

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
 Data File : VN070242.D
 Acq On : 20 Dec 2021 15:54
 Operator : JC/MD
 Sample : M5044-08
 Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DA-8-4.5

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

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
 Title : SW846 8260

Signal : TIC: VN070242.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.045	1861	1885	1904	rBV3	214620	672453	1.01%	0.147%
2	7.144	1905	1922	1942	rVB2	265377	723978	1.09%	0.158%
3	7.844	2168	2183	2202	rVB2	301081	717544	1.08%	0.157%
4	8.021	2228	2249	2257	rBV	902614	2139995	3.23%	0.468%
5	8.080	2259	2271	2290	rVV2	2175603	5766993	8.70%	1.260%
6	8.174	2292	2306	2330	rVB	708134	1845160	2.78%	0.403%
7	8.295	2331	2351	2372	rBV	896248	2078384	3.13%	0.454%
8	8.437	2385	2404	2435	rBV	1102425	2689763	4.06%	0.588%
9	8.614	2436	2470	2495	rBV	2763893	8038911	12.13%	1.757%
10	8.826	2527	2549	2573	rBV3	741597	1835340	2.77%	0.401%
11	8.965	2582	2601	2625	rBV2	3480685	7952413	12.00%	1.738%
12	9.054	2627	2634	2649	rVV2	428492	876289	1.32%	0.191%
13	9.456	2752	2784	2795	rBV3	1392567	3672803	5.54%	0.803%
14	9.510	2796	2804	2821	rVV2	792835	1543174	2.33%	0.337%
15	9.883	2928	2943	2965	rVB	2196401	4622579	6.97%	1.010%
16	10.014	2966	2992	3006	rBV2	3102783	7264871	10.96%	1.588%
17	10.078	3006	3016	3046	rVB2	1421520	3795318	5.72%	0.829%
18	10.215	3048	3067	3092	rBV	1392430	3270917	4.93%	0.715%
19	10.368	3114	3124	3137	rVB	1441281	2534442	3.82%	0.554%
20	10.441	3137	3151	3162	rBV	4988490	9348325	14.10%	2.043%
21	10.505	3162	3175	3202	rVV	9549189	18172764	27.41%	3.971%
22	10.623	3204	3219	3233	rVB2	1354462	2705414	4.08%	0.591%
23	10.880	3297	3315	3333	rVV7	697856	2362382	3.56%	0.516%
24	11.151	3395	3416	3432	rBV5	550465	1633519	2.46%	0.357%
25	11.524	3546	3555	3581	rVB2	1423377	3248677	4.90%	0.710%
26	11.626	3582	3593	3615	rBV	1090020	1981574	2.99%	0.433%
27	11.744	3622	3637	3653	rBV	5483925	9833171	14.83%	2.149%
28	11.843	3660	3674	3695	rVB	13912059	23750843	35.82%	5.190%
29	11.950	3696	3714	3740	rBV2	33164537	66296996	100.00%	14.488%
30	12.278	3819	3836	3857	rVB	16554681	29079743	43.86%	6.355%
31	12.578	3936	3948	3960	rBV	2540708	4415358	6.66%	0.965%
32	12.728	3993	4004	4027	rVB	4547822	9159687	13.82%	2.002%
33	12.919	4063	4075	4086	rBV	5348877	8566343	12.92%	1.872%
34	12.980	4086	4098	4106	rBV	13871630	23862658	35.99%	5.215%
35	13.058	4119	4127	4142	rVB	8356401	13720390	20.70%	2.998%
36	13.219	4174	4187	4203	rBV	7251895	12302628	18.56%	2.688%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070242.D
Acq On : 20 Dec 2021 15:54
Operator : JC/MD
Sample : M5044-08
Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-8-4.5

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

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Title : SW846 8260

37	13.367	4228	4242	4271	rVB2	30264678	51996480	78.43%	11.363%
38	13.493	4275	4289	4301	rBV3	689343	1797288	2.71%	0.393%
39	13.557	4306	4313	4324	rVB	931028	1390510	2.10%	0.304%
40	13.675	4345	4357	4361	rVV	5762723	9400876	14.18%	2.054%
41	13.704	4363	4368	4398	rVB	8338120	14333525	21.62%	3.132%
42	13.839	4406	4418	4421	rBV	2501970	3697622	5.58%	0.808%
43	13.871	4422	4430	4439	rVV3	6641366	10595073	15.98%	2.315%
44	13.997	4469	4477	4489	rVB3	564076	887370	1.34%	0.194%
45	14.067	4492	4503	4514	rVB	1573011	2519459	3.80%	0.551%
46	14.134	4515	4528	4530	rBV2	3602185	5051231	7.62%	1.104%
47	14.214	4548	4558	4571	rVB	5133915	7975300	12.03%	1.743%
48	14.278	4575	4582	4588	rVV	625318	998238	1.51%	0.218%
49	14.324	4590	4599	4613	rVB3	2360353	4081876	6.16%	0.892%
50	14.458	4639	4649	4660	rVB	1050059	1631985	2.46%	0.357%
51	14.539	4668	4679	4685	rBV	2274563	3441521	5.19%	0.752%
52	14.576	4686	4693	4703	rVV	3149841	4777874	7.21%	1.044%
53	14.619	4703	4709	4718	rVB2	961808	1263967	1.91%	0.276%
54	14.807	4769	4779	4790	rBV3	2428602	4200646	6.34%	0.918%
55	14.927	4806	4824	4836	rBV4	3064575	7580741	11.43%	1.657%
56	14.981	4838	4844	4860	rVB2	784008	1503862	2.27%	0.329%
57	15.083	4874	4882	4898	rVB3	507280	858120	1.29%	0.188%
58	15.196	4914	4924	4951	rVB5	1244372	3447582	5.20%	0.753%
59	15.308	4955	4966	4980	rVB6	771288	1631809	2.46%	0.357%
60	15.504	5026	5039	5054	rVB	2944791	5555380	8.38%	1.214%
61	15.804	5139	5151	5170	rVB2	534194	1105575	1.67%	0.242%
62	16.614	5438	5453	5480	rVB	1481959	3408451	5.14%	0.745%

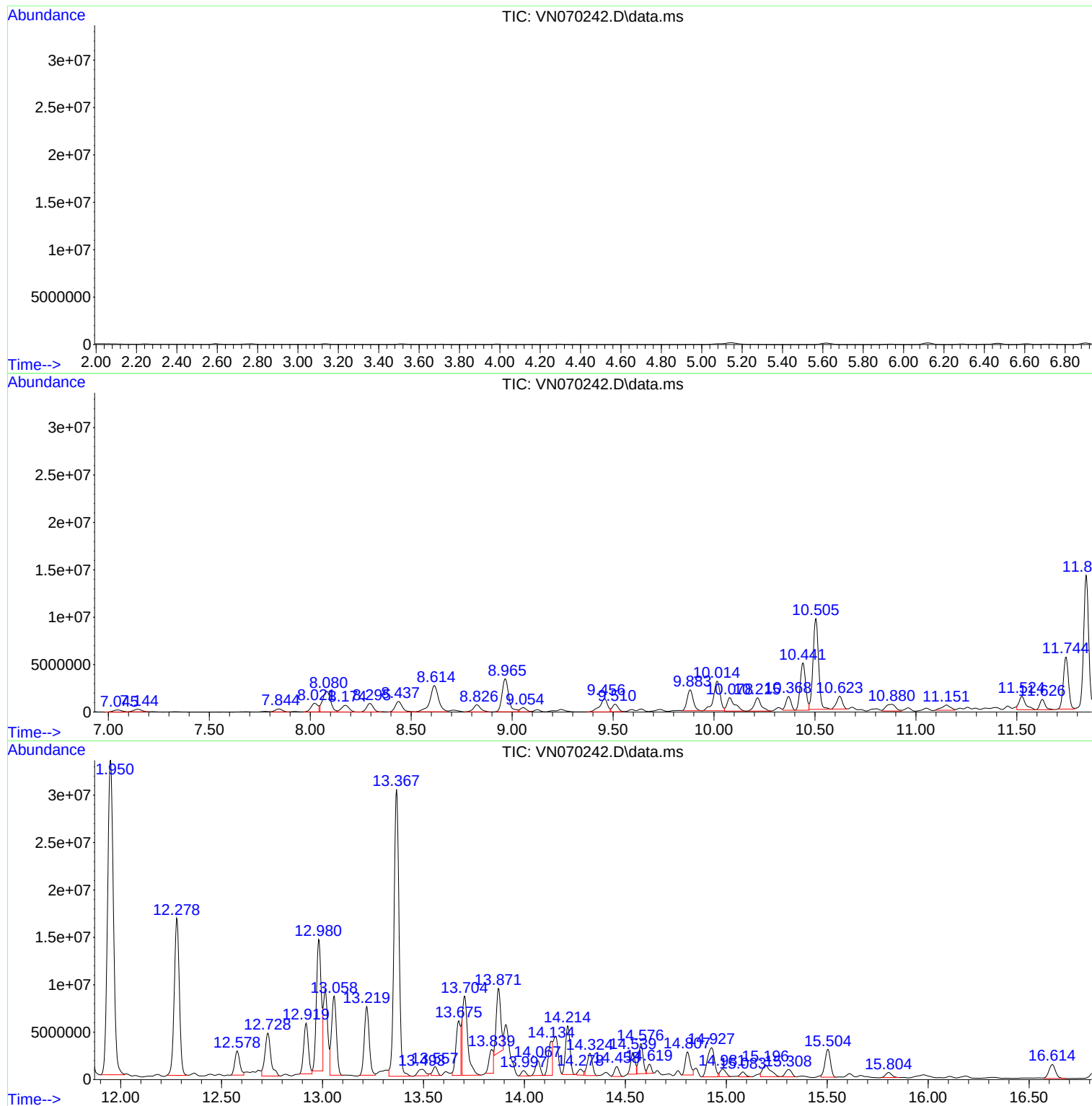
Sum of corrected areas: 457614160

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070242.D
Acq On : 20 Dec 2021 15:54
Operator : JC/MD
Sample : M5044-08
Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-8-4.5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070242.D
Acq On : 20 Dec 2021 15:54
Operator : JC/MD
Sample : M5044-08
Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-8-4.5

