

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN110423\
 Data File : VN079908.D
 Acq On : 04 Nov 2023 21:15
 Operator : JC\MD
 Sample : 05102-10 20X
 Misc : 3.28g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 67S-SB14-1216

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\82N110123W.M
 Title : SW846 8260

Signal : TIC: VN079908.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	51	57	67	rBV	35857	83481	4.25%	0.466%
2	3.236	212	218	230	rVB7	11620	31995	1.63%	0.179%
3	5.341	570	576	590	rVB5	14069	45597	2.32%	0.255%
4	5.818	655	657	667	rVB2	13182	22991	1.17%	0.128%
5	7.330	906	914	924	rVB3	8492	22560	1.15%	0.126%
6	8.171	1046	1057	1061	rBV	247336	583667	29.74%	3.260%
7	8.229	1061	1067	1079	rVV	354621	892078	45.45%	4.983%
8	8.329	1079	1084	1096	rVB5	12883	30060	1.53%	0.168%
9	8.447	1096	1104	1112	rBV2	32650	77273	3.94%	0.432%
10	8.582	1119	1127	1137	rVB	259815	594315	30.28%	3.320%
11	8.718	1142	1150	1157	rVV6	12746	31829	1.62%	0.178%
12	8.794	1157	1163	1168	rVV5	11133	24376	1.24%	0.136%
13	8.859	1168	1174	1182	rVB3	21856	44573	2.27%	0.249%
14	9.106	1206	1216	1231	rBV	575327	1170939	59.66%	6.540%
15	9.606	1284	1301	1315	rBV2	115420	290541	14.80%	1.623%
16	9.782	1323	1331	1336	rBV5	13067	25365	1.29%	0.142%
17	9.865	1340	1345	1355	rVB5	9240	21843	1.11%	0.122%
18	10.012	1363	1370	1376	rVB3	12905	26241	1.34%	0.147%
19	10.241	1405	1409	1417	rVB5	16072	31532	1.61%	0.176%
20	10.341	1419	1426	1438	rBV4	28703	73155	3.73%	0.409%
21	10.571	1457	1465	1471	rBV	1023893	1862294	94.88%	10.402%
22	10.635	1471	1476	1482	rVB	346109	623561	31.77%	3.483%
23	10.753	1489	1496	1503	rVB6	25476	62815	3.20%	0.351%
24	10.918	1518	1524	1532	rVB2	26026	52501	2.67%	0.293%
25	11.006	1532	1539	1547	rBV7	17325	43329	2.21%	0.242%
26	11.088	1549	1553	1560	rVB4	12815	24910	1.27%	0.139%
27	11.176	1560	1568	1574	rBV2	44780	82861	4.22%	0.463%
28	11.276	1579	1585	1593	rVB2	21496	40179	2.05%	0.224%
29	11.353	1593	1598	1602	rBV5	12087	20907	1.07%	0.117%
30	11.423	1602	1610	1614	rVV4	39267	74470	3.79%	0.416%
31	11.470	1614	1618	1625	rVB2	74863	134283	6.84%	0.750%
32	11.576	1631	1636	1641	rBV2	31035	45774	2.33%	0.256%
33	11.641	1641	1647	1651	rBV3	27044	50163	2.56%	0.280%
34	11.747	1660	1665	1672	rBV	33592	56814	2.89%	0.317%
35	11.870	1678	1686	1696	rBV	933532	1698307	86.53%	9.486%
36	11.970	1697	1703	1707	rBV2	80587	138840	7.07%	0.775%

