

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020322\
 Data File : VN070930.D
 Acq On : 3 Feb 2022 15:17
 Operator : JC/MD
 Sample : N1381-05 10X
 Misc : 6.56g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DB-11(15-20)-02-02-22

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\82N020222W.M
 Title : SW846 8260

Signal : TIC: VN070930.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.021	2225	2249	2260	rBV	486610	1165442	25.68%	3.238%
2	8.086	2260	2273	2300	rVB	994886	2279827	50.23%	6.334%
3	8.437	2382	2404	2428	rBV	596025	1360636	29.98%	3.781%
4	8.968	2577	2602	2633	rBV	1401438	2920161	64.34%	8.114%
5	9.459	2757	2785	2801	rBV3	109543	260644	5.74%	0.724%
6	9.874	2926	2940	2956	rVB6	22912	45726	1.01%	0.127%
7	10.110	3021	3028	3044	rVB3	27656	51254	1.13%	0.142%
8	10.204	3047	3063	3073	rBV5	23185	56825	1.25%	0.158%
9	10.440	3133	3151	3185	rBV	2342340	4538819	100.00%	12.611%
10	10.612	3204	3215	3235	rVB8	61547	166932	3.68%	0.464%
11	10.781	3267	3278	3292	rVB2	102905	190048	4.19%	0.528%
12	10.878	3299	3314	3328	rBV4	54695	129373	2.85%	0.359%
13	10.966	3338	3347	3358	rVB3	40629	67659	1.49%	0.188%
14	11.052	3368	3379	3393	rVB	112712	189875	4.18%	0.528%
15	11.154	3405	3417	3433	rBV2	65246	141172	3.11%	0.392%
16	11.223	3434	3443	3451	rBV4	51752	82700	1.82%	0.230%
17	11.293	3459	3469	3478	rBV	183593	268440	5.91%	0.746%
18	11.347	3479	3489	3502	rVB2	248897	436056	9.61%	1.212%
19	11.454	3518	3529	3539	rBV3	144183	239196	5.27%	0.665%
20	11.551	3557	3565	3581	rVB3	115036	204365	4.50%	0.568%
21	11.623	3582	3592	3602	rBV3	55047	90391	1.99%	0.251%
22	11.744	3621	3637	3661	rBV	2193283	3941715	86.84%	10.952%
23	11.881	3680	3688	3694	rBV3	55618	82850	1.83%	0.230%
24	11.926	3696	3705	3717	rVB7	93882	186500	4.11%	0.518%
25	11.988	3718	3728	3736	rBV2	230698	402568	8.87%	1.119%
26	12.253	3813	3827	3842	rBV6	311640	731931	16.13%	2.034%
27	12.369	3861	3870	3880	rVB2	377473	580486	12.79%	1.613%
28	12.420	3883	3889	3891	rBV5	64580	64849	1.43%	0.180%
29	12.455	3894	3902	3905	rBV3	231203	291635	6.43%	0.810%
30	12.731	3992	4005	4021	rVB	1840908	3125950	68.87%	8.685%
31	12.913	4059	4073	4085	rVB2	429267	1077653	23.74%	2.994%
32	13.055	4113	4126	4137	rBV9	350275	788539	17.37%	2.191%
33	13.197	4173	4179	4187	rVB3	176379	221528	4.88%	0.616%
34	13.675	4344	4357	4378	rVB	2120059	3747230	82.56%	10.412%
35	13.999	4468	4478	4487	rBV5	670089	1104563	24.34%	3.069%
36	14.214	4551	4558	4570	rVB2	638092	975049	21.48%	2.709%

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Title : SW846 8260

37	14.509	4659	4668	4675	rBV5	576451	926644	20.42%	2.575%
38	14.917	4810	4820	4835	rVB3	902057	1771178	39.02%	4.921%
39	16.614	5444	5453	5498	rVB3	388923	1084459	23.89%	3.013%

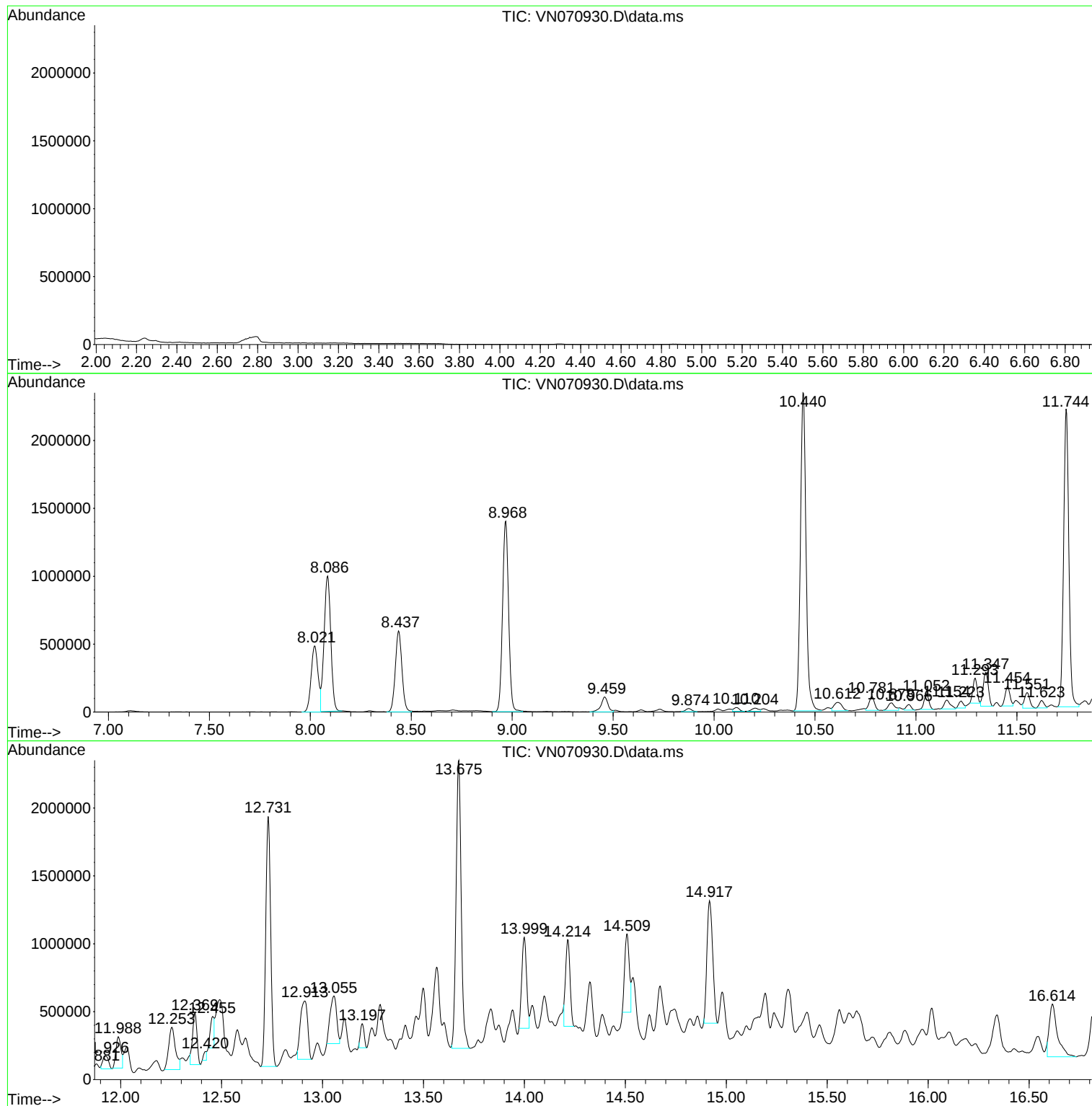
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020222W.M
Quant Title : SW846 8260