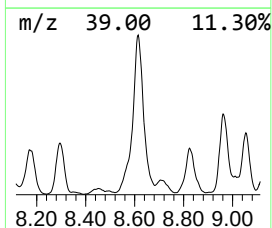
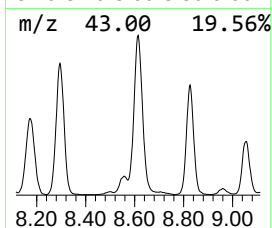
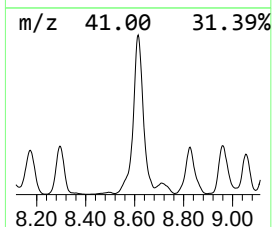
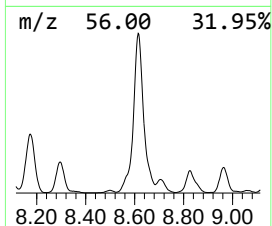
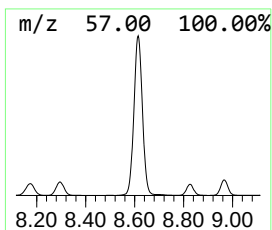
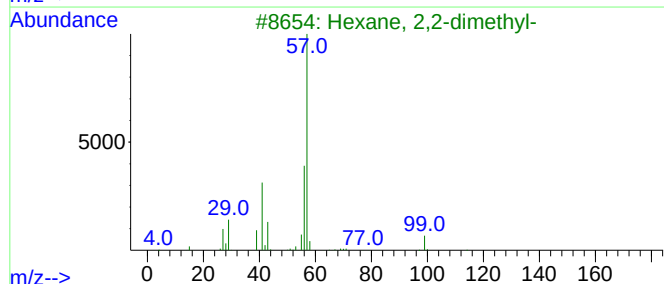
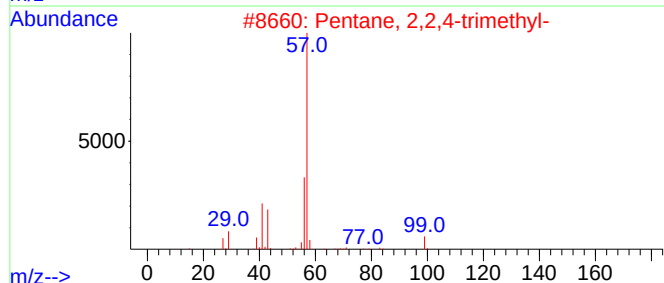
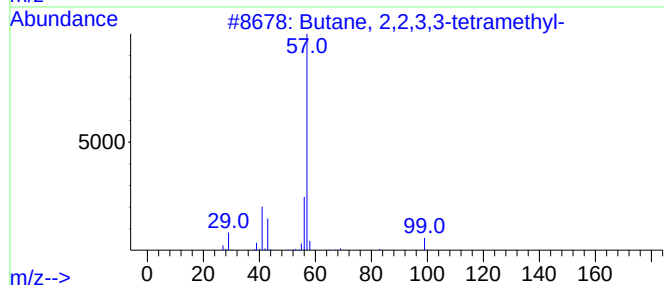
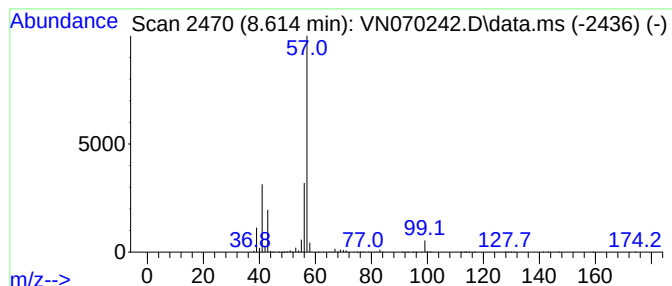
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2,2,3,3-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.614	50.54 ug/l	8038910	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070242.D
Acq On : 20 Dec 2021 15:54
Operator : JC/MD
Sample : M5044-08
Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-8-4.5

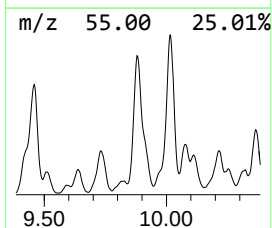
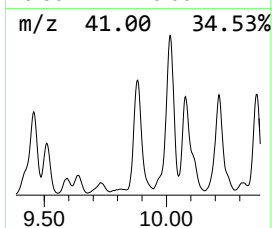
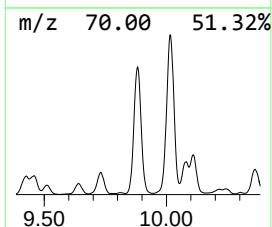
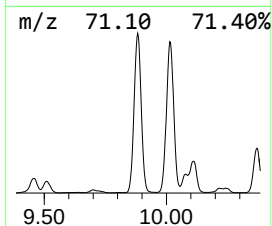
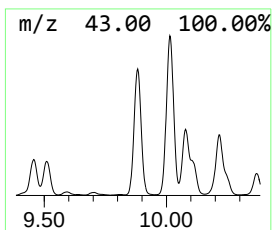
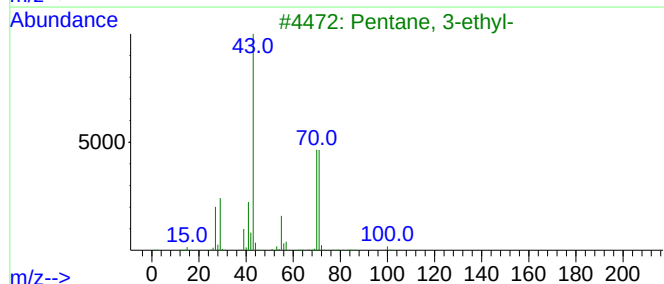
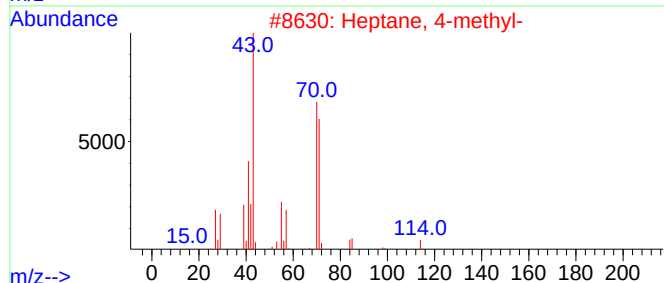
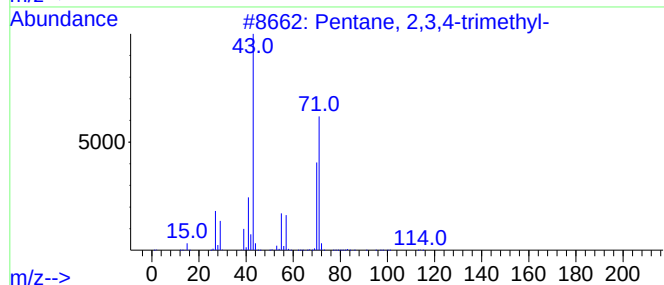
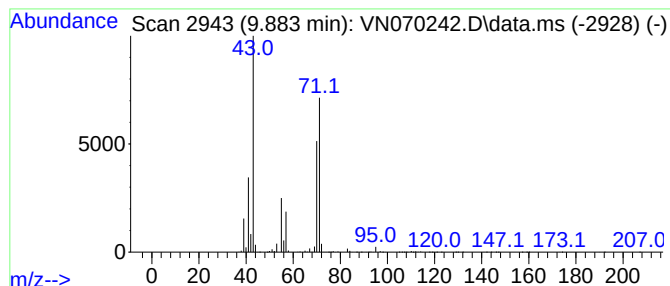
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 2,3,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.883	29.06 ug/l	4622580	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3			Pentane, 3-ethyl-	100	C7H16	000617-78-7	78
4			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	74
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070242.D
Acq On : 20 Dec 2021 15:54
Operator : JC/MD
Sample : M5044-08
Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-8-4.5

