

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN081722\  
 Data File : VN073982.D  
 Acq On : 17 Aug 2022 17:36  
 Operator : JC\MD  
 Sample : N4204-25 10X  
 Misc : 5.0mL/MSVOA\_N/WATER  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 MW-5

Integration Parameters: RTEINT.P  
 Integrator: RTE  
 Smoothing : 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\_N\methods\82N081522W.M  
 Title : SW846 8260

Signal : TIC: VN073982.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.081	195	203	212	rBV2	75800	168337	6.01%	0.602%
2	3.475	257	270	281	rBV4	20020	67963	2.43%	0.243%
3	3.657	292	301	314	rVB	39126	93073	3.32%	0.333%
4	3.828	323	330	338	rBV3	14079	35120	1.25%	0.126%
5	3.928	338	347	359	rVB2	80703	219490	7.84%	0.785%
6	4.187	380	391	409	rBV4	21803	83536	2.98%	0.299%
7	4.887	497	510	519	rBV	57873	183918	6.57%	0.658%
8	4.998	519	529	535	rVV3	22078	79755	2.85%	0.285%
9	5.104	538	547	559	rVB3	42476	170209	6.08%	0.609%
10	5.292	568	579	594	rVB4	34715	126447	4.51%	0.452%
11	5.534	603	620	640	rBV3	160288	575329	20.54%	2.057%
12	6.381	751	764	776	rBV2	16919	48745	1.74%	0.174%
13	6.522	778	788	796	rBV4	12218	37974	1.36%	0.136%
14	6.610	796	803	814	rVV3	12348	36025	1.29%	0.129%
15	6.816	830	838	848	rBV4	10379	32986	1.18%	0.118%
16	7.069	870	881	890	rVV2	55159	154751	5.53%	0.553%
17	7.239	902	910	920	rBV2	27388	78080	2.79%	0.279%
18	7.769	994	1000	1009	rVB3	22593	54254	1.94%	0.194%
19	7.951	1018	1031	1037	rBV	412130	1021531	36.47%	3.653%
20	8.016	1037	1042	1053	rVV	789107	1835728	65.54%	6.564%
21	8.104	1053	1057	1071	rVB4	27503	68899	2.46%	0.246%
22	8.380	1093	1104	1114	rBV3	609401	1745030	62.30%	6.240%
23	8.469	1114	1119	1122	rVV2	25834	59933	2.14%	0.214%
24	8.533	1122	1130	1143	rVB4	71217	278705	9.95%	0.997%
25	8.904	1184	1193	1205	rBV	1020623	2105736	75.18%	7.530%
26	9.392	1264	1276	1283	rBV5	29277	88207	3.15%	0.315%
27	9.739	1328	1335	1342	rBV8	11303	30933	1.10%	0.111%
28	9.822	1342	1349	1358	rVB	53358	106849	3.81%	0.382%
29	9.916	1358	1365	1366	rBV3	24919	44023	1.57%	0.157%
30	9.951	1366	1371	1380	rVB	118966	248525	8.87%	0.889%
31	10.139	1396	1403	1406	rBV5	14684	30920	1.10%	0.111%
32	10.310	1427	1432	1436	rVV3	21612	35929	1.28%	0.128%
33	10.380	1436	1444	1451	rVV	1430012	2579951	92.11%	9.225%
34	10.445	1451	1455	1469	rVB	154161	299167	10.68%	1.070%
35	10.798	1508	1515	1524	rBV5	11980	28894	1.03%	0.103%
36	10.886	1524	1530	1540	rVB3	17474	34904	1.25%	0.125%

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 ClientSampleId :  
 MW-5

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

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37	11.074	1556	1562	1571	rVB	83612	146539	5.23%	0.524%
38	11.527	1634	1639	1646	rBV2	14286	30982	1.11%	0.111%
39	11.686	1657	1666	1675	rBV	1519889	2613923	93.33%	9.347%
40	11.786	1675	1683	1693	rVV	1015964	1713444	61.18%	6.127%
41	11.898	1694	1702	1713	rVB	288189	565300	20.18%	2.021%
42	12.521	1800	1808	1818	rBV	511355	841996	30.06%	3.011%
43	12.674	1825	1834	1845	rVB	1293490	2208778	78.86%	7.898%
44	12.862	1858	1866	1873	rVB	532733	845823	30.20%	3.024%
45	12.957	1876	1882	1886	rVV	37326	62459	2.23%	0.223%
46	12.998	1886	1889	1896	rVB3	34179	54735	1.95%	0.196%
47	13.162	1910	1917	1925	rBV	89909	148404	5.30%	0.531%
48	13.439	1955	1964	1970	rBV3	28309	64355	2.30%	0.230%
49	13.615	1986	1994	2007	rBV	1668300	2800826	100.00%	10.015%
50	13.780	2015	2022	2023	rBV	80868	106624	3.81%	0.381%
51	13.815	2023	2028	2034	rVV	704286	1161741	41.48%	4.154%
52	13.857	2034	2035	2046	rVV4	37686	75308	2.69%	0.269%
53	13.945	2046	2050	2055	rVB3	18468	28552	1.02%	0.102%
54	14.009	2055	2061	2066	rBV	59976	93577	3.34%	0.335%
55	14.157	2079	2086	2092	rBV	191917	287408	10.26%	1.028%
56	14.215	2092	2096	2100	rVV	24140	41405	1.48%	0.148%
57	14.268	2100	2105	2112	rVB2	96031	154252	5.51%	0.552%
58	14.480	2131	2141	2151	rBV	131418	228364	8.15%	0.817%
59	14.751	2181	2187	2193	rBV	80486	131997	4.71%	0.472%
60	14.868	2198	2207	2213	rVV3	182028	394008	14.07%	1.409%
61	15.133	2246	2252	2256	rBV2	30942	48646	1.74%	0.174%
62	15.245	2265	2271	2277	rVB4	22115	50048	1.79%	0.179%
63	15.439	2297	2304	2310	rVB2	65117	122067	4.36%	0.436%
64	16.733	2518	2524	2533	rVB4	23690	54591	1.95%	0.195%