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Peak Location: TOP

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

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37	12.070	1712	1720	1726	rBV	259679	501946	25.57%	2.804%
38	12.294	1751	1758	1764	rBV6	16401	34999	1.78%	0.195%
39	12.400	1765	1776	1784	rBV2	100661	282477	14.39%	1.578%
40	12.482	1785	1790	1796	rVB2	83335	141143	7.19%	0.788%
41	12.594	1796	1809	1813	rBV5	56395	190642	9.71%	1.065%
42	12.700	1822	1827	1831	rBV2	53764	97067	4.95%	0.542%
43	12.741	1831	1834	1835	rVV2	25157	30003	1.53%	0.168%
44	12.776	1836	1840	1842	rVV2	46622	77527	3.95%	0.433%
45	12.853	1846	1853	1862	rVB	780899	1370541	69.83%	7.655%
46	13.035	1877	1884	1890	rVB	126829	246868	12.58%	1.379%
47	13.100	1890	1895	1899	rBV6	34353	61221	3.12%	0.342%
48	13.182	1902	1909	1913	rVV4	47117	101954	5.19%	0.569%
49	13.264	1921	1923	1927	rVB2	28212	29535	1.50%	0.165%
50	13.323	1927	1933	1934	rBV3	32181	52277	2.66%	0.292%
51	13.400	1942	1946	1954	rVB	91461	153567	7.82%	0.858%
52	13.488	1958	1961	1964	rBV2	18733	24024	1.22%	0.134%
53	13.582	1974	1977	1979	rBV3	22516	25621	1.31%	0.143%
54	13.617	1980	1983	1986	rVV2	20651	28461	1.45%	0.159%
55	13.723	1998	2001	2004	rBV4	38510	46499	2.37%	0.260%
56	13.794	2007	2013	2030	rVB2	951780	1962722	100.00%	10.963%
57	13.947	2035	2039	2043	rBV3	52731	82830	4.22%	0.463%
58	14.000	2044	2048	2052	rBV3	56772	95483	4.86%	0.533%
59	14.117	2063	2068	2073	rBV8	72935	156977	8.00%	0.877%
60	14.335	2099	2105	2109	rBV	185604	303181	15.45%	1.693%
61	14.447	2119	2124	2129	rVB2	79473	139890	7.13%	0.781%
62	14.582	2143	2147	2150	rBV4	51723	82256	4.19%	0.459%
63	14.635	2151	2156	2157	rBV2	77333	114752	5.85%	0.641%
64	14.735	2170	2173	2178	rVB4	43881	57876	2.95%	0.323%
65	14.929	2202	2206	2210	rBV	78050	140048	7.14%	0.782%
66	15.047	2219	2226	2243	rVB6	203191	780056	39.74%	4.357%
67	15.323	2269	2273	2278	rVB3	62993	97907	4.99%	0.547%
68	15.435	2289	2292	2300	rVB4	65162	149979	7.64%	0.838%
69	15.600	2315	2320	2323	rBV2	105147	184263	9.39%	1.029%
70	15.641	2323	2327	2333	rVB	103477	194822	9.93%	1.088%
71	15.947	2372	2379	2387	rBV7	74172	213768	10.89%	1.194%
72	16.023	2389	2392	2401	rVB8	40146	100081	5.10%	0.559%
73	16.617	2490	2493	2500	rVB4	55043	89757	4.57%	0.501%
74	16.782	2515	2521	2522	rBV3	231653	323901	16.50%	1.809%

