

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042121\
 Data File : VX021794.D
 Acq On : 21 Apr 2021 15:49
 Operator : JC/MD
 Sample : M2079-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-06

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\82X042021W.M
 Title : SW846 8260

Signal : TIC: VX021794.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.343	35	42	45	rBV6	3842	10732	1.16%	0.124%
2	2.825	277	285	289	rBV2	11650	25406	2.76%	0.294%
3	3.154	331	339	348	rBB4	9309	23856	2.59%	0.276%
4	4.282	514	524	532	rBV2	14721	44499	4.83%	0.515%
5	4.373	532	539	552	rVB4	11392	31699	3.44%	0.367%
6	5.208	667	676	689	rVB8	3704	14215	1.54%	0.165%
7	5.464	706	718	728	rBV	104341	300061	32.56%	3.474%
8	5.629	735	745	752	rBV	168466	484248	52.55%	5.607%
9	5.696	752	756	767	rVB3	47522	127258	13.81%	1.473%
10	5.891	779	788	800	rBV7	4197	15123	1.64%	0.175%
11	6.031	800	811	819	rVV	103614	274080	29.74%	3.173%
12	6.111	819	824	836	rVV2	19035	51324	5.57%	0.594%
13	6.318	838	858	869	rVV	102490	334776	36.33%	3.876%
14	6.434	869	877	884	rVB4	5814	16294	1.77%	0.189%
15	6.830	932	942	952	rBV	269644	640394	69.49%	7.415%
16	7.427	1030	1040	1050	rBV6	13035	39349	4.27%	0.456%
17	7.549	1053	1060	1065	rBV2	10493	21296	2.31%	0.247%
18	7.616	1065	1071	1074	rVV3	10035	20447	2.22%	0.237%
19	7.659	1074	1078	1083	rVV	8518	17097	1.86%	0.198%
20	7.824	1098	1105	1112	rVB5	5296	10457	1.13%	0.121%
21	8.037	1130	1140	1150	rVB	86608	175332	19.03%	2.030%
22	8.159	1150	1160	1168	rBV	120381	250796	27.21%	2.904%
23	8.549	1218	1224	1234	rVB4	8595	18870	2.05%	0.218%
24	8.696	1234	1248	1258	rBV	565690	921586	100.00%	10.671%
25	9.013	1296	1300	1306	rVB5	4472	9274	1.01%	0.107%
26	9.147	1314	1322	1327	rVB2	6639	13419	1.46%	0.155%
27	9.202	1327	1331	1335	rBV	12514	19300	2.09%	0.223%
28	10.092	1472	1477	1496	rVB	522102	739614	80.25%	8.564%
29	10.232	1496	1500	1505	rBV	11050	14275	1.55%	0.165%
30	10.342	1510	1518	1523	rVB	11940	20836	2.26%	0.241%
31	11.000	1621	1626	1633	rBV	171510	214774	23.30%	2.487%
32	11.122	1640	1646	1658	rVB	439930	582704	63.23%	6.747%
33	11.341	1677	1682	1690	rVB	340788	404683	43.91%	4.686%
34	11.652	1729	1733	1737	rBV	14226	18536	2.01%	0.215%
35	11.786	1752	1755	1759	rVB	9041	11327	1.23%	0.131%
36	11.902	1768	1774	1776	rBV	36374	46651	5.06%	0.540%

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37	11.927	1776	1778	1783	rVB	33394	37887	4.11%	0.439%
38	12.061	1794	1800	1808	rBV	602786	723873	78.55%	8.381%
39	12.280	1831	1836	1842	rVV	408745	514116	55.79%	5.953%
40	12.353	1842	1848	1855	rVV2	63062	93114	10.10%	1.078%
41	12.445	1858	1863	1868	rVV	36558	47101	5.11%	0.545%
42	12.512	1868	1874	1879	rVB2	15348	23836	2.59%	0.276%
43	12.652	1891	1897	1900	rBV	230607	273566	29.68%	3.168%
44	12.683	1900	1902	1906	rVV	18049	20044	2.17%	0.232%
45	12.737	1906	1911	1919	rVV2	122358	179837	19.51%	2.082%
46	12.878	1926	1934	1939	rVB3	6563	10935	1.19%	0.127%
47	12.957	1939	1947	1953	rBV	147247	190119	20.63%	2.201%
48	13.061	1960	1964	1972	rVB2	13291	20276	2.20%	0.235%
49	13.152	1972	1979	1981	rBV4	12052	19574	2.12%	0.227%
50	13.207	1985	1988	1996	rVB	34854	45718	4.96%	0.529%
51	13.329	2004	2008	2014	rVB3	38083	55892	6.06%	0.647%
52	13.408	2018	2021	2026	rVV	9243	14530	1.58%	0.168%
53	13.463	2026	2030	2034	rVB3	10680	13718	1.49%	0.159%
54	13.585	2045	2050	2052	rBV	11905	15534	1.69%	0.180%
55	13.615	2052	2055	2059	rVB2	22324	26227	2.85%	0.304%
56	13.676	2059	2065	2068	rBV3	9177	16576	1.80%	0.192%
57	13.713	2068	2071	2076	rVB2	14264	20077	2.18%	0.232%
58	13.817	2078	2088	2097	rBV	117461	152807	16.58%	1.769%
59	13.969	2105	2113	2116	rBV5	6127	10167	1.10%	0.118%
60	14.115	2132	2137	2142	rBV	10879	13998	1.52%	0.162%
61	14.256	2154	2160	2164	rBV2	8468	14606	1.58%	0.169%
62	14.359	2171	2177	2181	rBV	22802	30215	3.28%	0.350%
63	14.414	2181	2186	2190	rVB	7684	10376	1.13%	0.120%
64	14.822	2246	2253	2262	rVB	33353	47170	5.12%	0.546%
65	16.389	2503	2510	2520	rVB2	15898	30117	3.27%	0.349%

