

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063022\
 Data File : VN073261.D
 Acq On : 30 Jun 2022 13:22
 Operator : JC\MD
 Sample : N3554-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 152140-SPC-01-20

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\82N062822W.M
 Title : SW846 8260

Signal : TIC: VN073261.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.251	904	912	919	rBV5	7174	19170	1.46%	0.188%
2	7.951	1021	1031	1036	rBV	201818	486039	36.90%	4.763%
3	8.016	1036	1042	1062	rVB	375562	860233	65.31%	8.431%
4	8.369	1093	1102	1114	rBV	215186	487553	37.02%	4.778%
5	8.898	1183	1192	1209	rBV	512404	1091025	82.83%	10.693%
6	10.381	1434	1444	1455	rBV	703033	1317145	100.00%	12.909%
7	10.910	1529	1534	1541	rVB2	15553	27474	2.09%	0.269%
8	11.680	1657	1665	1679	rBV	720874	1281611	97.30%	12.560%
9	12.669	1826	1833	1843	rBV	585499	967442	73.45%	9.481%
10	12.992	1881	1888	1892	rBV5	7028	15279	1.16%	0.150%
11	13.610	1986	1993	2003	rBV	728289	1224578	92.97%	12.002%
12	13.933	2042	2048	2053	rBV4	37252	64742	4.92%	0.635%
13	14.039	2062	2066	2069	rBV6	10564	17419	1.32%	0.171%
14	14.086	2069	2074	2080	rVV8	7611	19713	1.50%	0.193%
15	14.192	2089	2092	2096	rVB5	12202	17103	1.30%	0.168%
16	14.257	2097	2103	2108	rBV5	36197	67966	5.16%	0.666%
17	14.316	2108	2113	2121	rBV6	33552	79900	6.07%	0.783%
18	14.445	2129	2135	2139	rBV6	38172	68679	5.21%	0.673%
19	14.557	2149	2154	2157	rBV2	57784	88522	6.72%	0.868%
20	14.604	2157	2162	2165	rVV4	35661	63428	4.82%	0.622%
21	14.692	2173	2177	2182	rVB5	12435	23633	1.79%	0.232%
22	14.763	2183	2189	2190	rBV6	10597	20923	1.59%	0.205%
23	14.792	2190	2194	2198	rVB5	27999	51793	3.93%	0.508%
24	14.845	2198	2203	2208	rBV2	39085	89005	6.76%	0.872%
25	14.904	2210	2213	2221	rVB4	36207	79630	6.05%	0.780%
26	15.045	2232	2237	2238	rBV4	21870	29905	2.27%	0.293%
27	15.127	2246	2251	2259	rBV2	85595	166554	12.65%	1.632%
28	15.233	2264	2269	2278	rVB6	56673	135289	10.27%	1.326%
29	15.315	2280	2283	2290	rVB8	34914	61059	4.64%	0.598%
30	15.392	2291	2296	2306	rBV5	82346	190740	14.48%	1.869%
31	15.492	2307	2313	2316	rBV5	39123	84505	6.42%	0.828%
32	15.574	2325	2327	2333	rVB6	36212	62584	4.75%	0.613%
33	15.704	2345	2349	2352	rBV4	23398	40142	3.05%	0.393%
34	15.810	2364	2367	2372	rVB6	35249	51963	3.95%	0.509%
35	16.021	2400	2403	2409	rVB3	42925	72143	5.48%	0.707%
36	16.092	2410	2415	2423	rBV4	38107	90697	6.89%	0.889%

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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\82N062822W.M

Title : SW846 8260

37	16.245	2435	2441	2447	rBV6	49332	119086	9.04%	1.167%
38	16.380	2459	2464	2468	rBV3	42916	65668	4.99%	0.644%
39	16.457	2472	2477	2483	rVV2	94109	189319	14.37%	1.855%
40	16.527	2484	2489	2493	rVV3	29139	50068	3.80%	0.491%
41	16.592	2496	2500	2505	rVB2	44054	75384	5.72%	0.739%
42	16.721	2516	2522	2531	rBV2	55844	188416	14.30%	1.847%