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



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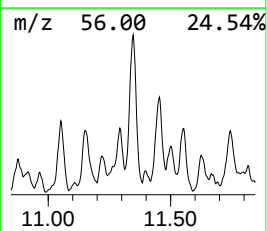
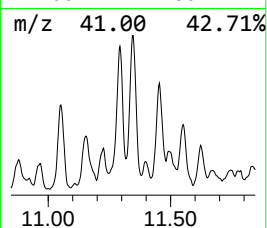
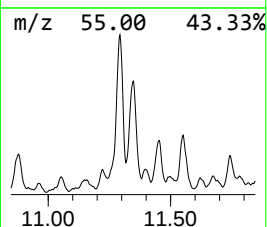
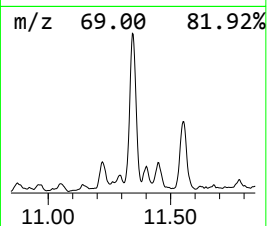
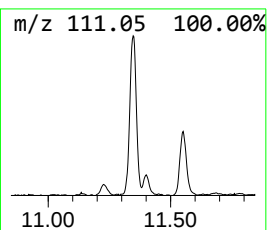
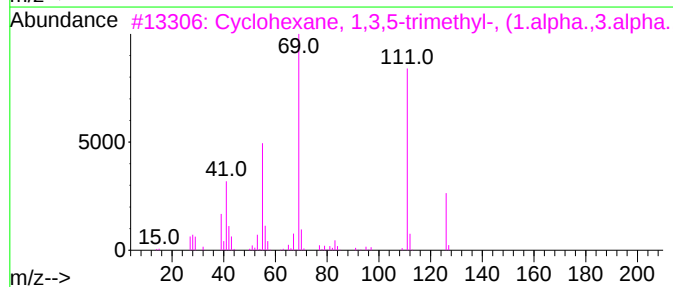
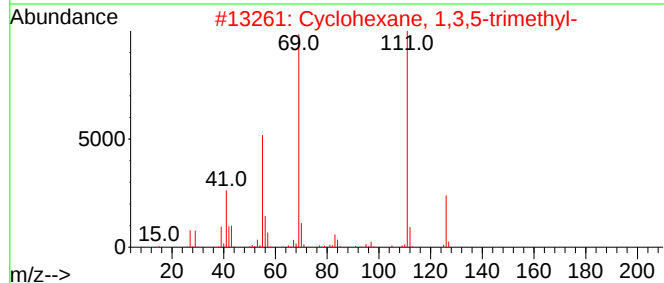
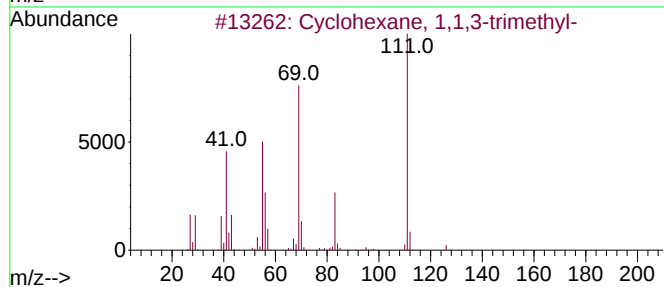
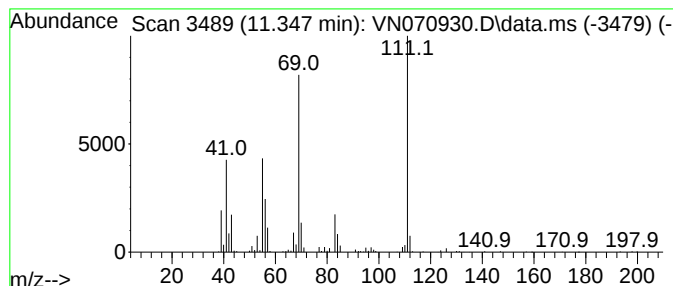
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020222W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.347	5.53 ug/l	436056	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	90
2			Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	72
3			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	72
4			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	72
5			1,1,4-Trimethylcyclohexane	126	C9H18	007094-27-1	64



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Instrument :
MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