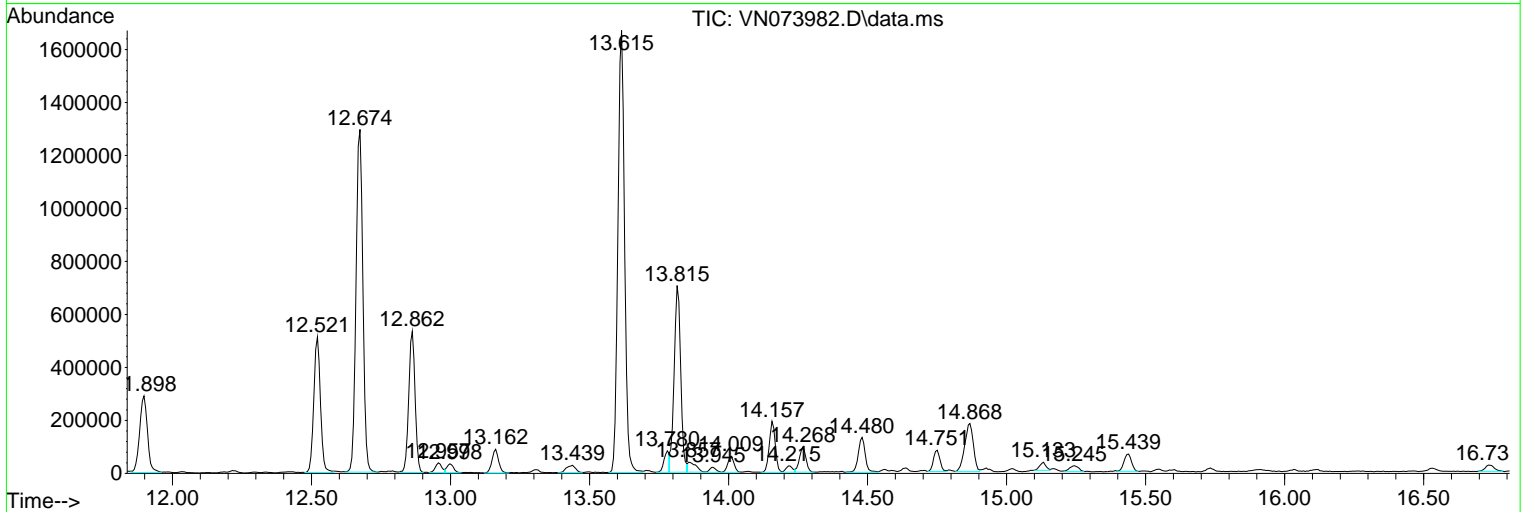
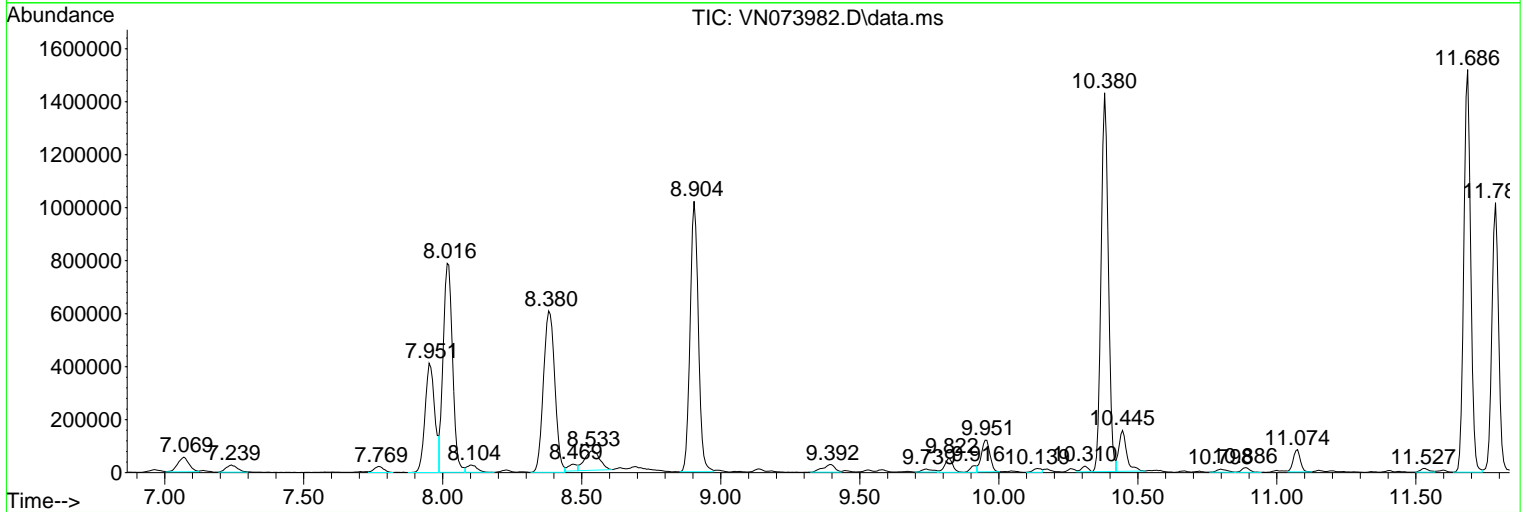
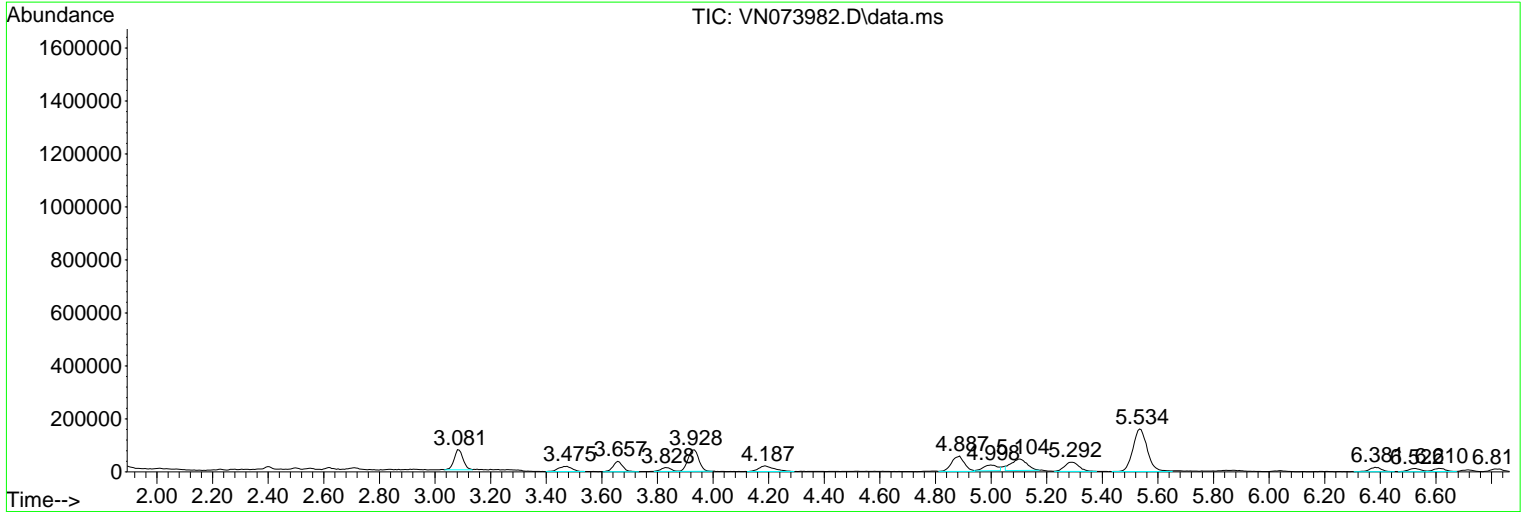
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 ClientSampleId :  
 MW-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N081522W.M  
 Quant Title : SW846 8260

