

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
 Data File : VN074270.D
 Acq On : 02 Sep 2022 03:19
 Operator : JC\MD
 Sample : N4354-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-22

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\82N083022W.M
 Title : SW846 8260

Signal : TIC: VN074270.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	49	58	64	rBV4	38600	71477	5.94%	0.634%
2	2.405	82	88	95	rBV3	35797	74758	6.22%	0.663%
3	3.087	196	204	213	rVB2	118930	269006	22.37%	2.384%
4	3.457	258	267	276	rVB4	14131	35204	2.93%	0.312%
5	4.999	524	529	531	rVV4	7986	12534	1.04%	0.111%
6	5.110	538	548	563	rVB5	33886	130465	10.85%	1.156%
7	5.275	568	576	578	rBV3	25022	49148	4.09%	0.436%
8	5.534	606	620	637	rBV2	51755	194608	16.19%	1.725%
9	6.410	757	769	778	rBV5	7578	27384	2.28%	0.243%
10	7.063	869	880	891	rVB2	60909	192696	16.03%	1.708%
11	7.951	1021	1031	1036	rBV	164578	390356	32.47%	3.460%
12	8.016	1036	1042	1053	rVV3	339251	817509	67.99%	7.246%
13	8.098	1054	1056	1066	rVB5	15389	31053	2.58%	0.275%
14	8.381	1093	1104	1115	rBV4	330883	948410	78.88%	8.406%
15	8.634	1145	1147	1157	rVB7	10249	19068	1.59%	0.169%
16	8.904	1182	1193	1205	rBV	418656	869709	72.33%	7.708%
17	9.398	1266	1277	1283	rBV7	17861	53656	4.46%	0.476%
18	9.822	1344	1349	1356	rVB3	13178	25066	2.08%	0.222%
19	9.904	1358	1363	1367	rVV3	13938	26466	2.20%	0.235%
20	9.951	1367	1371	1381	rVB3	24994	45846	3.81%	0.406%
21	10.139	1397	1403	1408	rBV6	12574	26688	2.22%	0.237%
22	10.263	1418	1424	1429	rBV4	9569	16913	1.41%	0.150%
23	10.381	1436	1444	1452	rBV	651660	1202355	100.00%	10.657%
24	10.439	1452	1454	1459	rVB3	11404	14913	1.24%	0.132%
25	10.581	1468	1478	1484	rVV4	33628	68207	5.67%	0.605%
26	10.657	1484	1491	1497	rVB2	32671	57392	4.77%	0.509%
27	10.792	1508	1514	1522	rBV6	13204	30006	2.50%	0.266%
28	11.063	1558	1560	1566	rVB3	9111	15686	1.30%	0.139%
29	11.528	1632	1639	1644	rBV2	11541	20566	1.71%	0.182%
30	11.686	1658	1666	1674	rBV	602558	1091504	90.78%	9.674%
31	11.786	1676	1683	1690	rVB2	100940	174285	14.50%	1.545%
32	11.886	1695	1700	1706	rBV3	15460	36561	3.04%	0.324%
33	12.516	1801	1807	1815	rBV2	58002	94632	7.87%	0.839%
34	12.669	1825	1833	1843	rBV	479755	825345	68.64%	7.315%
35	12.857	1860	1865	1871	rVB	50984	78283	6.51%	0.694%
36	13.157	1911	1916	1921	rBV2	23096	34473	2.87%	0.306%

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37	13.304	1936	1941	1946	rVB2	14291	19961	1.66%	0.177%
38	13.422	1954	1961	1969	rBV4	18220	45702	3.80%	0.405%
39	13.610	1986	1993	2003	rBV	581158	983255	81.78%	8.715%
40	13.710	2006	2010	2016	rVB5	10654	13820	1.15%	0.122%
41	13.780	2016	2022	2023	rBV2	32926	50574	4.21%	0.448%
42	13.816	2023	2028	2033	rVV	282445	470488	39.13%	4.170%
43	13.857	2033	2035	2040	rVV4	16266	22153	1.84%	0.196%
44	13.939	2043	2049	2054	rBV3	20676	34122	2.84%	0.302%
45	14.004	2054	2060	2066	rBV2	53041	82334	6.85%	0.730%
46	14.216	2090	2096	2099	rBV4	32067	54999	4.57%	0.487%
47	14.269	2099	2105	2110	rVV	151611	253406	21.08%	2.246%
48	14.321	2110	2114	2120	rVB7	7495	17509	1.46%	0.155%
49	14.398	2120	2127	2131	rBV5	20596	37036	3.08%	0.328%
50	14.474	2131	2140	2144	rBV2	92724	151800	12.63%	1.345%
51	14.516	2144	2147	2152	rVB	58632	82605	6.87%	0.732%
52	14.698	2174	2178	2181	rBV4	12034	18277	1.52%	0.162%
53	14.745	2181	2186	2191	rVV4	26869	44630	3.71%	0.396%
54	14.786	2191	2193	2199	rVB4	12032	15348	1.28%	0.136%
55	14.868	2199	2207	2212	rBV2	75898	139412	11.59%	1.236%
56	14.927	2212	2217	2223	rVB5	18275	35981	2.99%	0.319%
57	15.016	2226	2232	2236	rBV3	35193	60968	5.07%	0.540%
58	15.127	2244	2251	2255	rBV5	42031	81853	6.81%	0.725%
59	15.233	2261	2269	2280	rVB6	31504	90455	7.52%	0.802%
60	15.433	2290	2303	2309	rBV	63456	144306	12.00%	1.279%
61	15.492	2309	2313	2317	rVV5	9952	17255	1.44%	0.153%
62	15.533	2317	2320	2323	rVV4	12765	22099	1.84%	0.196%
63	15.568	2324	2326	2334	rVB10	11991	24578	2.04%	0.218%
64	15.721	2348	2352	2359	rBV7	9913	21044	1.75%	0.187%
65	16.027	2400	2404	2409	rBV5	7528	14648	1.22%	0.130%
66	16.104	2412	2417	2425	rVB7	11163	25800	2.15%	0.229%
67	16.251	2438	2442	2449	rBV8	7583	13256	1.10%	0.117%
68	16.521	2484	2488	2499	rVB8	7102	19003	1.58%	0.168%
69	16.733	2516	2524	2533	rBV3	44582	101702	8.46%	0.901%

