

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
 Data File : VN068308.D
 Acq On : 25 Aug 2021 18:55
 Operator : JC/MD
 Sample : M3529-01
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31113

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\82N081721W.M
 Title : SW846 8260

Signal : TIC: VN068308.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.291	831	858	900	rBV	599977	1802862	2.38%	0.936%
2	8.086	2261	2273	2297	rVB	598219	1379704	1.82%	0.716%
3	8.458	2384	2412	2438	rBV5	789855	2211033	2.92%	1.147%
4	8.971	2584	2603	2624	rBV	820066	1701884	2.25%	0.883%
5	10.070	2987	3013	3032	rBV	900643	1660055	2.20%	0.862%
6	10.285	3066	3093	3104	rBV2	429071	1085685	1.44%	0.563%
7	10.443	3136	3152	3164	rBV	1226740	2286873	3.02%	1.187%
8	10.508	3164	3176	3206	rVB	1956645	3668348	4.85%	1.904%
9	11.146	3400	3414	3429	rBV	1741321	3096644	4.10%	1.607%
10	11.224	3430	3443	3459	rVV	1936600	3707694	4.90%	1.924%
11	11.747	3623	3638	3648	rBV	1371087	2471498	3.27%	1.283%
12	11.918	3687	3702	3707	rVV2	2486329	4338614	5.74%	2.252%
13	11.950	3709	3714	3735	rVV	2848364	4841899	6.40%	2.513%
14	12.055	3737	3753	3782	rVB	3073862	6048520	8.00%	3.139%
15	12.288	3825	3840	3854	rBV4	2559991	5230257	6.92%	2.714%
16	12.530	3917	3930	3940	rBV	1189801	2128908	2.82%	1.105%
17	12.586	3943	3951	3991	rVB8	684904	1586357	2.10%	0.823%
18	12.734	3992	4006	4017	rBV	1244343	2153397	2.85%	1.118%
19	12.790	4017	4027	4044	rVB2	751437	1326115	1.75%	0.688%
20	12.924	4064	4077	4089	rBV	650209	1113371	1.47%	0.578%
21	13.055	4118	4126	4138	rVB3	788623	1395971	1.85%	0.724%
22	13.155	4157	4163	4176	rVB2	600893	906450	1.20%	0.470%
23	13.230	4176	4191	4208	rVB5	596228	1292772	1.71%	0.671%
24	13.324	4209	4226	4232	rBV4	585016	1191224	1.58%	0.618%
25	13.369	4234	4243	4253	rVV	2442406	4257488	5.63%	2.210%
26	13.420	4254	4262	4273	rVV	1215268	2023039	2.68%	1.050%
27	13.678	4345	4358	4364	rBV	1749054	3036530	4.02%	1.576%
28	13.879	4422	4433	4467	rVB3	730882	1848976	2.45%	0.960%
29	14.058	4485	4500	4518	rVB	17106563	28797584	38.08%	14.945%
30	14.426	4624	4637	4659	rBV4	777000	1689000	2.23%	0.877%
31	14.919	4808	4821	4837	rBV3	617354	1392790	1.84%	0.723%
32	14.997	4837	4850	4865	rVV	1945013	3341451	4.42%	1.734%
33	15.083	4867	4882	4901	rVB	2725525	4855916	6.42%	2.520%
34	15.188	4908	4921	4935	rBV4	391612	848972	1.12%	0.441%
35	15.509	5015	5041	5059	rBV2	38818326	75617126	100.00%	39.243%
36	15.606	5060	5077	5095	rVB	1244304	2829425	3.74%	1.468%

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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\82N081721W.M
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37	16.620	5439	5455	5483	rVB	1567589	3524849	4.66%	1.829%
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Sum of corrected areas: 192689281

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Quant Title : SW846 8260

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



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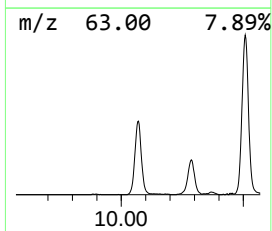
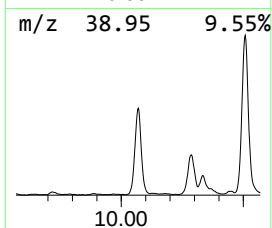
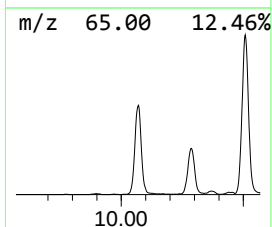
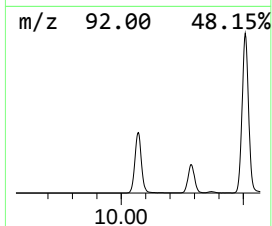
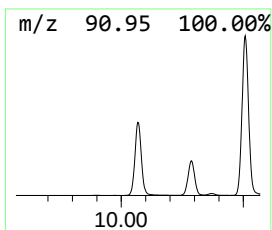
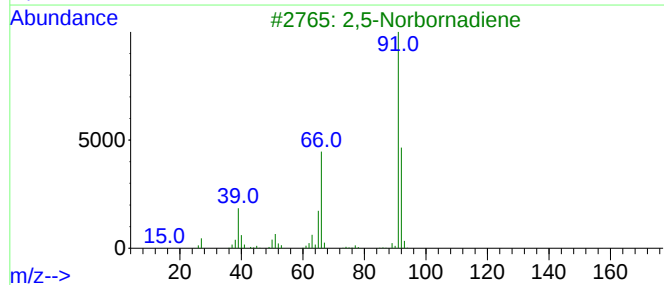
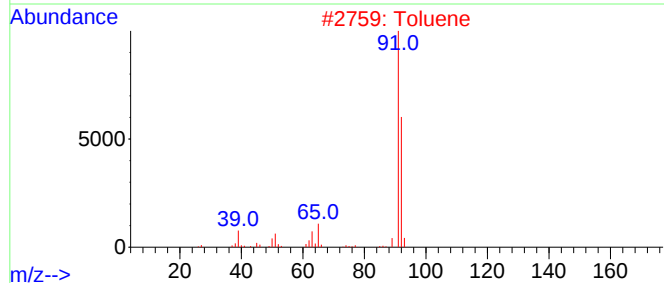
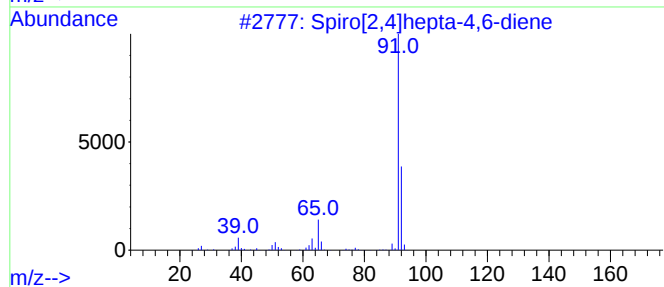
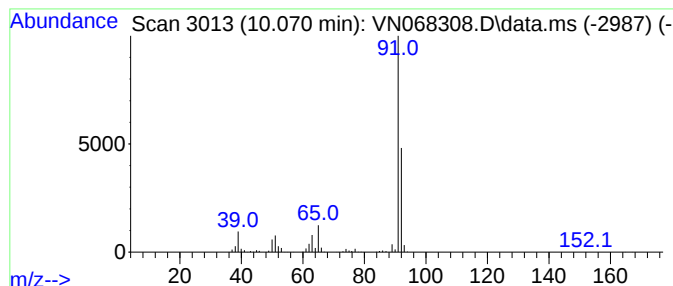
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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