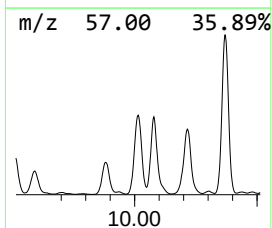
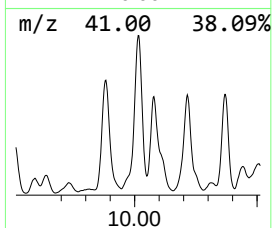
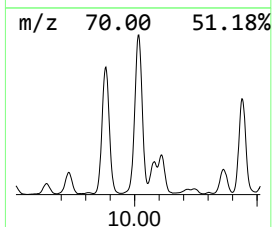
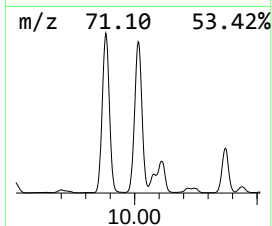
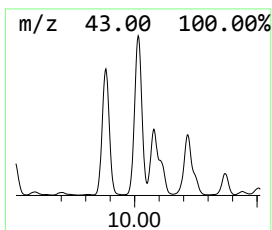
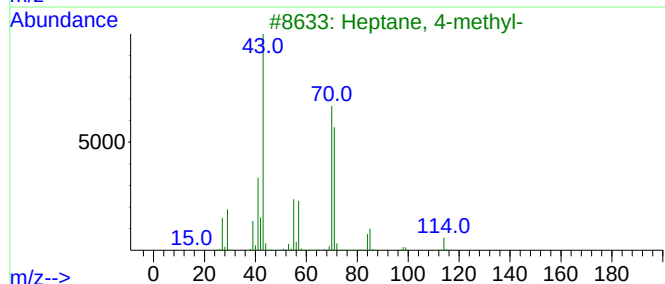
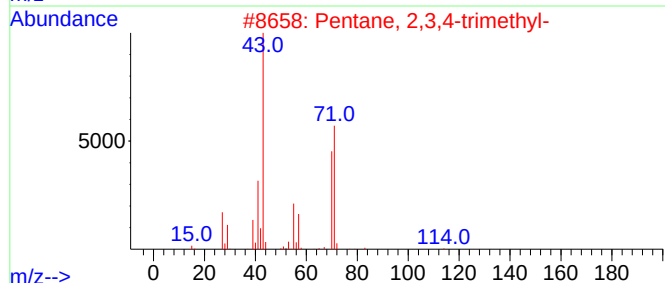
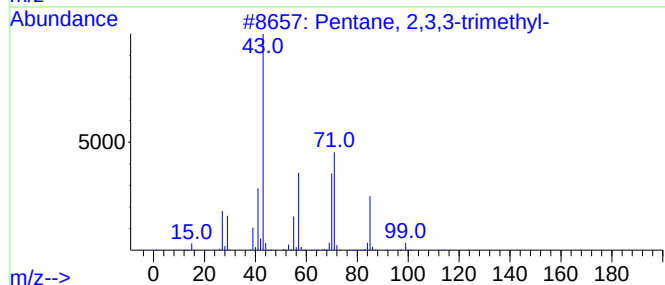
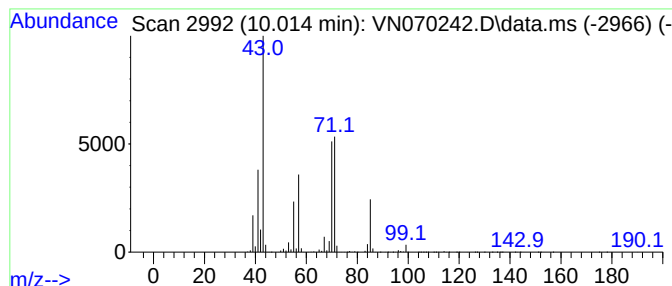
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	45.68 ug/l	7264870	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	81
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	72
4			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	59
5			Diisooamyl ether	158	C10H22O	000544-01-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070242.D
Acq On : 20 Dec 2021 15:54
Operator : JC/MD
Sample : M5044-08
Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-8-4.5

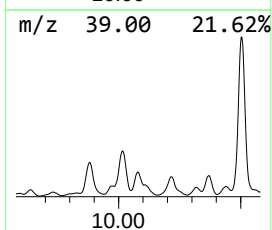
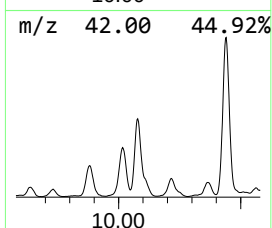
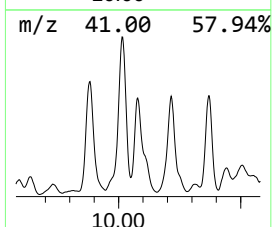
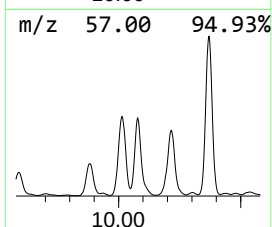
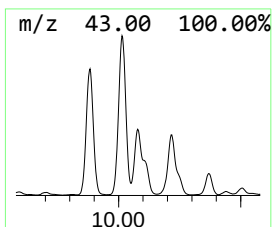
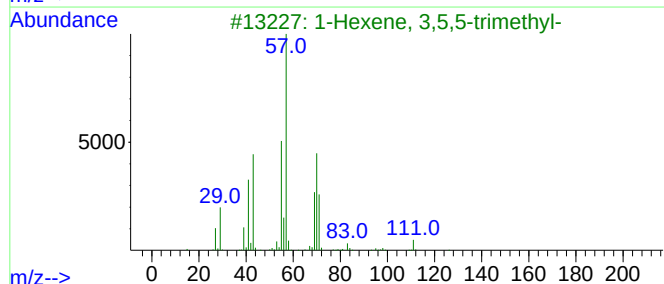
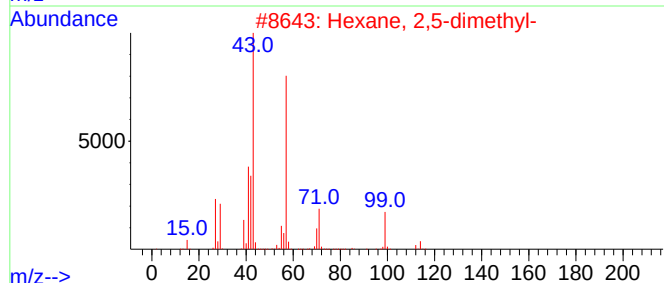
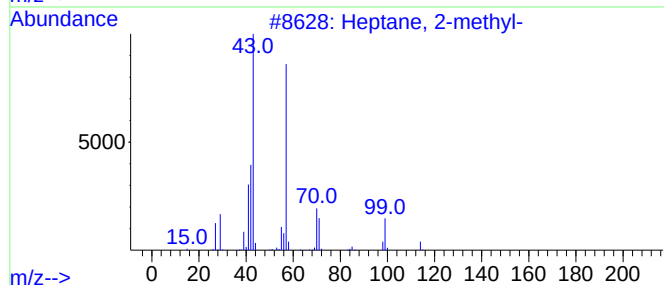
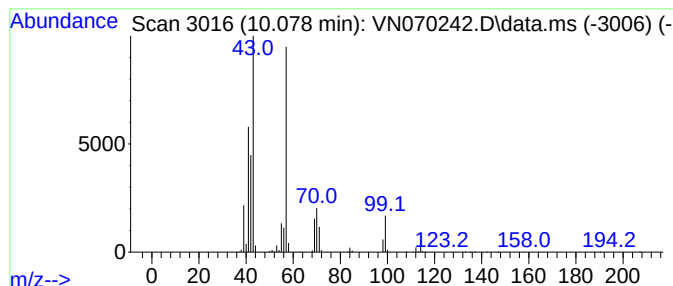
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 4 Heptane, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.079	23.86 ug/l	3795320	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2-methyl-	114	C8H18	000592-27-8	91
2			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	64
3			1-Hexene, 3,5,5-trimethyl-	126	C9H18	004316-65-8	43
4			2-Piperidinone	99	C5H9NO	000675-20-7	40
5			Cyclohexanol, 4-methyl-	114	C7H14O	000589-91-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070242.D
Acq On : 20 Dec 2021 15:54
Operator : JC/MD
Sample : M5044-08
Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-8-4.5