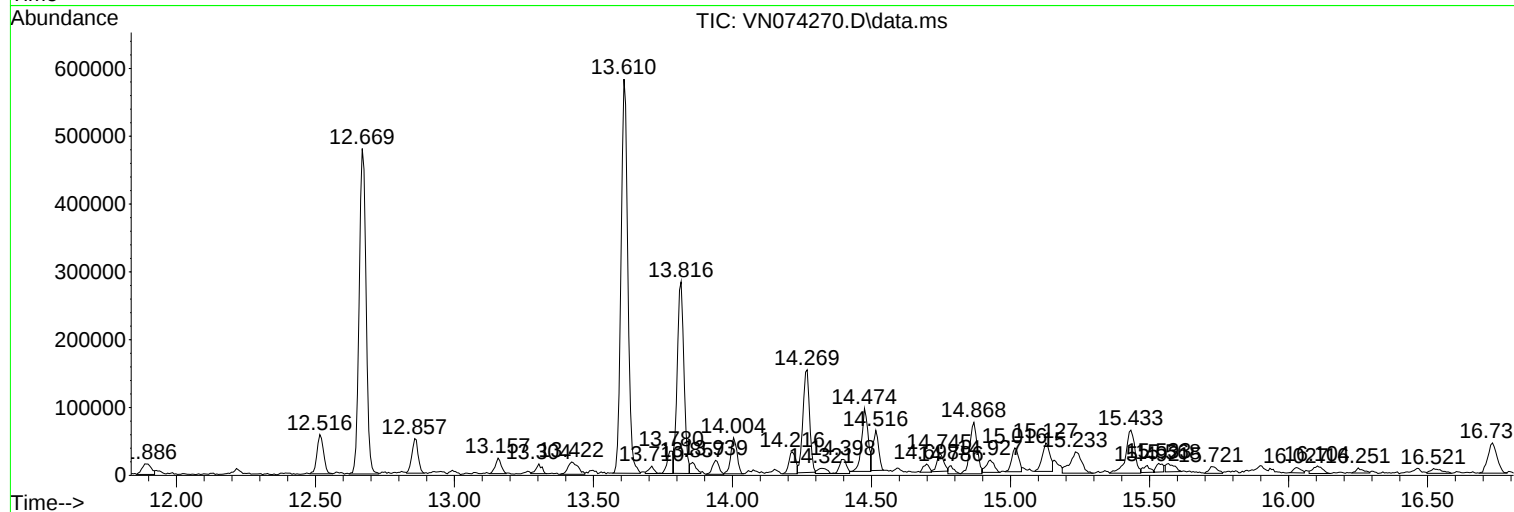
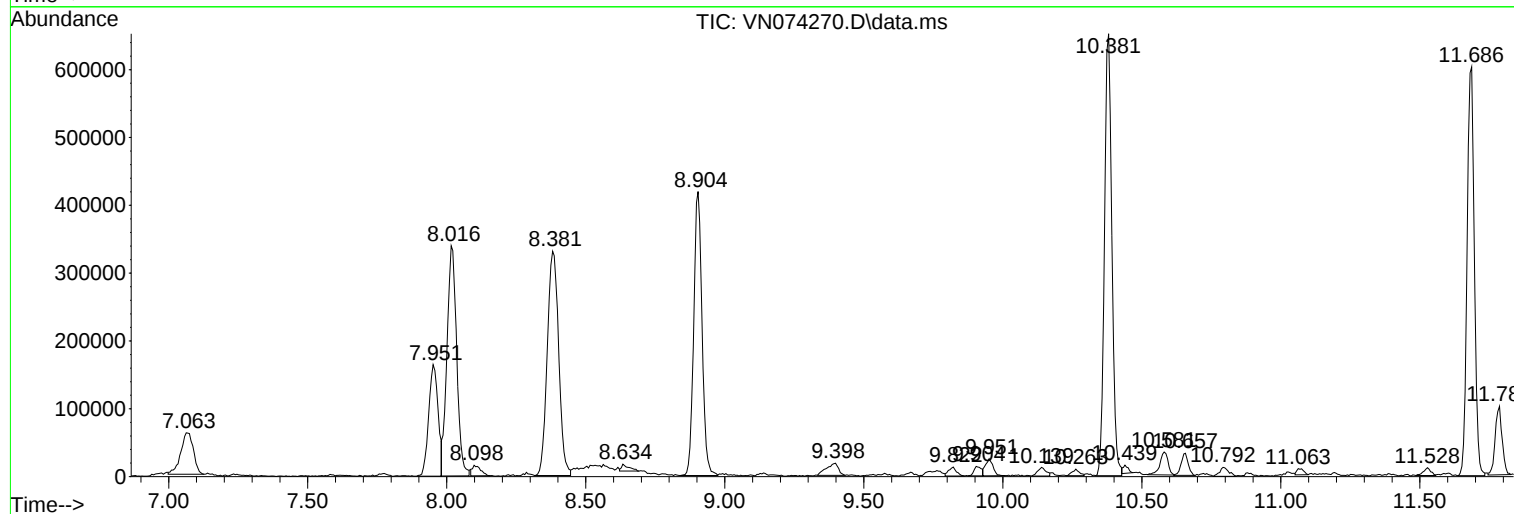
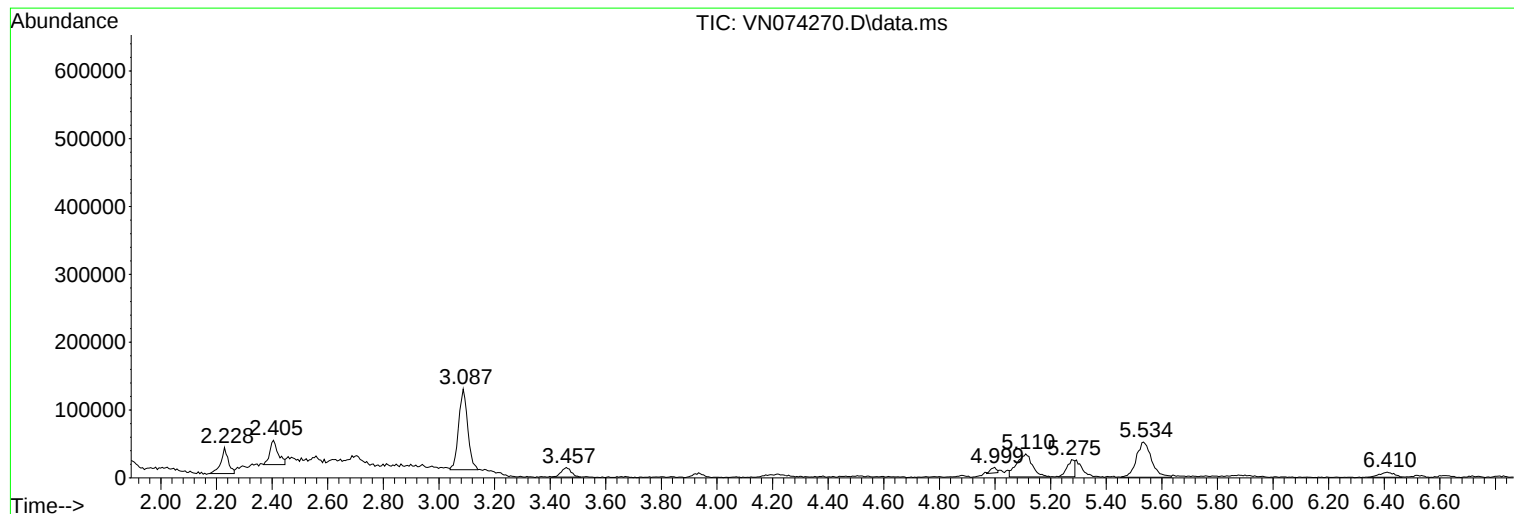
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-22