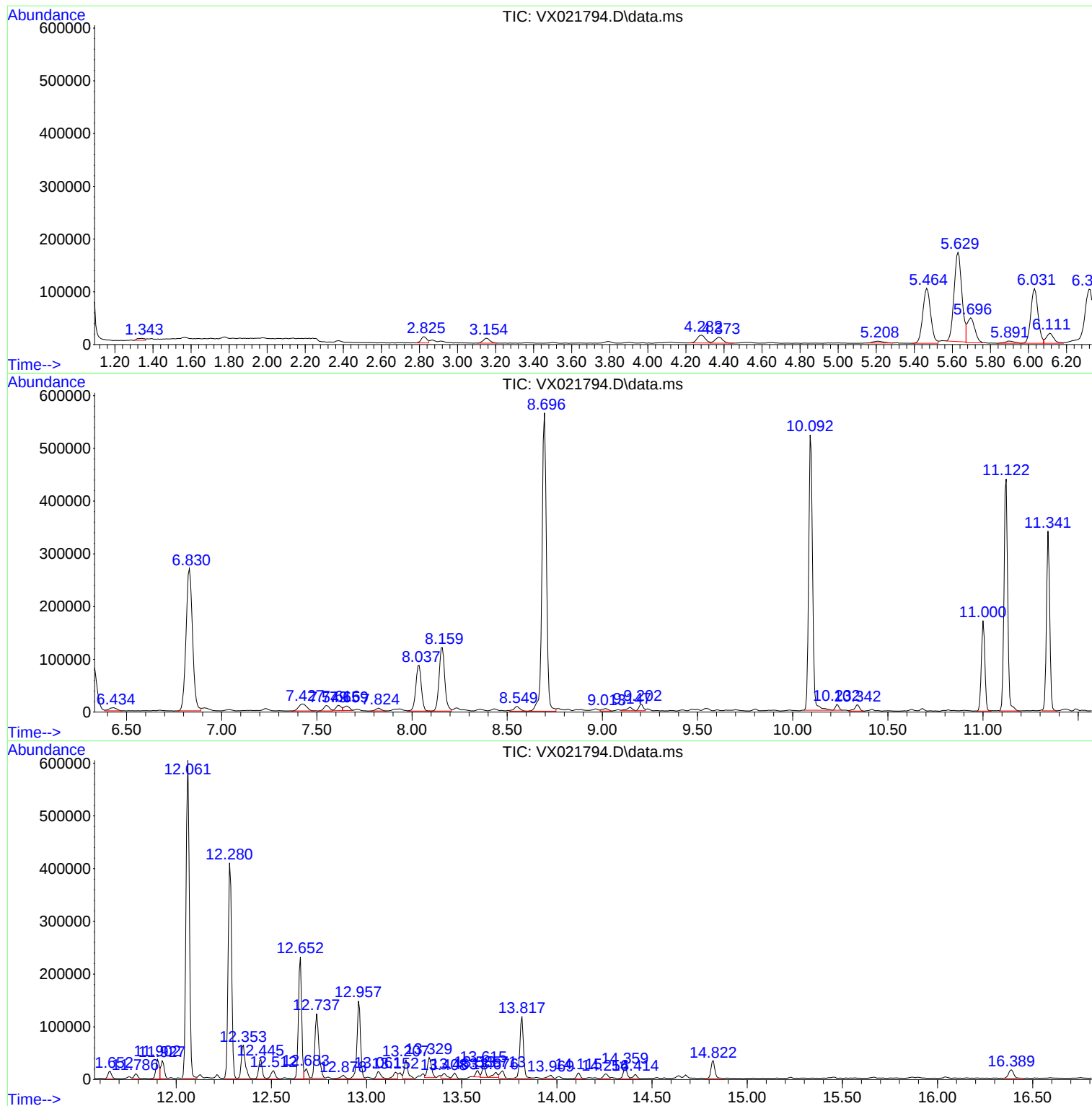
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Quant Title : SW846 8260

