

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071024\
 Data File : VN082855.D
 Acq On : 10 Jul 2024 15:13
 Operator : JC\MD
 Sample : P3184-01
 Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 COMP(00187-00189-00186)

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\82N070824W.M
 Title : SW846 8260

Signal : TIC: VN082855.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.518	85	96	100	rBV4	5438	15035	3.01%	0.411%
2	2.789	137	142	143	rBV2	5071	8197	1.64%	0.224%
3	7.471	929	938	947	rBV	3632	9444	1.89%	0.258%
4	8.165	1044	1056	1060	rBV2	73940	168195	33.72%	4.597%
5	8.218	1060	1065	1076	rVB	108455	240967	48.30%	6.586%
6	8.577	1117	1126	1137	rBV2	75899	171208	34.32%	4.679%
7	9.100	1205	1215	1225	rBV	169725	342102	68.58%	9.350%
8	10.012	1365	1370	1378	rVB3	3244	6347	1.27%	0.173%
9	10.147	1388	1393	1397	rBV2	3825	6640	1.33%	0.181%
10	10.565	1456	1464	1471	rBV	271348	498845	100.00%	13.634%
11	10.629	1471	1475	1483	rVB	13338	24192	4.85%	0.661%
12	11.865	1678	1685	1694	rBV	247852	439653	88.13%	12.016%
13	11.965	1697	1702	1707	rBV	4012	5328	1.07%	0.146%
14	12.070	1712	1720	1726	rBV3	13981	25857	5.18%	0.707%
15	12.400	1768	1776	1781	rVB4	6543	10792	2.16%	0.295%
16	12.853	1845	1853	1861	rBV	193174	325018	65.15%	8.883%
17	13.100	1890	1895	1898	rBV2	4982	7037	1.41%	0.192%
18	13.170	1904	1907	1912	rVB6	4286	6965	1.40%	0.190%
19	13.347	1930	1937	1943	rBV3	20842	36572	7.33%	1.000%
20	13.482	1954	1960	1965	rBV2	9274	14009	2.81%	0.383%
21	13.676	1987	1993	1998	rBV4	4577	9697	1.94%	0.265%
22	13.794	2006	2013	2023	rBV	273245	456777	91.57%	12.484%
23	14.023	2048	2052	2062	rVB7	6300	13494	2.71%	0.369%
24	14.117	2062	2068	2073	rBV4	8356	17706	3.55%	0.484%
25	14.247	2085	2090	2092	rBV6	5326	6511	1.31%	0.178%
26	14.270	2092	2094	2100	rVV4	5130	9679	1.94%	0.265%
27	14.329	2101	2104	2110	rVB3	6058	9717	1.95%	0.266%
28	14.441	2116	2123	2128	rBV2	14707	29380	5.89%	0.803%
29	14.523	2131	2137	2141	rBV5	5715	11282	2.26%	0.308%
30	14.576	2141	2146	2150	rBV7	4636	8101	1.62%	0.221%
31	14.623	2150	2154	2158	rBV4	14672	24977	5.01%	0.683%
32	14.658	2158	2160	2163	rVV4	6604	8442	1.69%	0.231%
33	14.688	2163	2165	2170	rVB3	7356	10089	2.02%	0.276%
34	14.735	2170	2173	2177	rBV5	8210	12277	2.46%	0.336%
35	14.794	2177	2183	2188	rBV7	10607	20373	4.08%	0.557%
36	14.847	2188	2192	2195	rBV6	6185	11091	2.22%	0.303%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071024\
Data File : VN082855.D
Acq On : 10 Jul 2024 15:13
Operator : JC\MD
Sample : P3184-01
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP(00187-00189-00186)

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\82N070824W.M
Title : SW846 8260

37	14.964	2209	2212	2218	rVB4	8813	14528	2.91%	0.397%
38	15.041	2218	2225	2227	rBV4	16584	35092	7.03%	0.959%
39	15.105	2232	2236	2241	rVB7	13783	25022	5.02%	0.684%
40	15.223	2251	2256	2260	rBV6	15523	30980	6.21%	0.847%
41	15.270	2260	2264	2268	rVV7	15889	25450	5.10%	0.696%
42	15.323	2268	2273	2279	rVV9	18878	42459	8.51%	1.160%
43	15.435	2287	2292	2298	rBV7	19487	43255	8.67%	1.182%
44	15.600	2316	2320	2328	rBV7	14497	33549	6.73%	0.917%
45	15.929	2371	2376	2378	rBV5	26666	53127	10.65%	1.452%
46	16.170	2413	2417	2423	rBV8	49635	112532	22.56%	3.076%
47	16.711	2504	2509	2515	rBV2	103617	220862	44.27%	6.036%