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



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 Misc : 5.0mL/MSVOA\_N/WATER  
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Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 MW-5

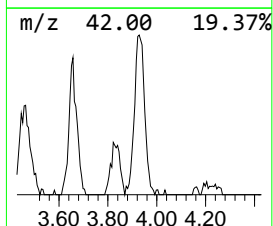
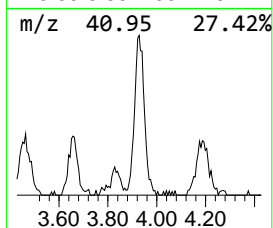
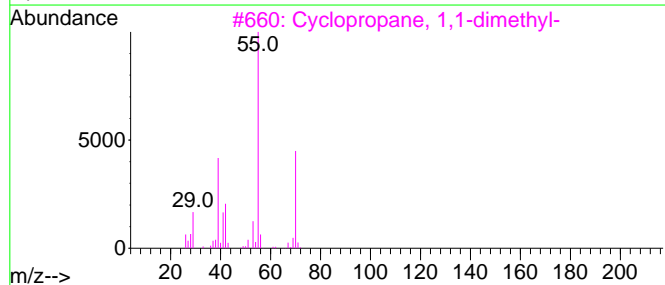
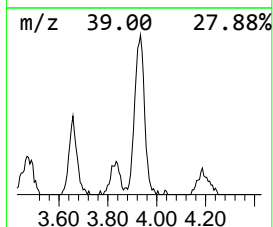
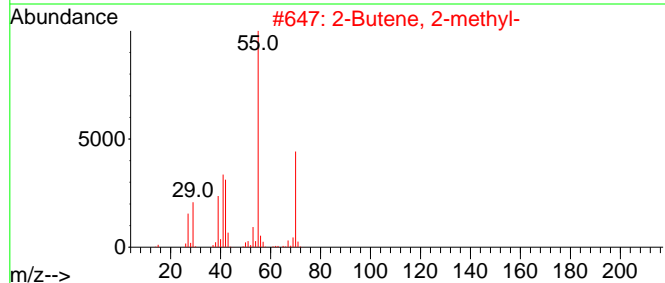
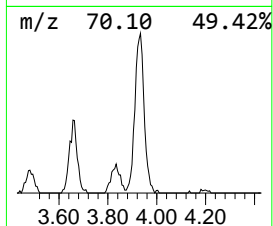
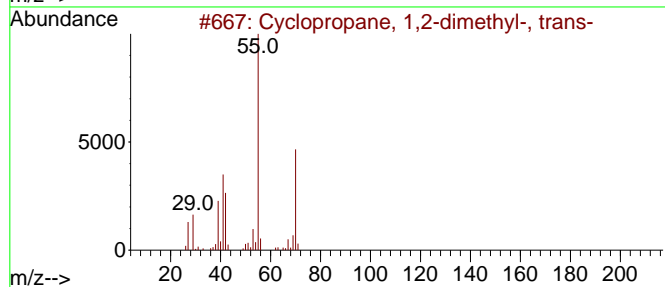
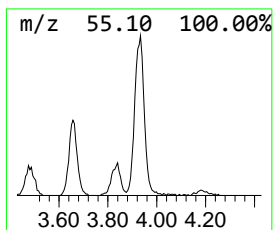
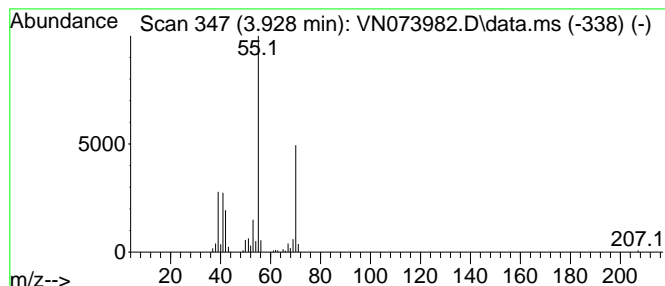
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N081522W.M  
 Quant Title : SW846 8260

