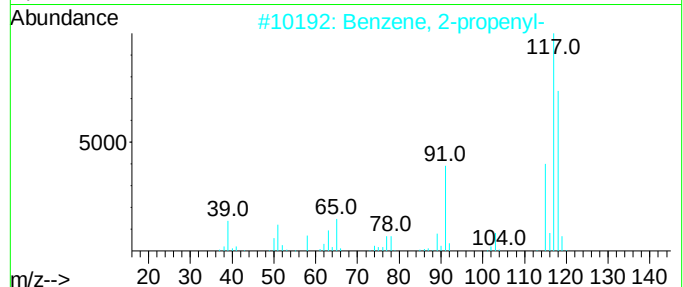
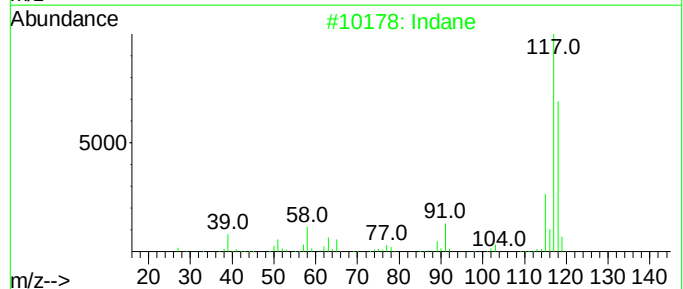
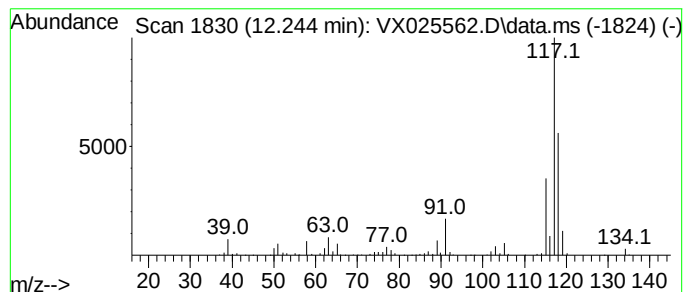
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 2 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	24.43 ug/l	180112	1,4-Dichlorobenzene-d4	12.024

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane		118	C9H10	000496-11-7	87
2	Benzene, 2-propenyl-		118	C9H10	000300-57-2	74
3	Benzene, 1-ethenyl-2-methyl-		118	C9H10	000611-15-4	74
4	Deltacyclene		118	C9H10	007785-10-6	50
5	Benzene, 1,1'-(1-ethenyl-1,3-pro...		222	C17H18	061141-97-7	50



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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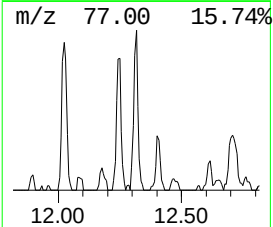
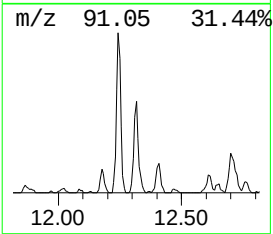
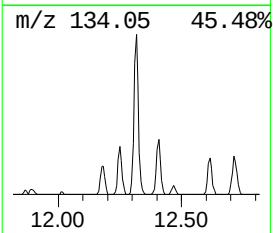
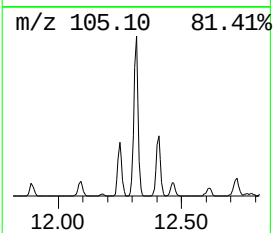
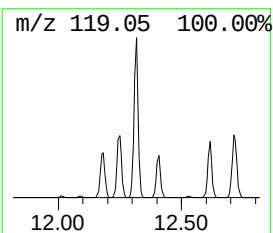
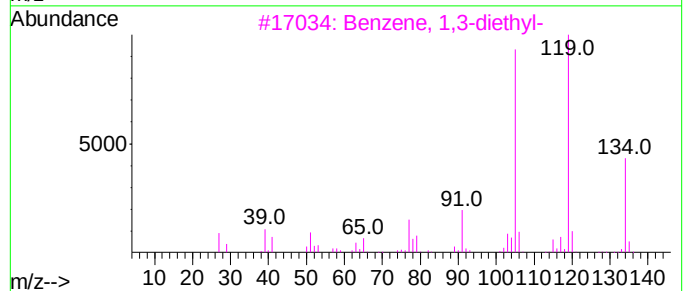
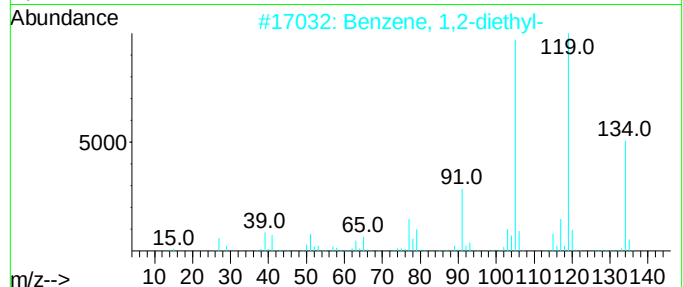
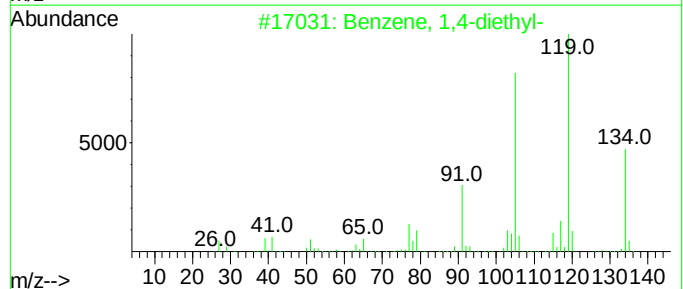
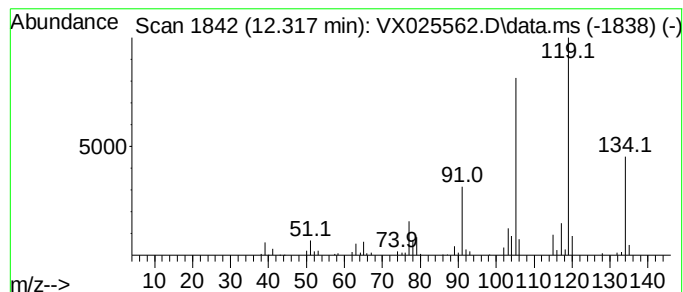
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1,4-diethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.317	9.31 ug/l	68616	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	96
2			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
3			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	95
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120621\
Data File : VX025562.D
Acq On : 06 Dec 2021 20:26
Operator : JC/MD
Sample : M4940-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