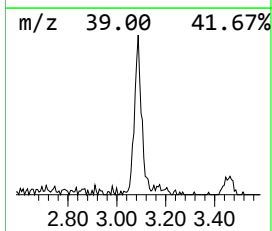
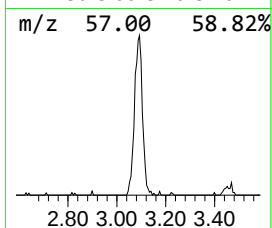
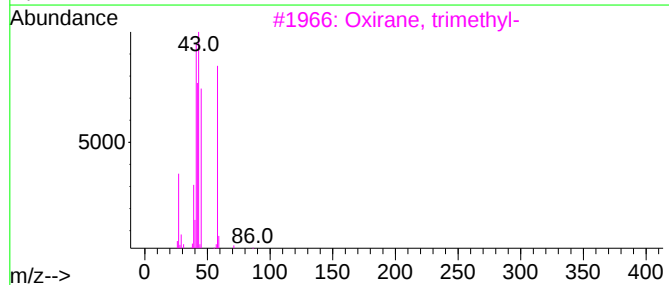
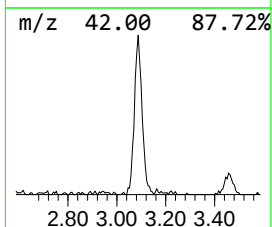
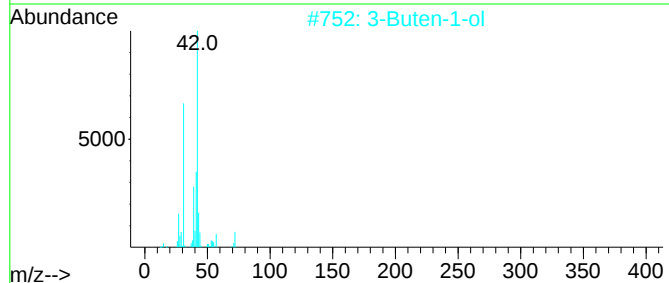
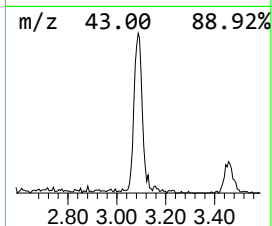
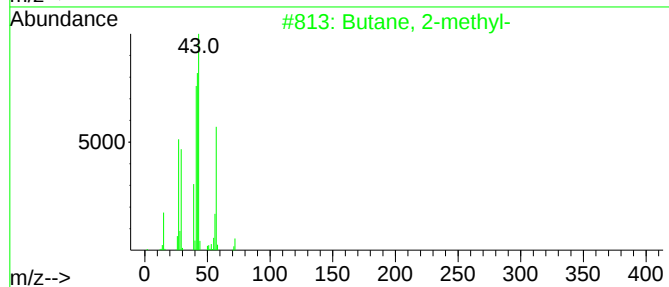
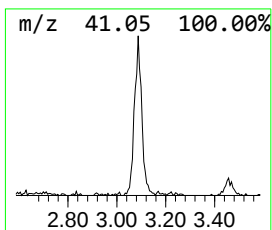
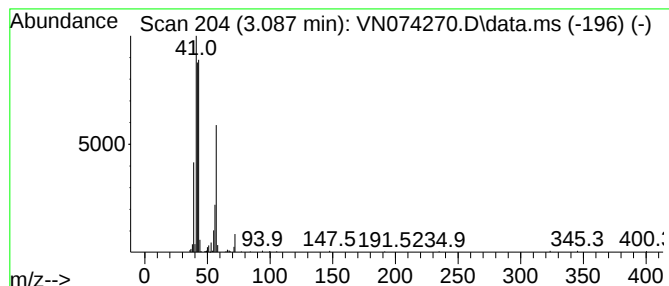
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	16.45 ug/l	269006	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methyl-	72	C5H12	000078-78-4	68
2		3-Buten-1-ol	72	C4H8O	000627-27-0	38
3		Oxirane, trimethyl-	86	C5H10O	005076-19-7	38
4		Pentane	72	C5H12	000109-66-0	38
5		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	25