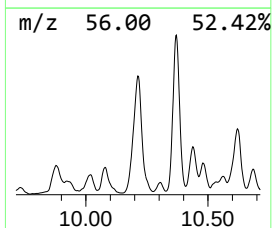
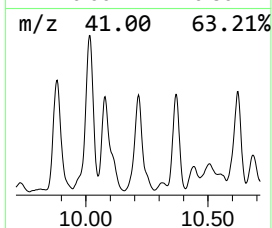
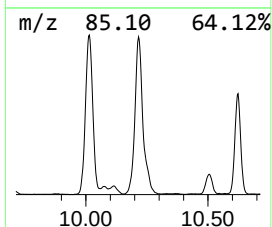
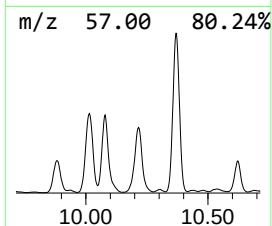
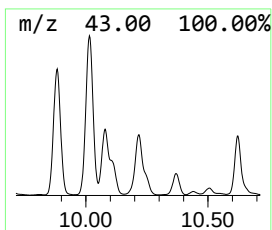
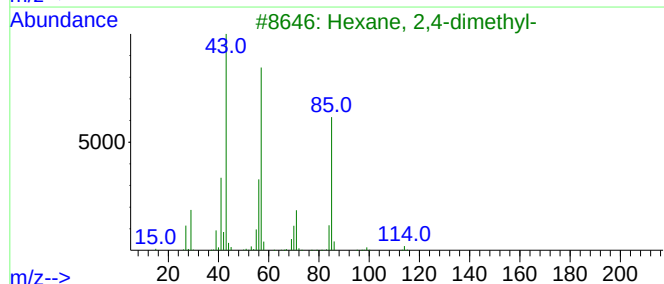
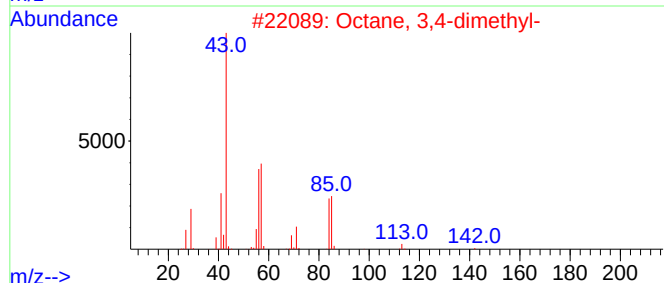
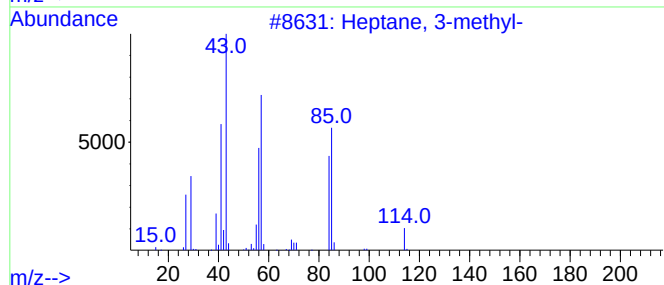
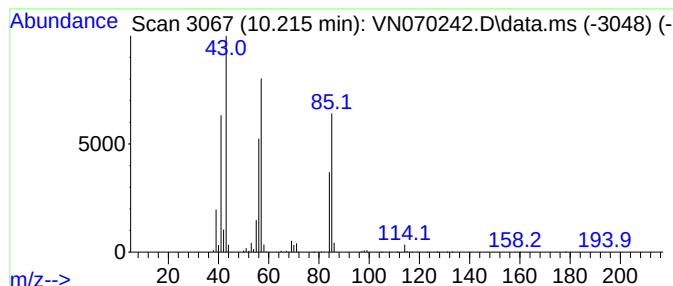
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 5 Heptane, 3-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.215	20.57 ug/l	3270920	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-methyl-	114	C8H18	000589-81-1	90
2			Octane, 3,4-dimethyl-	142	C10H22	015869-92-8	72
3			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	72
4			Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	53
5			Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070242.D
Acq On : 20 Dec 2021 15:54
Operator : JC/MD
Sample : M5044-08
Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-8-4.5

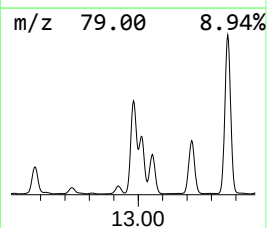
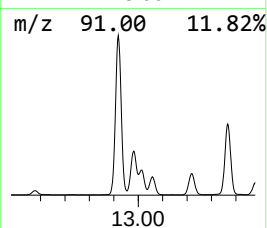
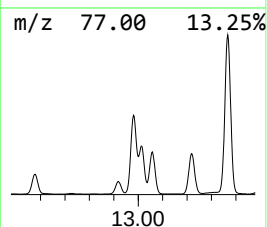
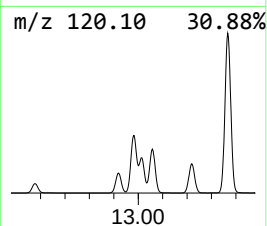
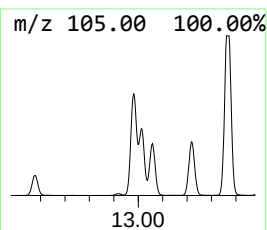
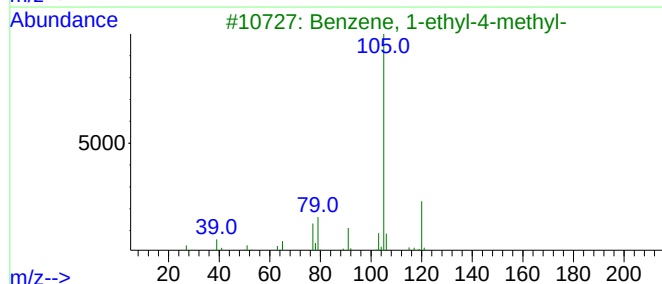
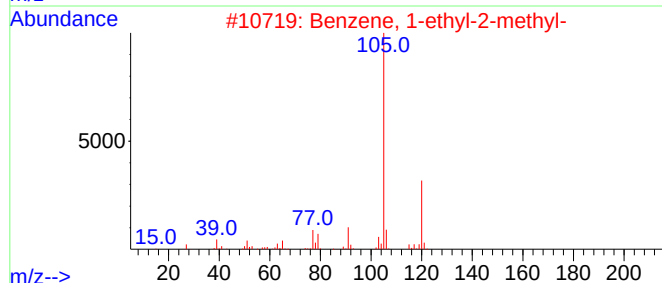
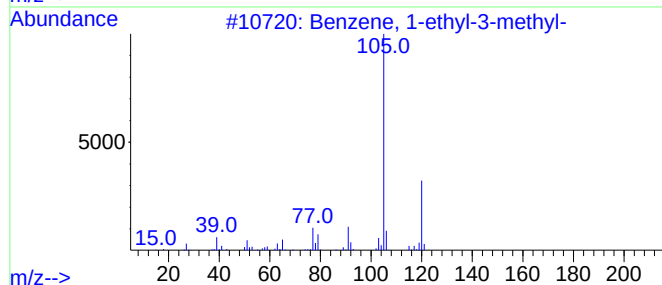
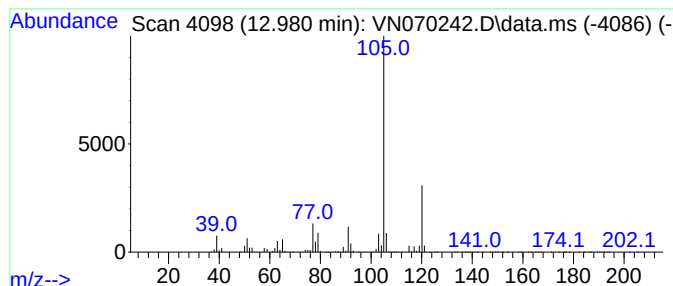
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	126.92 ug/l	23862700	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070242.D
Acq On : 20 Dec 2021 15:54
Operator : JC/MD
Sample : M5044-08
Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-8-4.5