Sum of corrected areas: 17903340

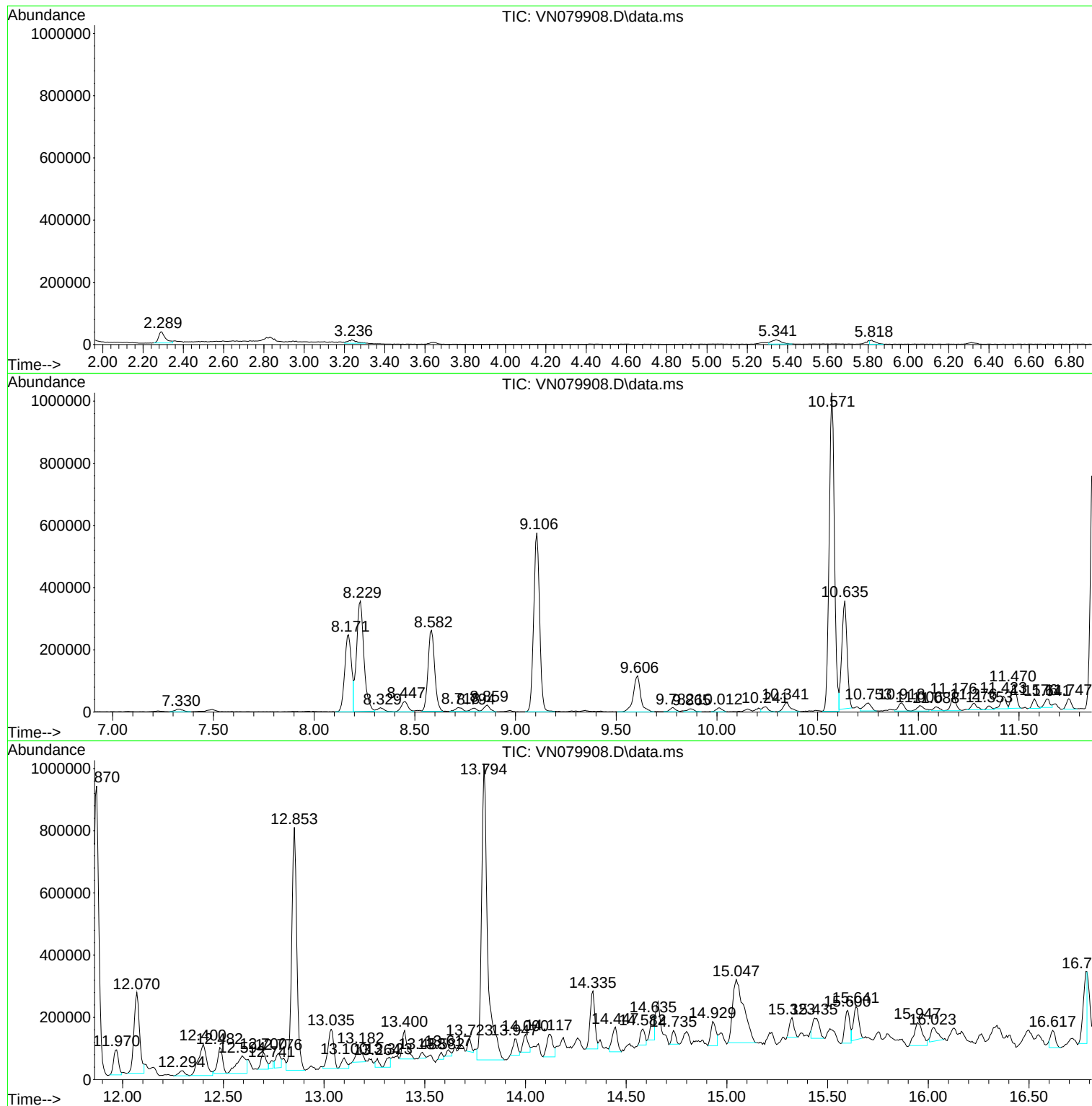
Instrument :
MSVOA_N
ClientSampleId :
67S-SB14-1216

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Instrument :
MSVOA_N
ClientSampleId :
67S-SB14-1216

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110123W.M
Quant Title : SW846 8260

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



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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
67S-SB14-1216