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



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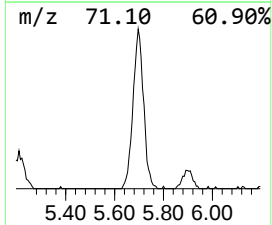
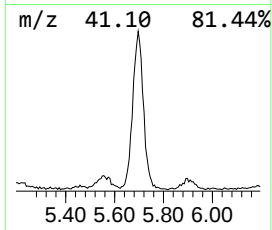
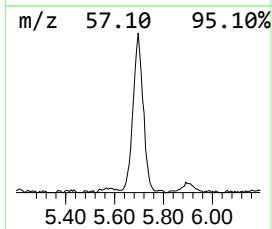
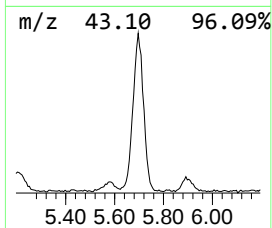
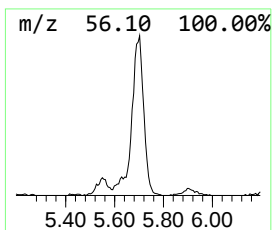
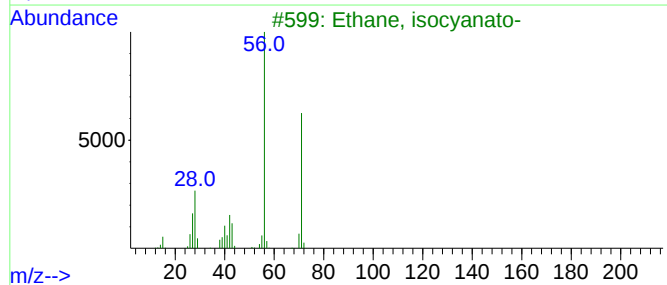
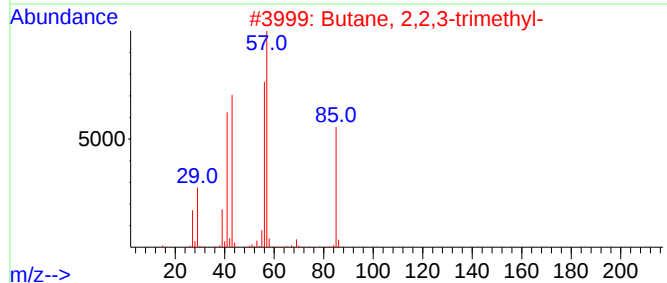
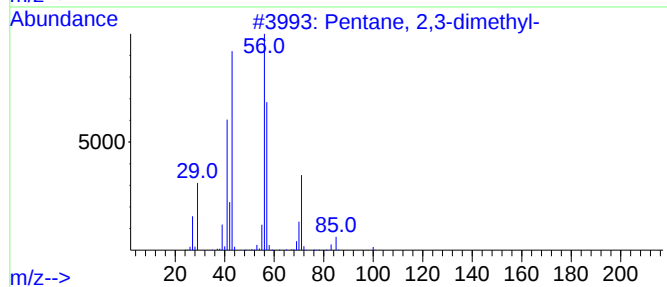
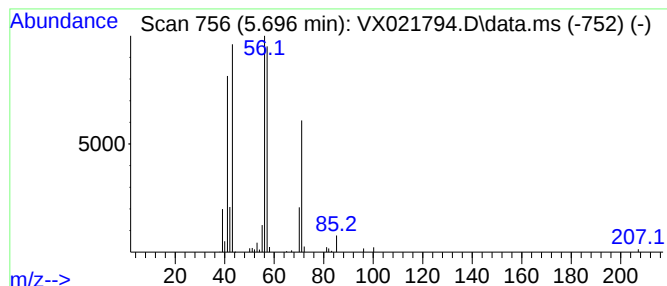
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.696	13.14 ug/l	127258	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	83
2			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	50
3			Ethane, isocyanato-	71	C3H5NO	000109-90-0	50
4			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	38
5			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	38



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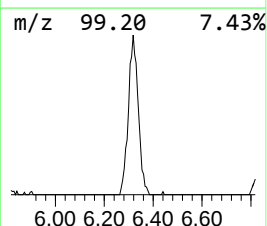
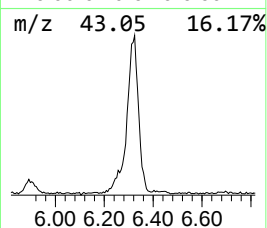
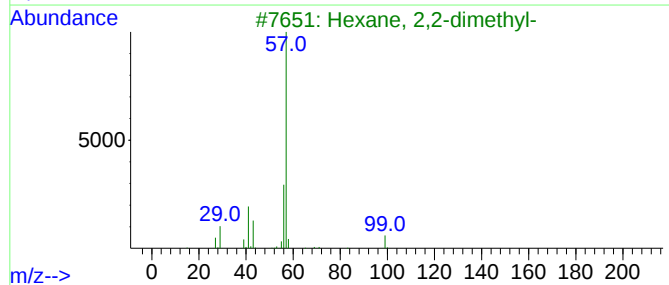
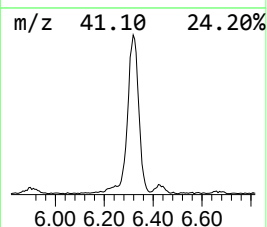
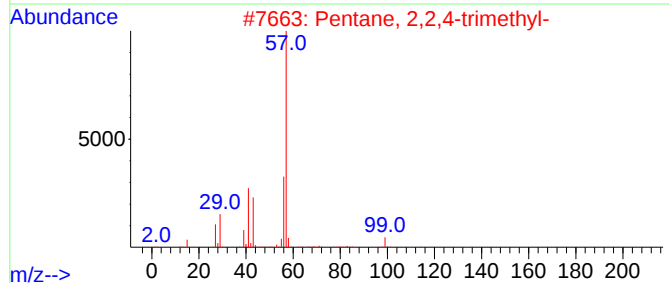
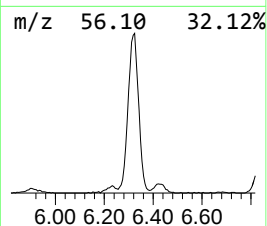
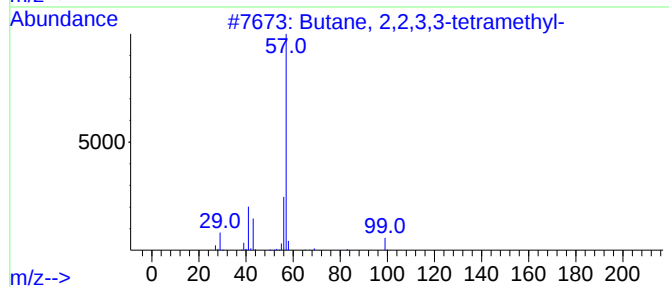
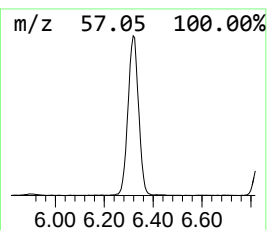
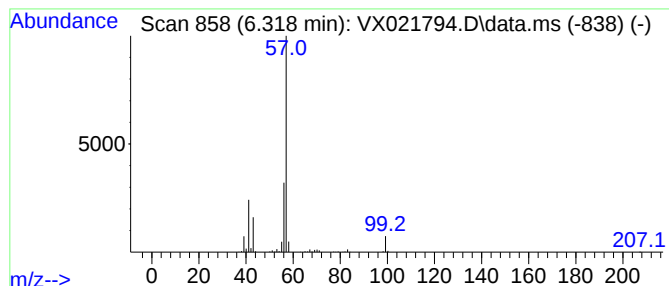
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2,2,3,3-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.318	26.14 ug/l	334776	1,4-Difluorobenzene	6.830

