

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
 Data File : VN073134.D
 Acq On : 26 Jun 2022 02:54
 Operator : JC\MD
 Sample : N3494-16
 Misc : 5.66g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SP-EXC-1-6

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\82N061722W.M
 Title : SW846 8260

Signal : TIC: VN073134.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.945	1019	1030	1035	rBV	253321	643033	1.42%	0.576%
2	8.010	1035	1041	1049	rVB	495617	1134931	2.50%	1.017%
3	8.375	1093	1103	1114	rBV3	514318	1356461	2.99%	1.215%
4	8.898	1184	1192	1205	rBV	674532	1427244	3.15%	1.279%
5	10.375	1436	1443	1452	rBV	1037532	2006923	4.43%	1.798%
6	11.281	1591	1597	1603	rBV	464716	793769	1.75%	0.711%
7	11.486	1627	1632	1641	rVB2	263454	506343	1.12%	0.454%
8	11.710	1659	1670	1678	rBV2	5781105	11972278	26.40%	10.726%
9	11.875	1692	1698	1702	rBV5	242986	587295	1.29%	0.526%
10	12.192	1745	1752	1758	rBV2	520708	1219619	2.69%	1.093%
11	12.304	1768	1771	1775	rVB	404585	588920	1.30%	0.528%
12	12.392	1781	1786	1787	rBV3	379359	543882	1.20%	0.487%
13	12.669	1828	1833	1838	rBV	1022060	1762572	3.89%	1.579%
14	12.833	1856	1861	1868	rBV4	719525	1277486	2.82%	1.145%
15	12.916	1869	1875	1881	rVV7	376099	835042	1.84%	0.748%
16	12.992	1882	1888	1902	rVB7	613108	2391099	5.27%	2.142%
17	13.133	1908	1912	1916	rVB2	419422	585658	1.29%	0.525%
18	13.222	1923	1927	1939	rVB3	809852	1475145	3.25%	1.322%
19	13.539	1978	1981	1985	rVB4	389332	532952	1.18%	0.477%
20	13.610	1989	1993	2002	rVB2	1220018	2650147	5.84%	2.374%
21	13.757	2014	2018	2031	rVB6	549550	1681287	3.71%	1.506%
22	13.927	2042	2047	2053	rVB3	1731783	3190986	7.04%	2.859%
23	14.151	2081	2085	2090	rVB	1276111	1773364	3.91%	1.589%
24	14.251	2098	2102	2108	rVB4	560000	1060512	2.34%	0.950%
25	14.322	2111	2114	2120	rVB5	501091	866986	1.91%	0.777%
26	14.404	2121	2128	2130	rBV5	321232	811209	1.79%	0.727%
27	14.445	2130	2135	2137	rVV2	1165369	1936657	4.27%	1.735%
28	14.474	2138	2140	2149	rVB3	1284476	2136309	4.71%	1.914%
29	14.557	2150	2154	2157	rBV	657042	927020	2.04%	0.831%
30	14.610	2158	2163	2168	rBV4	951881	1724200	3.80%	1.545%
31	14.792	2191	2194	2199	rBV3	464590	633049	1.40%	0.567%
32	14.851	2199	2204	2210	rBV3	1451737	3317981	7.32%	2.973%
33	14.910	2210	2214	2221	rVB4	1517895	2931707	6.46%	2.627%
34	15.127	2247	2251	2255	rVB3	1103621	1727187	3.81%	1.547%
35	15.239	2265	2270	2275	rBV4	841207	1625796	3.58%	1.457%
36	15.433	2292	2303	2310	rBV	21369468	45352475	100.00%	40.632%

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ClientSampleId :
SP-EXC-1-6

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\82N061722W.M
Title : SW846 8260

37	15.810	2362	2367	2372	rBV4	915900	1669804	3.68%	1.496%
38	16.380	2460	2464	2470	rVB2	713061	1174799	2.59%	1.053%
39	16.727	2517	2523	2533	rBV5	969232	2785632	6.14%	2.496%