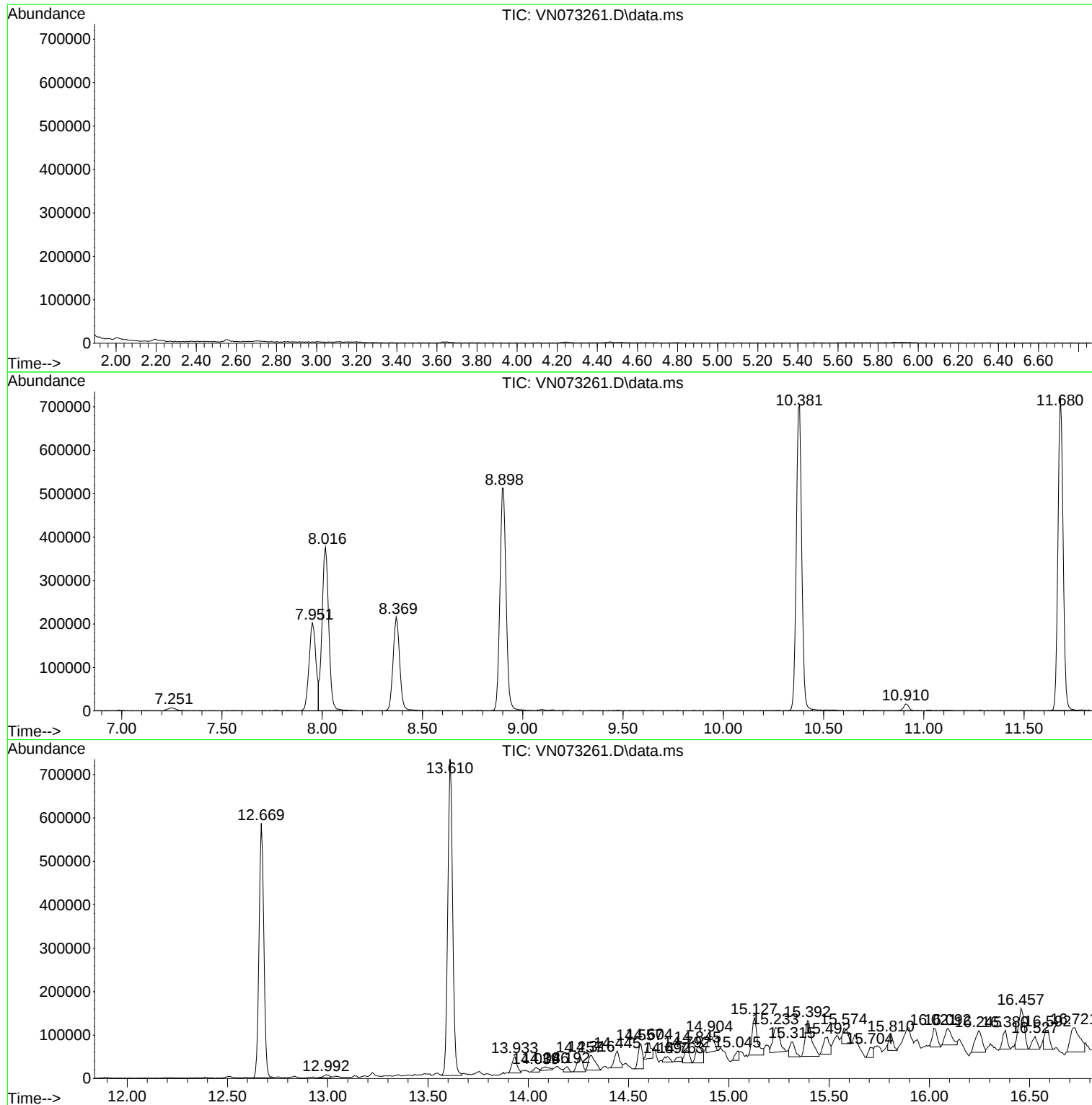
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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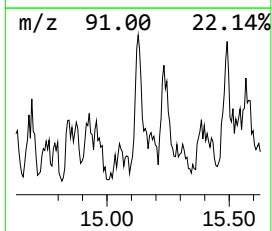
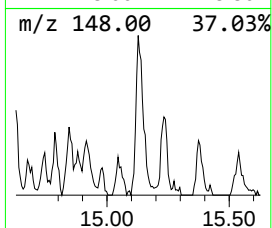
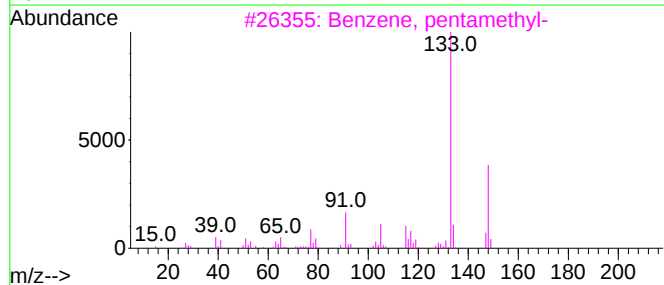
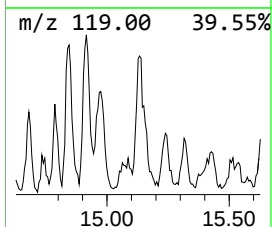
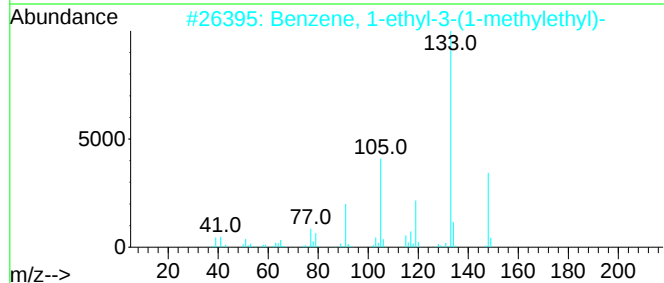
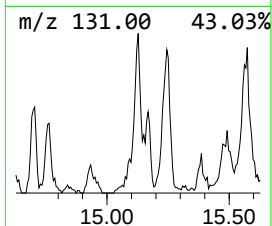
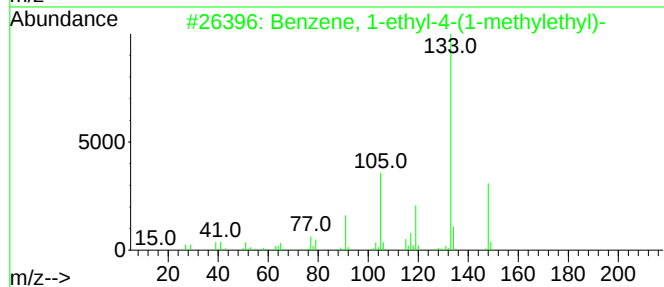
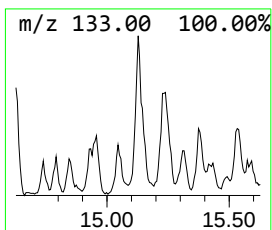
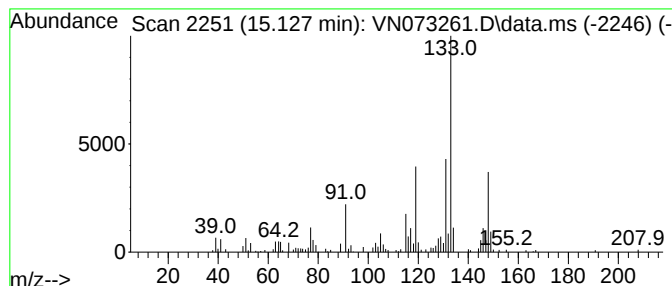
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-4-(1-methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	6.80 ug/l	166554	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	58
2			Benzene, 1-ethyl-3-(1-methylethyl)-	148	C11H16	004920-99-4	52
3			Benzene, pentamethyl-	148	C11H16	000700-12-9	49
4			Benzene, 1,3-dimethyl-5-(1-methy...	148	C11H16	004706-90-5	47
5			Phenol, 2-(2-methyl-2-propenyl)-	148	C10H12O	020944-88-1	46