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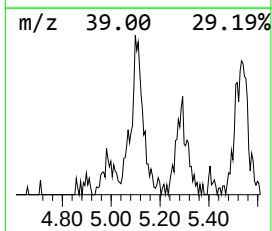
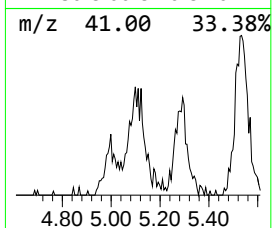
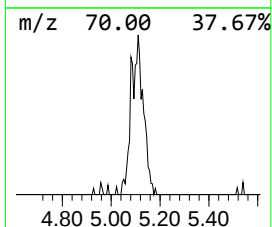
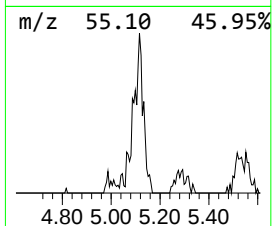
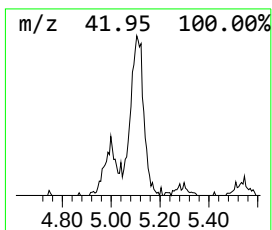
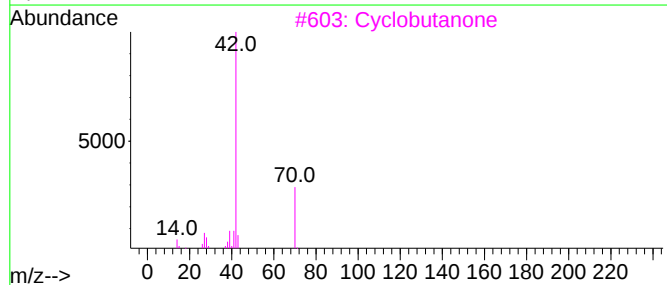
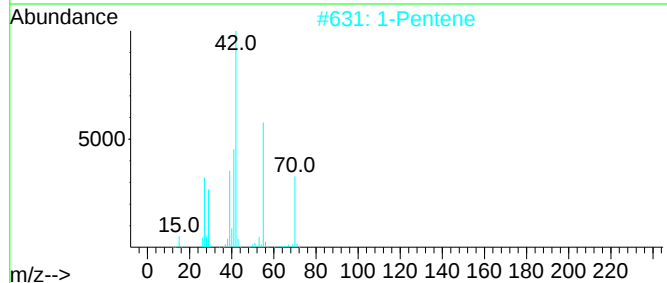
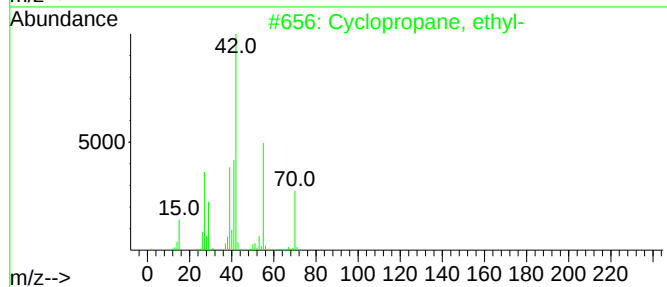
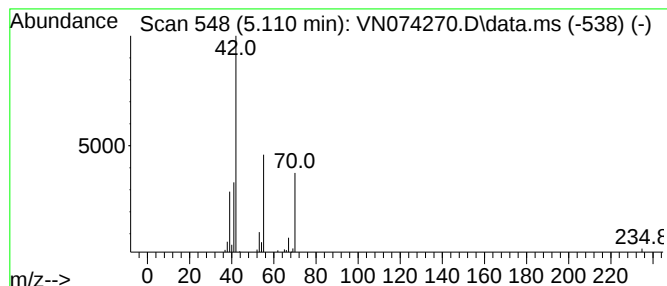
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclopropane, ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	7.98 ug/l	130465	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopropane, ethyl-	70	C5H10	001191-96-4	72
2		1-Pentene	70	C5H10	000109-67-1	56
3		Cyclobutanone	70	C4H6O	001191-95-3	9
4		Cyclopentane	70	C5H10	000287-92-3	9
5		Aziridine, 2-ethyl-	71	C4H9N	002549-67-9	9