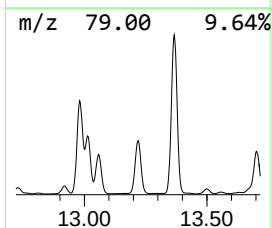
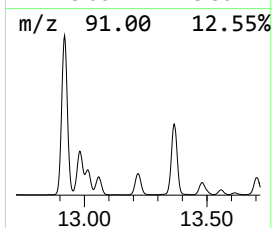
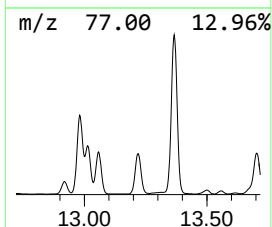
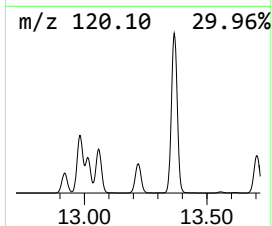
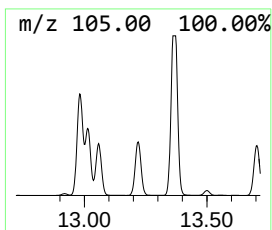
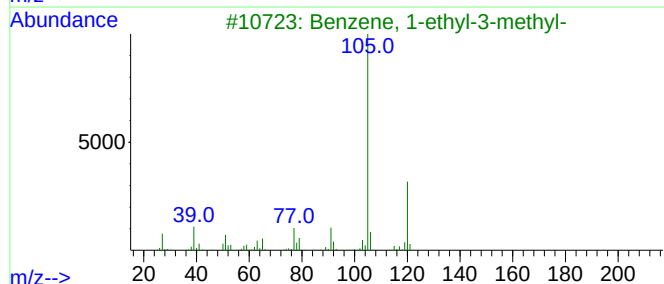
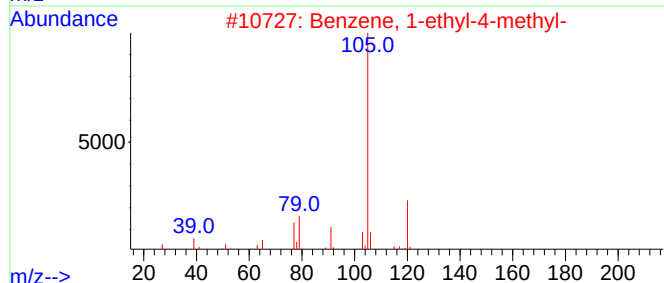
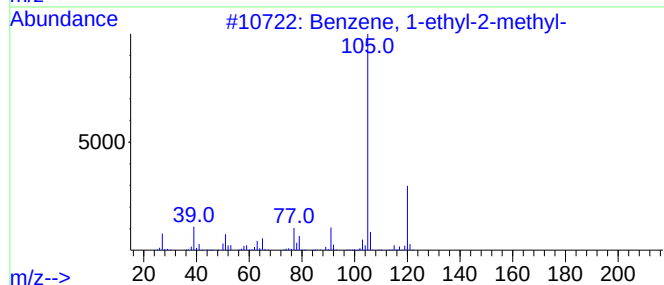
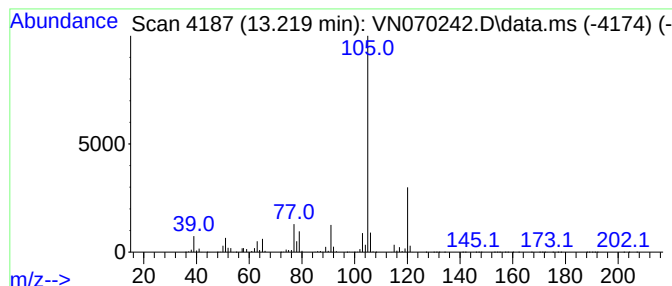
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.219	65.43 ug/l	12302600	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070242.D
Acq On : 20 Dec 2021 15:54
Operator : JC/MD
Sample : M5044-08
Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-8-4.5

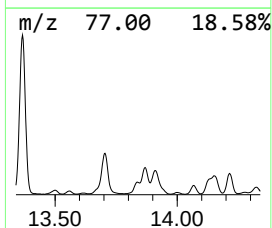
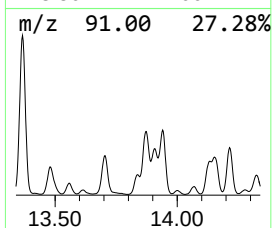
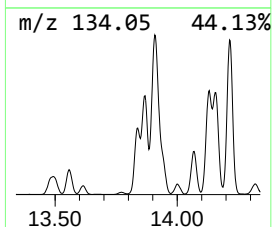
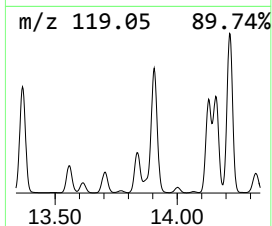
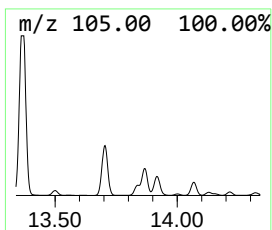
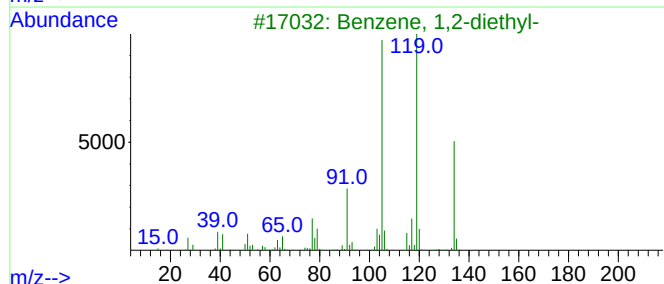
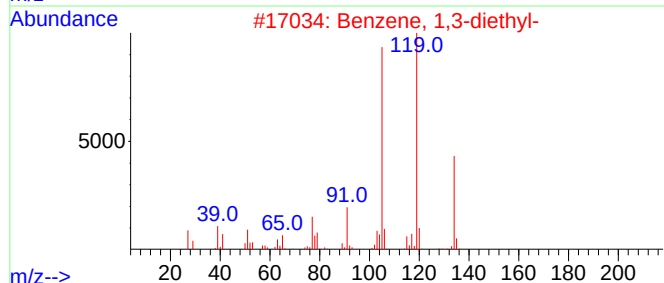
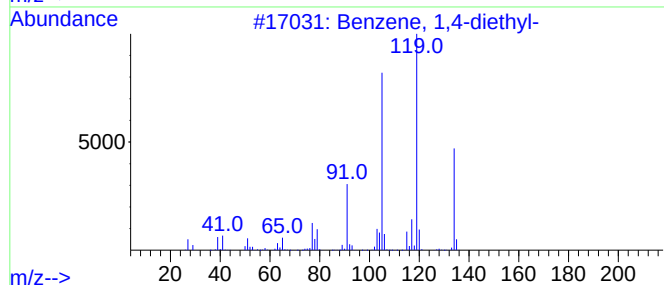
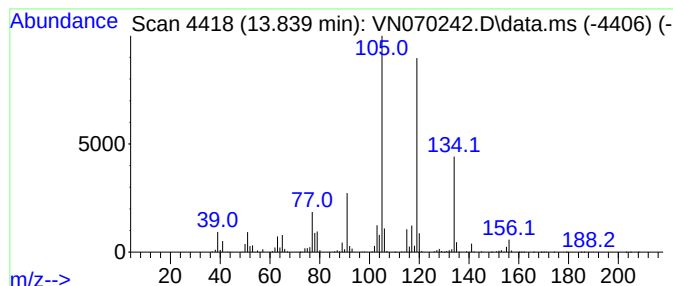
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,4-diethyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	19.67 ug/l	3697620	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	97
2			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	97
3			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070242.D
Acq On : 20 Dec 2021 15:54
Operator : JC/MD
Sample : M5044-08
Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-8-4.5

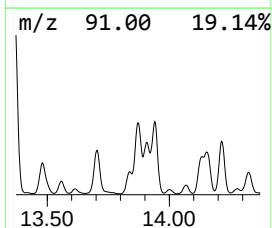
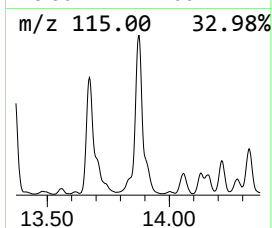
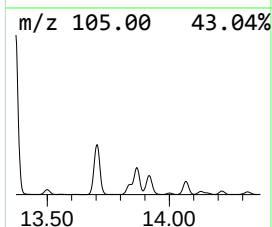
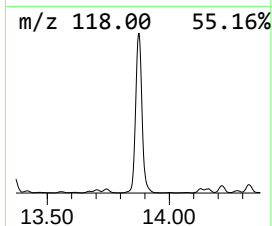
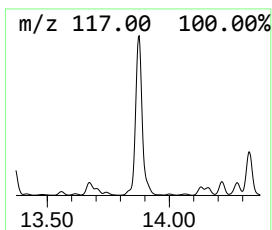
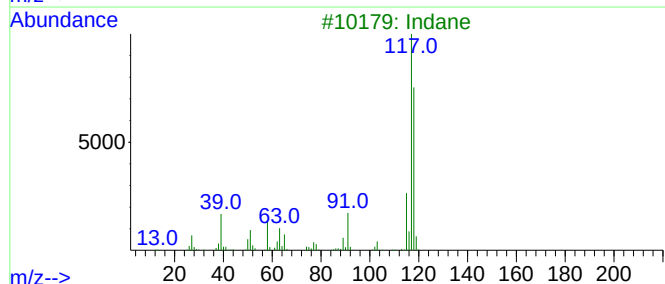
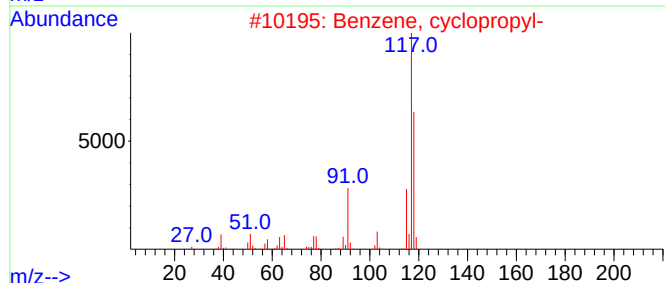
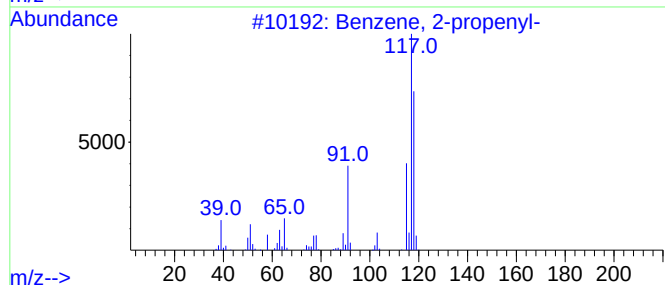
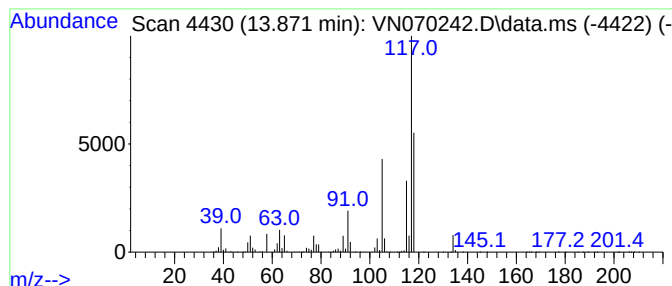
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 2-propenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	56.35 ug/l	10595100	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
3			Indane	118	C9H10	000496-11-7	76
4			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	70
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070242.D
Acq On : 20 Dec 2021 15:54
Operator : JC/MD
Sample : M5044-08
Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-8-4.5