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



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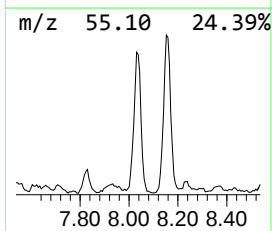
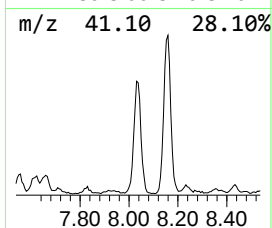
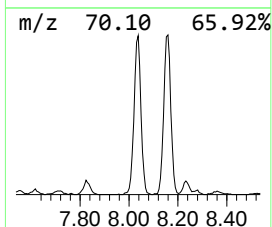
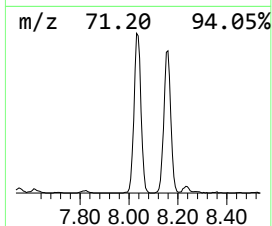
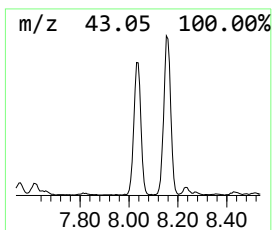
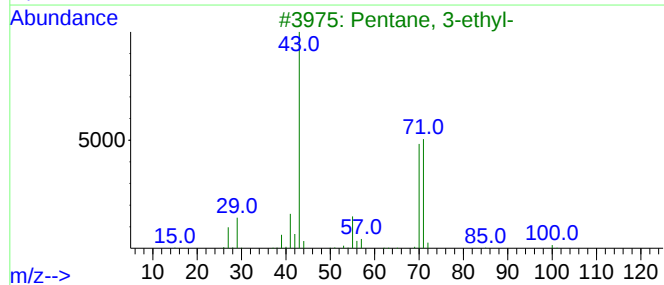
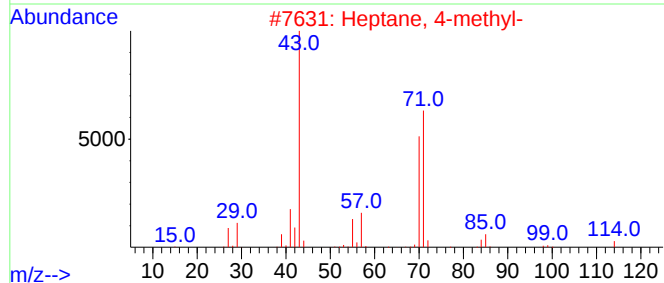
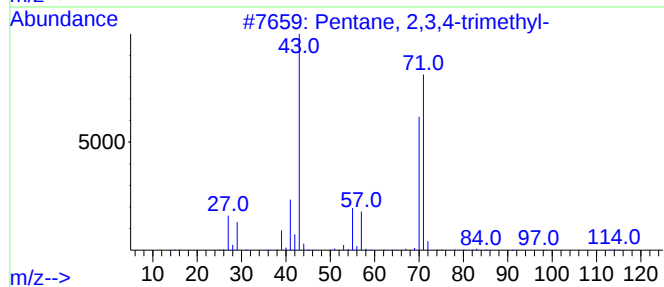
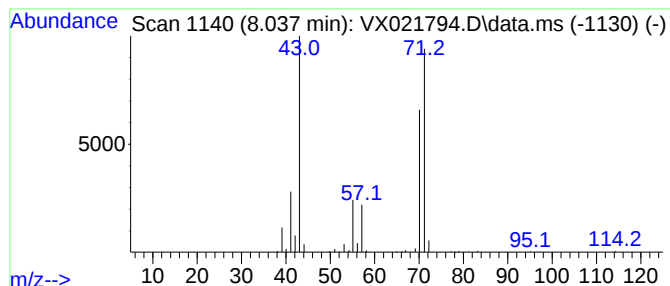
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane, 2,3,4-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.037	13.69 ug/l	175332	1,4-Difluorobenzene	6.830

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
4			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	78
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	78