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

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 Peak Number 1 Cyclopropane, 1,2-dimethyl-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.928	5.98 ug/l	219490	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	91
2		2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
3		Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	87
4		2-Methyl-1-butene	70	C5H10	000563-46-2	83
5		1-Butene, 3-methyl-	70	C5H10	000563-45-1	80



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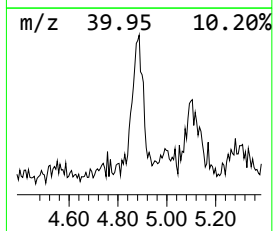
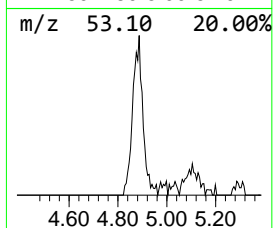
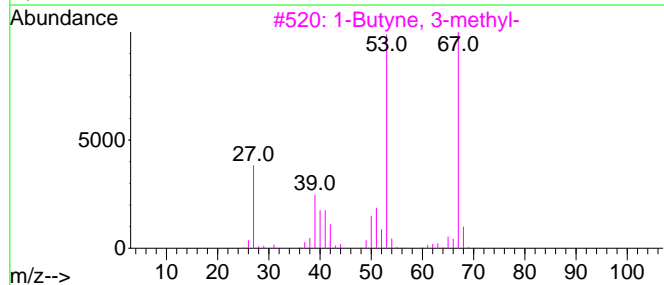
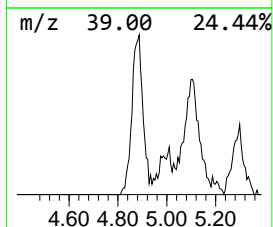
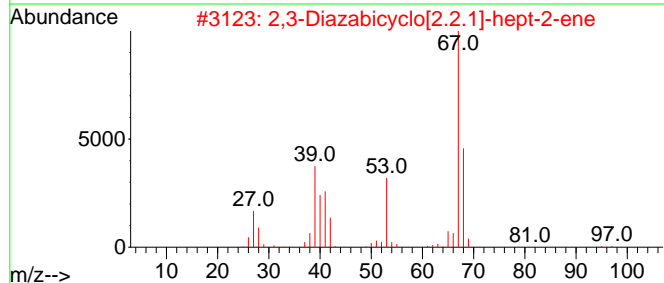
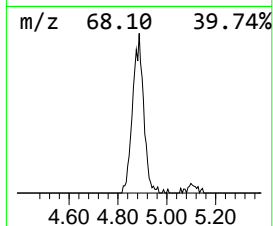
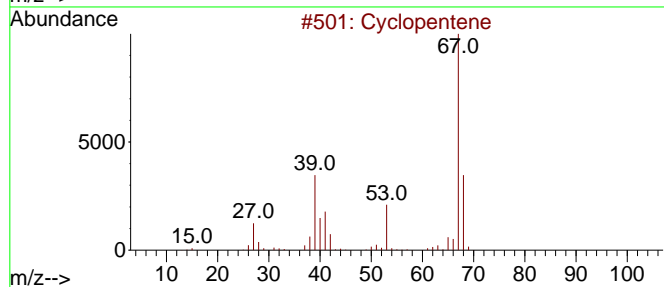
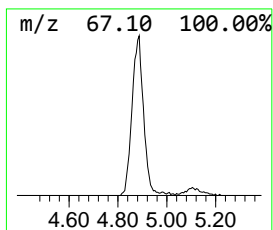
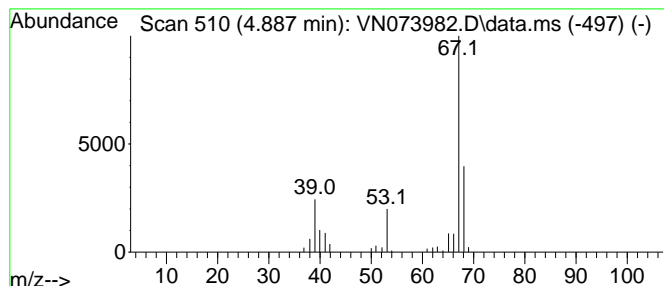
TIC Library : C:\Database\NIST20.L  
 TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
 Peak Number 2 Cyclopentene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.887	5.01 ug/l	183918	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentene	68	C5H8	000142-29-0	91
2		2,3-Diazabicyclo[2.2.1]-hept-2-ene	96	C5H8N2	002721-32-6	64
3		1-Butyne, 3-methyl-	68	C5H8	000598-23-2	59
4		1,3-Pentadiene, (Z)-	68	C5H8	001574-41-0	58
5		1,3-Pentadiene	68	C5H8	000504-60-9	53