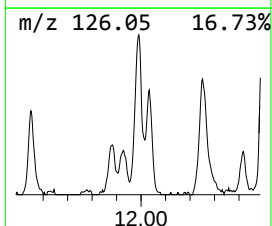
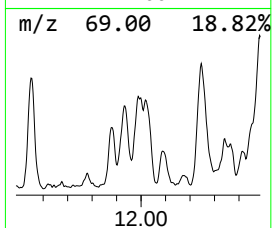
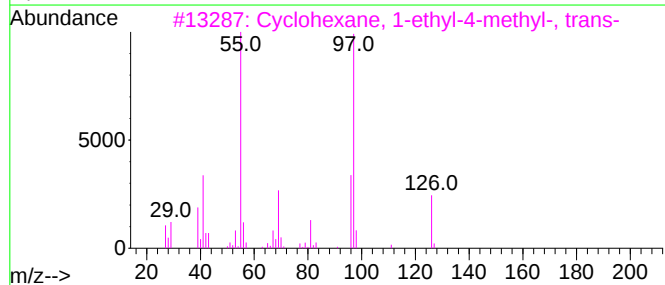
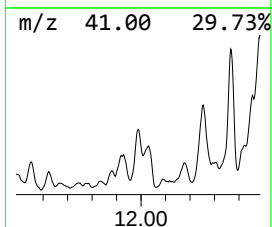
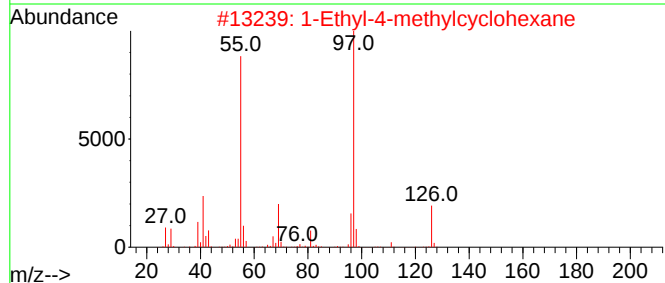
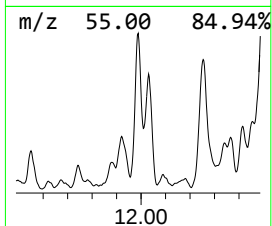
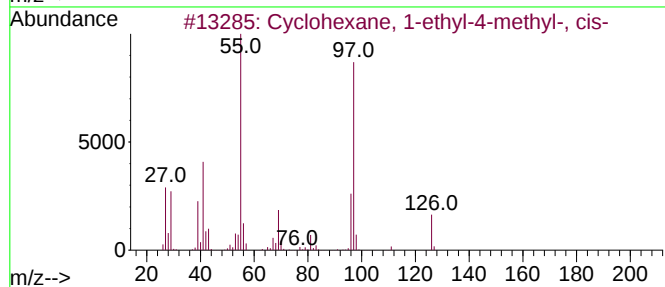
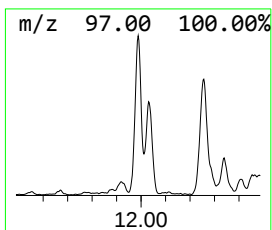
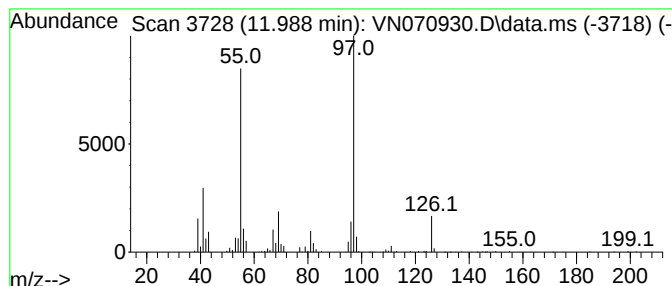
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020222W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.988	5.11 ug/l	402568	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	93
2			1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	91
3			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	90
4			Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	83
5			Sulfurous acid, cyclohexylmethyl...	402	C23H46O3S	1000309-22-4	72



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Misc : 6.56g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

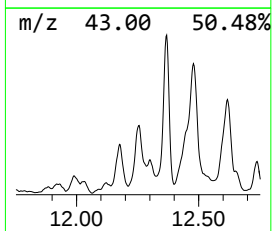
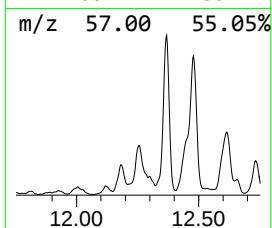
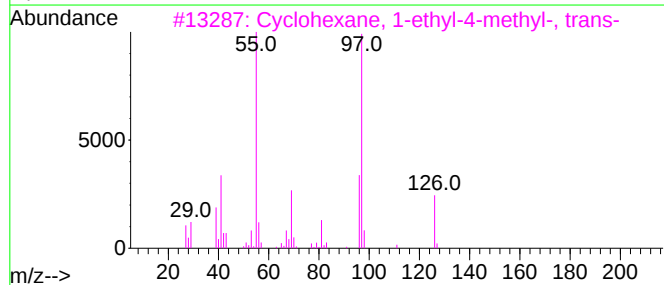
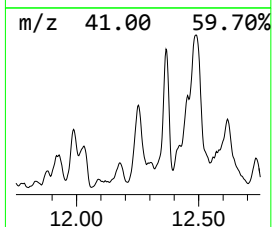
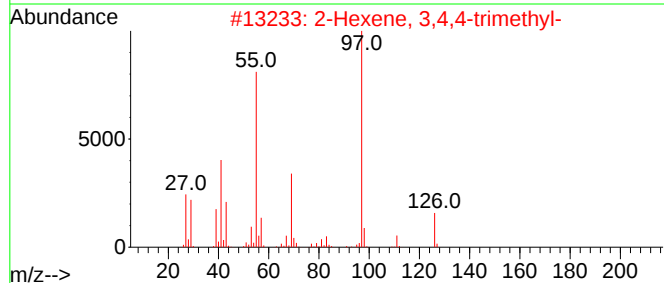
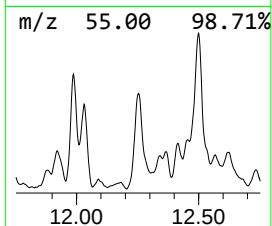
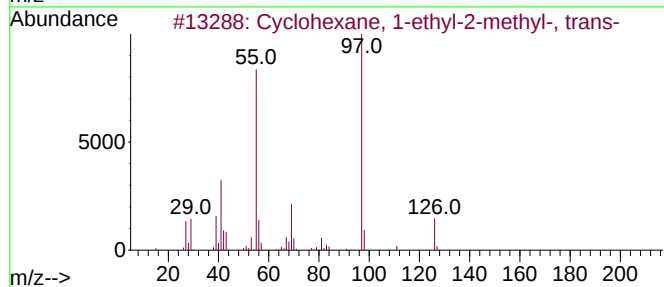
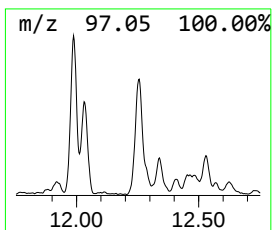
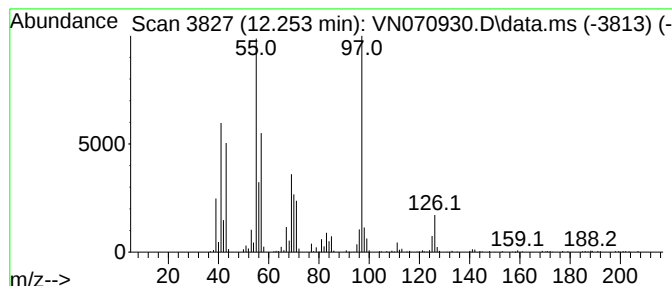
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020222W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclohexane, 1-ethyl-2-meth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.253	9.28 ug/l	731931	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	52
2			2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	52
3			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	52
4			Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	50
5			3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	50