Peak Number 1 Spiro[2,4]hepta-4,6-diene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.070	48.77 ug/l	1660060	1,4-Difluorobenzene	8.971

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	91
2			Toluene	92	C7H8	000108-88-3	91
3			2,5-Norbornadiene	92	C7H8	000121-46-0	91
4			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	91
5			Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	83



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Instrument :
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ClientSampleId :
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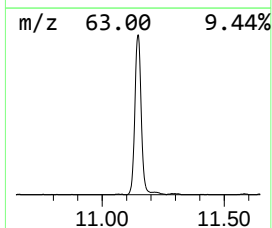
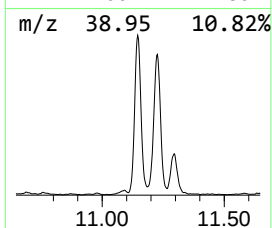
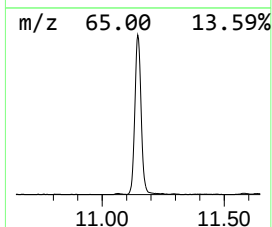
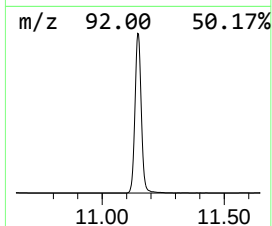
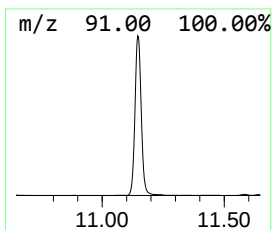
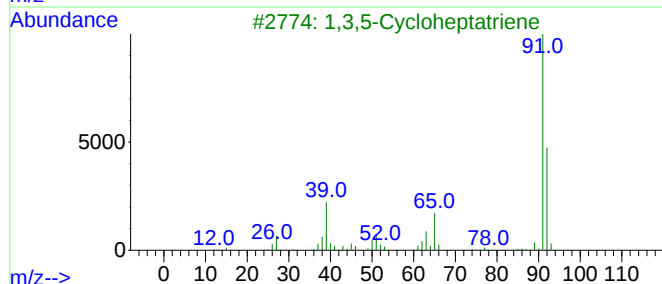
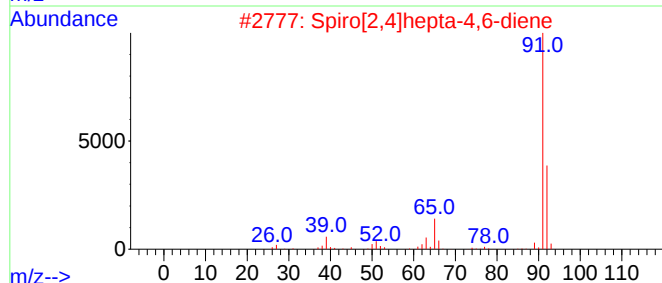
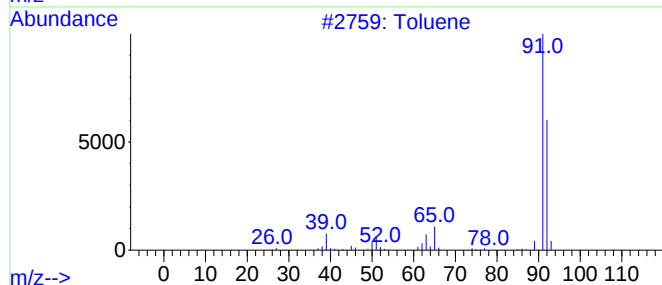
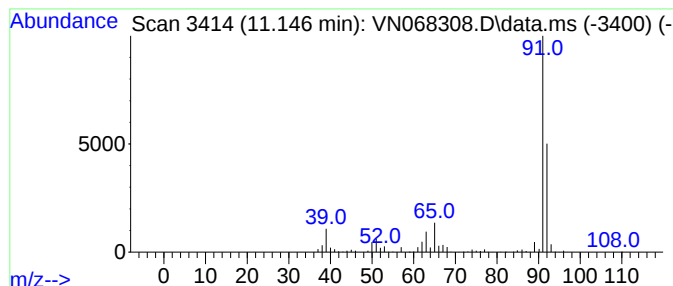
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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