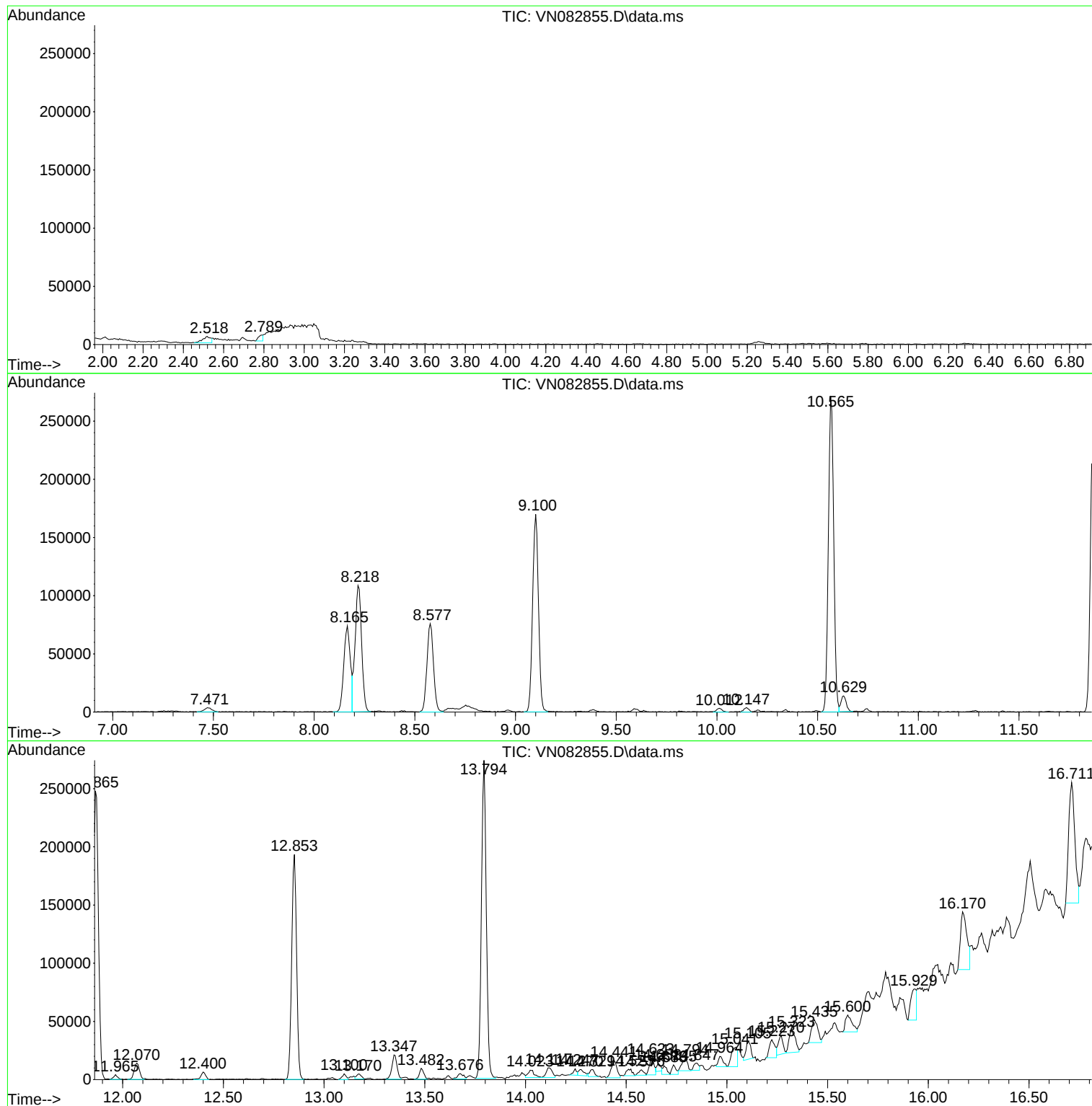
Sum of corrected areas: 3658852

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071024\
Data File : VN082855.D
Acq On : 10 Jul 2024 15:13
Operator : JC\MD
Sample : P3184-01
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP(00187-00189-00186)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071024\
Data File : VN082855.D
Acq On : 10 Jul 2024 15:13
Operator : JC\MD
Sample : P3184-01
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP(00187-00189-00186)