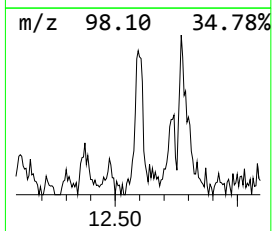
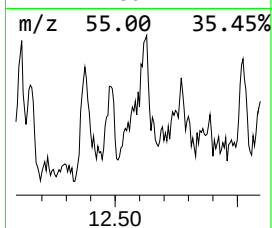
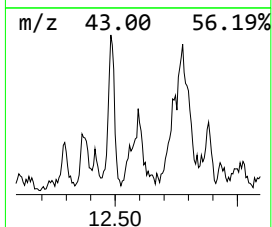
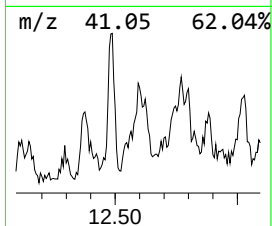
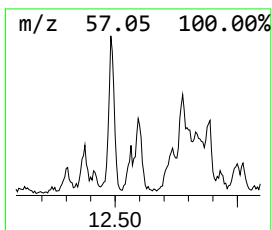
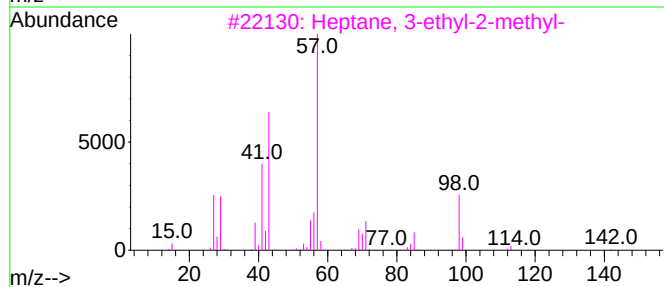
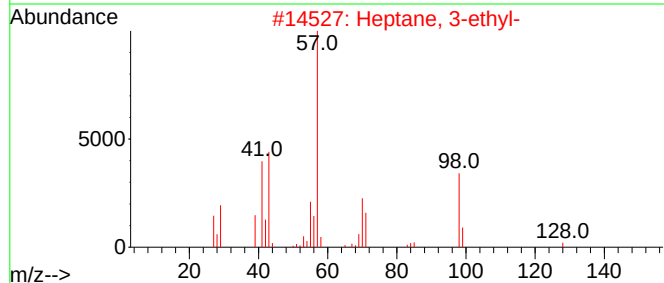
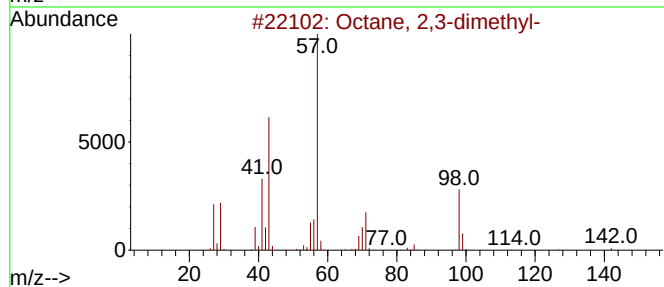
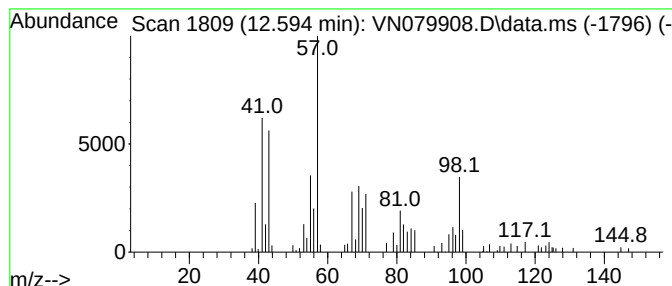
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110123W.M
Quant Title : SW846 8260

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

Peak Number 1 Octane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.594	5.61 ug/l	190642	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50
2			Heptane, 3-ethyl-	128	C9H20	015869-80-4	49
3			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	47
4			2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	43
5			Acetic acid, trichloro-, nonyl e...	288	C11H19Cl3O2	065611-32-7	38