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Instrument :
MSVOA_N
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152140-SPC-01-20

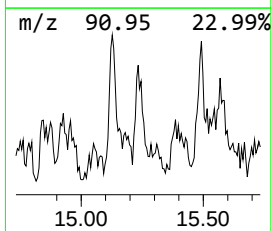
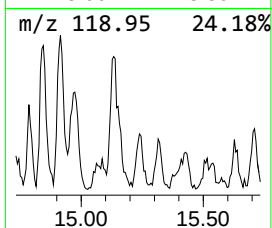
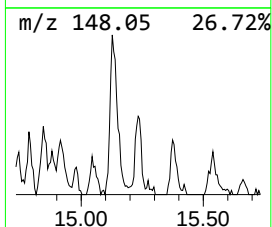
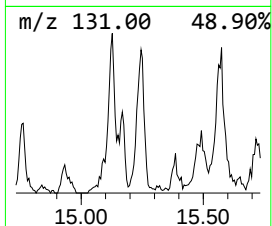
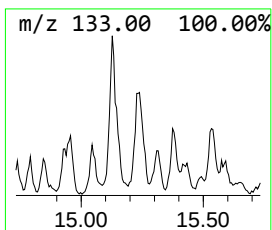
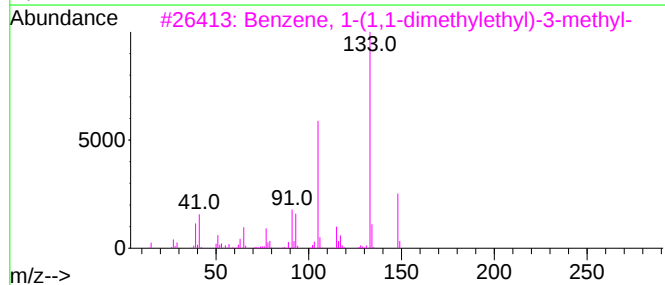
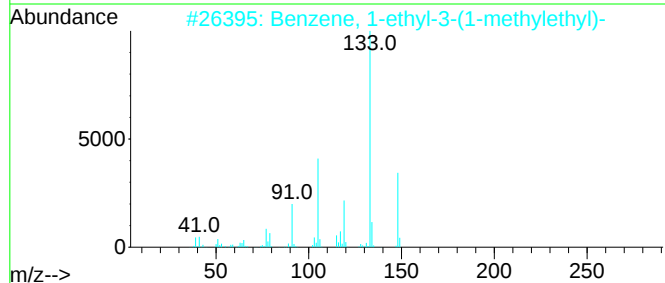
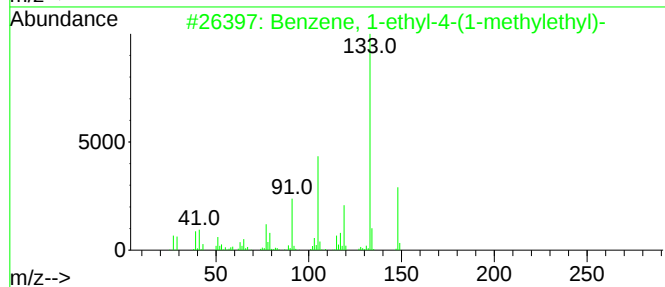
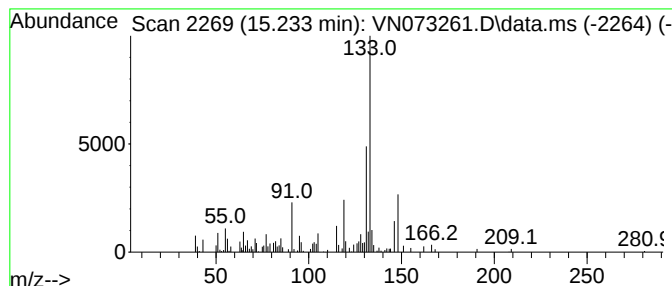
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1-ethyl-3-(1-methy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.233	5.52 ug/l	135289	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	52
2			Benzene, 1-ethyl-3-(1-methylethyl)-	148	C11H16	004920-99-4	52
3			Benzene, 1-(1,1-dimethylethyl)-3-methyl-	148	C11H16	001075-38-3	49
4			Benzene, 1,4-diethyl-2-methyl-	148	C11H16	013632-94-5	46
5			4-tert-Butyltoluene	148	C11H16	000098-51-1	46