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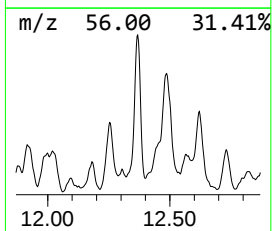
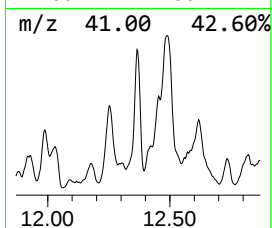
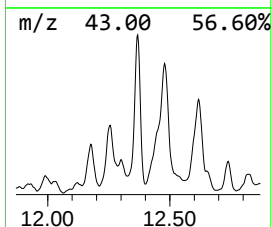
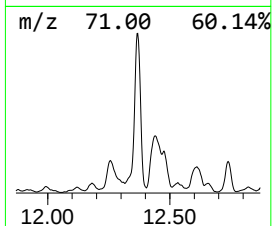
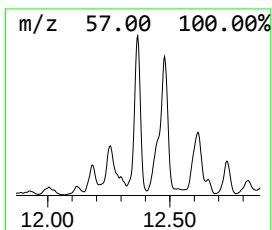
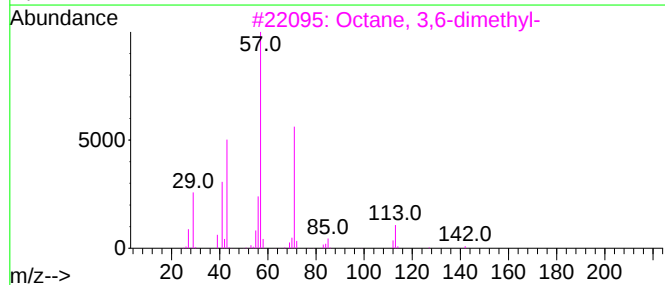
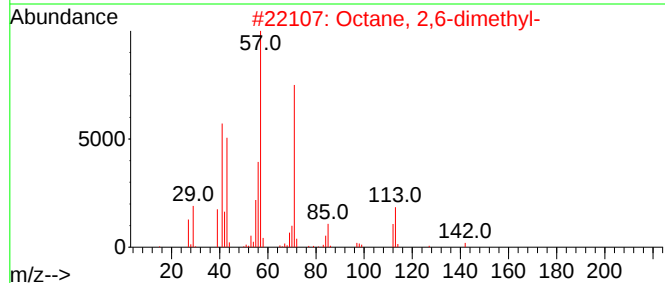
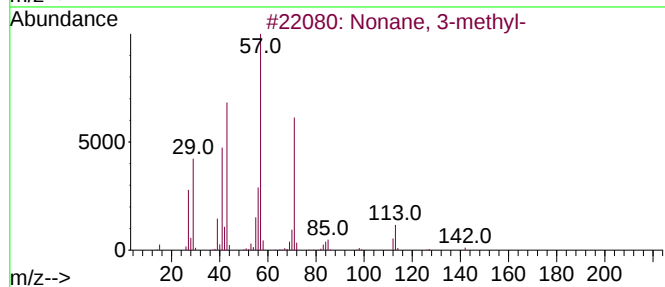
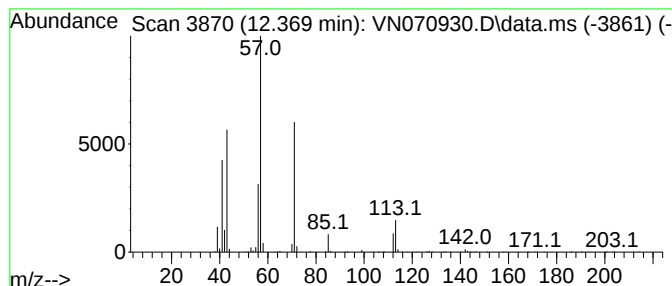
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020222W.M
Quant Title : SW846 8260

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

Peak Number 4 Nonane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.369	7.36 ug/l	580486	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 3-methyl-	142	C10H22	005911-04-6	91
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	90
3			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	86
4			Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	64
5			3-Hexanone, 2,2-dimethyl-	128	C8H16O	005405-79-8	53