Peak Number 2 1,3,5-Cycloheptatriene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.146	62.65 ug/l	3096640	Chlorobenzene-d5	11.747

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Toluene	92	C7H8	000108-88-3	91
2			Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	90
3			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	87
4			2,5-Norbornadiene	92	C7H8	000121-46-0	80
5			1,6-Heptadien-3-yne	92	C7H8	005150-80-1	72



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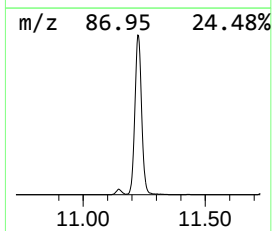
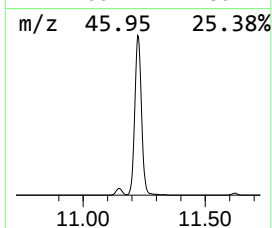
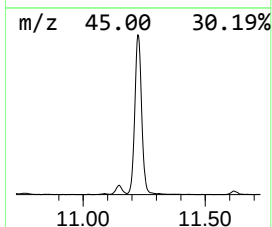
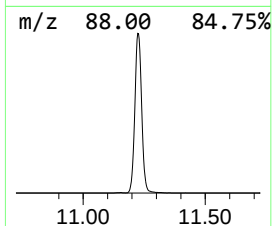
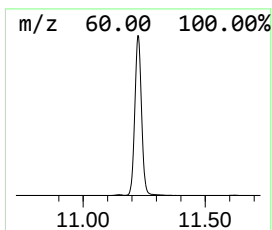
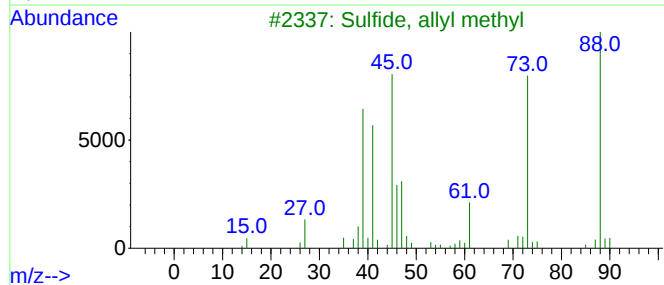
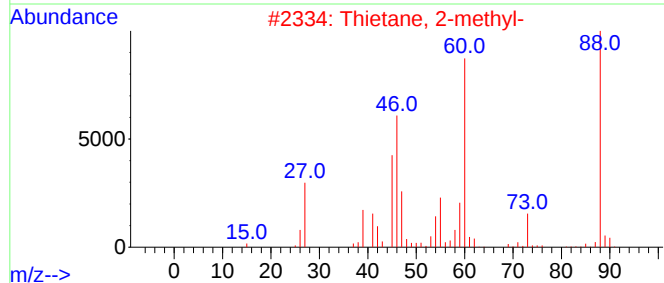
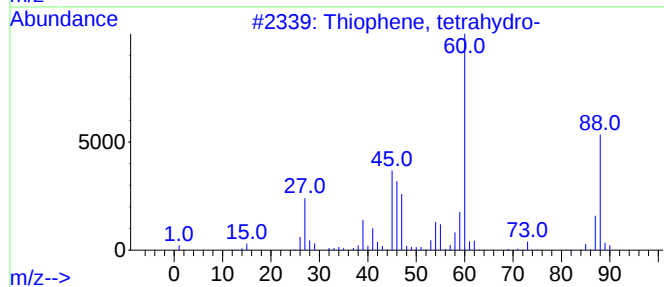
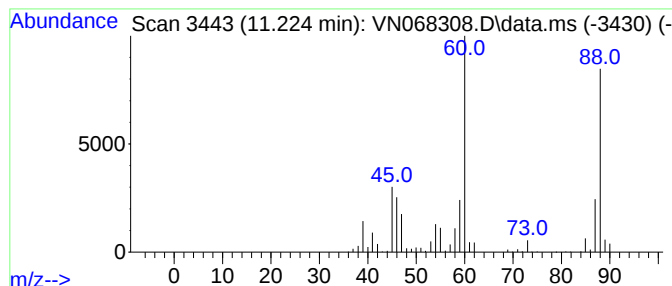
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Thiophene, tetrahydro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.224	75.01 ug/l	3707690	Chlorobenzene-d5	11.747

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-	88	C4H8S	000110-01-0	95
2			Thietane, 2-methyl-	88	C4H8S	017837-41-1	74
3			Sulfide, allyl methyl	88	C4H8S	010152-76-8	43
4			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	36
5			2,2-Dimethylthiirane	88	C4H8S	003772-13-2	25



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ALS Vial : 21 Sample Multiplier: 1