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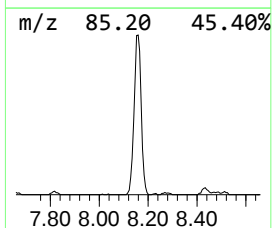
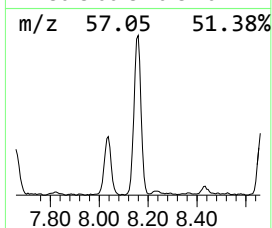
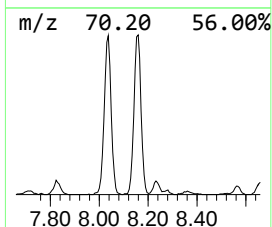
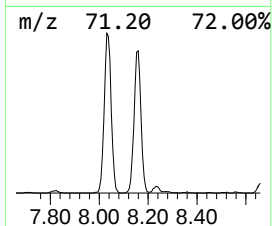
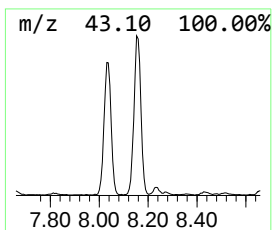
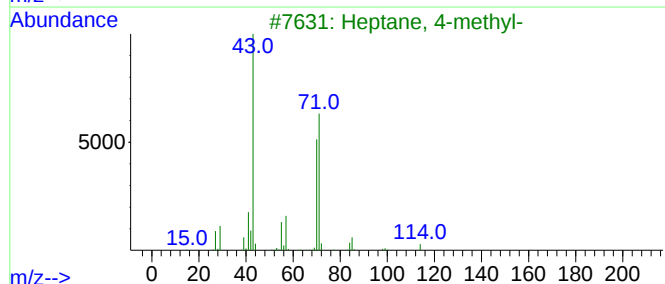
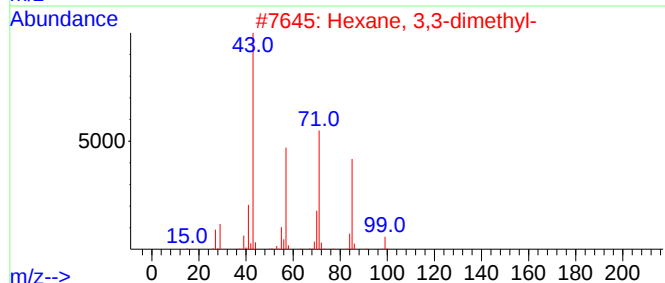
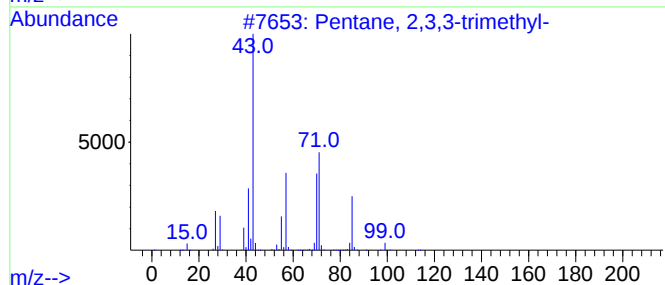
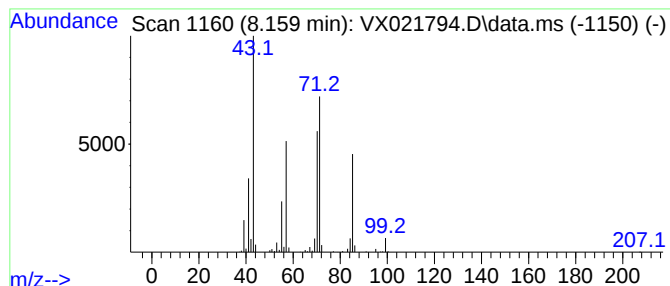
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2,3,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.159	19.58 ug/l	250796	1,4-Difluorobenzene	6.830

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	53
4			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	50
5			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	50