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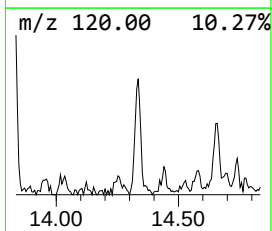
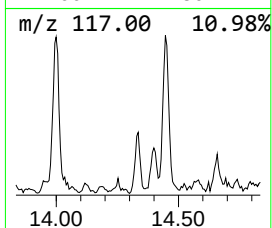
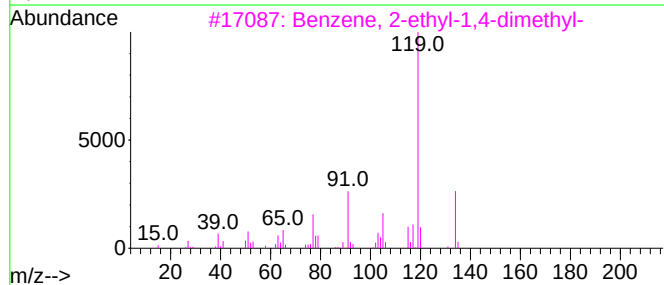
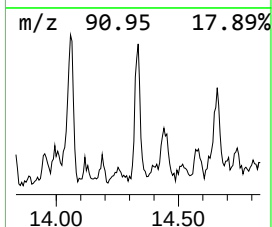
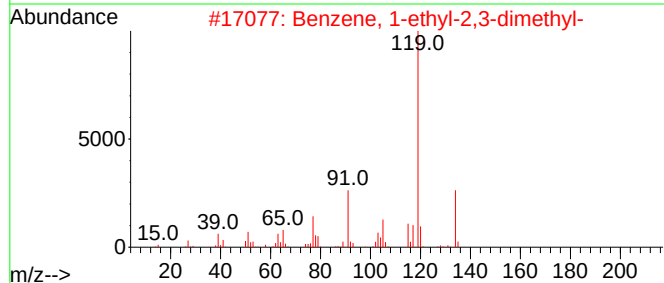
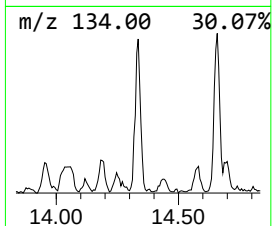
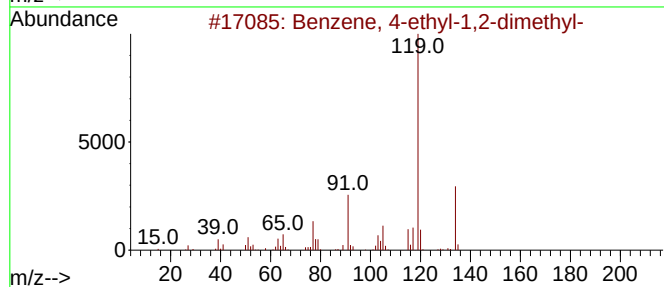
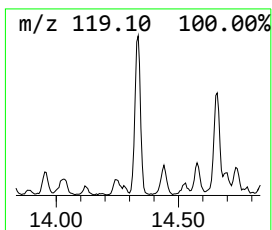
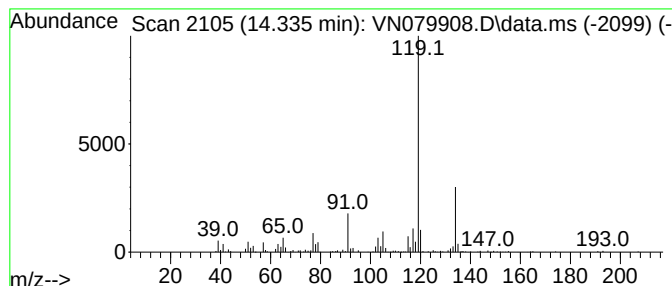
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110123W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.335	7.72 ug/l	303181	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
3			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
4			o-Cymene	134	C10H14	000527-84-4	94
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	91