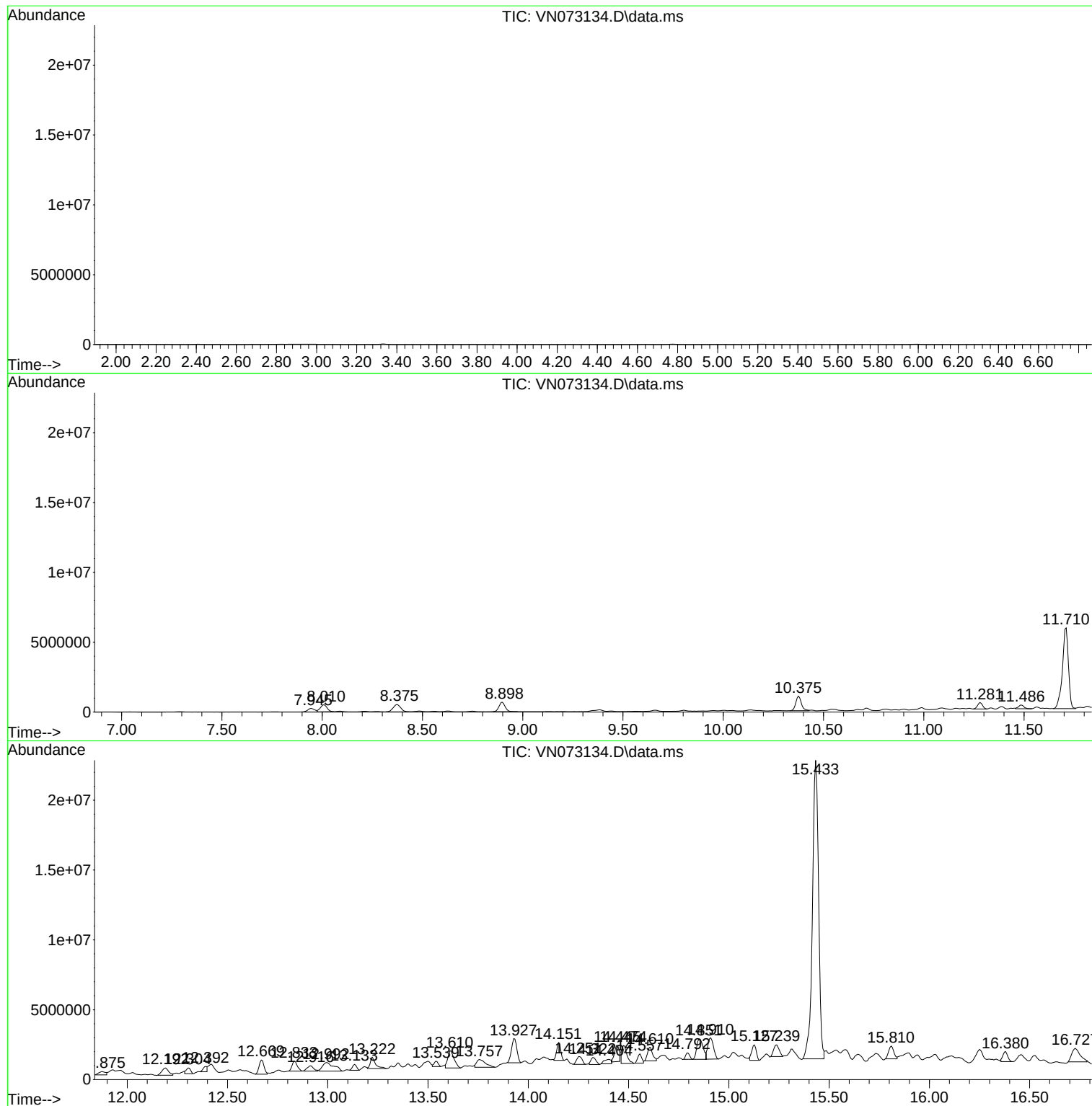
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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



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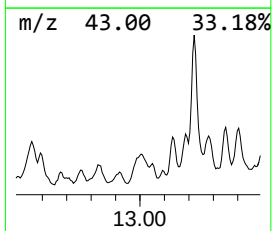
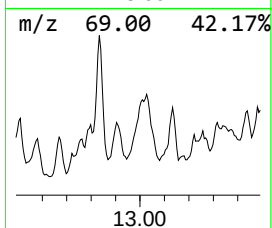
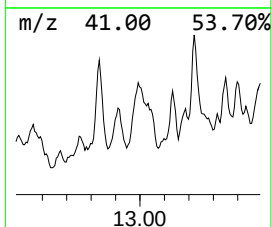
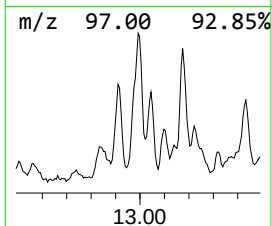
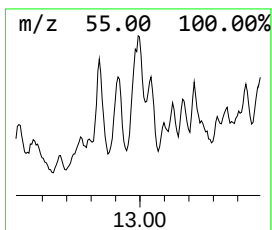
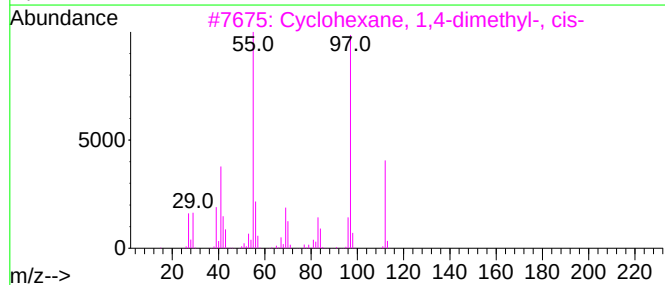
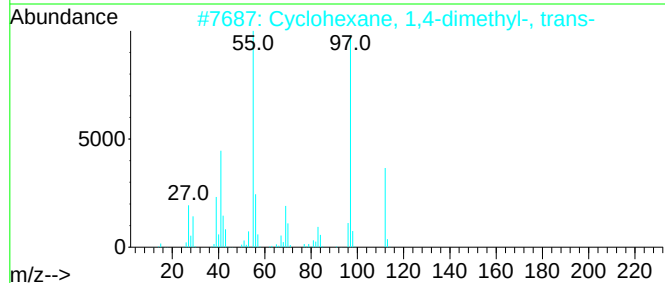
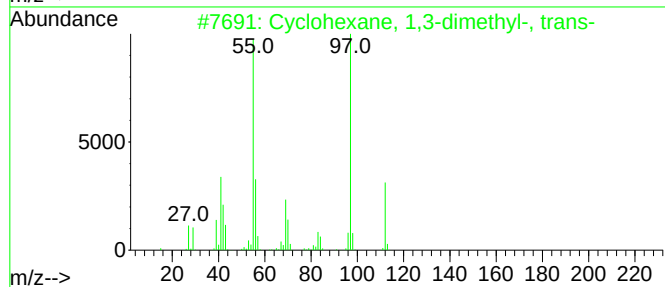
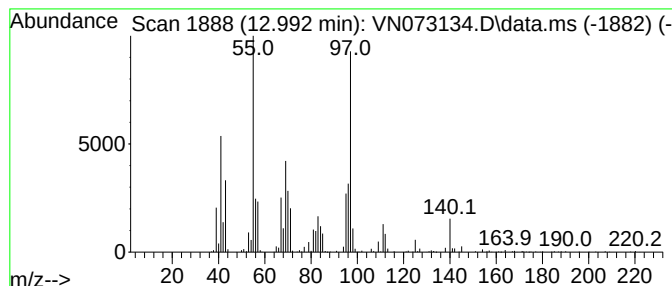
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown12.992 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.992	45.11 ug/l	2391100	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	46
2			Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	46
3			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	46
4			Cycloheptane, methyl-	112	C8H16	004126-78-7	46
5			Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	46