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ClientSampleId :
MW-06

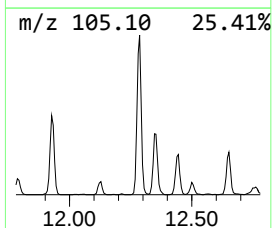
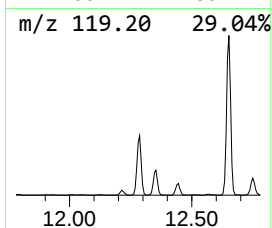
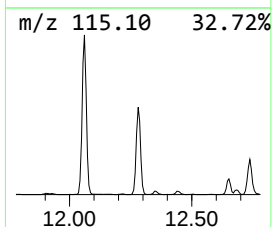
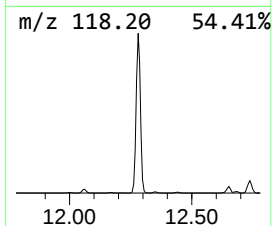
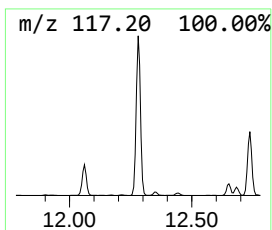
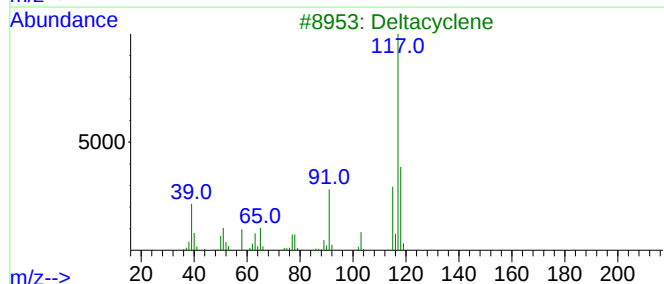
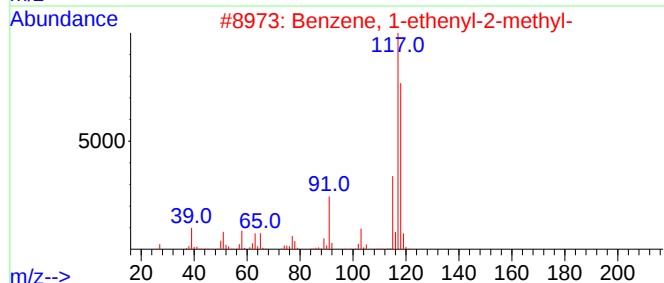
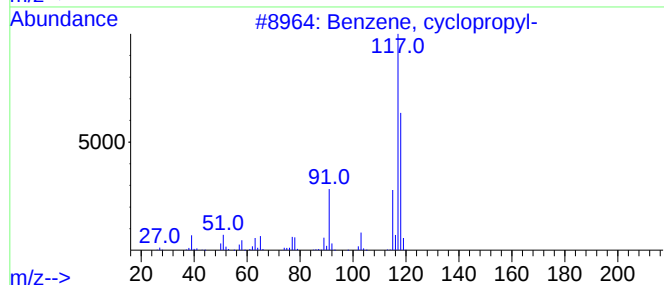
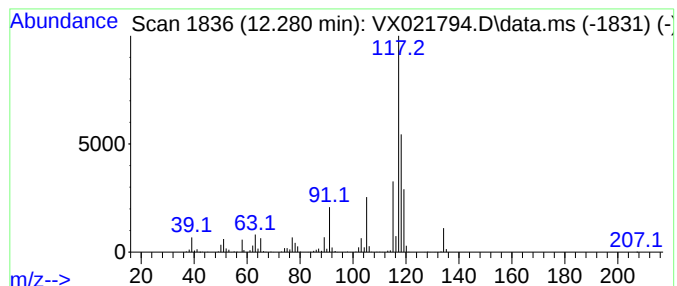
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, cyclopropyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.280	35.51 ug/l	514116	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, cyclopropyl-	118	C9H10	000873-49-4	91
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	91
3			Deltacyclene	118	C9H10	007785-10-6	64
4			Indane	118	C9H10	000496-11-7	64
5			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042121\
Data File : VX021794.D
Acq On : 21 Apr 2021 15:49
Operator : JC/MD
Sample : M2079-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

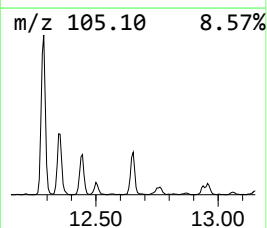
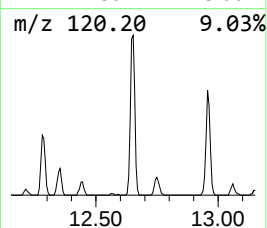
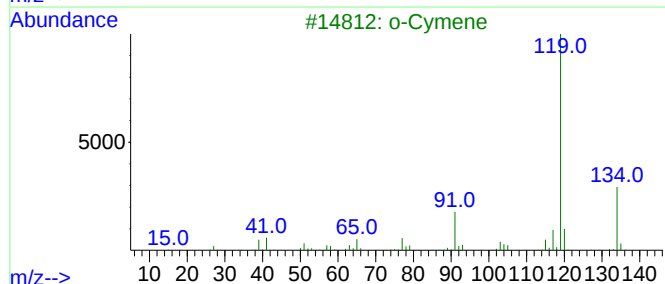
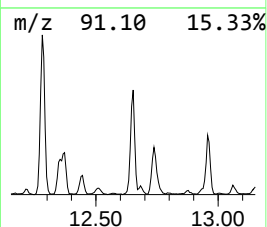
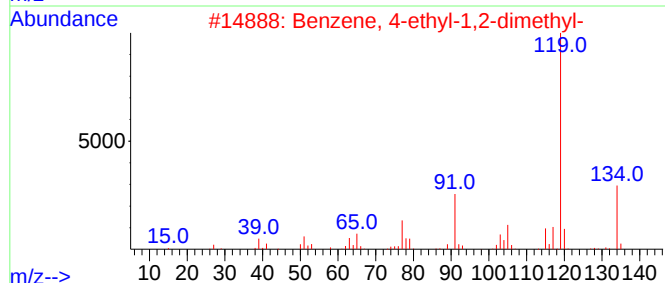
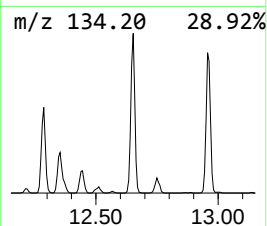
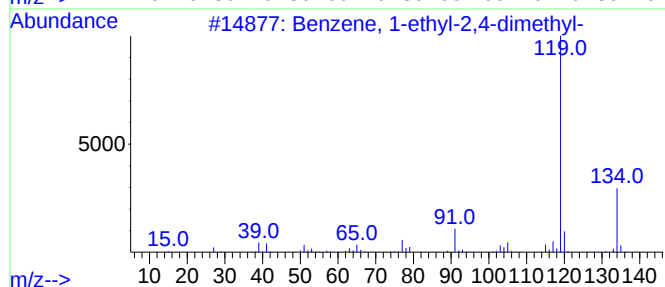
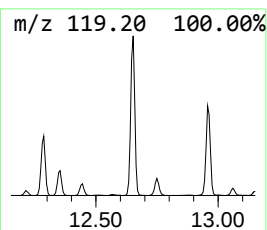
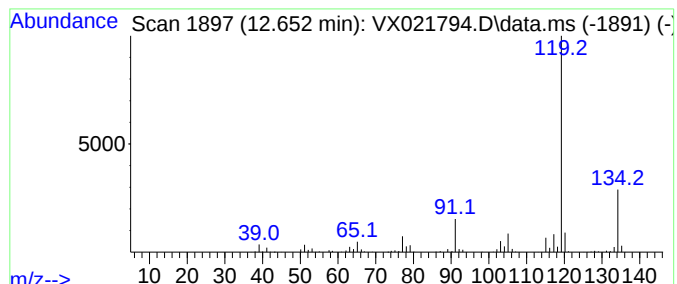
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.652	18.90 ug/l	273566	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			o-Cymene	134	C10H14	000527-84-4	95
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042121\
Data File : VX021794.D
Acq On : 21 Apr 2021 15:49
Operator : JC/MD
Sample : M2079-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