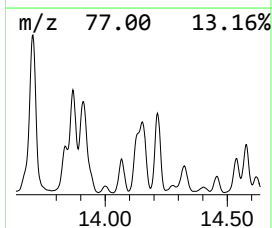
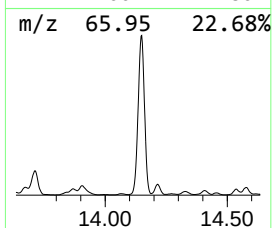
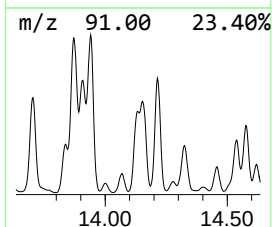
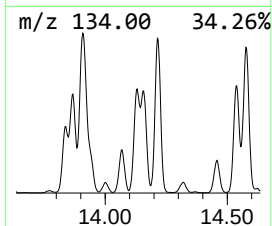
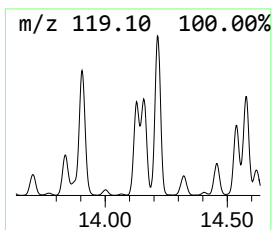
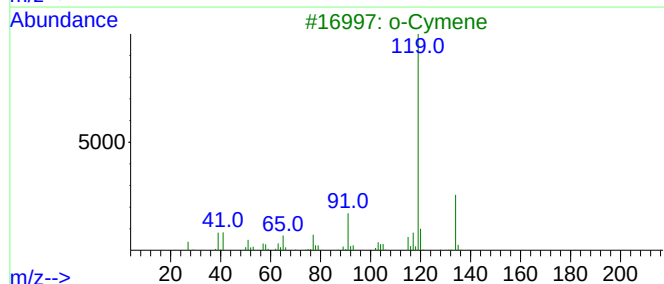
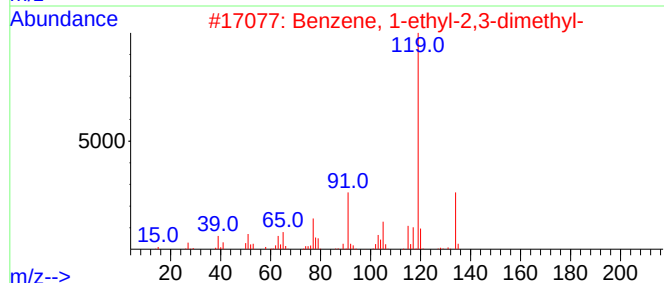
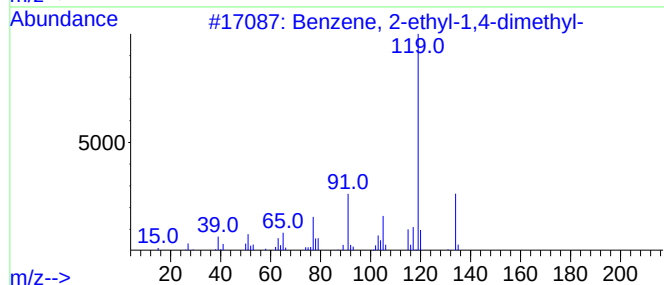
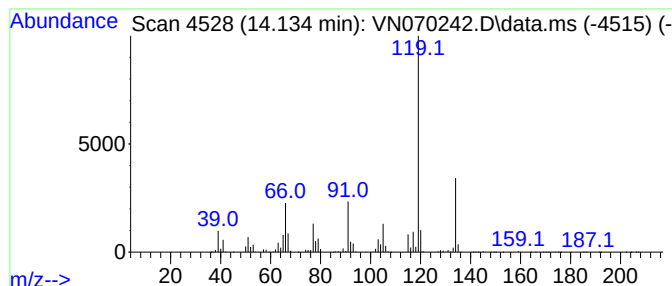
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.134	26.87 ug/l	5051230	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	92
2			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	92
3			o-Cymene	134	C10H14	000527-84-4	91
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	91
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070242.D
Acq On : 20 Dec 2021 15:54
Operator : JC/MD
Sample : M5044-08
Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-8-4.5

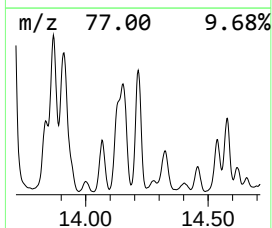
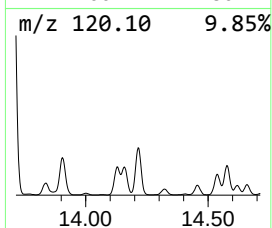
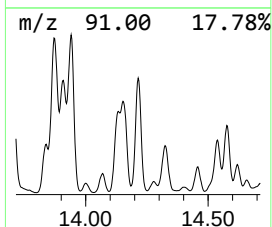
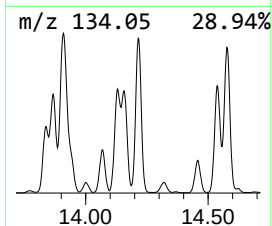
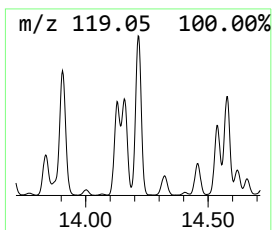
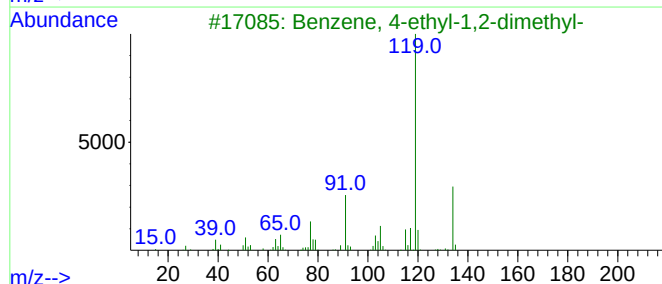
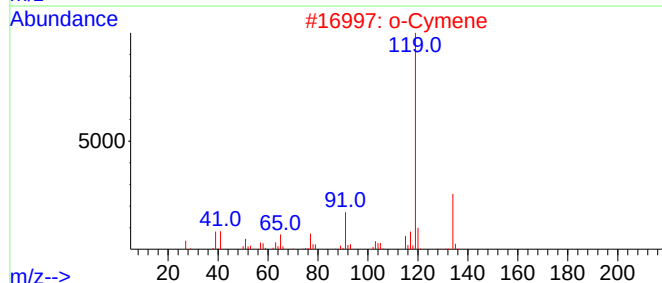
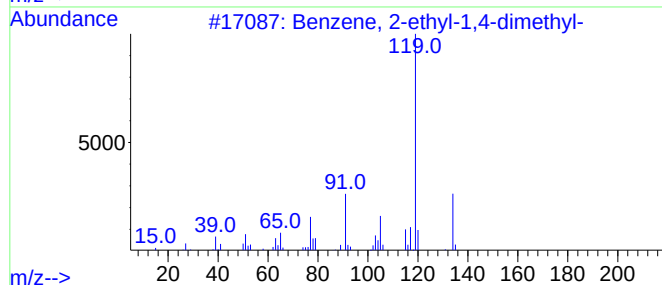
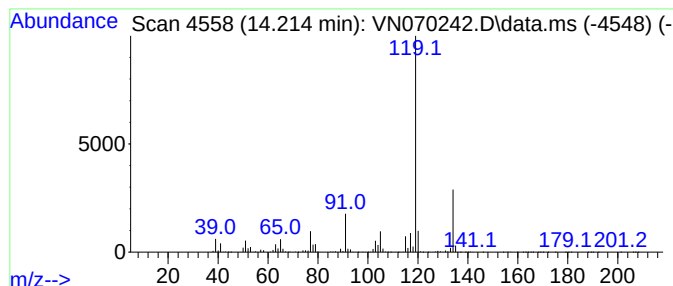
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 11 o-Cymene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.214	42.42 ug/l	7975300	1,4-Dichlorobenzene-d4	13.672