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 Sample : N4204-25 10X  
 Misc : 5.0mL/MSVOA\_N/WATER  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 MW-5

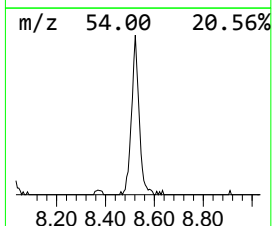
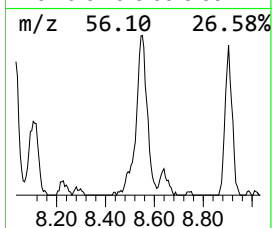
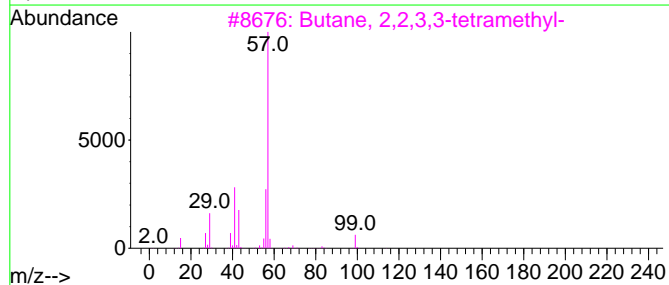
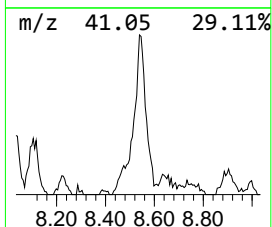
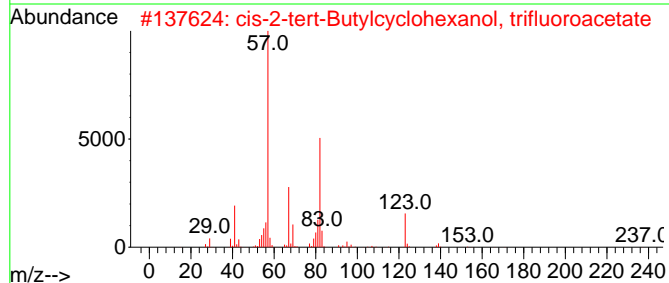
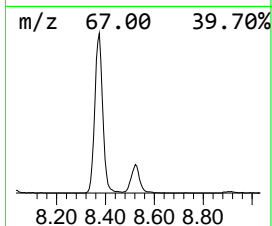
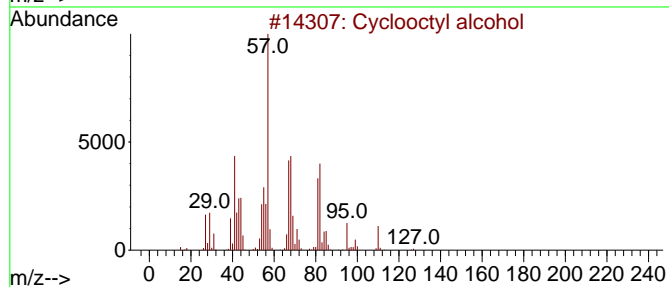
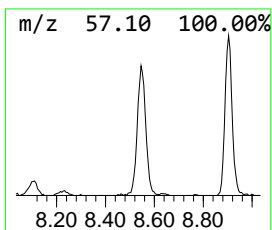
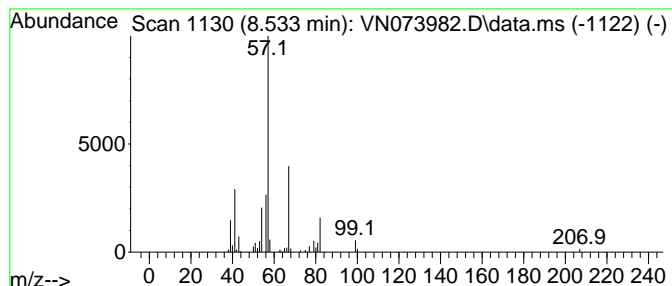
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N081522W.M  
 Quant Title : SW846 8260

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

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 Peak Number 3 Cyclooctyl alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.533	6.62 ug/l	278705	1,4-Difluorobenzene	8.904

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclooctyl alcohol	128	C8H16O	000696-71-9	56
2		cis-2-tert-Butylcyclohexanol, tr...	252	C12H19F3O2	1000467-27-6	25
3		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	10
4		2-Hexen-1-ol, (E)-	100	C6H12O	000928-95-0	9
5		Cyclohexanol	100	C6H12O	000108-93-0	9



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 Misc : 5.0mL/MSVOA\_N/WATER  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 MW-5