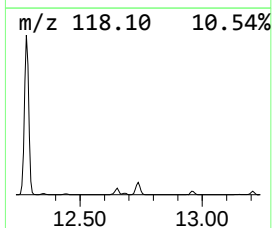
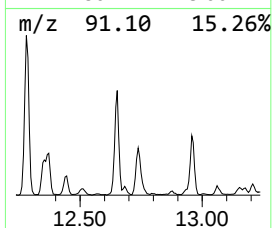
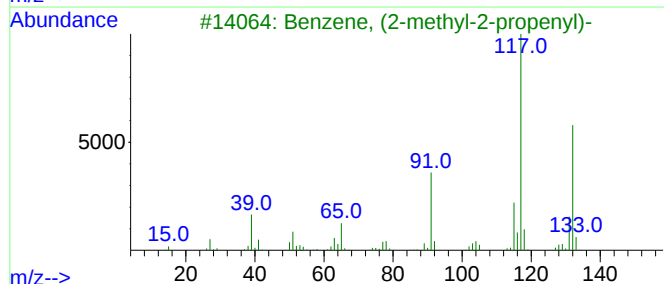
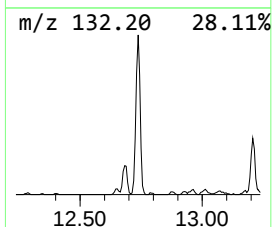
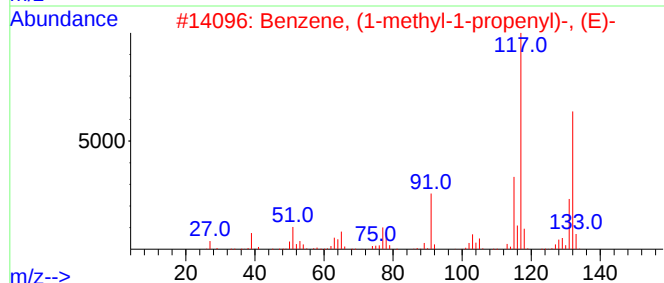
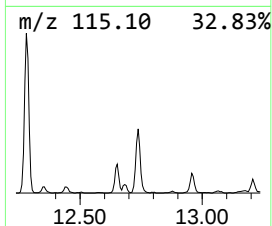
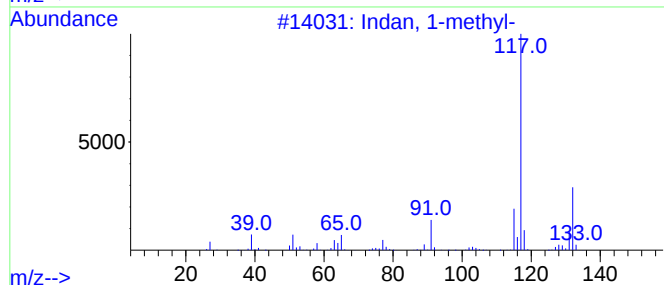
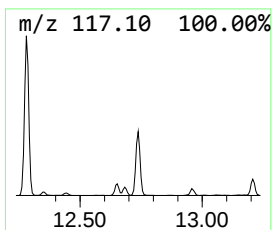
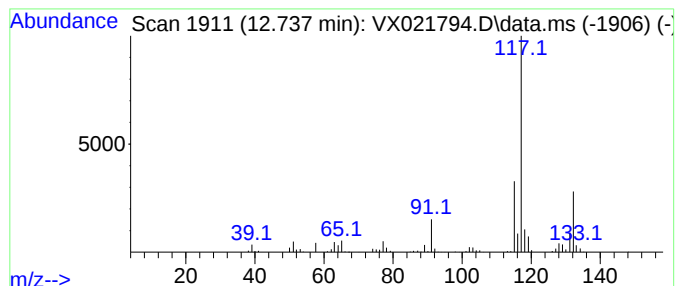
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

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

Peak Number 7 Indan, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.738	12.42 ug/l	179837	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	93
2			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
3			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	87
4			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	86
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042121\
Data File : VX021794.D
Acq On : 21 Apr 2021 15:49
Operator : JC/MD
Sample : M2079-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