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DB-11(15-20)-02-02-22

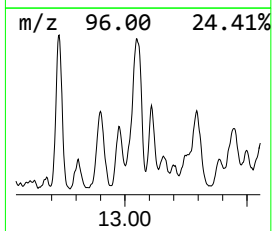
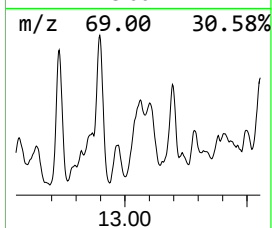
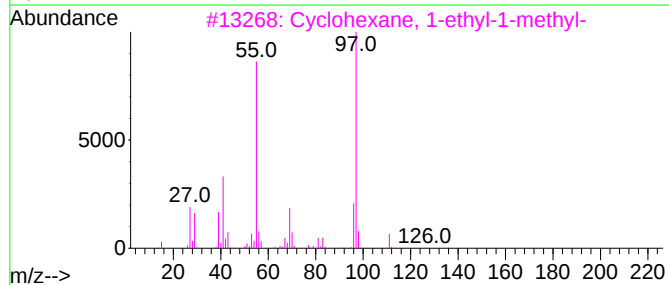
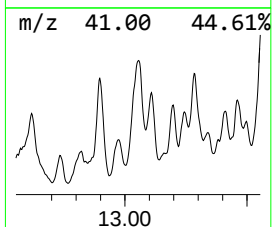
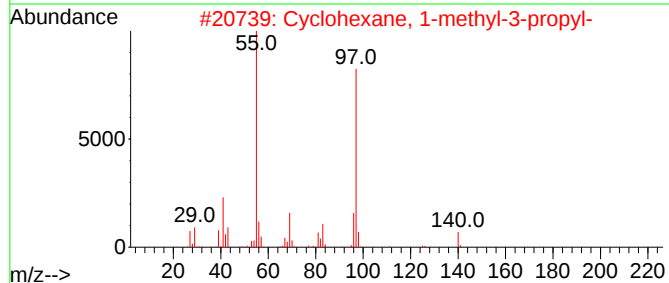
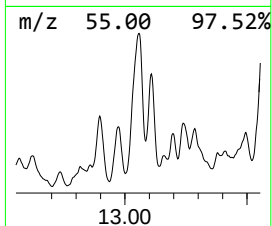
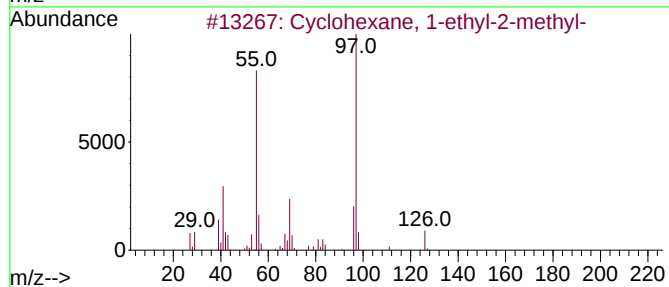
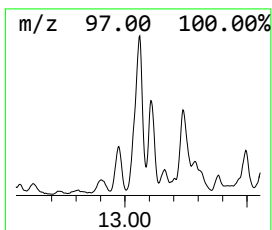
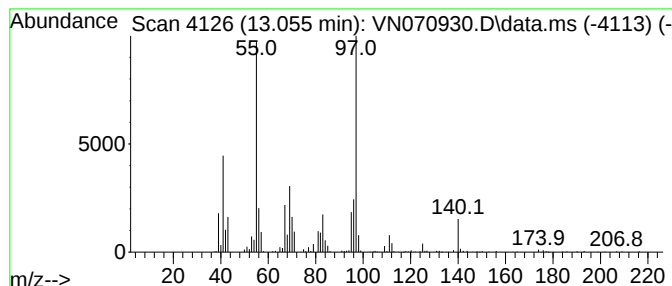
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Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.055	10.52 ug/l	788539	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	59
2			Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	58
3			Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	58
4			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	50
5			2,4-Dimethyl-1,5-diazabicyclo[3....	112	C6H12N2	100463-01-2	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020322\
Data File : VN070930.D
Acq On : 3 Feb 2022 15:17
Operator : JC/MD
Sample : N1381-05 10X
Misc : 6.56g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

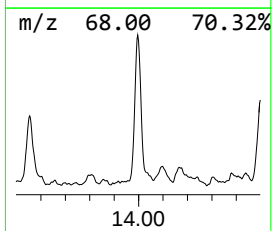
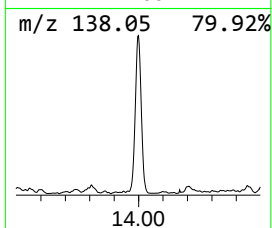
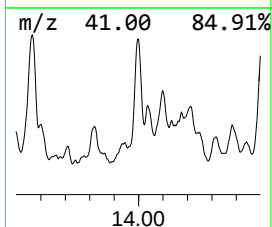
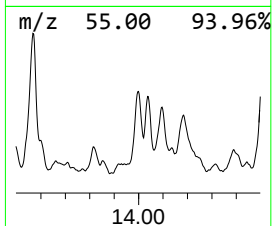
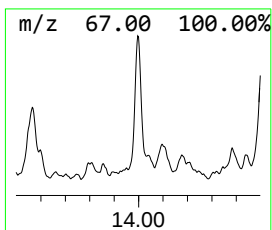
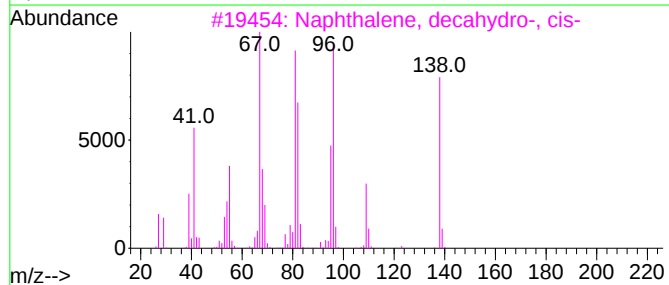
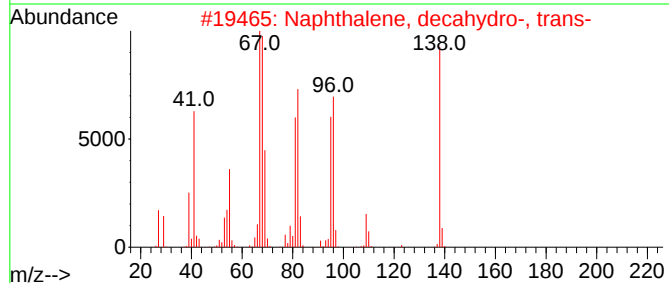
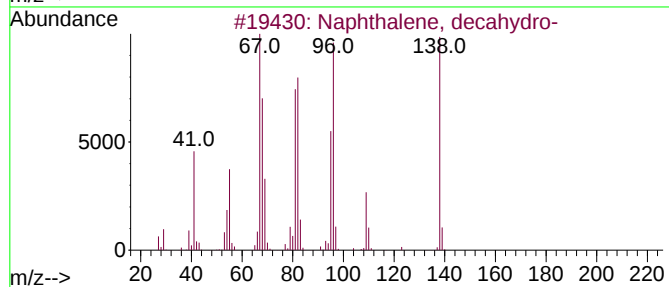
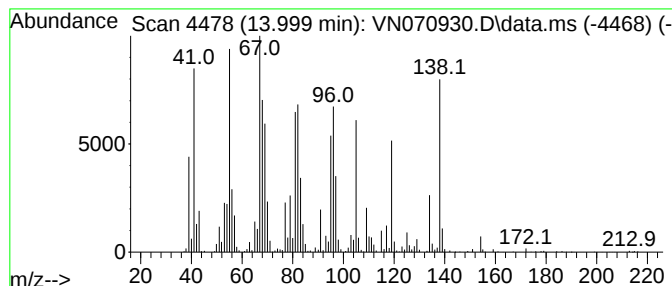
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, decahydro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.999	14.74 ug/l	1104560	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-	138	C10H18	000091-17-8	97
2			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	96
3			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	93
4			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-25-0	90
5			Spiro[4.5]decane	138	C10H18	000176-63-6	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020322\
Data File : VN070930.D
Acq On : 3 Feb 2022 15:17
Operator : JC/MD
Sample : N1381-05 10X
Misc : 6.56g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