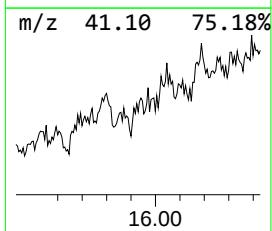
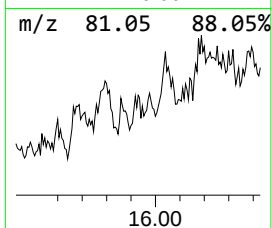
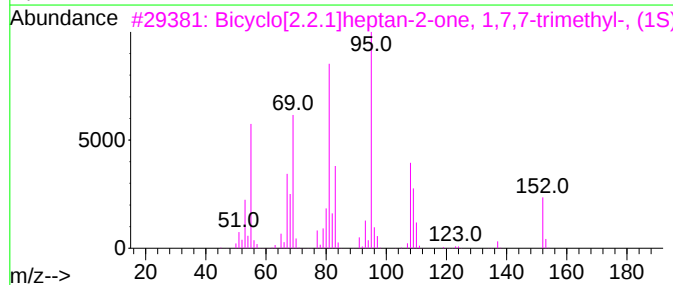
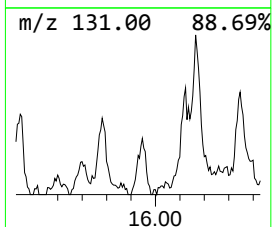
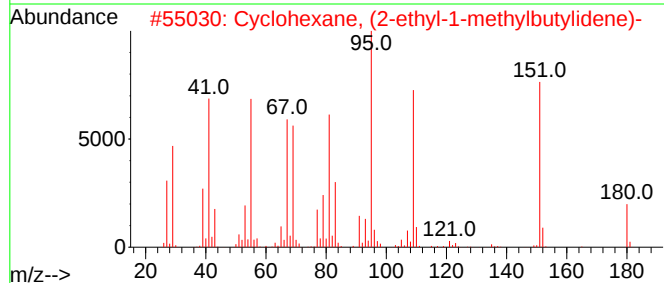
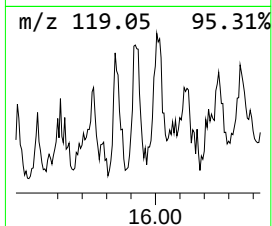
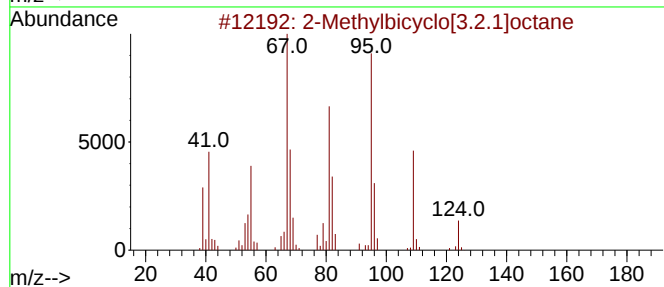
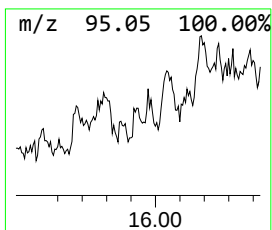
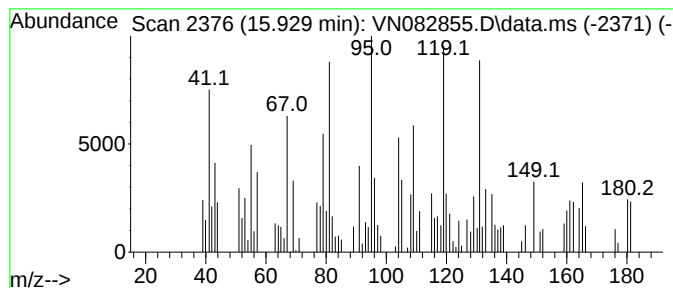
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown15.929 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.929	5.82 ug/l	53127	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methylbicyclo[3.2.1]octane	124	C9H16	1010215-28-0	38
2			Cyclohexane, (2-ethyl-1-methylbu...	180	C13H24	074810-41-6	30
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	25
4			Camphor	152	C10H16O	000076-22-2	22
5			5-(Furan-3-yl)-2-methylpent-1-en...	164	C10H12O2	080445-58-5	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071024\
Data File : VN082855.D
Acq On : 10 Jul 2024 15:13
Operator : JC\MD
Sample : P3184-01
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP(00187-00189-00186)