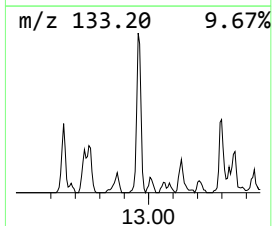
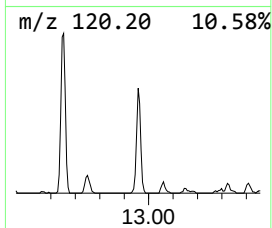
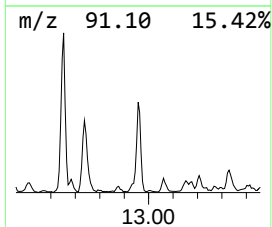
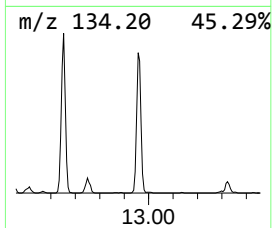
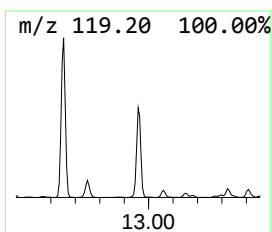
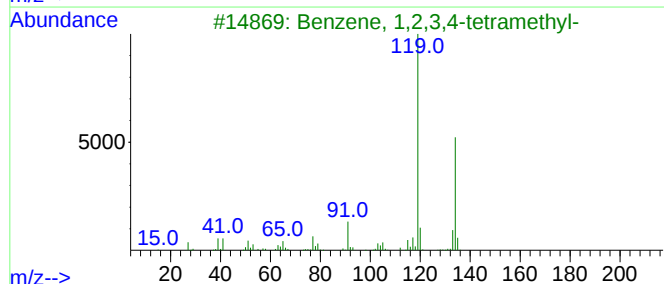
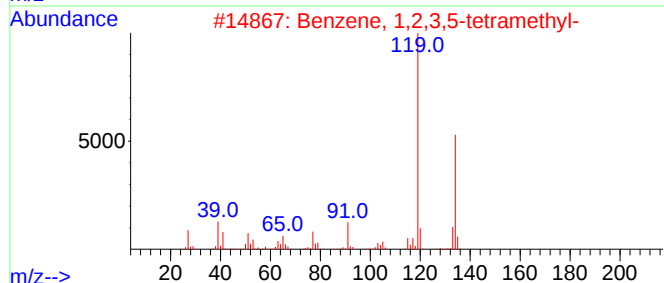
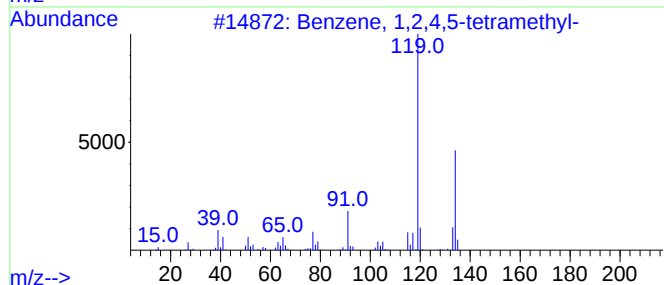
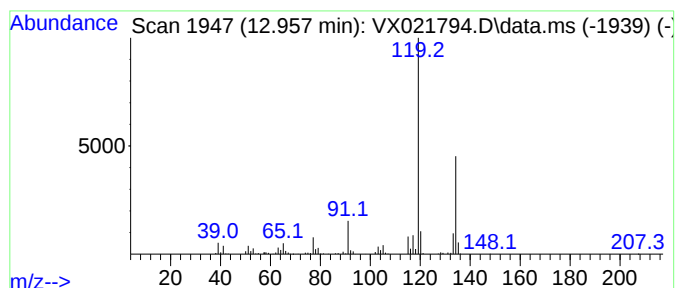
Instrument :
MSVOA_X
ClientSampleId :
MW-06

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.957	13.13 ug/l	190119	1,4-Dichlorobenzene-d4		12.061	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-		134	C10H14	000095-93-2	97
2	Benzene, 1,2,3,5-tetramethyl-		134	C10H14	000527-53-7	97
3	Benzene, 1,2,3,4-tetramethyl-		134	C10H14	000488-23-3	97
4	o-Cymene		134	C10H14	000527-84-4	95
5	Benzene, 1-ethyl-2,4-dimethyl-		134	C10H14	000874-41-9	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042121\
Data File : VX021794.D
Acq On : 21 Apr 2021 15:49
Operator : JC/MD
Sample : M2079-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
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
Pentane, 2,3-di...	5.696	13.1	ug/l	127258	1	5.629	484248	50.0
Butane, 2,2,3,3...	6.318	26.1	ug/l	334776	2	6.830	640394	50.0
Pentane, 2,3,4-...	8.037	13.7	ug/l	175332	2	6.830	640394	50.0
Pentane, 2,3,3-...	8.159	19.6	ug/l	250796	2	6.830	640394	50.0
Benzene, cyclop...	12.280	35.5	ug/l	514116	4	12.061	723873	50.0
Benzene, 1-ethy...	12.652	18.9	ug/l	273566	4	12.061	723873	50.0
Indan, 1-methyl-	12.738	12.4	ug/l	179837	4	12.061	723873	50.0
Benzene, 1,2,4,...	12.957	13.1	ug/l	190119	4	12.061	723873	50.0