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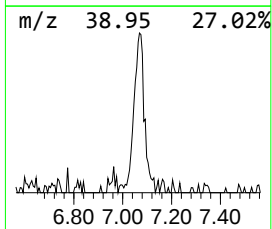
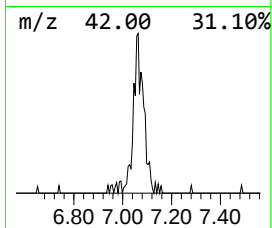
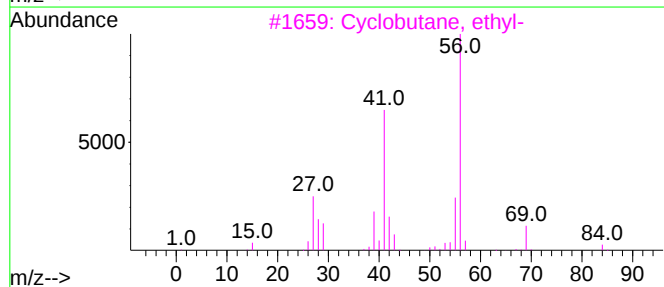
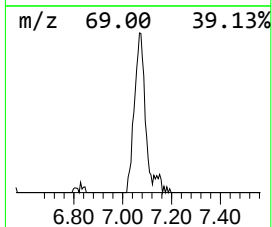
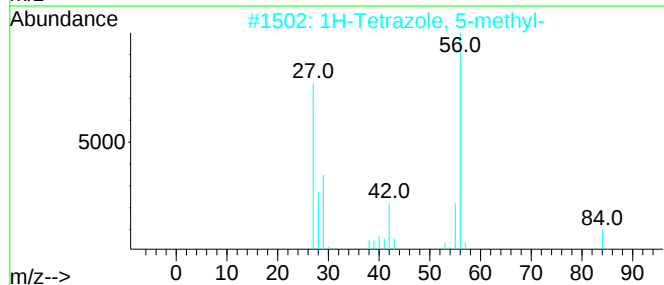
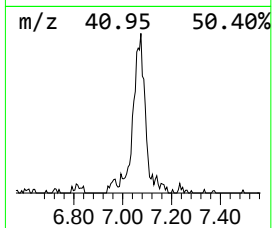
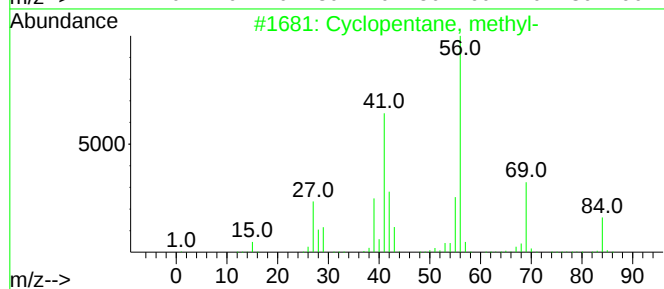
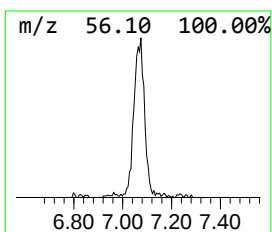
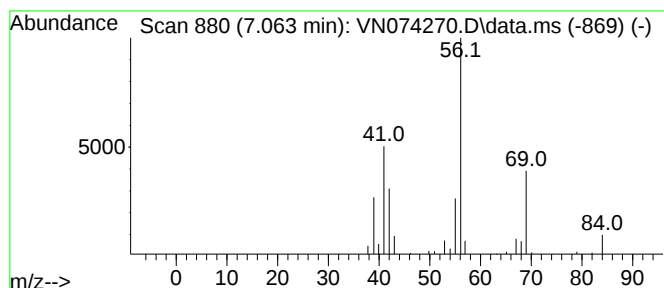
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Peak Number 3 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.063	11.79 ug/l	192696	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	86
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4			Cyclobutane, butyl-	112	C8H16	013152-44-8	64
5			Cyclobutane	56	C4H8	000287-23-0	49



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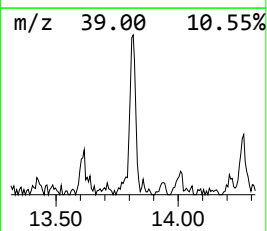
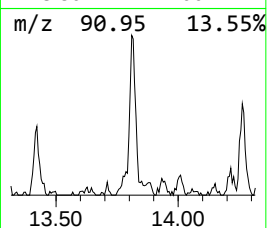
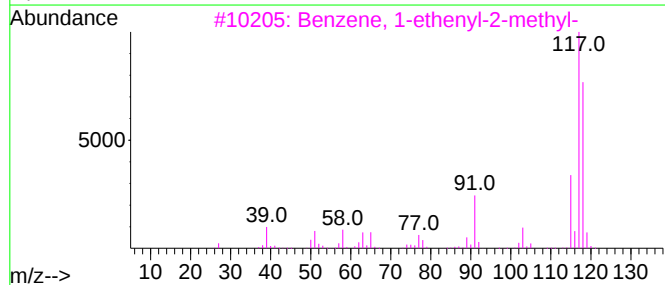
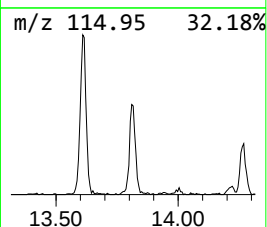
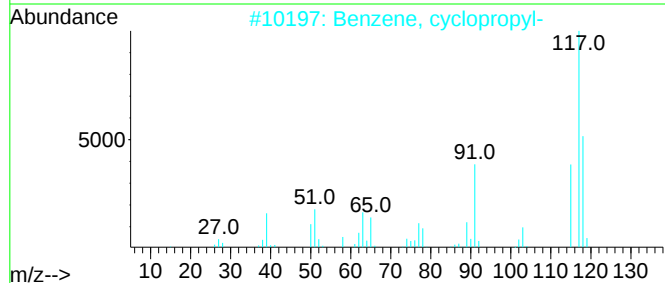
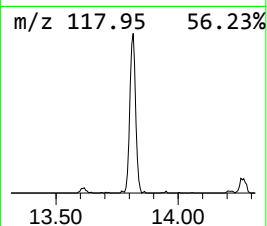
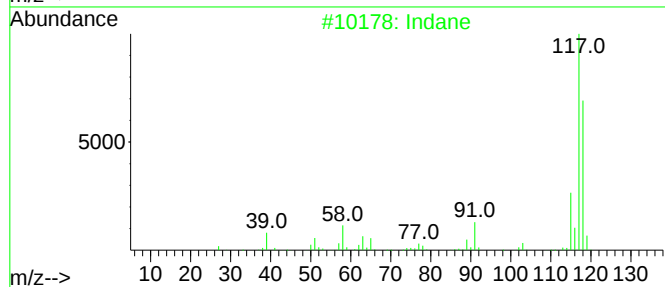
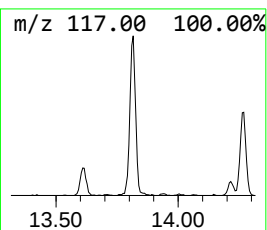
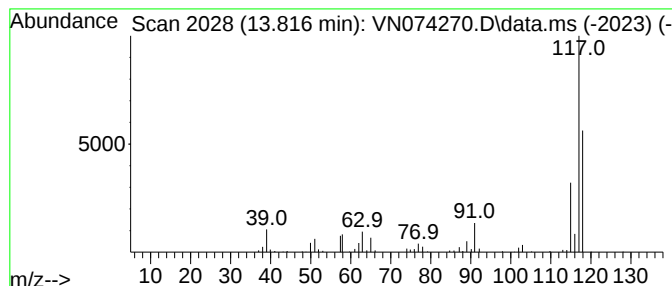
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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