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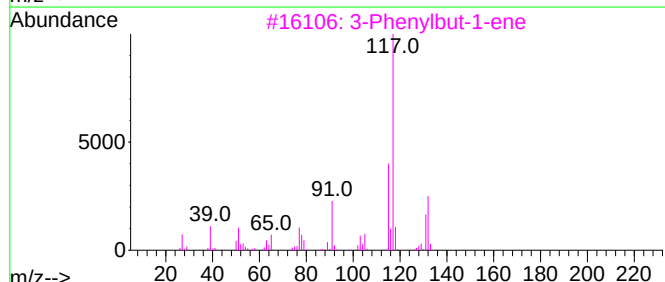
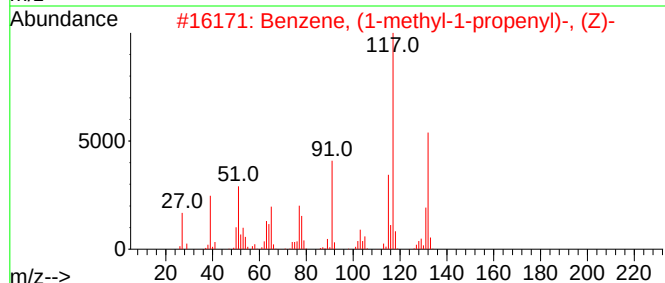
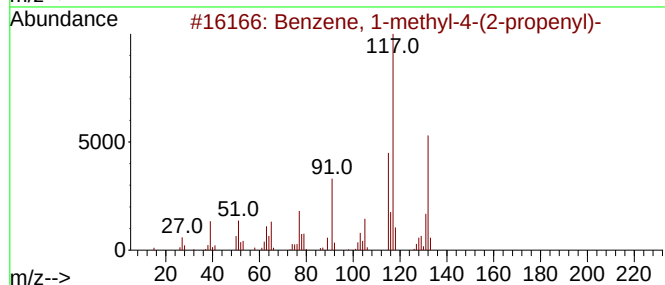
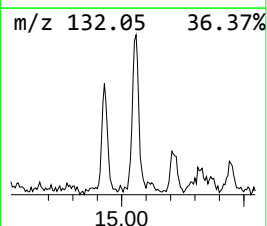
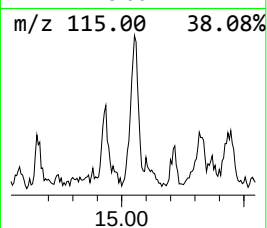
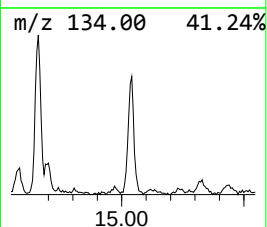
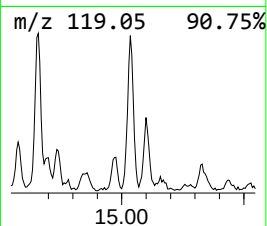
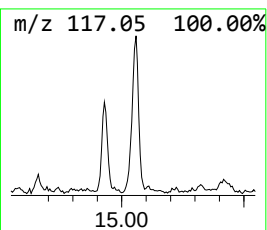
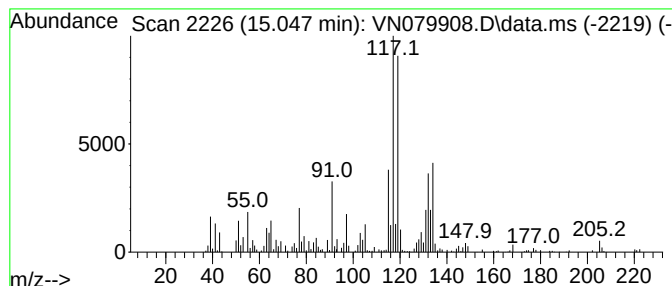
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Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-methyl-4-(2-prop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.047	19.87 ug/l	780056	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	89
2			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	64
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	50
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	50
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	50