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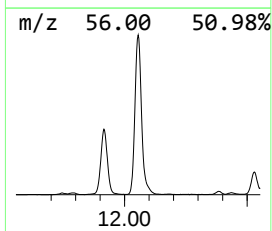
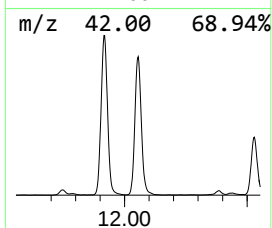
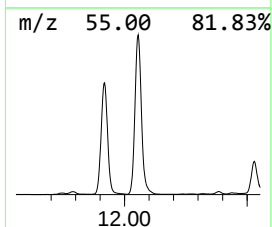
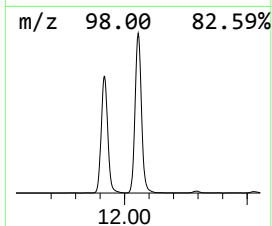
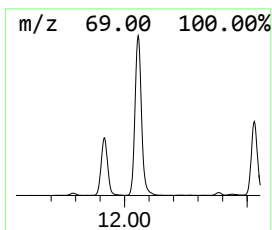
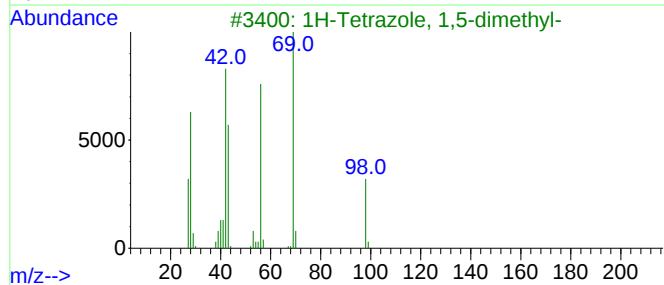
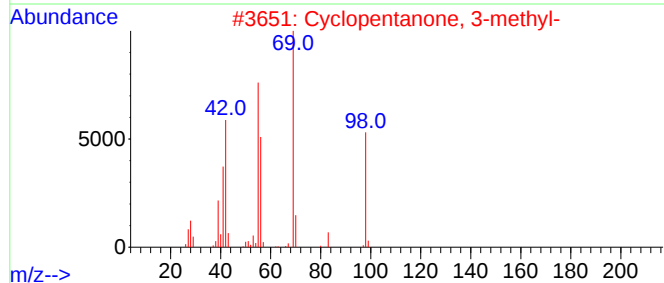
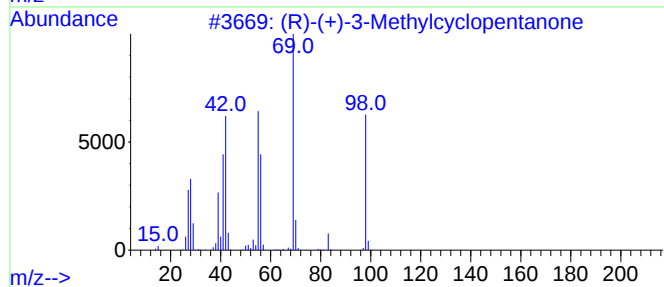
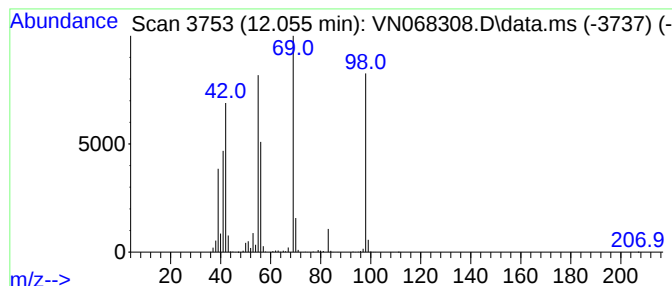
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (R)-(+)-3-Methylcyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.055	122.36 ug/l	6048520	Chlorobenzene-d5	11.747

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(R)-(+)-3-Methylcyclopentanone	98	C6H10O	006672-30-6	94
2			Cyclopentanone, 3-methyl-	98	C6H10O	001757-42-2	91
3			1H-Tetrazole, 1,5-dimethyl-	98	C3H6N4	005144-11-6	53
4			Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	43
5			(Z)-4-Methyl-2-hexene	98	C7H14	003683-19-0	43



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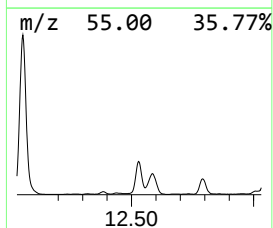
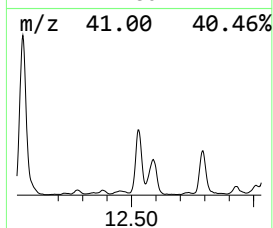
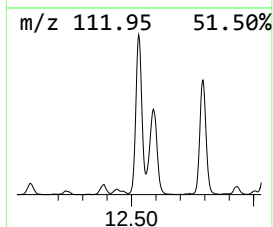
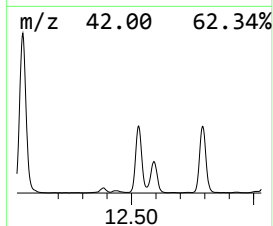
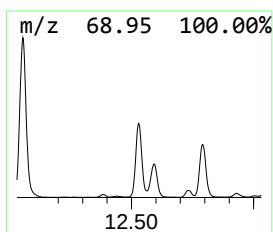
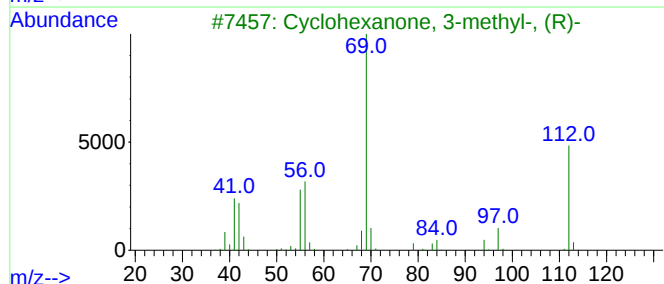
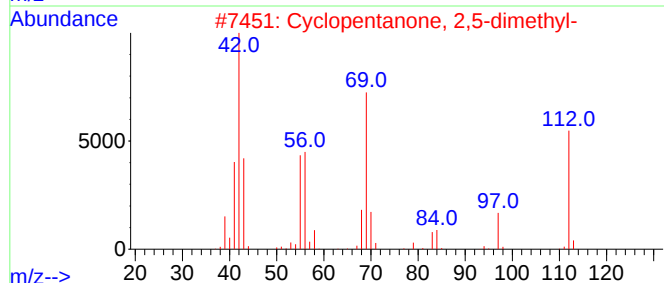
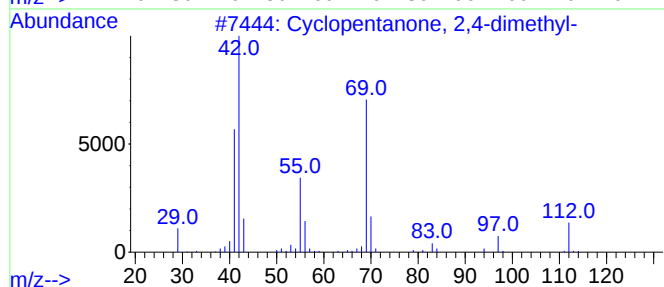
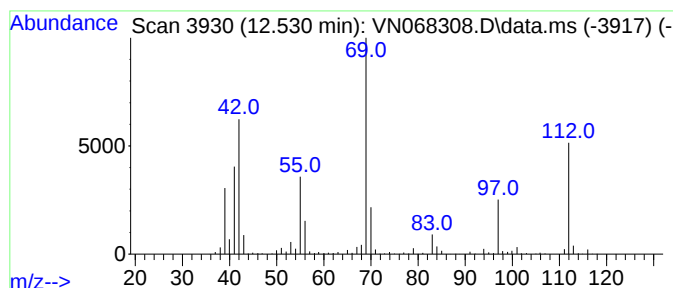
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Peak Number 5 Cyclopentanone, 2,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.530	43.07 ug/l	2128910	Chlorobenzene-d5	11.747