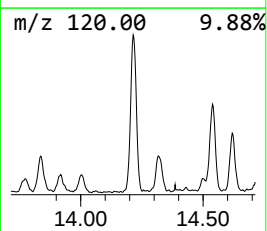
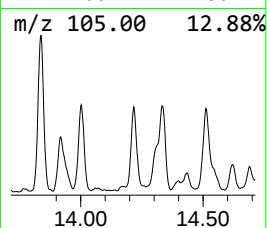
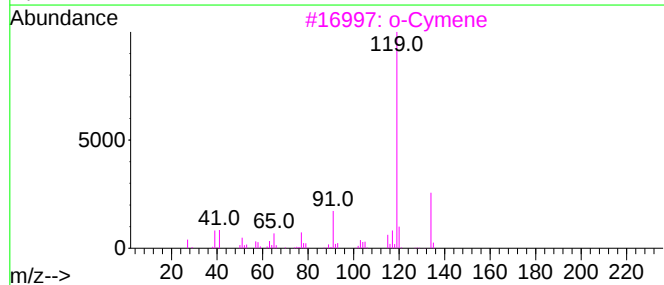
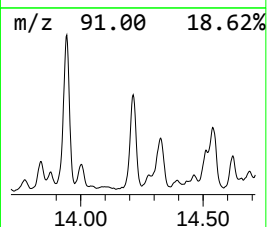
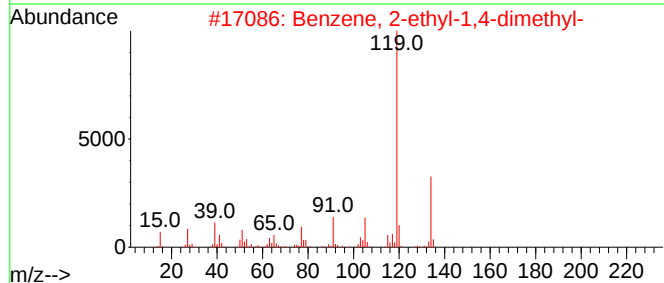
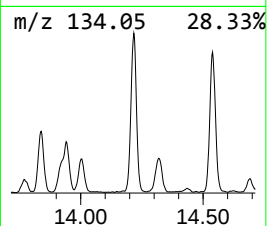
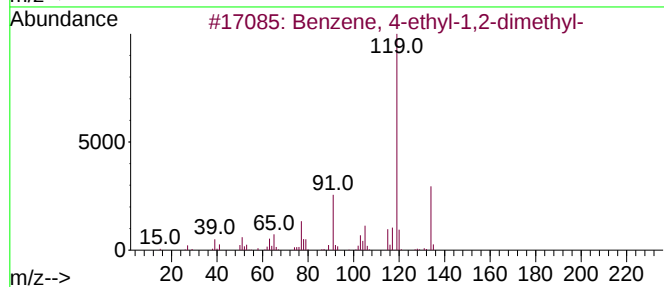
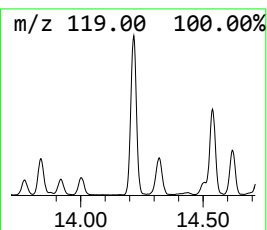
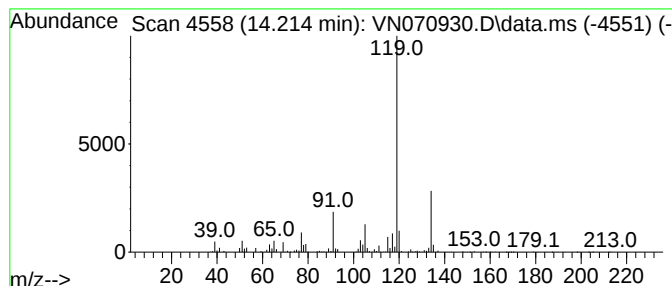
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.214	13.01 ug/l	975049	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
3			o-Cymene	134	C10H14	000527-84-4	95
4			p-Cymene	134	C10H14	000099-87-6	95
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020322\
Data File : VN070930.D
Acq On : 3 Feb 2022 15:17
Operator : JC/MD
Sample : N1381-05 10X
Misc : 6.56g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