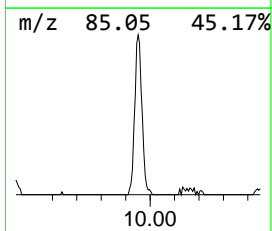
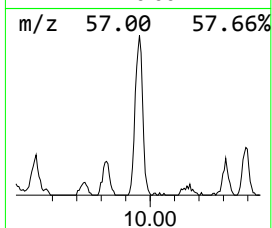
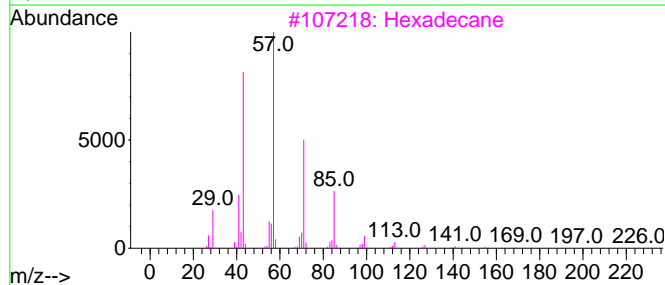
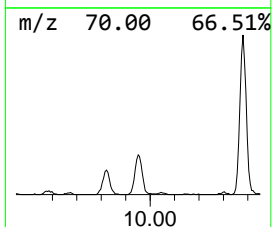
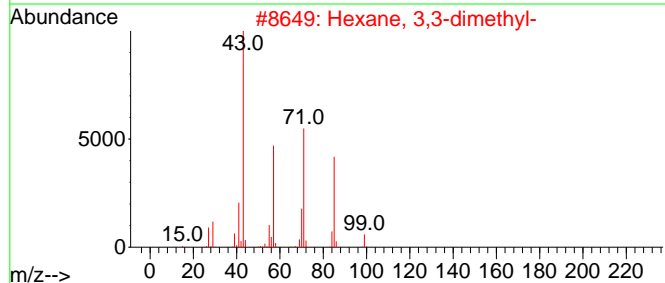
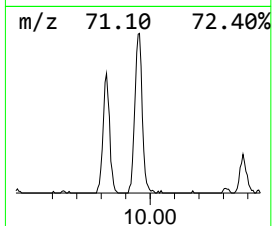
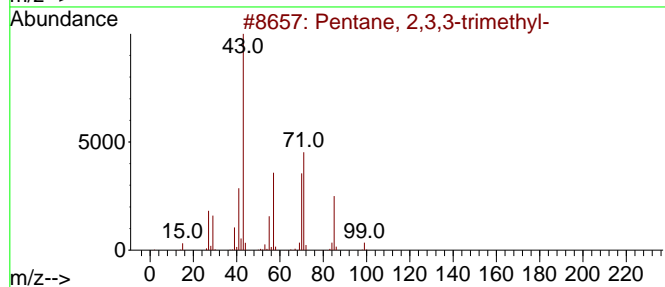
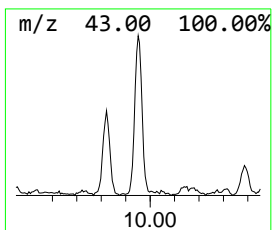
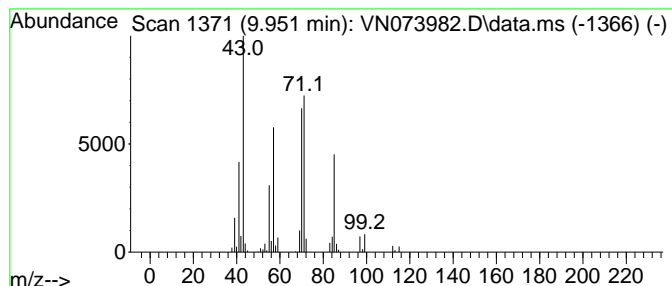
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 Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.951	5.90 ug/l	248525	1,4-Difluorobenzene	8.904

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	78
2		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53
3		Hexadecane	226	C16H34	000544-76-3	53
4		Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	50
5		Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN081722\  
 Data File : VN073982.D  
 Acq On : 17 Aug 2022 17:36  
 Operator : JC\MD  
 Sample : N4204-25 10X  
 Misc : 5.0mL/MSVOA\_N/WATER  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 MW-5

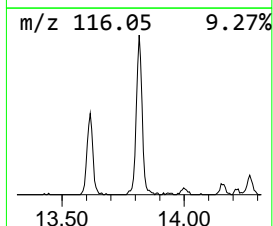
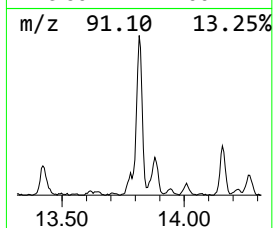
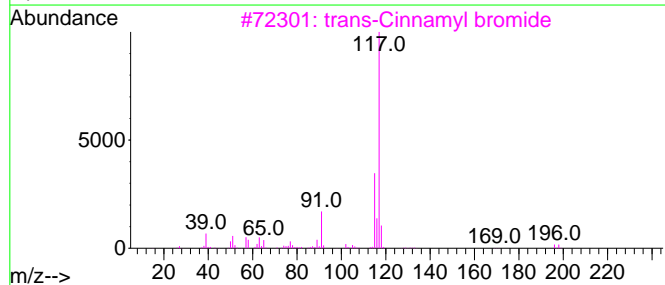
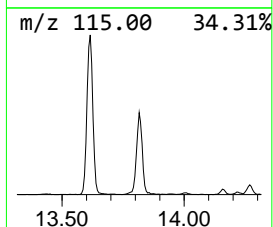
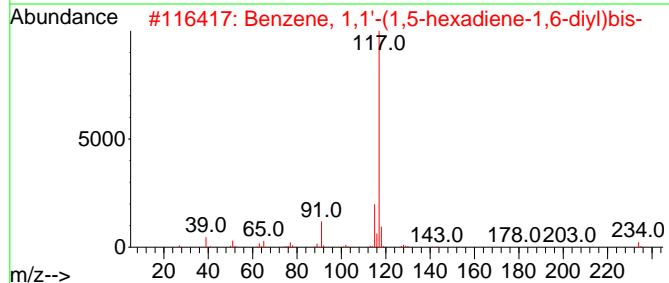
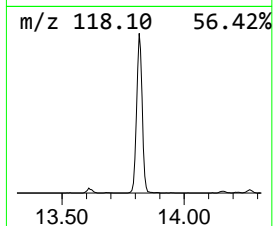
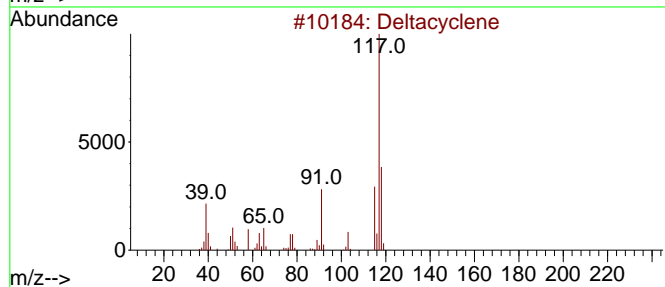
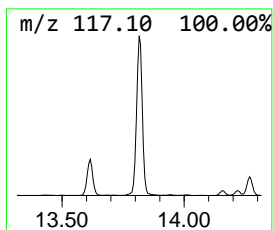
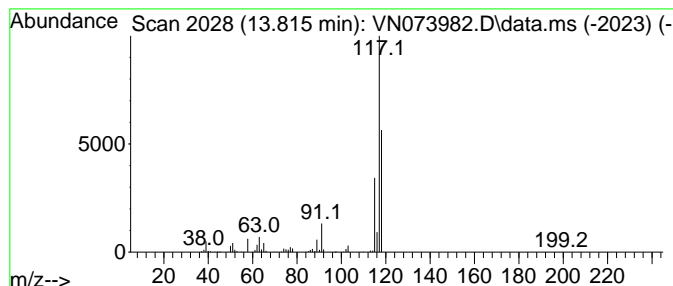
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 Quant Title : SW846 8260