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone, 2,4-dimethyl-	112	C7H12O	001121-33-1	91
2			Cyclopentanone, 2,5-dimethyl-	112	C7H12O	004041-09-2	86
3			Cyclohexanone, 3-methyl-, (R)-	112	C7H12O	013368-65-5	53
4			trans-3,4-Dimethylcyclopentanone	112	C7H12O	019550-73-3	53
5			1,3-Dimethyl-1H-pyrazol-5-ol	112	C5H8N2O	005203-77-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068308.D
Acq On : 25 Aug 2021 18:55
Operator : JC/MD
Sample : M3529-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31113

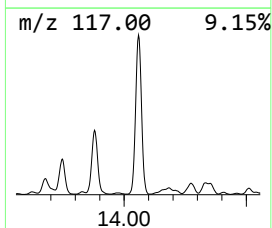
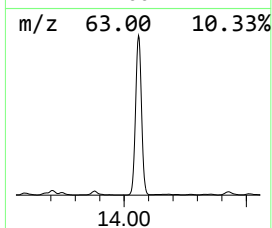
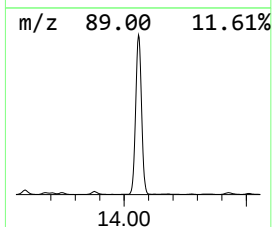
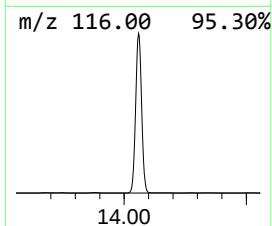
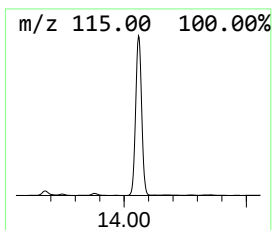
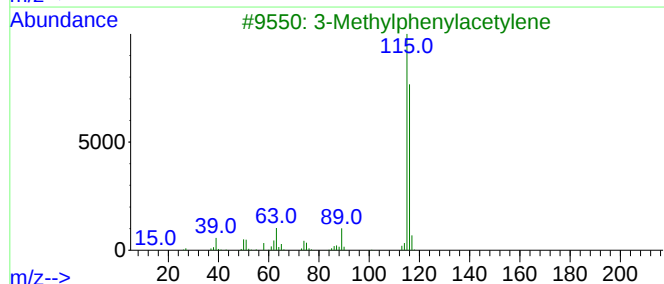
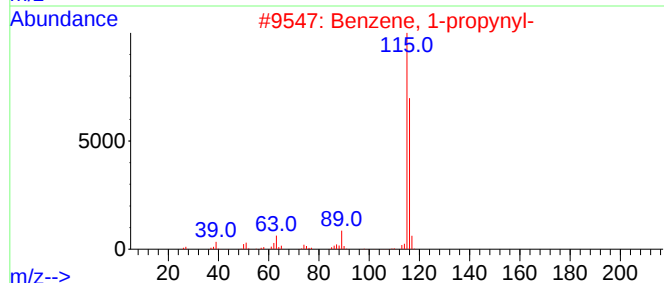
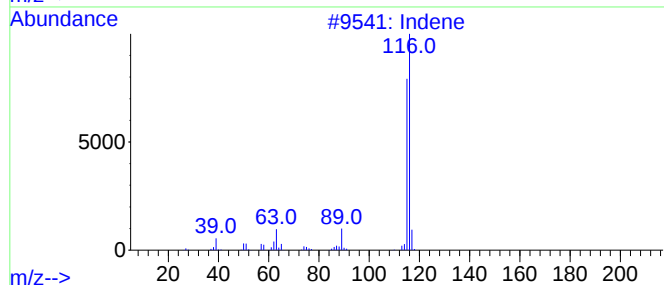
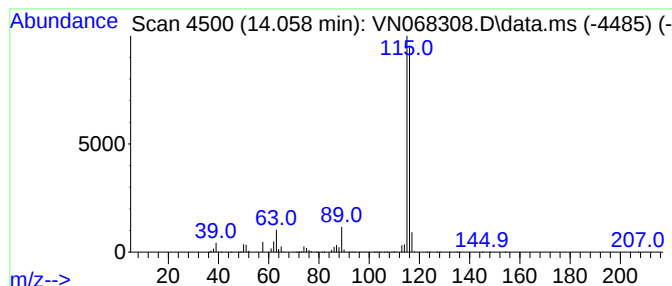
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Quant Title : SW846 8260

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

Peak Number 6 Indene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.058	474.19 ug/l	28797600	1,4-Dichlorobenzene-d4	13.678

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Indene	116	C9H8	000095-13-6	97
2		Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3		3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4		Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
5		Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068308.D
Acq On : 25 Aug 2021 18:55
Operator : JC/MD
Sample : M3529-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31113