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070242.D
Acq On : 20 Dec 2021 15:54
Operator : JC/MD
Sample : M5044-08
Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-8-4.5

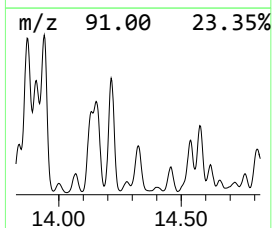
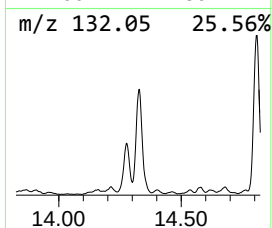
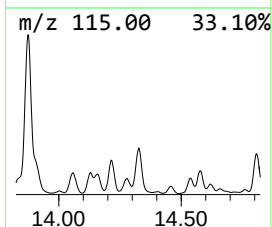
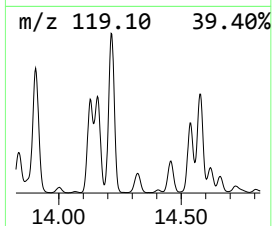
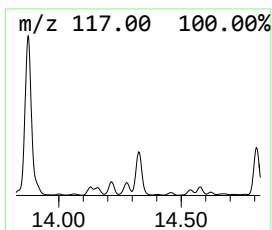
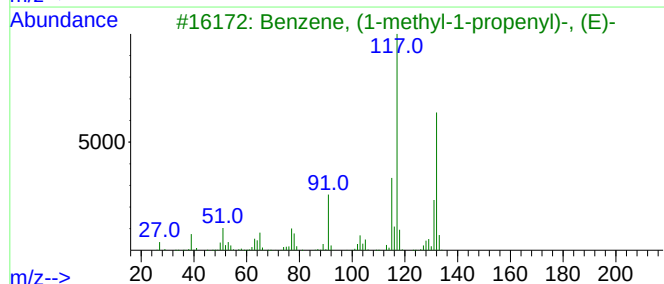
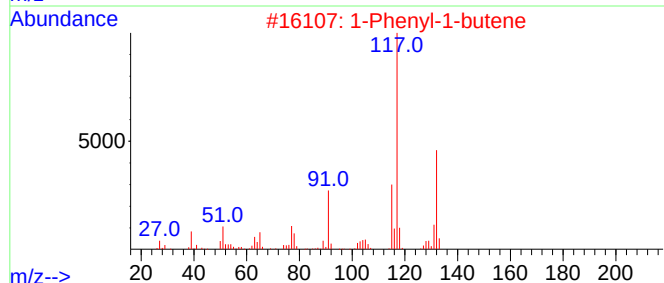
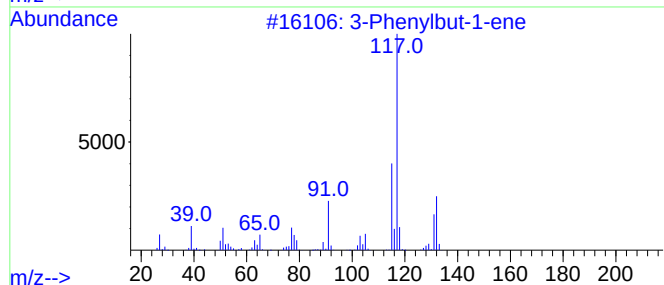
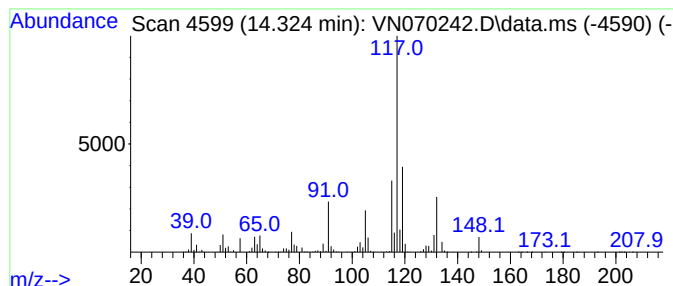
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 12 3-Phenylbut-1-ene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.324	21.71 ug/l	4081880	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Phenylbut-1-ene	132	C10H12	000934-10-1	64
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	64
3			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	64
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	62
5			Indan, 1-methyl-	132	C10H12	000767-58-8	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070242.D
Acq On : 20 Dec 2021 15:54
Operator : JC/MD
Sample : M5044-08
Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-8-4.5

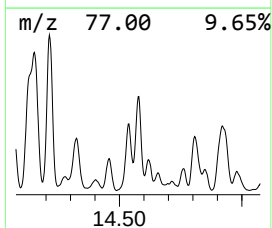
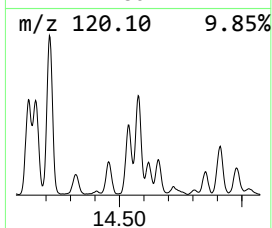
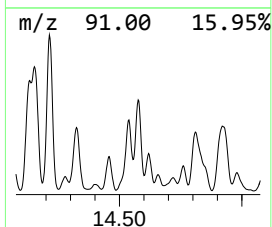
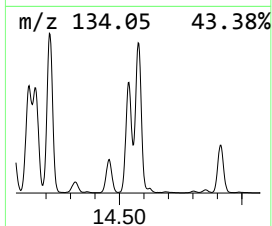
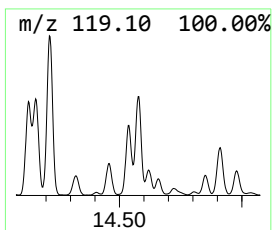
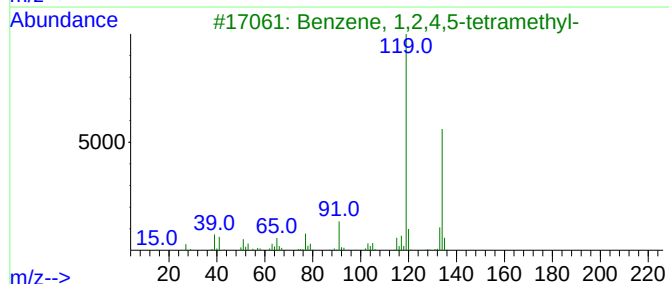
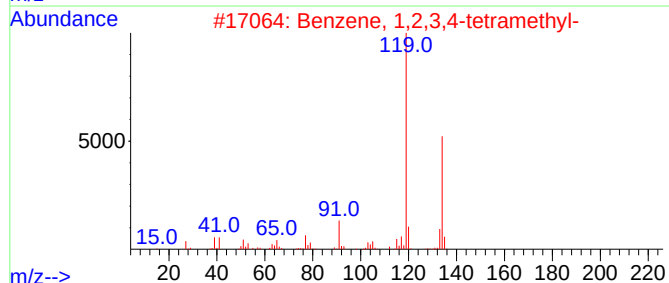
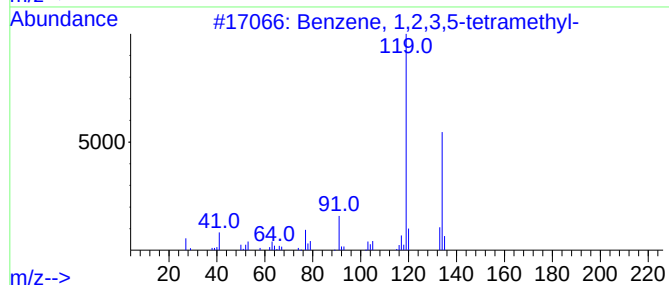
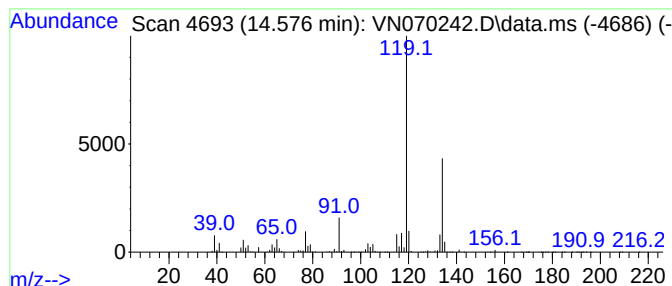
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 13 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.576	25.41 ug/l	4777870	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070242.D
Acq On : 20 Dec 2021 15:54
Operator : JC/MD
Sample : M5044-08
Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-8-4.5