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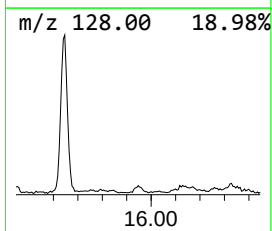
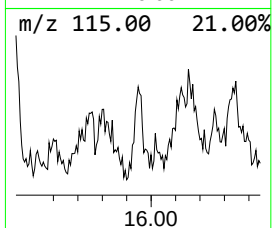
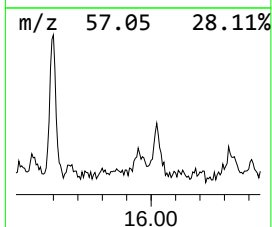
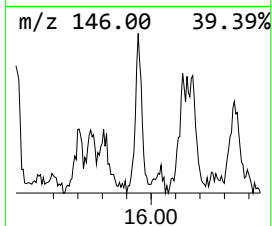
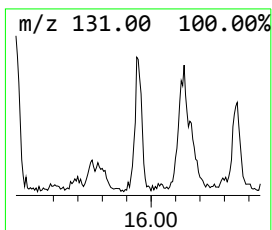
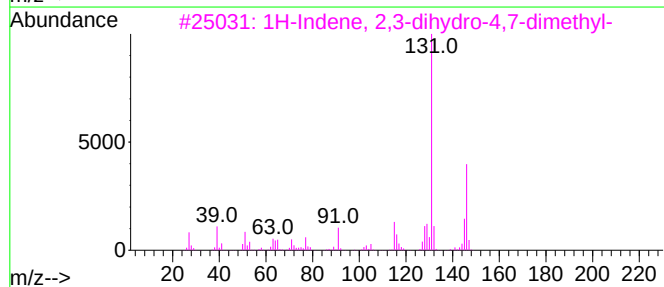
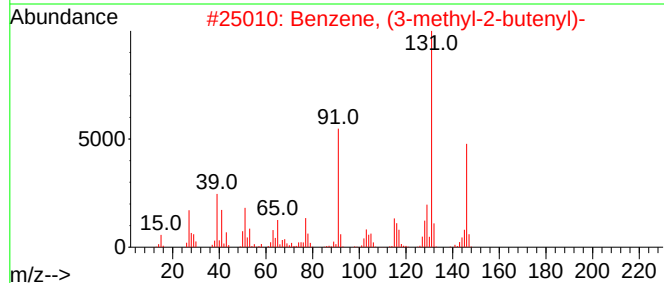
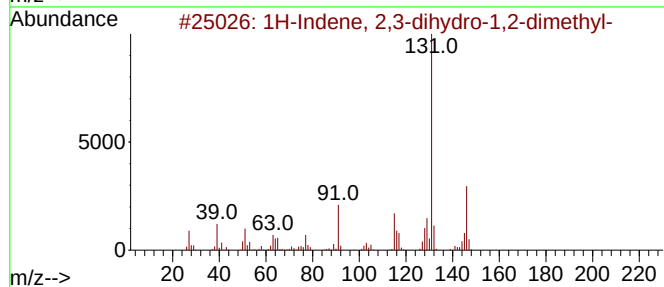
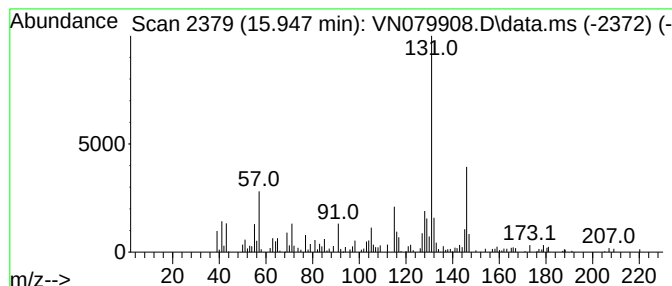
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Quant Title : SW846 8260

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

Peak Number 4 1H-Indene, 2,3-dihydro-1,2-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.947	5.45 ug/l	213768	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	91
2			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	90
3			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	90
4			Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	90
5			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN110423\
Data File : VN079908.D
Acq On : 04 Nov 2023 21:15
Operator : JC\MD
Sample : 05102-10 20X
Misc : 3.28g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
67S-SB14-1216