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

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 Peak Number 5 Deltacyclene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.815	20.74 ug/l	1161740	1,4-Dichlorobenzene-d4	13.615

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			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59
4			Indole	117	C8H7N	000120-72-9	46
5			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN081722\  
 Data File : VN073982.D  
 Acq On : 17 Aug 2022 17:36  
 Operator : JC\MD  
 Sample : N4204-25 10X  
 Misc : 5.0mL/MSVOA\_N/WATER  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 MW-5

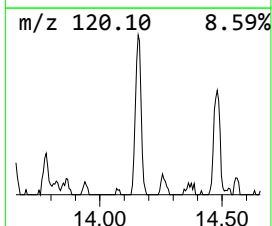
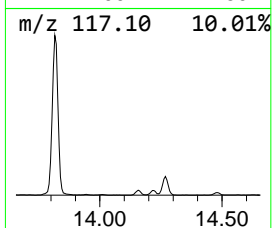
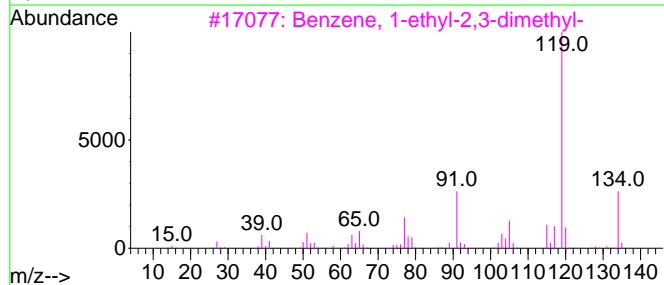
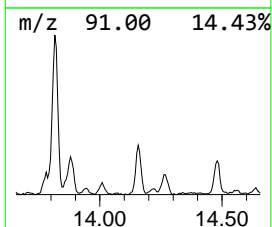
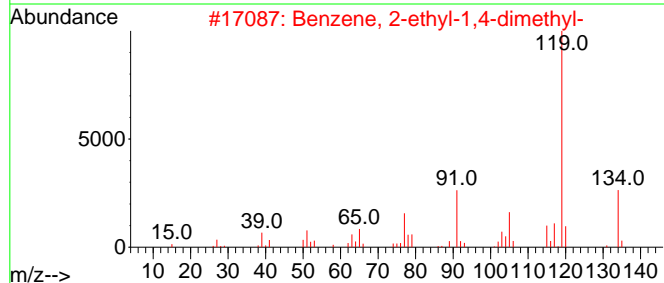
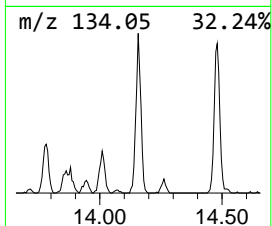
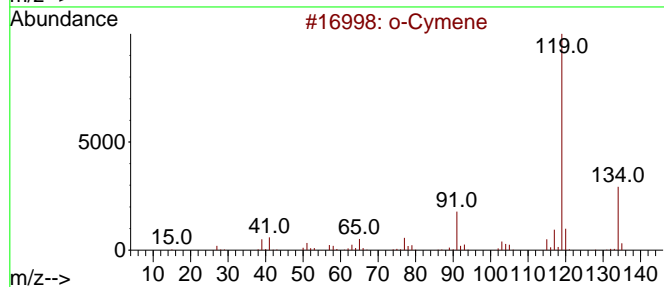
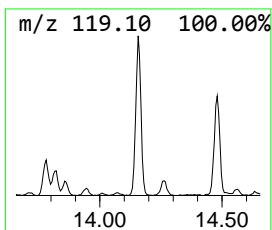
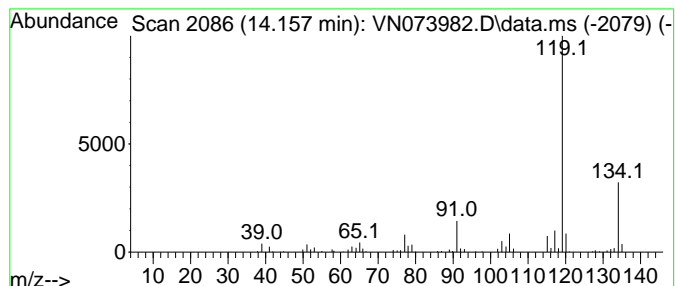
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 Quant Title : SW846 8260