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
152140-SPC-01-20

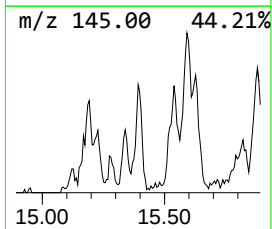
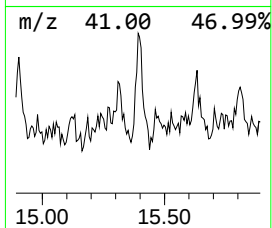
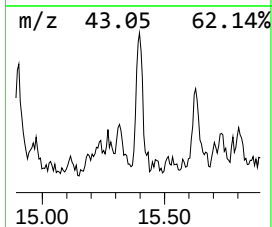
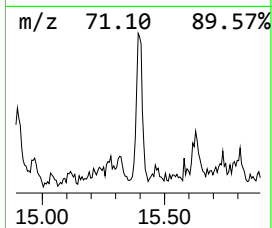
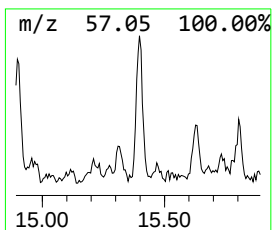
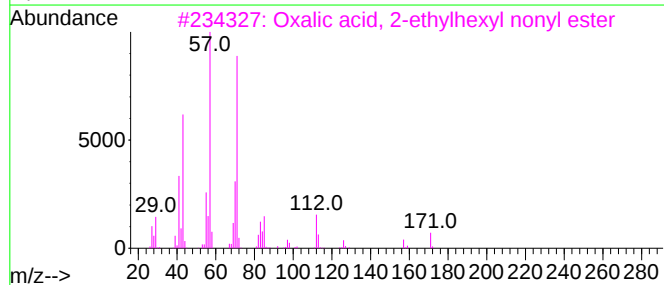
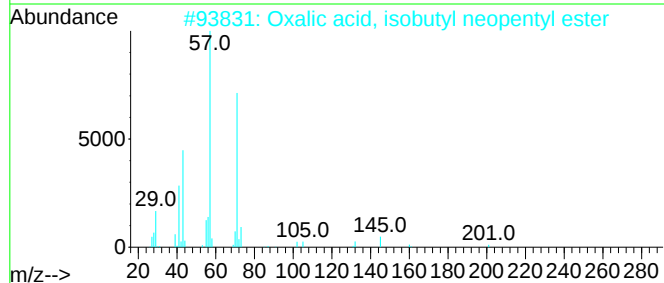
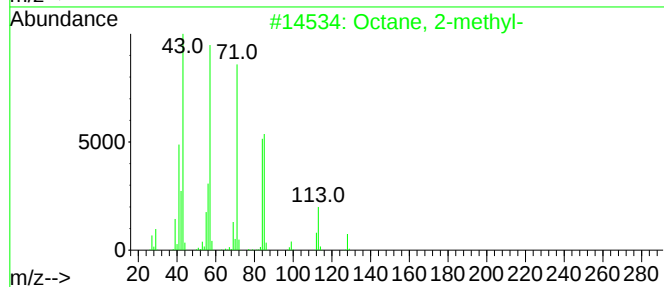
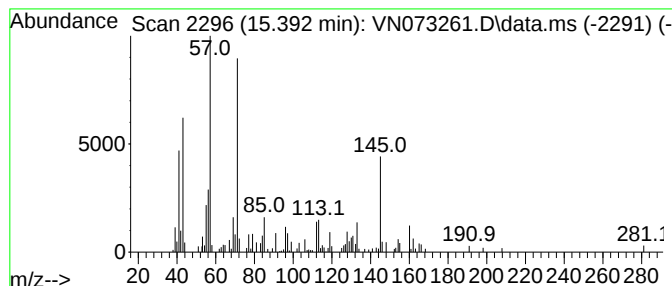
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 3 Octane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.392	7.79 ug/l	190740	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2-methyl-	128	C9H20	003221-61-2	45
2			Oxalic acid, isobutyl neopentyl ...	216	C11H20O4	1000309-72-6	43
3			Oxalic acid, 2-ethylhexyl nonyl ...	328	C19H36O4	1000309-39-2	38
4			3-Hexanone, 4-ethyl-	128	C8H16O	006137-12-8	38
5			Z-1-Methoxy-2-hexene	114	C7H14O	1000279-60-9	38