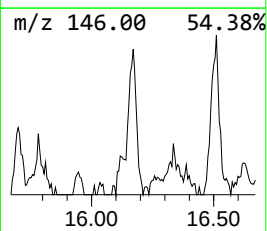
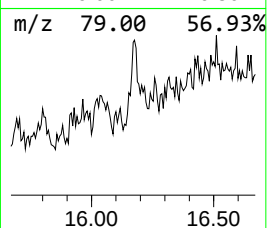
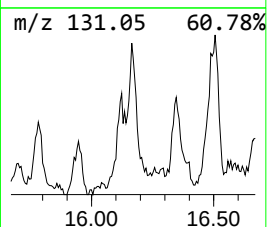
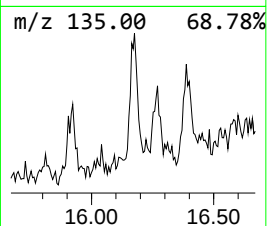
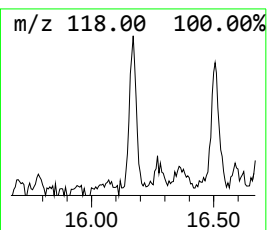
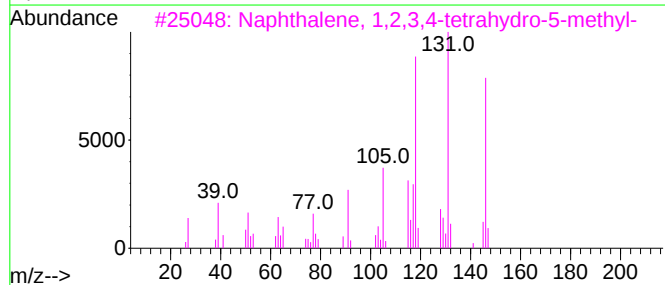
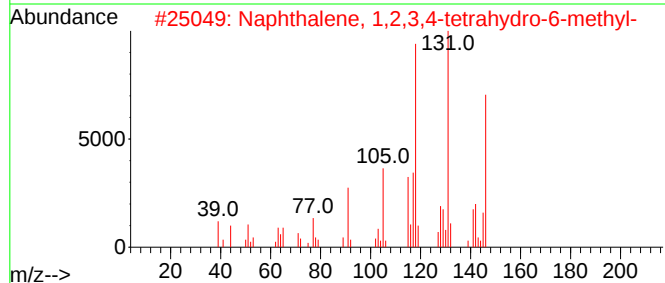
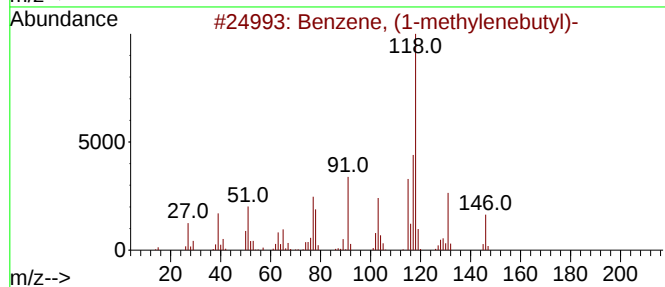
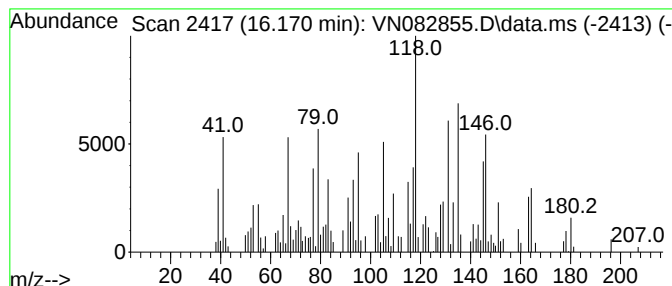
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, (1-methylenebutyl)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	12.32 ug/l	112532	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	50
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	49
3			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	46
4			Cinnoline, 1,2-dihydro-2-methyl-	146	C9H10N2	054063-10-4	45
5			1H-Pyrazole, 4,5-dihydro-3-phenyl-	146	C9H10N2	000936-48-1	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071024\
Data File : VN082855.D
Acq On : 10 Jul 2024 15:13
Operator : JC\MD
Sample : P3184-01
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP(00187-00189-00186)