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

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 Peak Number 6 o-Cymene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.156	5.13 ug/l	287408	1,4-Dichlorobenzene-d4	13.615

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		o-Cymene	134	C10H14	000527-84-4	97
2		Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
3		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN081722\  
 Data File : VN073982.D  
 Acq On : 17 Aug 2022 17:36  
 Operator : JC\MD  
 Sample : N4204-25 10X  
 Misc : 5.0mL/MSVOA\_N/WATER  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 MW-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N081522W.M  
 Quant Title : SW846 8260

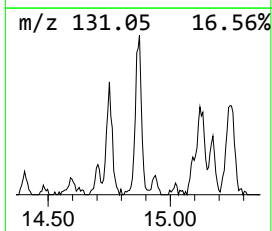
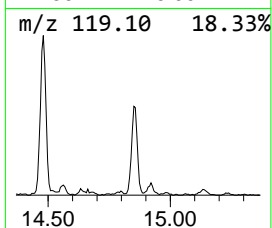
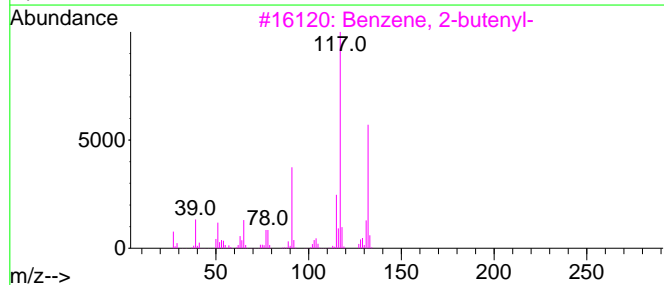
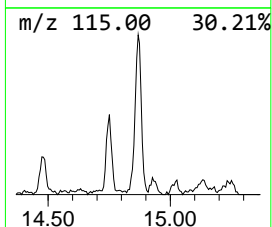
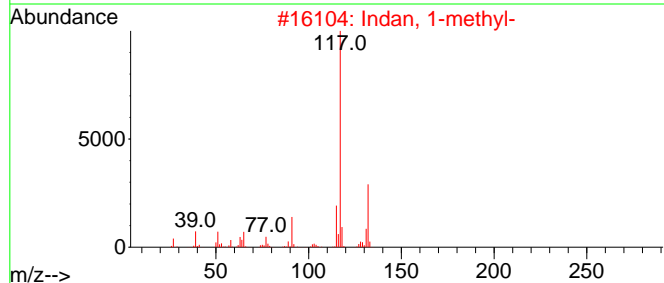
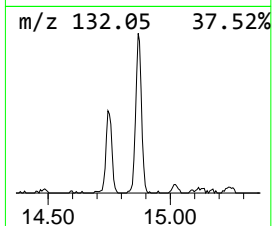
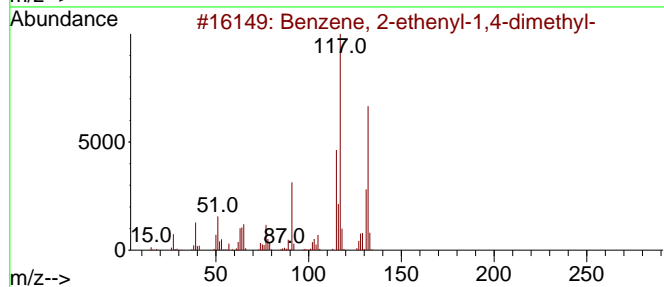
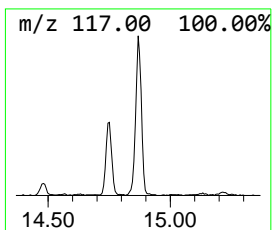
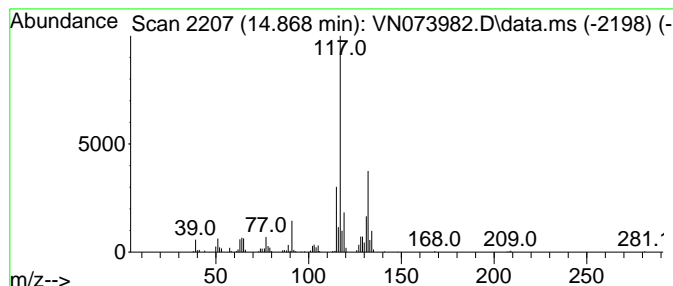
TIC Library : C:\Database\NIST20.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 7 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	7.03 ug/l	394008	1,4-Dichlorobenzene-d4	13.615

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2		Indan, 1-methyl-	132	C10H12	000767-58-8	87
3		Benzene, 2-butenyl-	132	C10H12	001560-06-1	83
4		Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	83
5		1-Phenyl-1-butene	132	C10H12	000824-90-8	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN081722\  
Data File : VN073982.D  
Acq On : 17 Aug 2022 17:36  
Operator : JC\MD  
Sample : N4204-25 10X  
Misc : 5.0mL/MSVOA\_N/WATER  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
MW-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N081522W.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclopropane, 1...	3.928	6.0	ug/l	219490	1	8.016	1835730	50.0
Cyclopentene	4.887	5.0	ug/l	183918	1	8.016	1835730	50.0
Cyclooctyl alcohol	8.533	6.6	ug/l	278705	2	8.904	2105740	50.0
Pentane, 2,3,3-...	9.951	5.9	ug/l	248525	2	8.904	2105740	50.0
Deltacyclene	13.815	20.7	ug/l	1161740	4	13.615	2800830	50.0
o-Cymene	14.156	5.1	ug/l	287408	4	13.615	2800830	50.0
Benzene, 2-ethe...	14.868	7.0	ug/l	394008	4	13.615	2800830	50.0