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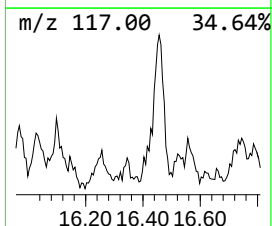
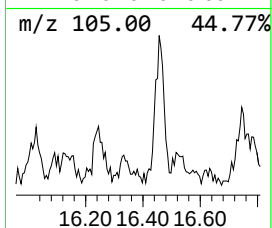
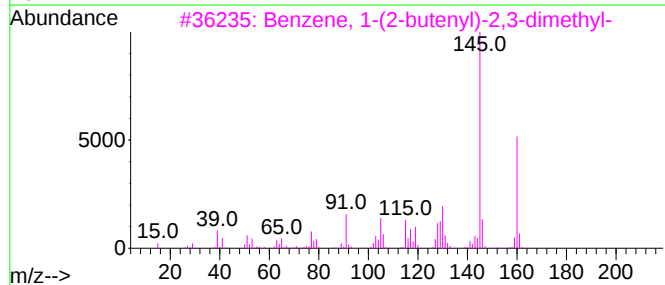
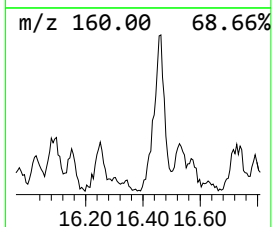
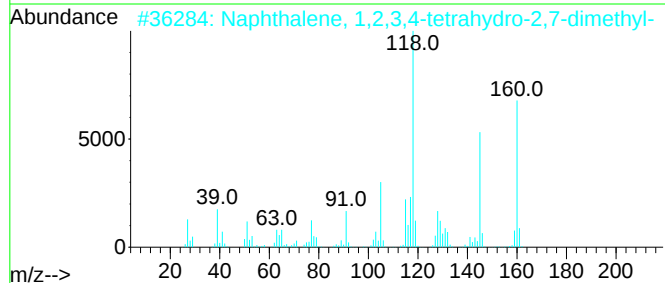
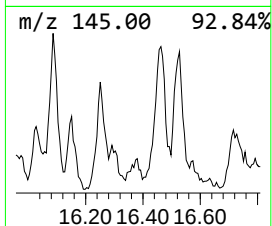
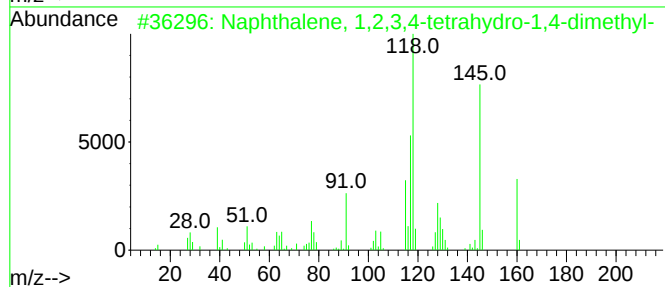
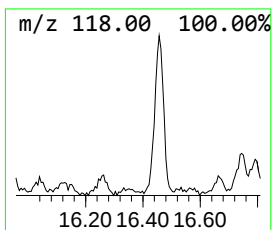
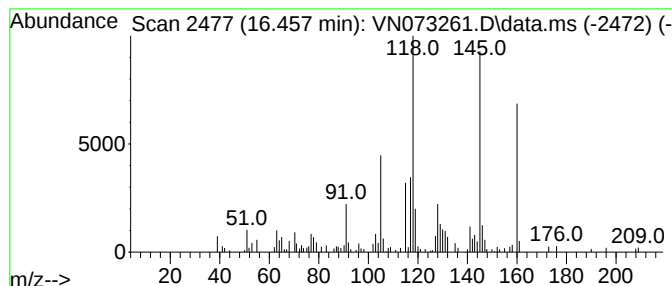
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Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.457	7.73 ug/l	189319	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	90
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	76
3			Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	64
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	020027-77-4	64
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	001076-61-5	64