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ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-6

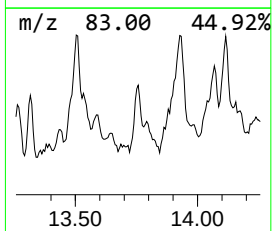
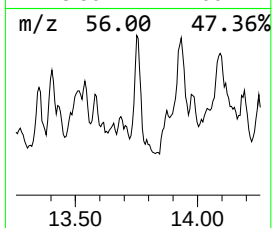
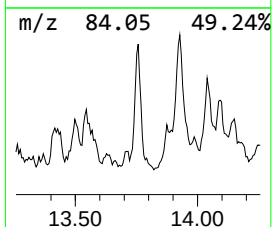
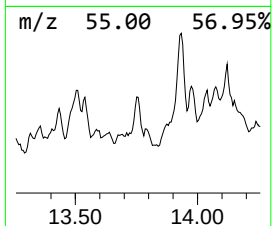
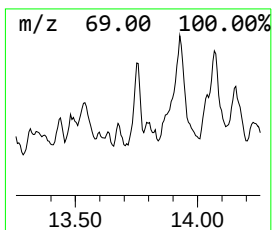
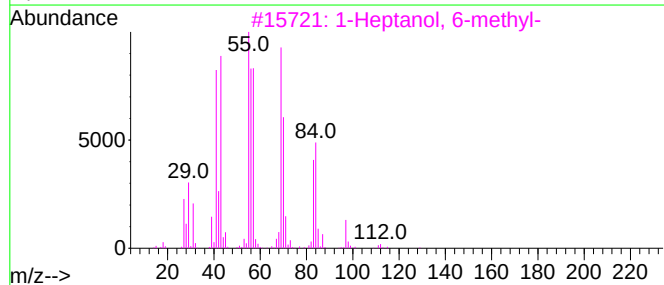
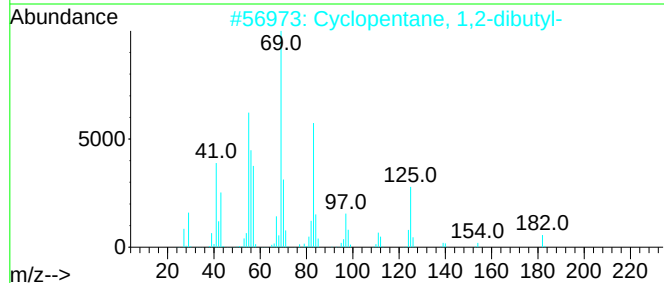
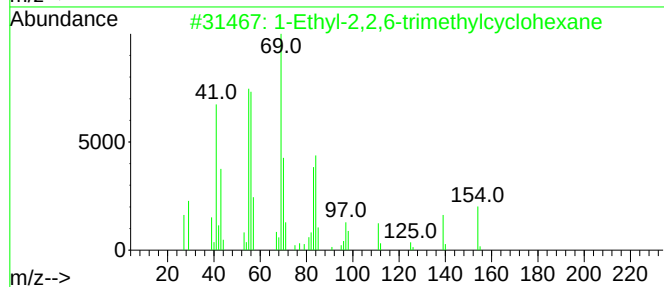
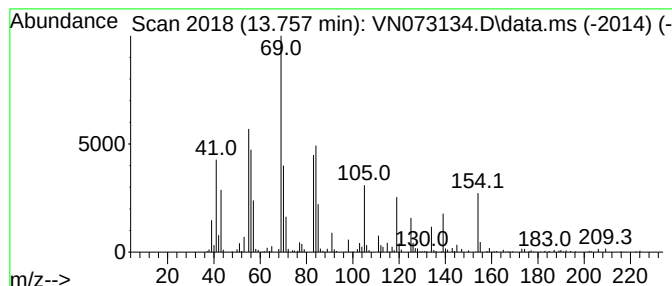
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Ethyl-2,2,6-trimethylcycl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.757	31.72 ug/l	1681290	1,4-Dichlorobenzene-d4	13.610

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Ethyl-2,2,6-trimethylcyclohexane	154	C11H22	071186-27-1	80
2		Cyclopentane, 1,2-dibutyl-	182	C13H26	062199-52-4	50
3		1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	43
4		6-Dodecene, (E)-	168	C12H24	007206-17-9	40
5		1-Hexene, 3,3,5-trimethyl-	126	C9H18	013427-43-5	38