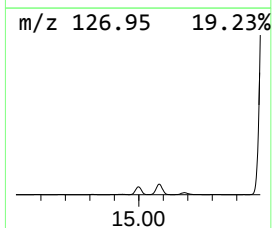
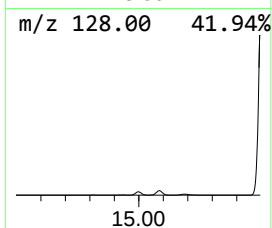
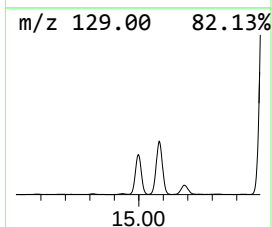
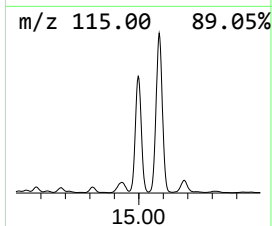
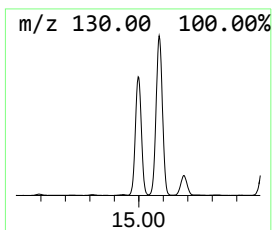
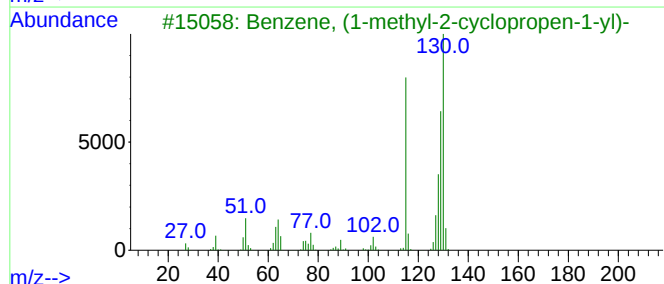
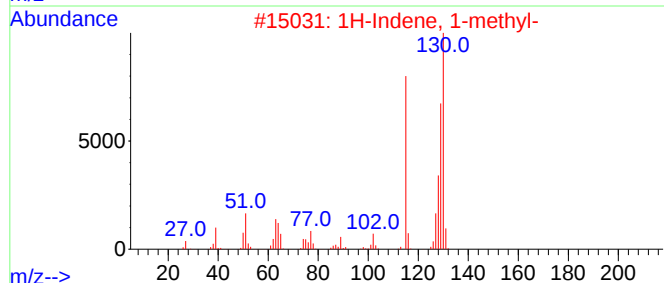
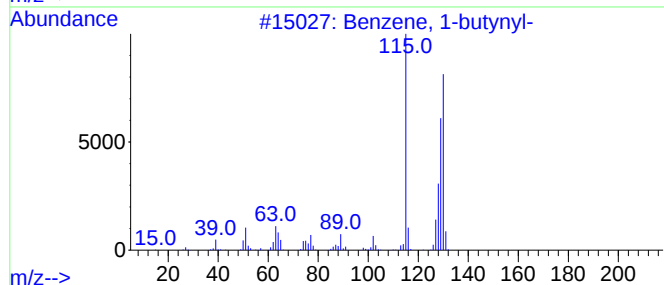
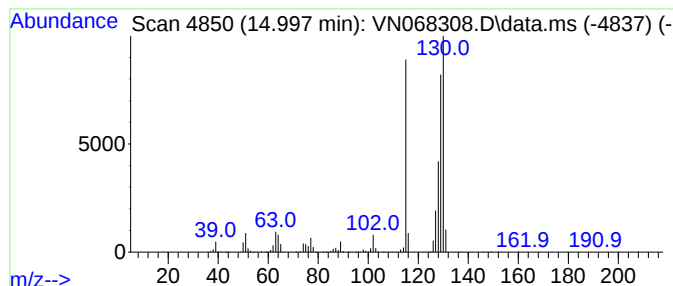
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-butynyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.997	55.02 ug/l	3341450	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-butynyl-	130	C10H10	000622-76-4	94
2			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	93
3			Benzene, (1-methyl-2-cyclopropen-1-yl)-	130	C10H10	065051-83-4	91
4			Benzene, 1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	90
5			2-Methylindene	130	C10H10	002177-47-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068308.D
Acq On : 25 Aug 2021 18:55
Operator : JC/MD
Sample : M3529-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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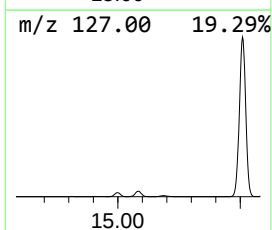
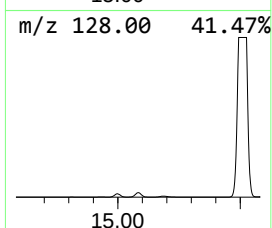
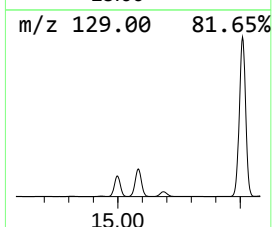
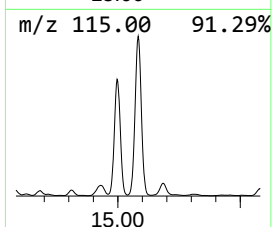
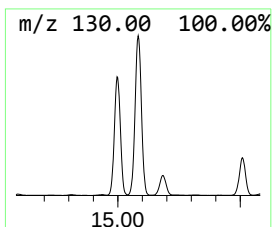
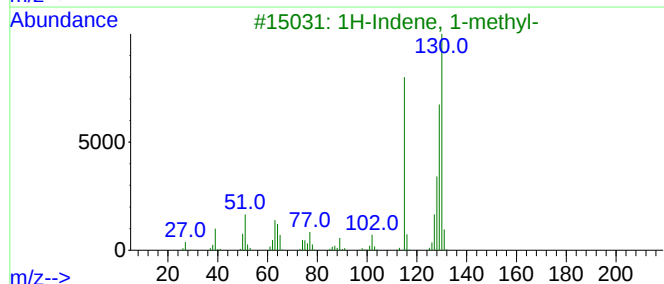
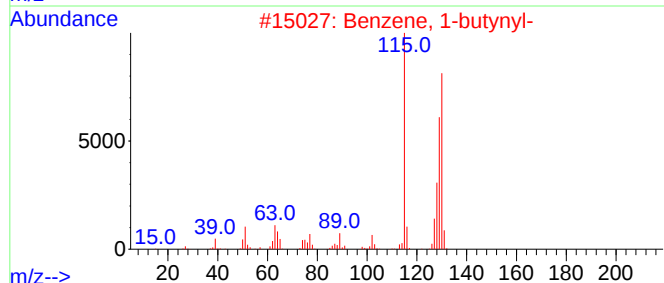
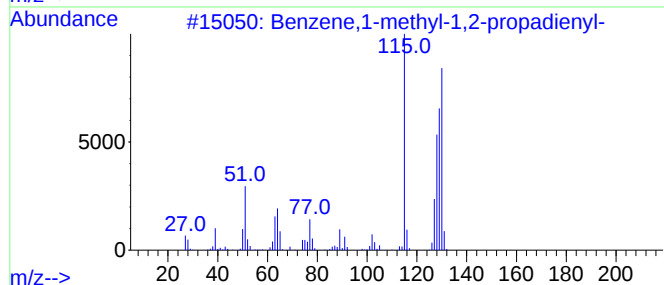
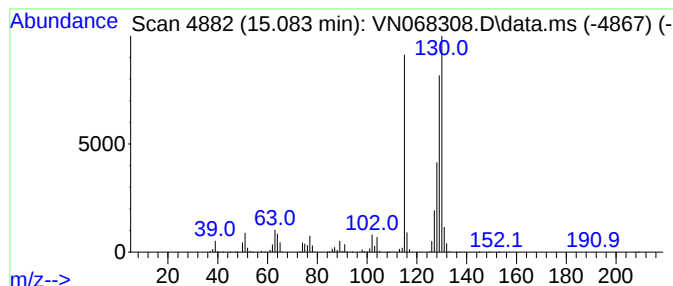
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Quant Title : SW846 8260