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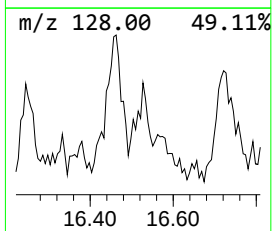
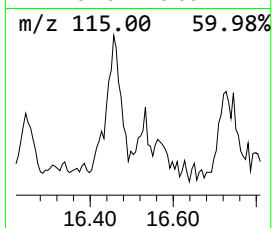
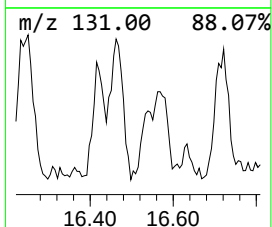
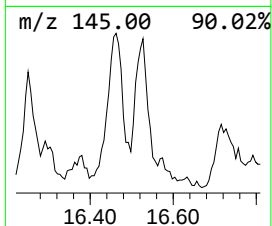
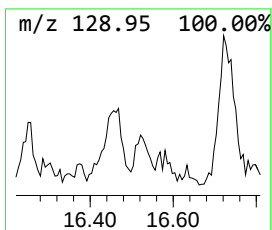
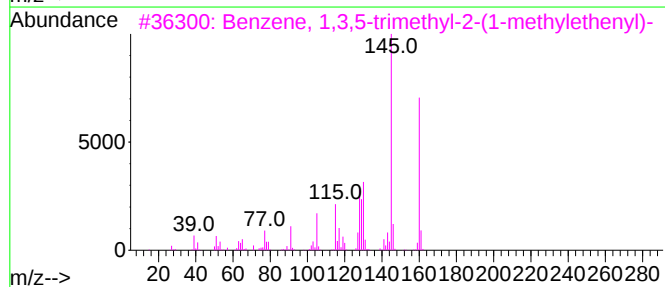
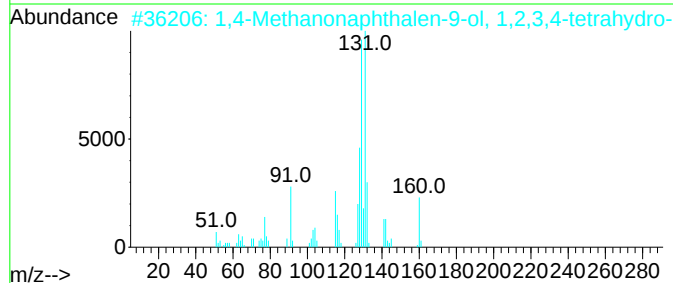
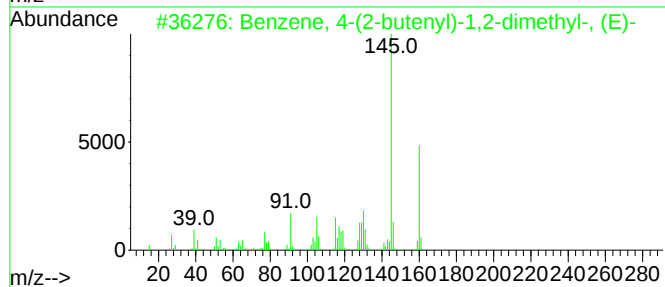
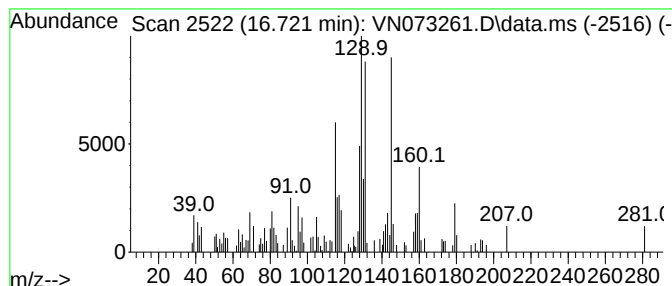
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 4-(2-butenyl)-1,2-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.721	7.69 ug/l	188416	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	55
2			1,4-Methanonaphthalen-9-ol, 1,2,...	160	C11H12O	001198-20-5	52
3			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	46
4			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	30
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063022\
Data File : VN073261.D
Acq On : 30 Jun 2022 13:22
Operator : JC\MD
Sample : N3554-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
152140-SPC-01-20

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.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
Benzene, 1-ethy...	15.127	6.8	ug/l	166554	4	13.610	1224580	50.0
Benzene, 1-ethy...	15.233	5.5	ug/l	135289	4	13.610	1224580	50.0
Octane, 2-methyl-	15.392	7.8	ug/l	190740	4	13.610	1224580	50.0
Naphthalene, 1,...	16.457	7.7	ug/l	189319	4	13.610	1224580	50.0
Benzene, 4-(2-b...	16.721	7.7	ug/l	188416	4	13.610	1224580	50.0