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Misc : 5.66g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-6

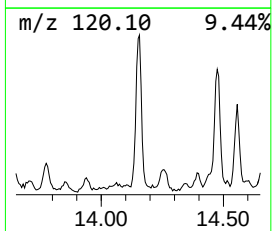
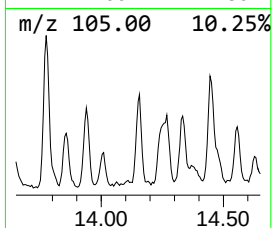
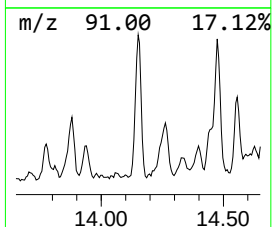
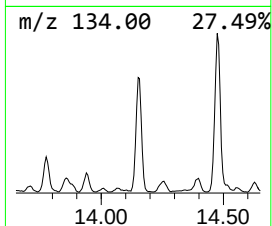
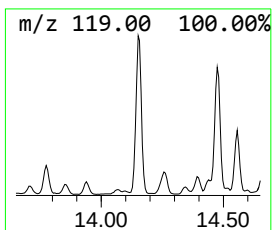
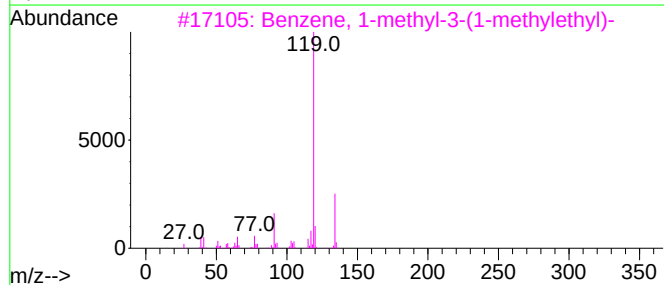
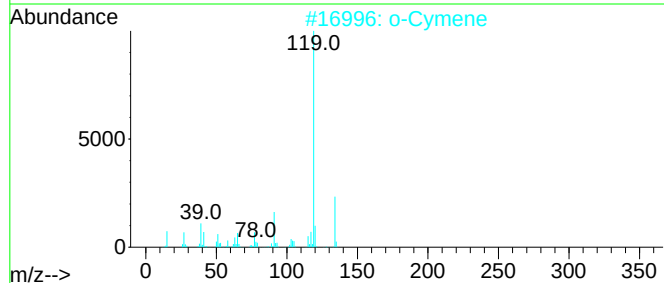
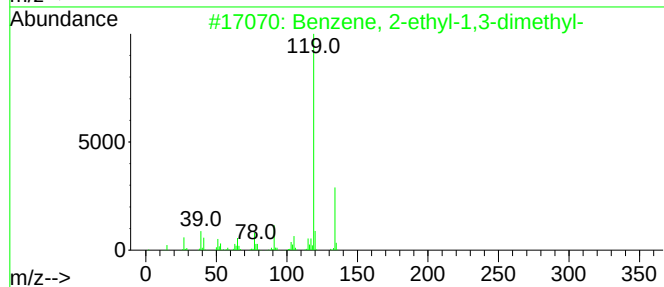
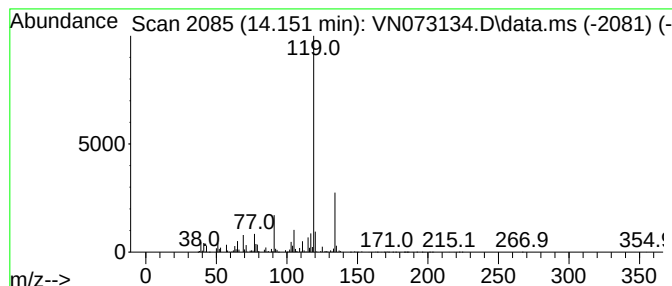
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 2-ethyl-1,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.151	33.46 ug/l	1773360	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
2			o-Cymene	134	C10H14	000527-84-4	95
3			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



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Instrument :
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ClientSampleId :
SP-EXC-1-6