Peak Number 4 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	23.93 ug/l	470488	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	94
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	68
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	59
5			Deltacyclene	118	C9H10	007785-10-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074270.D
Acq On : 02 Sep 2022 03:19
Operator : JC\MD
Sample : N4354-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-22

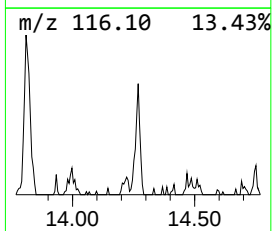
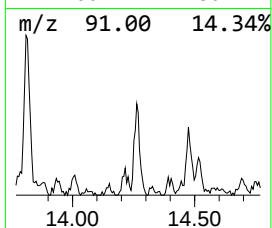
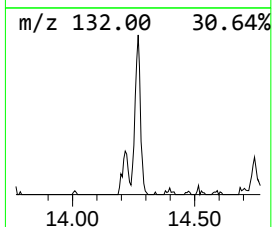
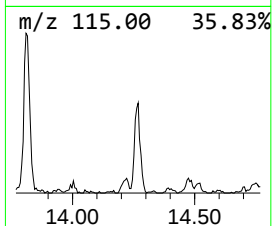
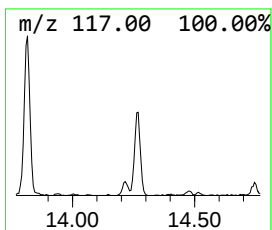
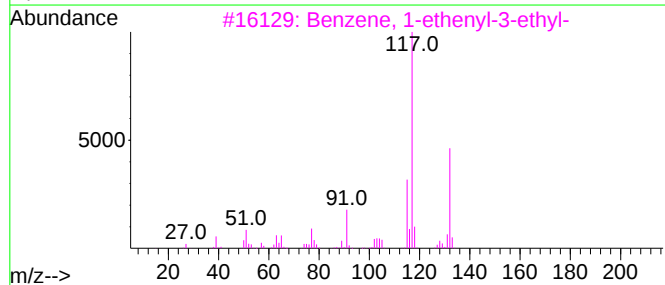
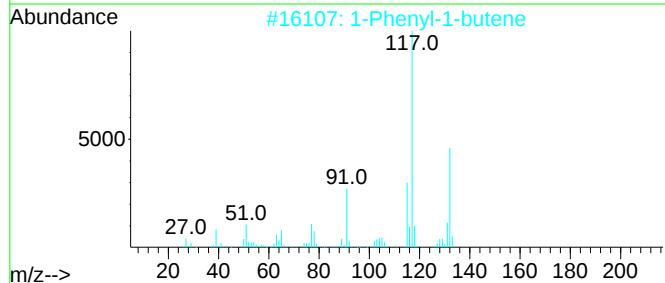
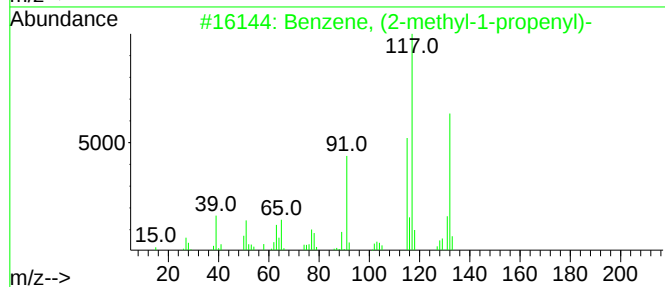
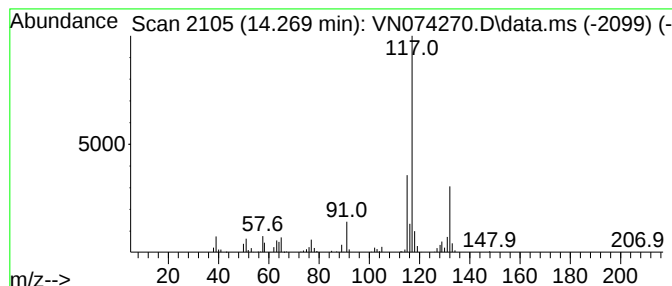
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, (2-methyl-1-propen... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.269	12.89 ug/l	253406	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	91
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	91
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074270.D
Acq On : 02 Sep 2022 03:19
Operator : JC\MD
Sample : N4354-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-22