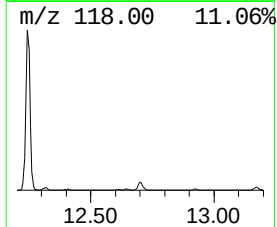
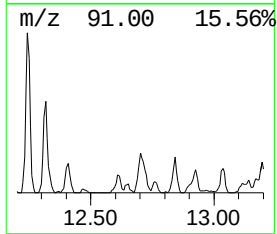
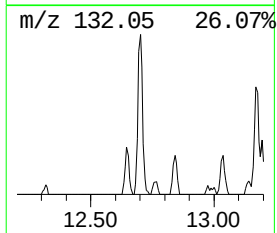
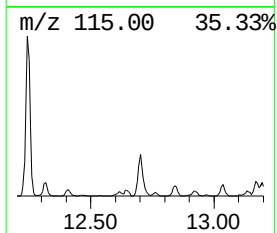
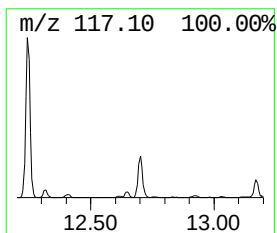
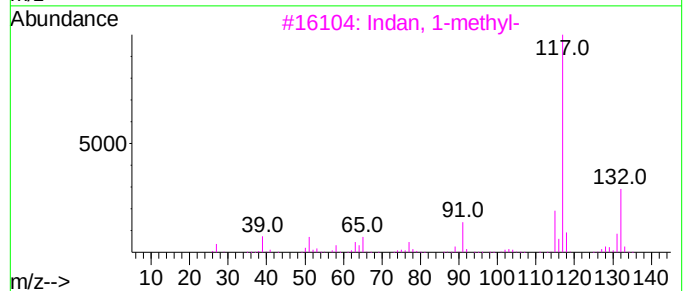
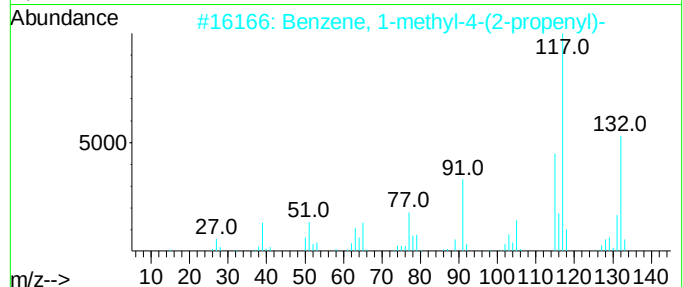
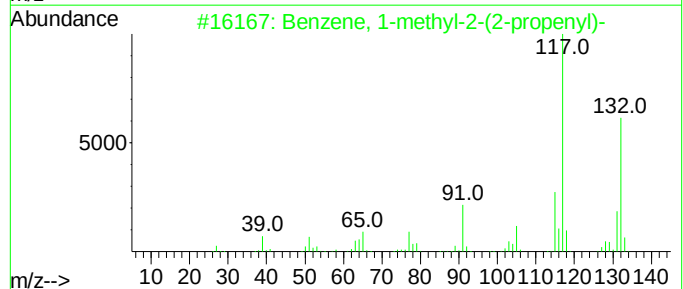
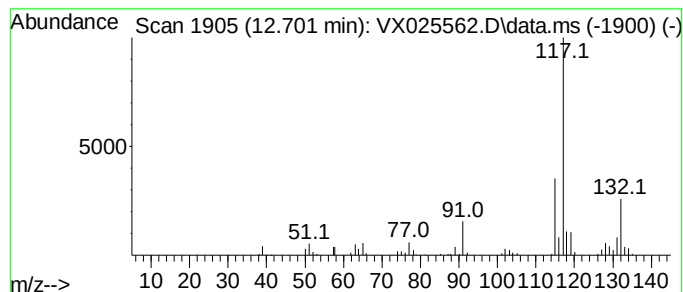
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	8.28 ug/l	61024	1,4-Dichlorobenzene-d4	12.024

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87
2		Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	87
3		Indan, 1-methyl-	132	C10H12	000767-58-8	87
4		1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	86
5		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120621\
Data File : VX025562.D
Acq On : 06 Dec 2021 20:26
Operator : JC/MD
Sample : M4940-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
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
Amylene hydrate	6.245	10.9	ug/l	79753	2	6.769	367169	50.0
Indane	12.244	24.4	ug/l	180112	4	12.024	368616	50.0
Benzene, 1,4-di...	12.317	9.3	ug/l	68616	4	12.024	368616	50.0
Benzene, 1-meth...	12.701	8.3	ug/l	61024	4	12.024	368616	50.0