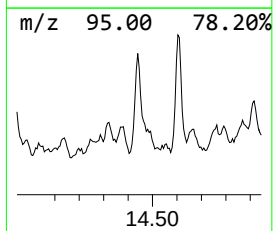
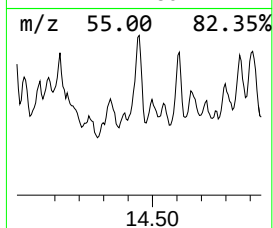
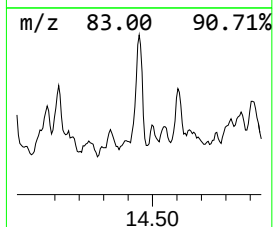
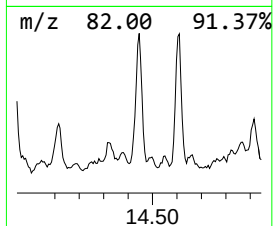
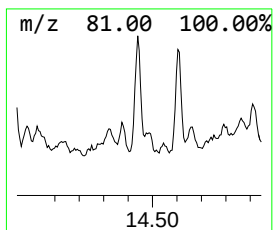
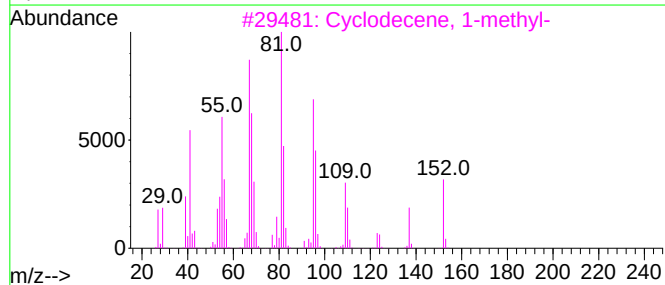
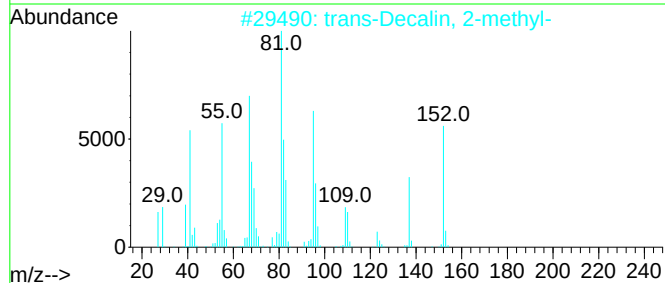
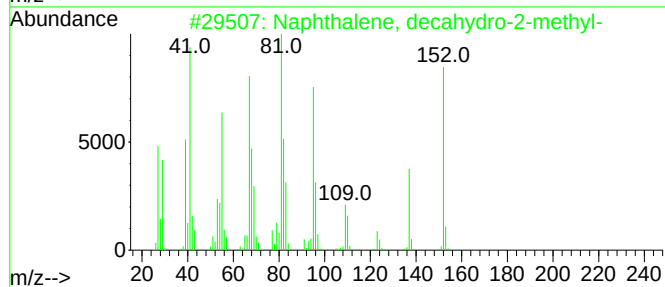
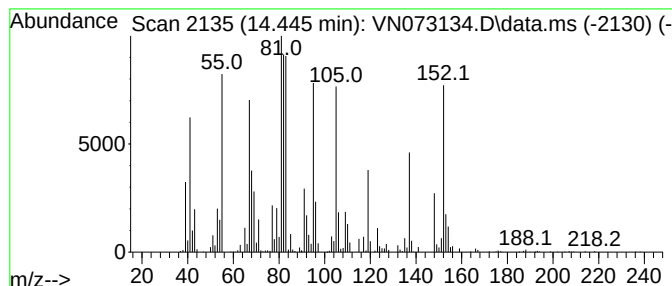
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, decahydro-2-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.445	36.54 ug/l	1936660	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	90
2			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	62
3			Cyclodecene, 1-methyl-	152	C11H20	066633-38-3	52
4			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	45
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	45



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MSVOA_N
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SP-EXC-1-6

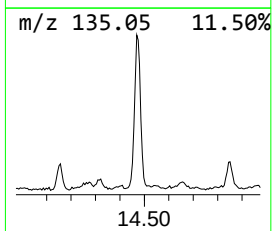
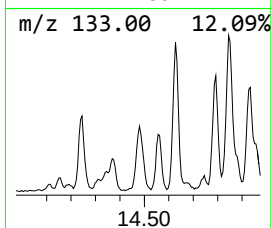
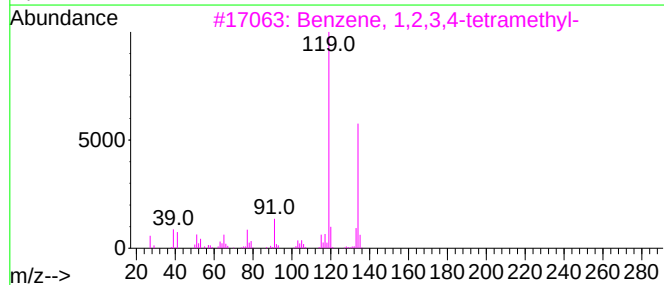
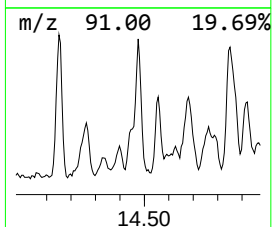
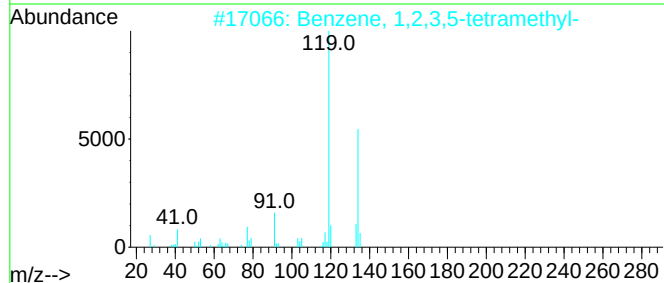
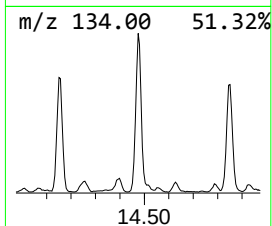
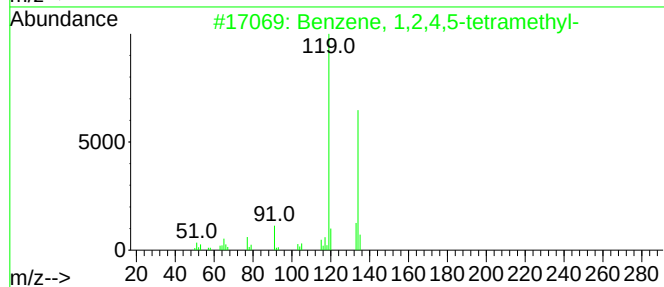
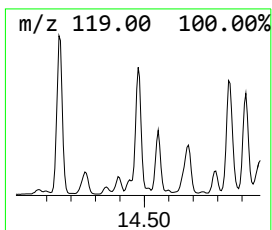
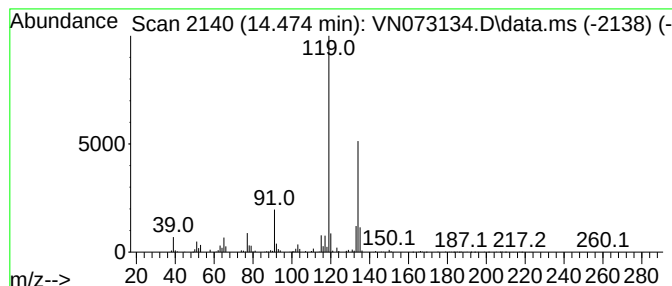
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.474	40.31 ug/l	2136310	1,4-Dichlorobenzene-d4	13.610