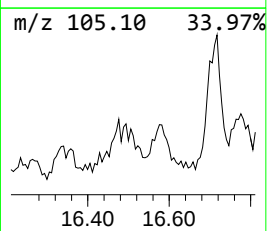
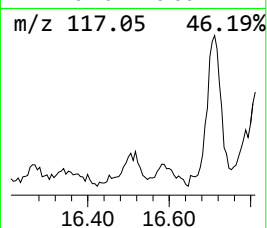
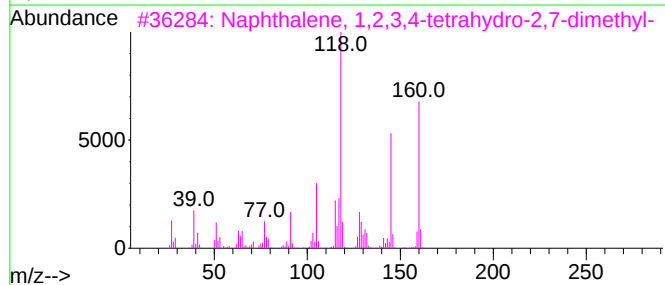
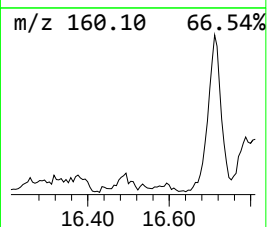
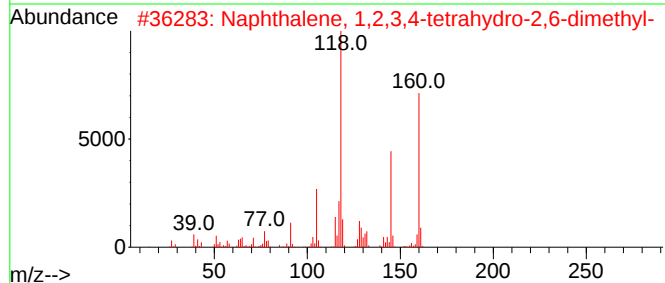
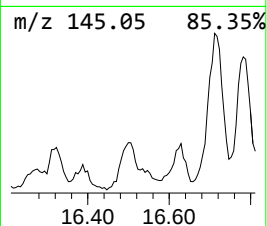
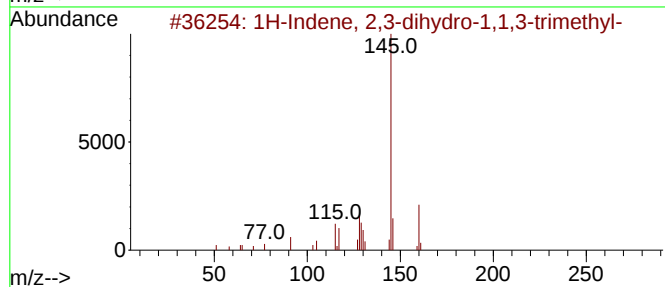
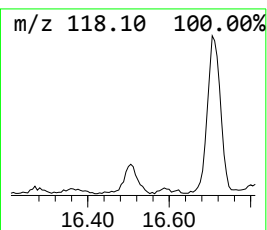
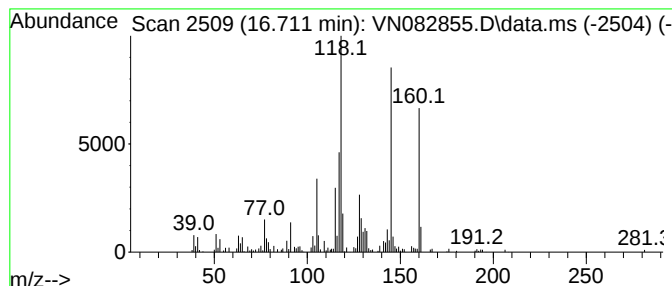
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.711	24.18 ug/l	220862	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	83
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	70
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	64
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	001076-61-5	55
5			4-(4-Methylphenyl)-1,6-heptadien...	201	C14H19N	1000486-01-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071024\
Data File : VN082855.D
Acq On : 10 Jul 2024 15:13
Operator : JC\MD
Sample : P3184-01
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP(00187-00189-00186)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.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
unknown15.929	15.929	5.8	ug/l	53127	4	13.794	456777	50.0
Benzene, (1-met...	16.170	12.3	ug/l	112532	4	13.794	456777	50.0
1H-Indene, 2,3-...	16.711	24.2	ug/l	220862	4	13.794	456777	50.0