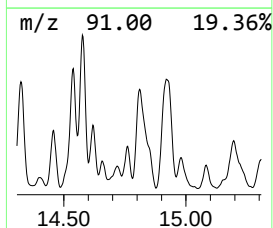
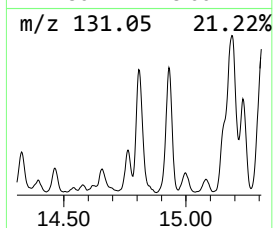
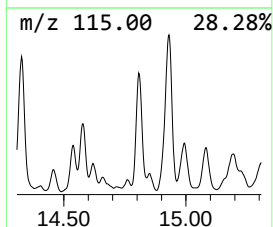
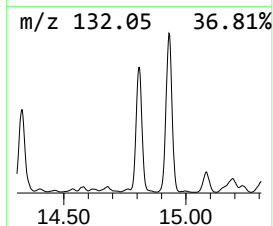
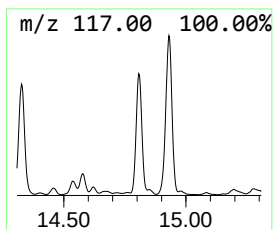
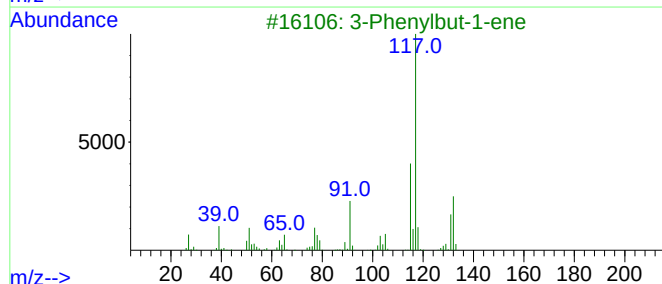
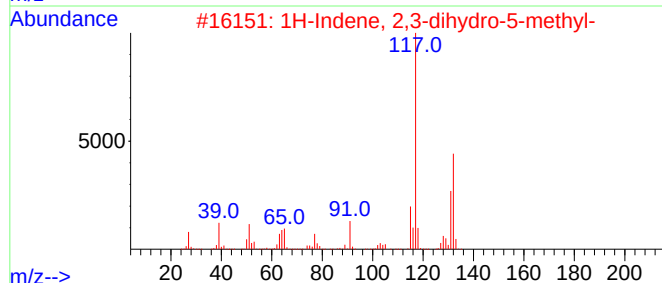
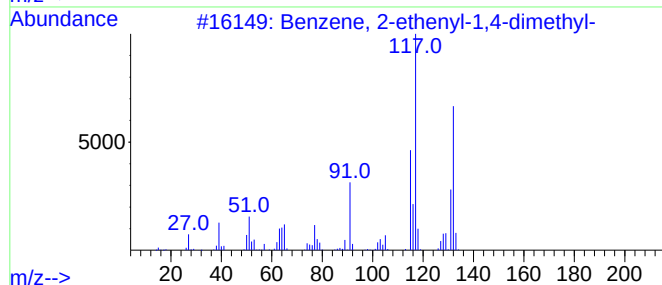
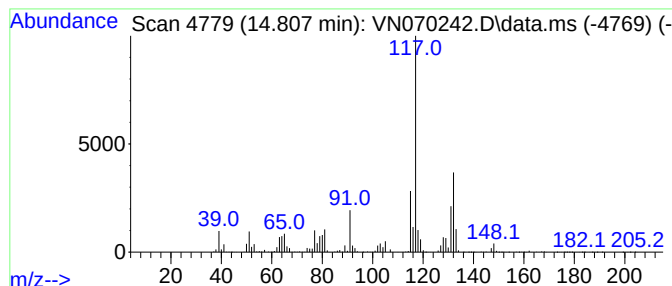
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 14 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.807	22.34 ug/l	4200650	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	87
5			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070242.D
Acq On : 20 Dec 2021 15:54
Operator : JC/MD
Sample : M5044-08
Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-8-4.5

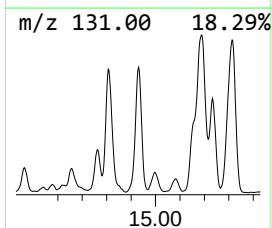
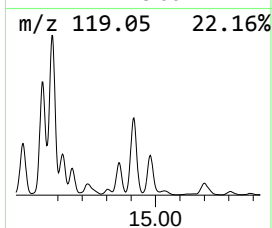
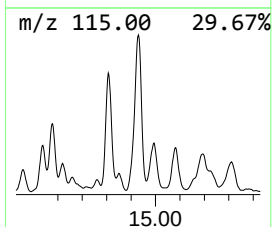
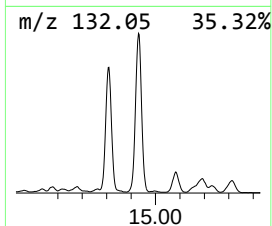
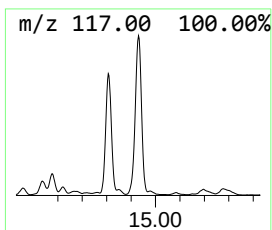
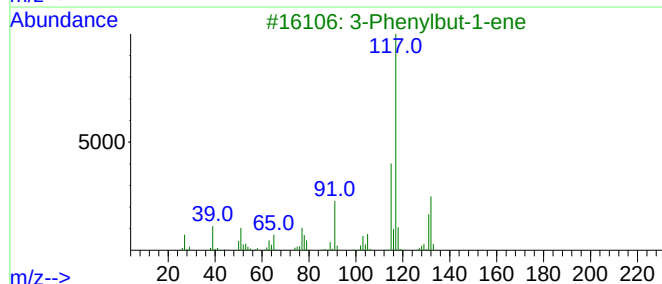
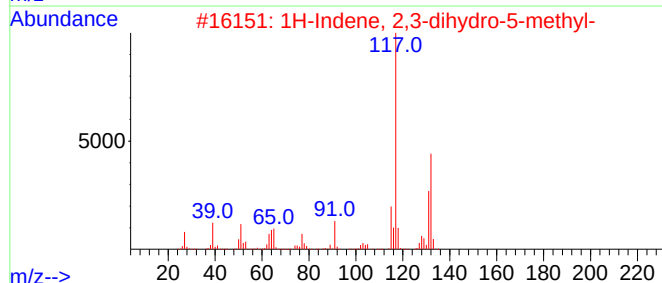
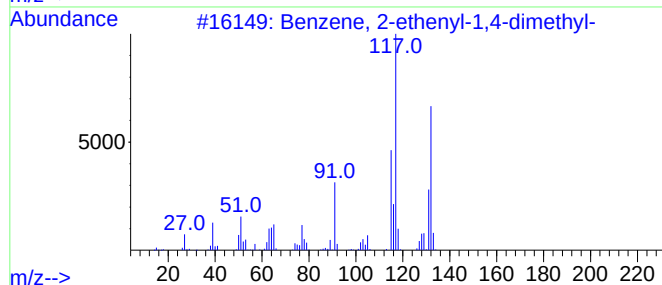
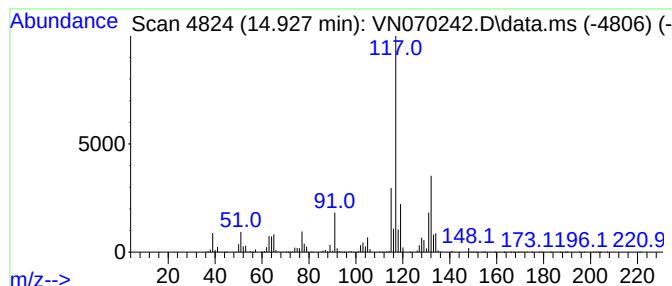
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 15 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.928	40.32 ug/l	7580740	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
4			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	83
5			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
 Data File : VN070242.D
 Acq On : 20 Dec 2021 15:54
 Operator : JC/MD
 Sample : M5044-08
 Misc : 4.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DA-8-4.5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.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, 2,2,3,3...	8.614	50.5	ug/l	8038910	2	8.965	7952410	50.0
Pentane, 2,3,4-...	9.883	29.1	ug/l	4622580	2	8.965	7952410	50.0
Pentane, 2,3,3-...	10.014	45.7	ug/l	7264870	2	8.965	7952410	50.0
Heptane, 2-methyl-	10.079	23.9	ug/l	3795320	2	8.965	7952410	50.0
Heptane, 3-methyl-	10.215	20.6	ug/l	3270920	2	8.965	7952410	50.0
Benzene, 1-ethy...	12.980	126.9	ug/l	23862700	4	13.672	9400880	50.0
Benzene, 1-ethy...	13.219	65.4	ug/l	12302600	4	13.672	9400880	50.0
Benzene, 1,4-di...	13.839	19.7	ug/l	3697620	4	13.672	9400880	50.0
Benzene, 2-prop...	13.871	56.4	ug/l	10595100	4	13.672	9400880	50.0
Benzene, 2-ethy...	14.134	26.9	ug/l	5051230	4	13.672	9400880	50.0
o-Cymene	14.214	42.4	ug/l	7975300	4	13.672	9400880	50.0
3-Phenylbut-1-ene	14.324	21.7	ug/l	4081880	4	13.672	9400880	50.0
Benzene, 1,2,3...	14.576	25.4	ug/l	4777870	4	13.672	9400880	50.0
Benzene, 2-ethe...	14.807	22.3	ug/l	4200650	4	13.672	9400880	50.0
1H-Indene, 2,3-...	14.928	40.3	ug/l	7580740	4	13.672	9400880	50.0