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	91
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	91
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	90
5			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073134.D
Acq On : 26 Jun 2022 02:54
Operator : JC\MD
Sample : N3494-16
Misc : 5.66g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-6

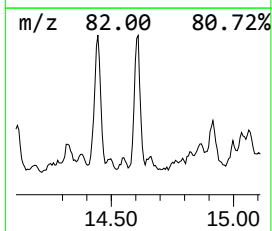
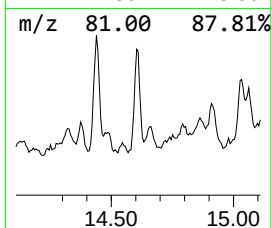
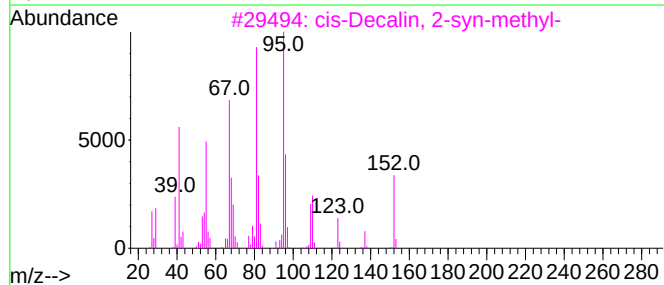
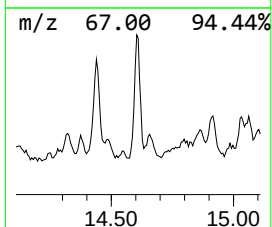
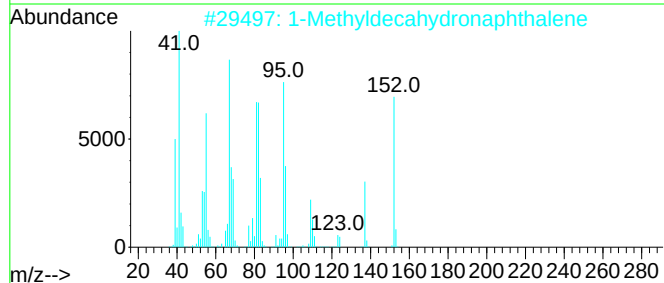
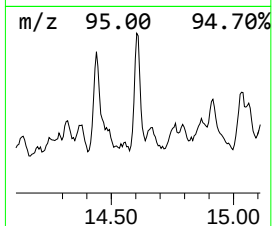
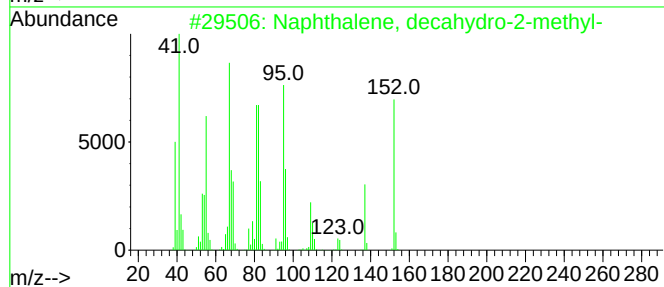
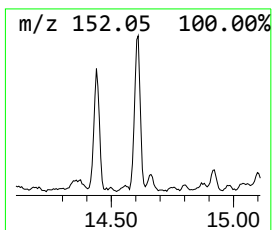
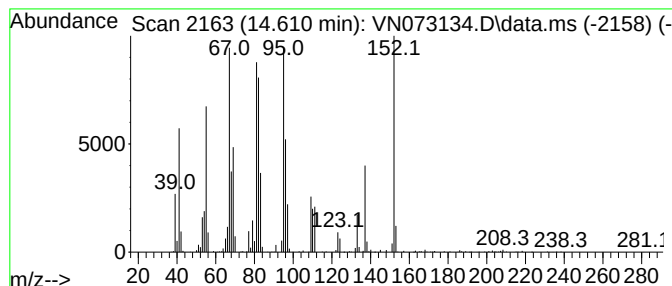
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Quant Title : SW846 8260