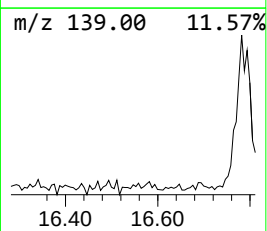
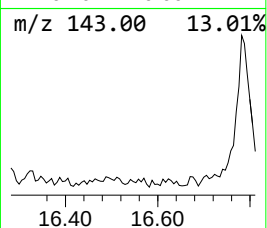
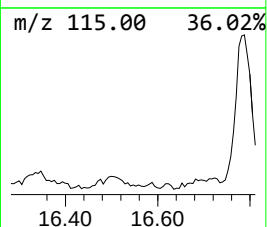
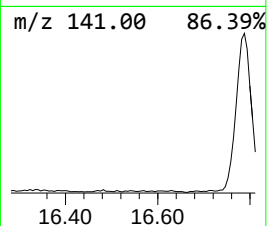
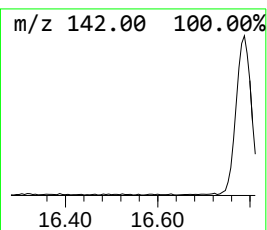
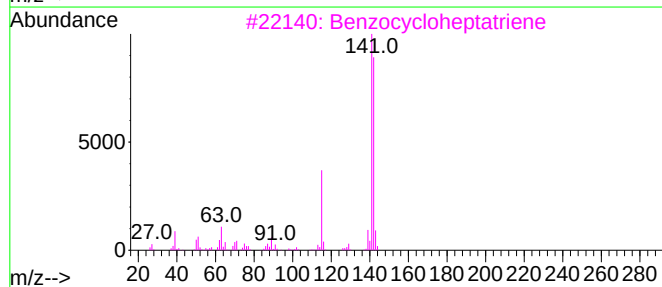
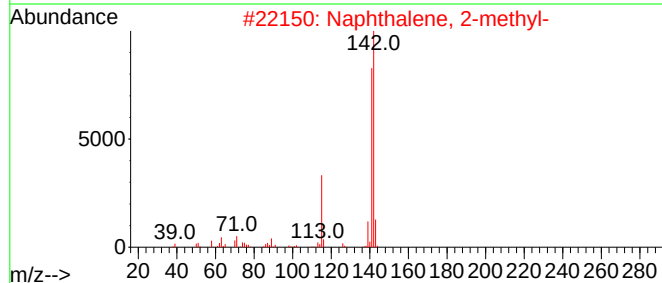
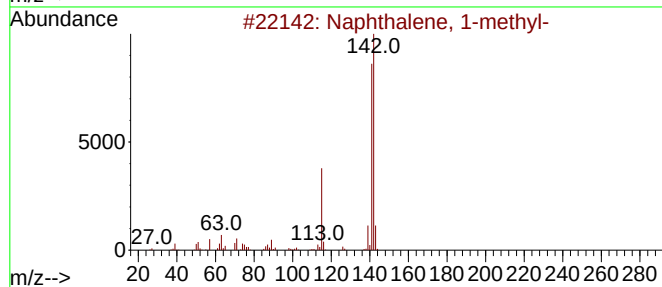
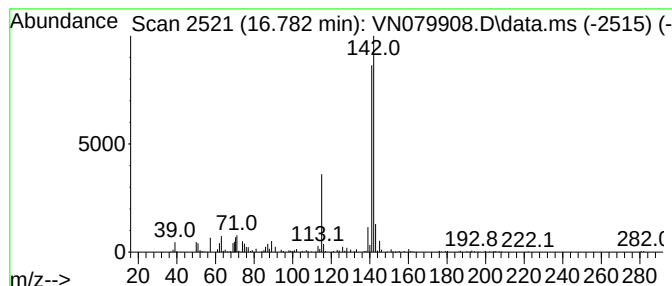
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110123W.M
Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.782	8.25 ug/l	323901	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN110423\
Data File : VN079908.D
Acq On : 04 Nov 2023 21:15
Operator : JC\MD
Sample : 05102-10 20X
Misc : 3.28g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
67S-SB14-1216

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110123W.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
Octane, 2,3-dim...	12.594	5.6	ug/l	190642	3	11.870	1698310	50.0
Benzene, 4-ethy...	14.335	7.7	ug/l	303181	4	13.794	1962720	50.0
Benzene, 1-meth...	15.047	19.9	ug/l	780056	4	13.794	1962720	50.0
1H-Indene, 2,3-...	15.947	5.5	ug/l	213768	4	13.794	1962720	50.0
Naphthalene, 1-...	16.782	8.3	ug/l	323901	4	13.794	1962720	50.0