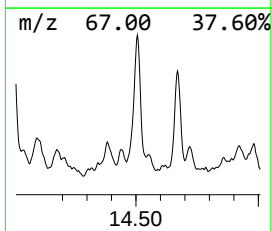
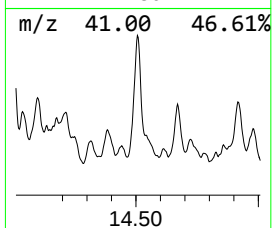
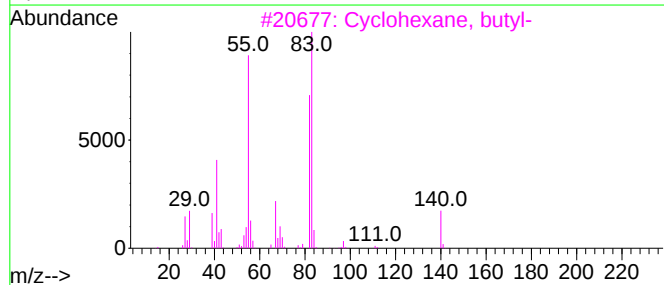
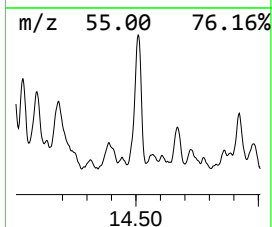
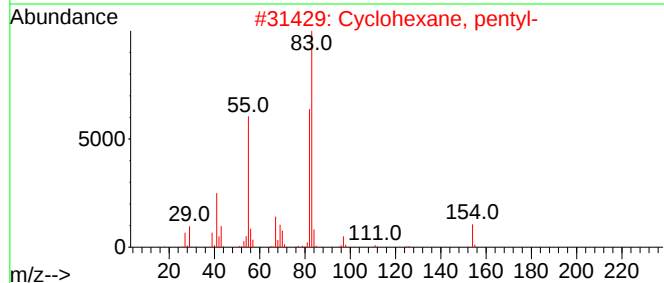
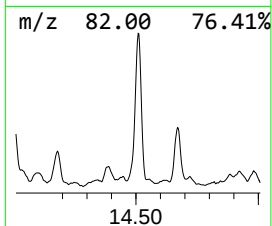
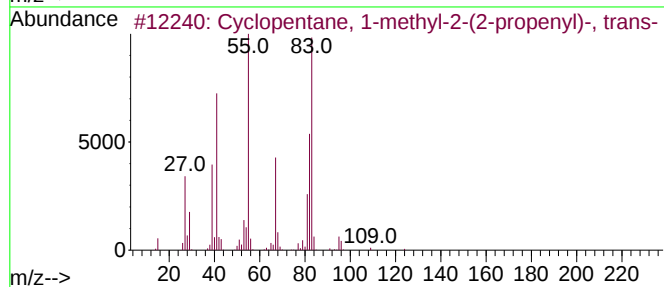
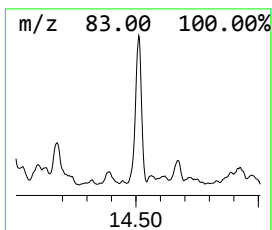
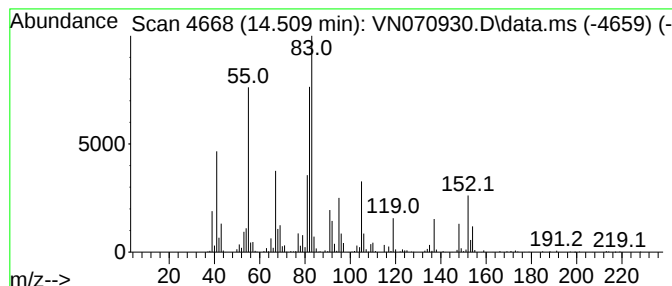
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Quant Title : SW846 8260

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

Peak Number 8 Cyclopentane, 1-methyl-2-(2... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.509	12.36 ug/l	926644	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1-methyl-2-(2-prop...	124	C9H16	050746-53-7	60
2			Cyclohexane, pentyl-	154	C11H22	004292-92-6	53
3			Cyclohexane, butyl-	140	C10H20	001678-93-9	47
4			3-Cyclohexyl-1-chloropropane	160	C9H17Cl	001124-62-5	47
5			Cyclohexane, undecyl-	238	C17H34	054105-66-7	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020322\
Data File : VN070930.D
Acq On : 3 Feb 2022 15:17
Operator : JC/MD
Sample : N1381-05 10X
Misc : 6.56g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

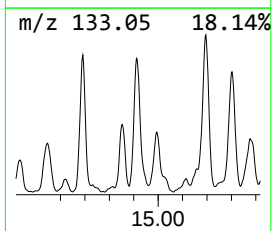
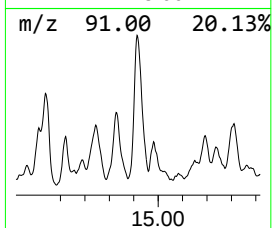
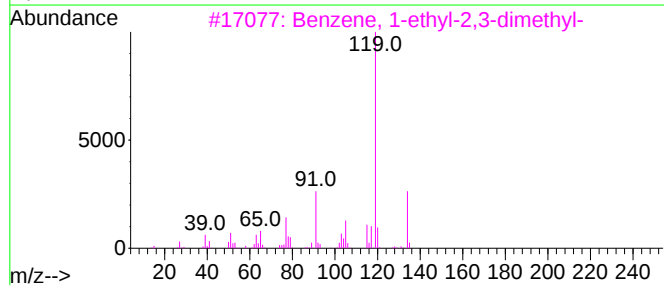
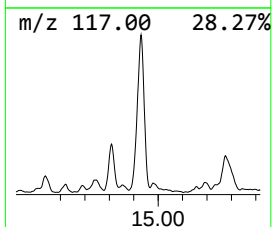
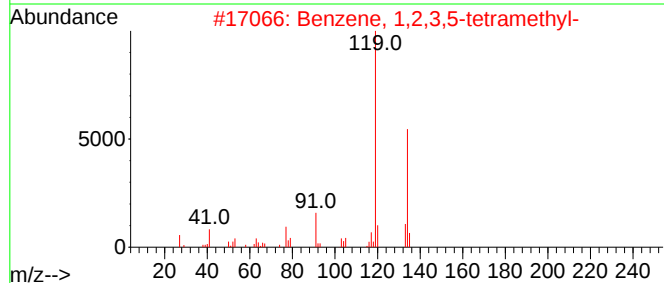
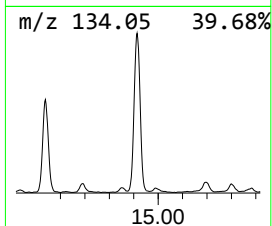
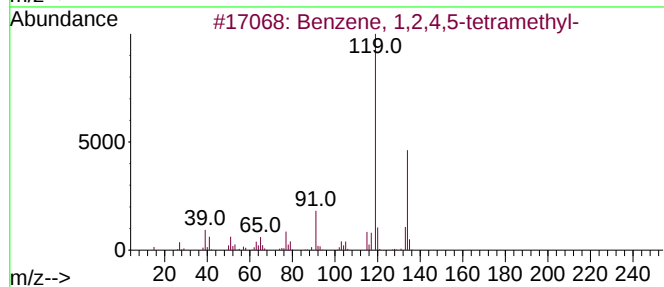
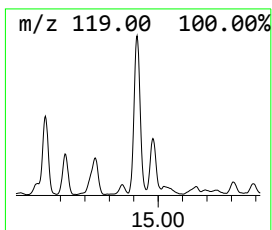
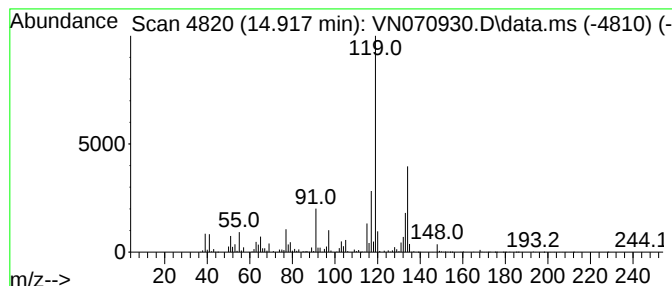
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.917	23.63 ug/l	1771180	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	93
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	76
3			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	76
4			p-Cymene	134	C10H14	000099-87-6	76
5			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020322\
Data File : VN070930.D
Acq On : 3 Feb 2022 15:17
Operator : JC/MD
Sample : N1381-05 10X
Misc : 6.56g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