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

Peak Number 6 1-Methyldecahydronaphthalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.610	32.53 ug/l	1724200	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	96
2			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	96
3			cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	76
4			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	70
5			Decalin, syn-1-methyl-, cis-	152	C11H20	1000158-89-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073134.D
Acq On : 26 Jun 2022 02:54
Operator : JC\MD
Sample : N3494-16
Misc : 5.66g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-6

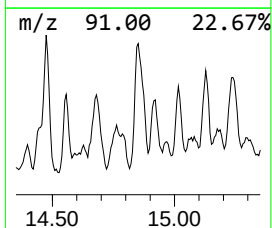
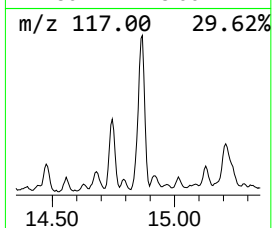
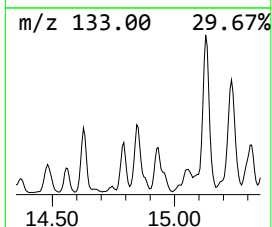
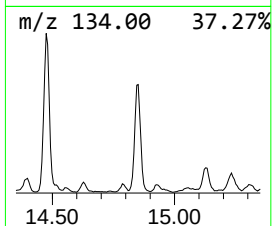
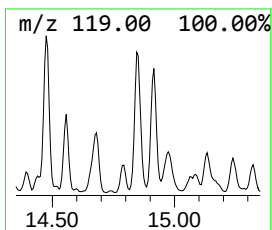
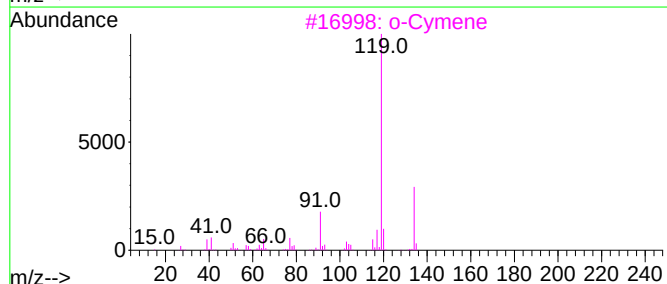
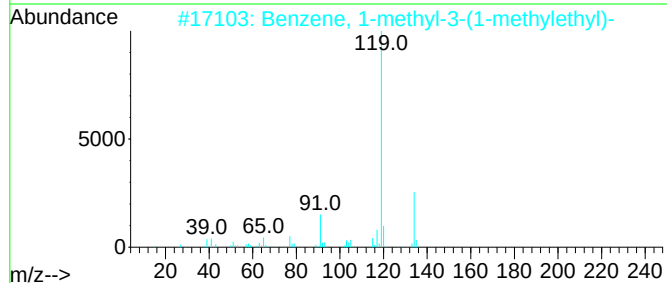
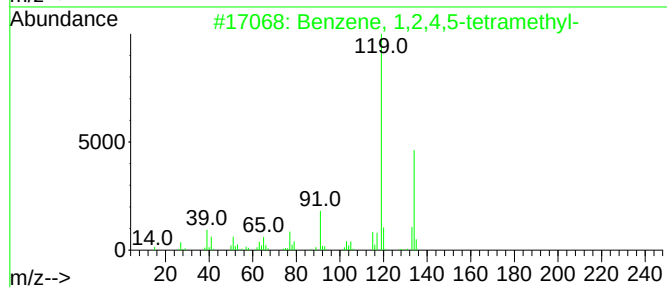
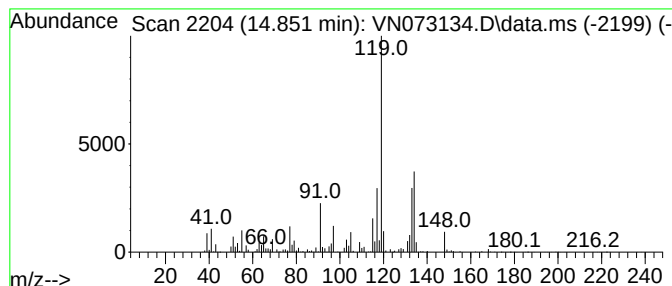
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-methyl-3-(1-meth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.851	62.60 ug/l	3317980	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	64
2			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	64
3			o-Cymene	134	C10H14	000527-84-4	64
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	64
5			p-Cymene	134	C10H14	000099-87-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073134.D
Acq On : 26 Jun 2022 02:54
Operator : JC\MD
Sample : N3494-16
Misc : 5.66g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-6