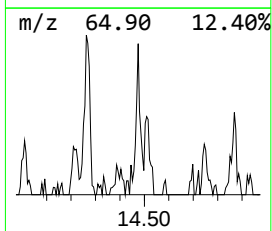
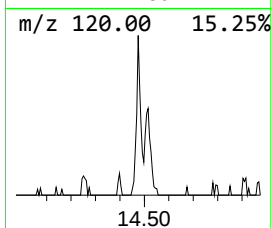
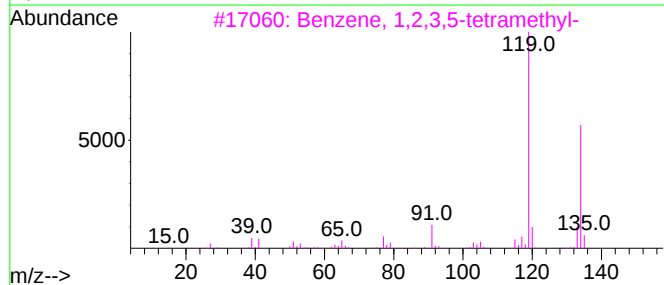
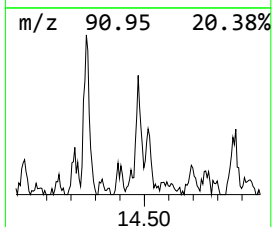
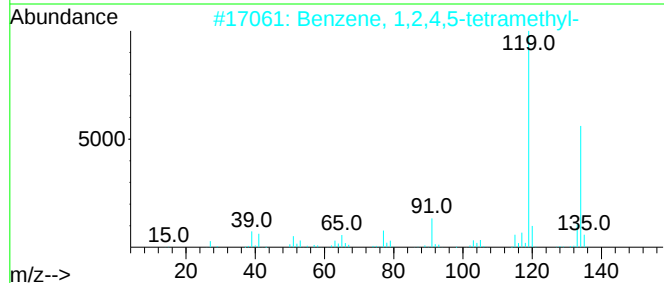
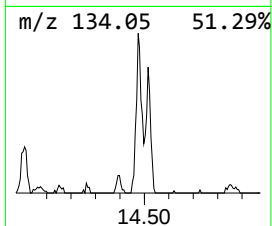
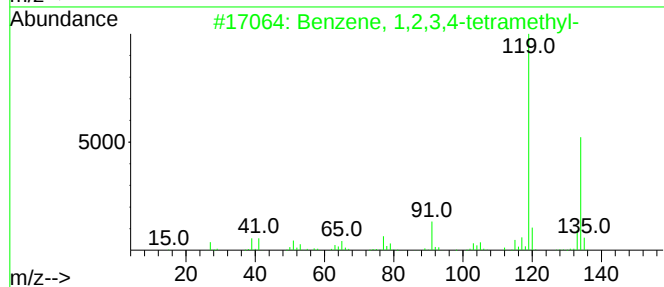
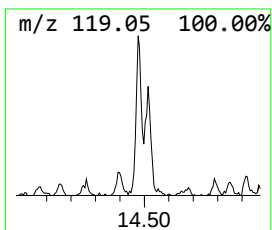
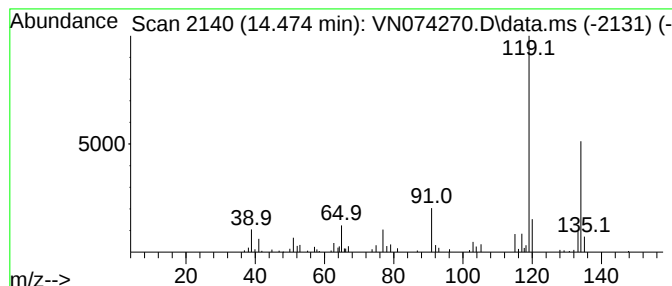
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.474	7.72 ug/l	151800	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	91
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	91
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074270.D
Acq On : 02 Sep 2022 03:19
Operator : JC\MD
Sample : N4354-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

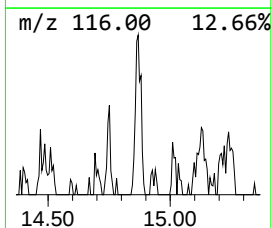
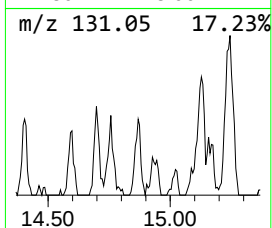
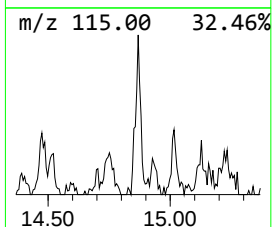
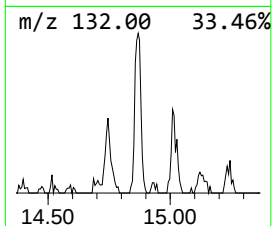
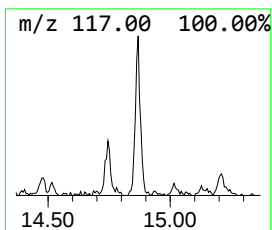
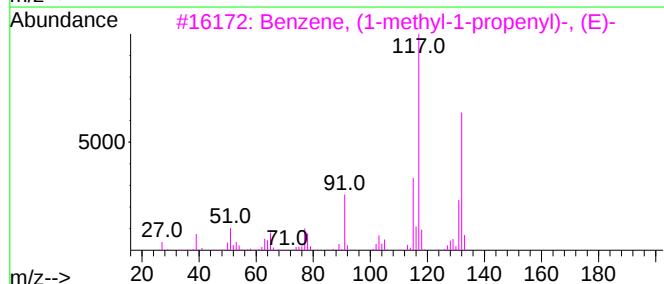
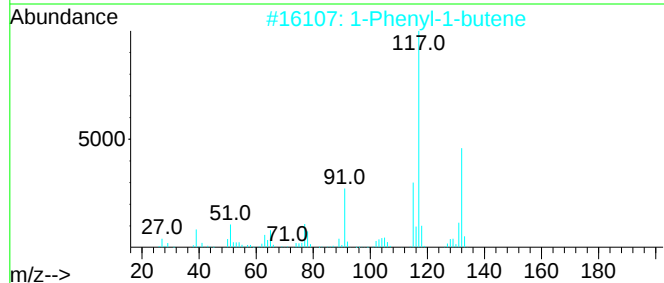
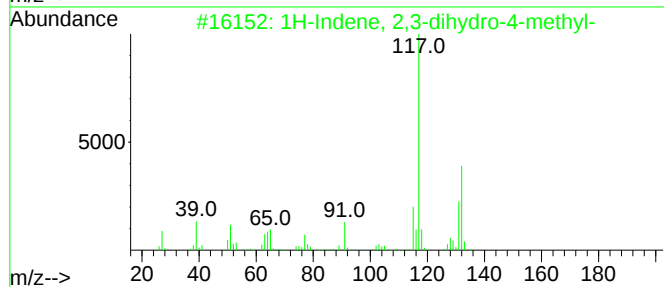
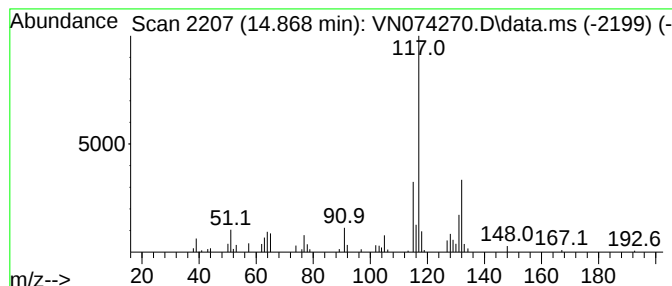
Instrument :
MSVOA_N
ClientSampleId :
MW-22