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

Peak Number 8 Benzene,1-methyl-1,2-propad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.083	79.96 ug/l	4855920	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	94
2			Benzene, 1-butyryl-	130	C10H10	000622-76-4	94
3			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	93
4			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	92
5			2-Methylindene	130	C10H10	002177-47-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068308.D
Acq On : 25 Aug 2021 18:55
Operator : JC/MD
Sample : M3529-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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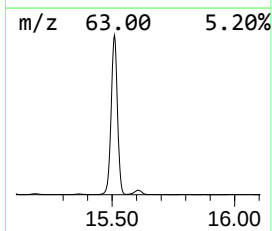
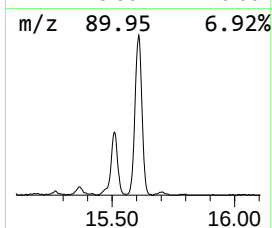
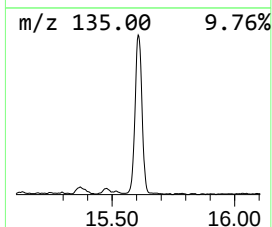
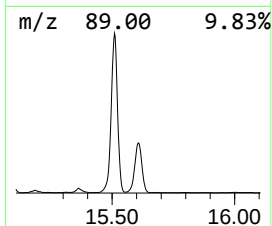
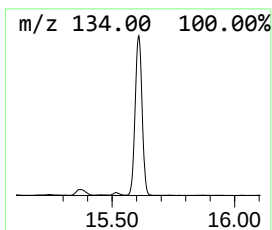
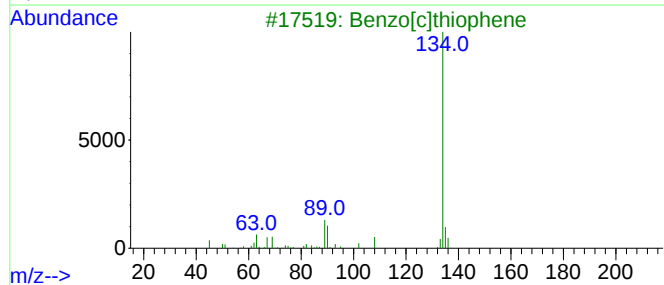
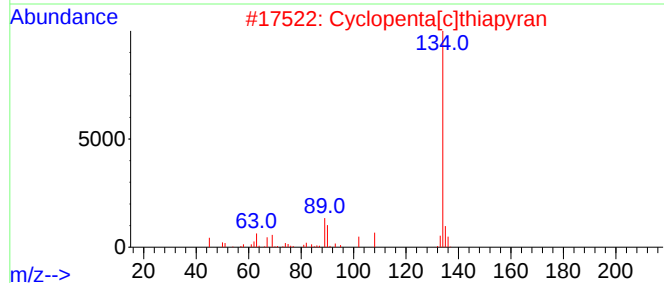
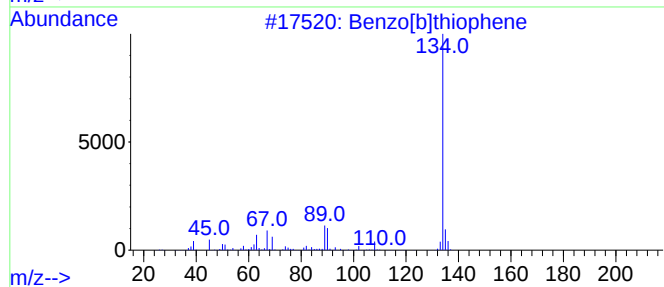
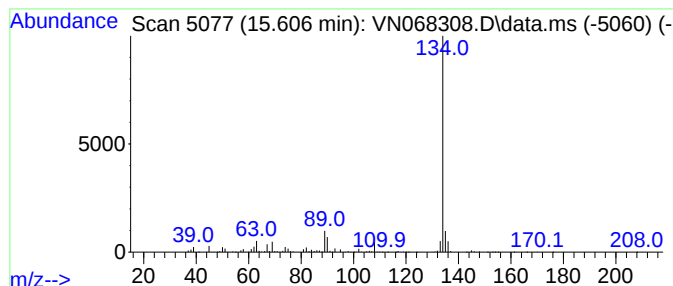
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Quant Title : SW846 8260