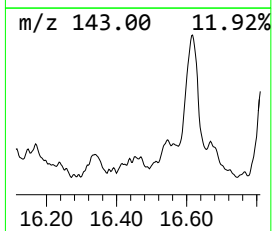
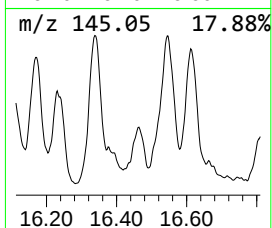
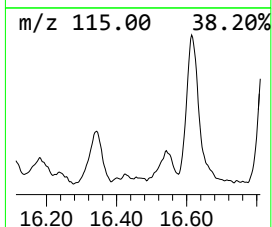
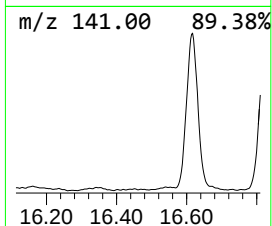
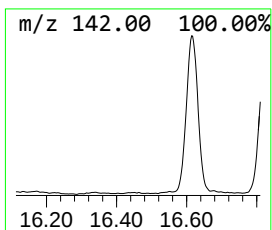
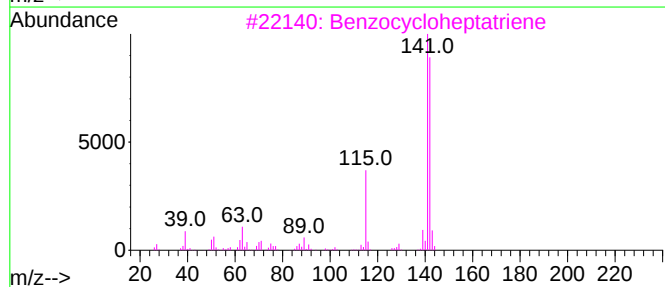
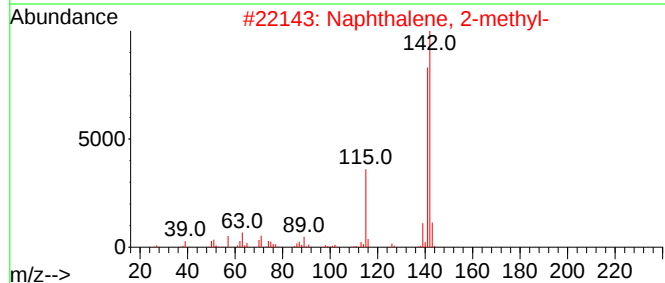
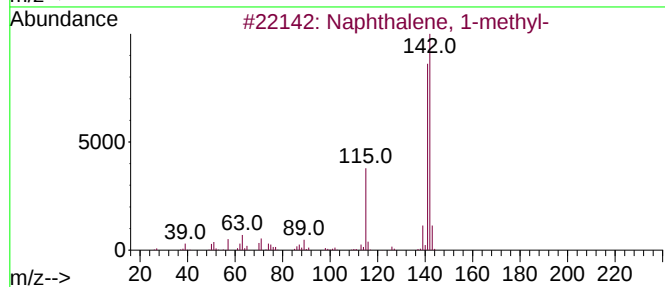
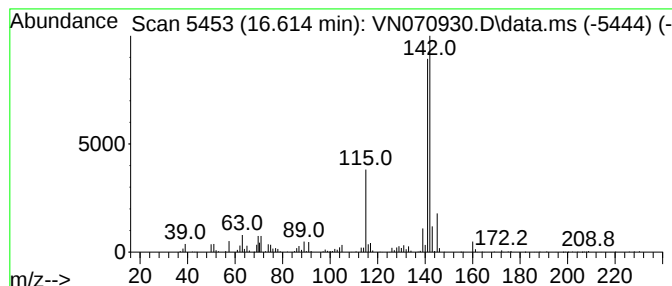
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.614	14.47 ug/l	1084460	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	93
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020322\
Data File : VN070930.D
Acq On : 3 Feb 2022 15:17
Operator : JC/MD
Sample : N1381-05 10X
Misc : 6.56g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DB-11(15-20)-02-02-22

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020222W.M
Quant Title : SW846 8260

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

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					#	RT	Resp	Conc
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Cyclohexane, 1-...	11.988	5.1	ug/l	402568	3	11.744	3941720	50.0
Cyclohexane, 1-...	12.253	9.3	ug/l	731931	3	11.744	3941720	50.0
Nonane, 3-methyl-	12.369	7.4	ug/l	580486	3	11.744	3941720	50.0
Cyclohexane, 1-...	13.055	10.5	ug/l	788539	4	13.675	3747230	50.0
Naphthalene, de...	13.999	14.7	ug/l	1104560	4	13.675	3747230	50.0
Benzene, 4-ethy...	14.214	13.0	ug/l	975049	4	13.675	3747230	50.0
Cyclopentane, 1...	14.509	12.4	ug/l	926644	4	13.675	3747230	50.0
Benzene, 1,2,4,...	14.917	23.6	ug/l	1771180	4	13.675	3747230	50.0
Naphthalene, 1-...	16.614	14.5	ug/l	1084460	4	13.675	3747230	50.0