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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

Peak Number 7 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.868	7.09 ug/l	139412	1,4-Dichlorobenzene-d4		13.610	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4-methyl-		132	C10H12	000824-22-6	94
2	1-Phenyl-1-butene		132	C10H12	000824-90-8	91
3	Benzene, (1-methyl-1-propenyl)-,...		132	C10H12	000768-00-3	91
4	Benzene, (1-methyl-1-propenyl)-,...		132	C10H12	000767-99-7	91
5	3-Phenylbut-1-ene		132	C10H12	000934-10-1	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074270.D
Acq On : 02 Sep 2022 03:19
Operator : JC\MD
Sample : N4354-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-22

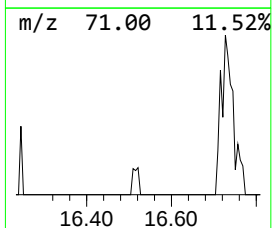
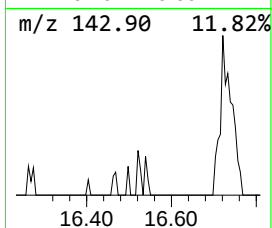
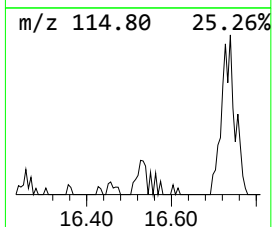
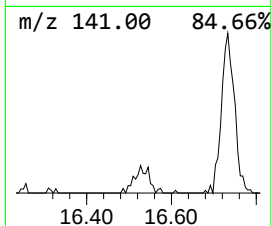
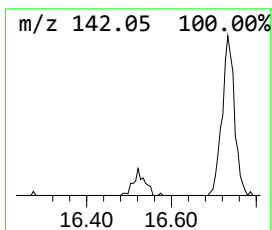
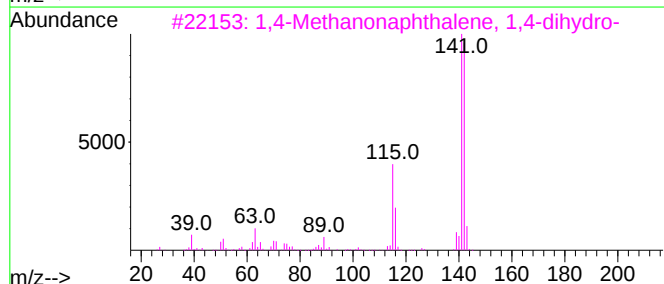
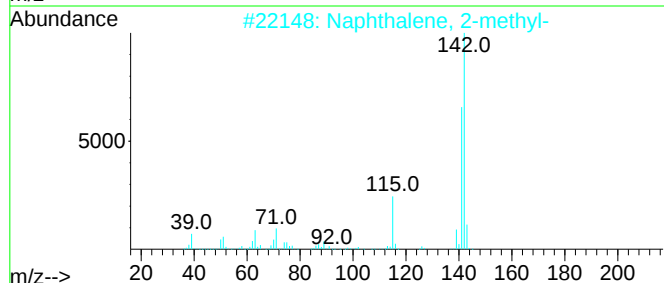
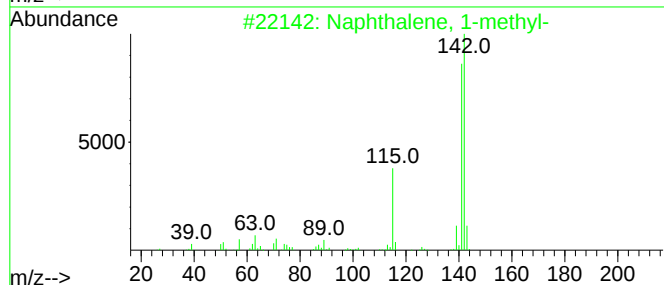
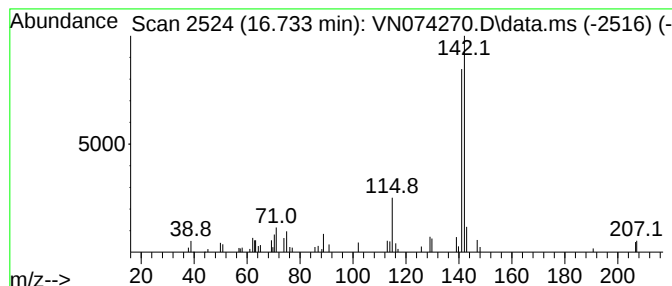
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Quant Title : SW846 8260

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

Peak Number 8 1,4-Methanonaphthalene, 1,4... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.733	5.17 ug/l	101702	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	87
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	87
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	83
4			Benzocycloheptatriene	142	C11H10	000264-09-5	80
5			Naphthalene, 1-(2-hydroxypropyl)	186	C13H14O	027653-13-0	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074270.D
Acq On : 02 Sep 2022 03:19
Operator : JC\MD
Sample : N4354-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-22

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.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
Butane, 2-methyl-	3.087	16.4	ug/l	269006	1	8.016	817509	50.0
Cyclopropane, e...	5.110	8.0	ug/l	130465	1	8.016	817509	50.0
Cyclopentane, m...	7.063	11.8	ug/l	192696	1	8.016	817509	50.0
Indane	13.816	23.9	ug/l	470488	4	13.610	983255	50.0
Benzene, (2-met...	14.269	12.9	ug/l	253406	4	13.610	983255	50.0
Benzene, 1,2,3,...	14.474	7.7	ug/l	151800	4	13.610	983255	50.0
1H-Indene, 2,3-...	14.868	7.1	ug/l	139412	4	13.610	983255	50.0
1,4-Methanonaph...	16.733	5.2	ug/l	101702	4	13.610	983255	50.0