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

Peak Number 9 Benzo[b]thiophene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.606	46.59 ug/l	2829430	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]thiophene	134	C8H6S	000095-15-8	91
2			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	91
3			Benzo[c]thiophene	134	C8H6S	000270-82-6	91
4			[1]Benzo[thieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	64
5			3-Deazaadenine	134	C6H6N4	006811-77-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068308.D
Acq On : 25 Aug 2021 18:55
Operator : JC/MD
Sample : M3529-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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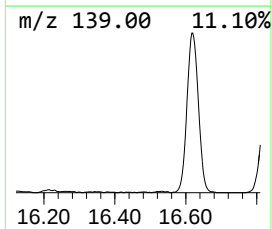
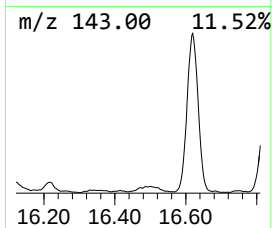
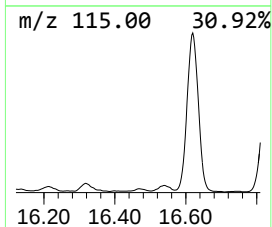
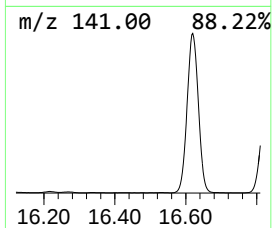
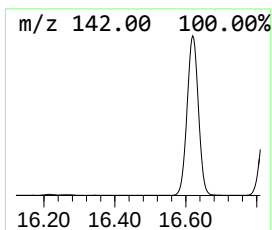
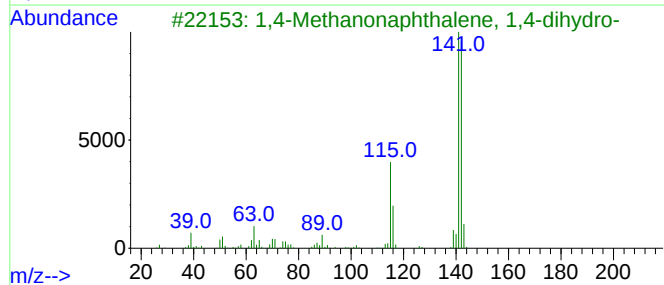
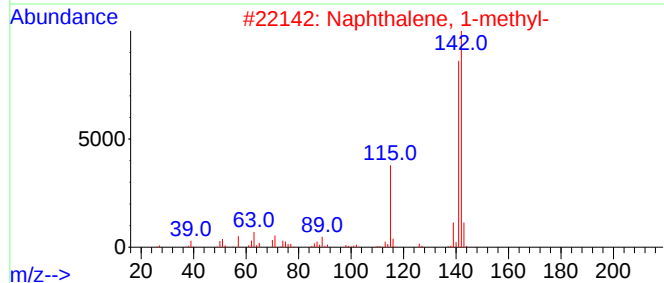
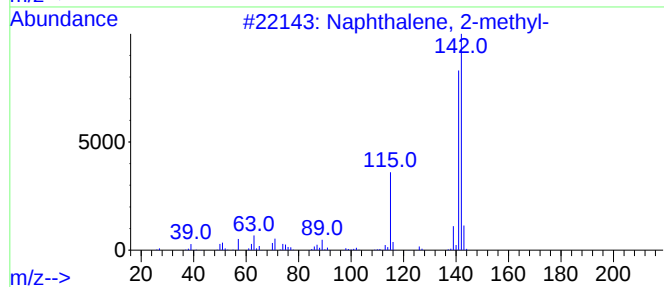
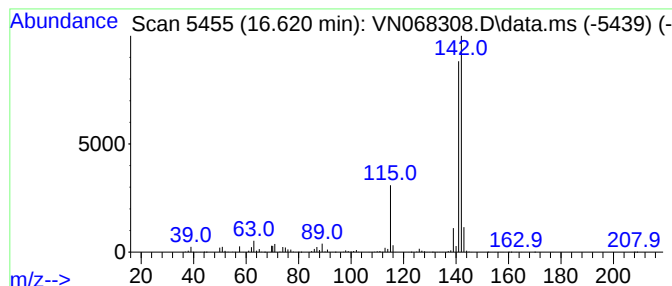
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.620	58.04 ug/l	3524850	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068308.D
Acq On : 25 Aug 2021 18:55
Operator : JC/MD
Sample : M3529-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.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
Spiro[2,4]hepta...	10.070	48.8	ug/l	1660060	2	8.971	1701880	50.0
1,3,5-Cyclohept...	11.146	62.6	ug/l	3096640	3	11.747	2471500	50.0
Thiophene, tetr...	11.224	75.0	ug/l	3707690	3	11.747	2471500	50.0
(R)-(+)-3-Methy...	12.055	122.4	ug/l	6048520	3	11.747	2471500	50.0
Cyclopentanone,...	12.530	43.1	ug/l	2128910	3	11.747	2471500	50.0
Indene	14.058	474.2	ug/l	28797600	4	13.678	3036530	50.0
Benzene, 1-buty...	14.997	55.0	ug/l	3341450	4	13.678	3036530	50.0
Benzene,1-methy...	15.083	80.0	ug/l	4855920	4	13.678	3036530	50.0
Benzo[b]thiophene	15.606	46.6	ug/l	2829430	4	13.678	3036530	50.0
Naphthalene, 1-...	16.620	58.0	ug/l	3524850	4	13.678	3036530	50.0