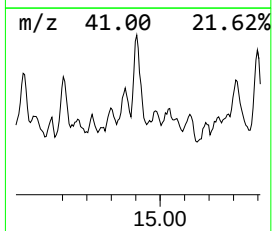
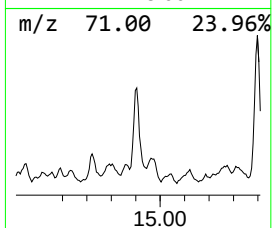
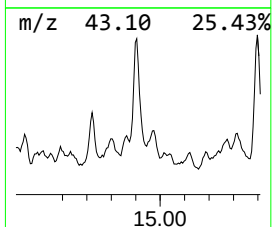
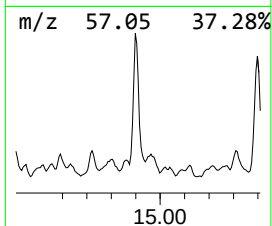
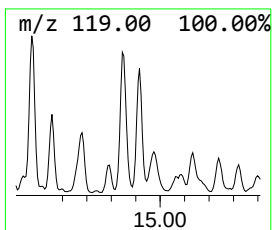
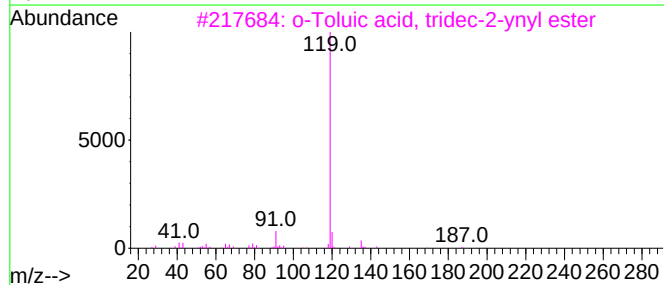
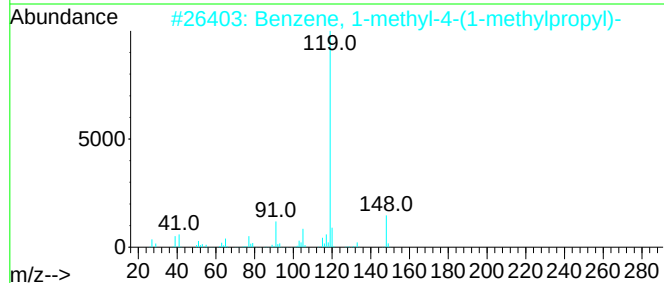
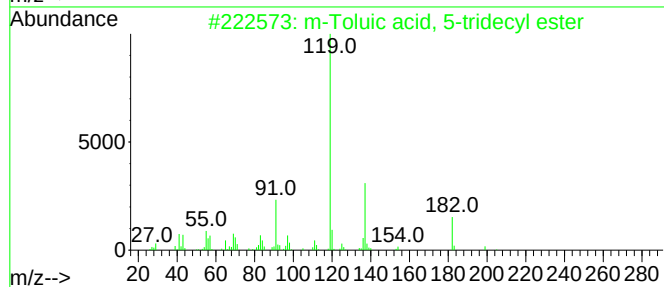
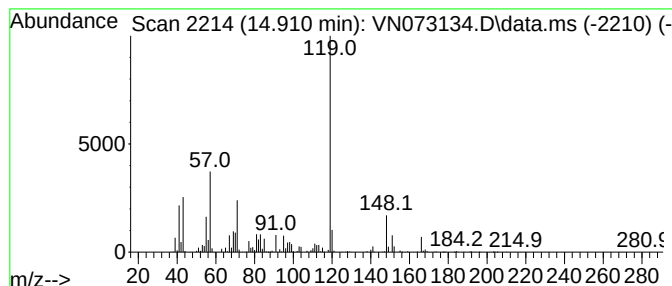
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Quant Title : SW846 8260

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

Peak Number 8 m-Toluic acid, 5-tridecyl e... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.910	55.31 ug/l	2931710	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			m-Toluic acid, 5-tridecyl ester	318	C21H34O2	1000299-78-1	53
2			Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	50
3			o-Toluic acid, tridec-2-ynyl ester	314	C21H30O2	1000292-51-7	47
4			m-Toluic acid, 2-ethylcyclohexyl...	246	C16H22O2	1000293-33-2	47
5			p-Menthane, 2,3-dibromo-8-phenyl-	372	C16H22Br2	1000152-61-6	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073134.D
Acq On : 26 Jun 2022 02:54
Operator : JC\MD
Sample : N3494-16
Misc : 5.66g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-6

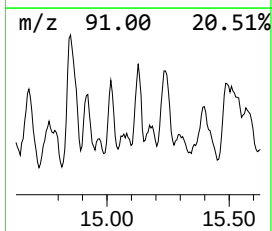
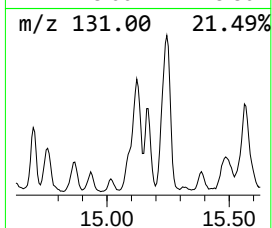
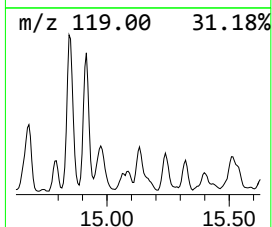
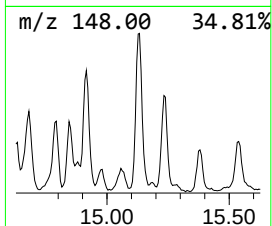
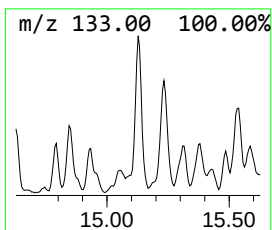
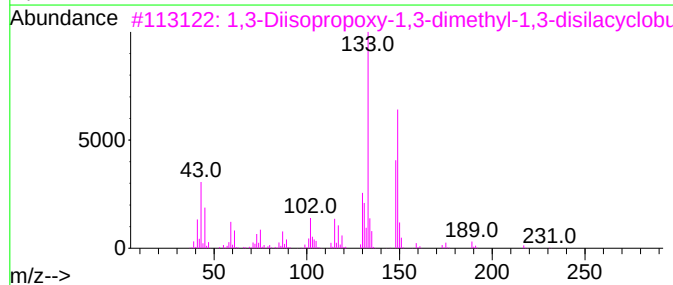
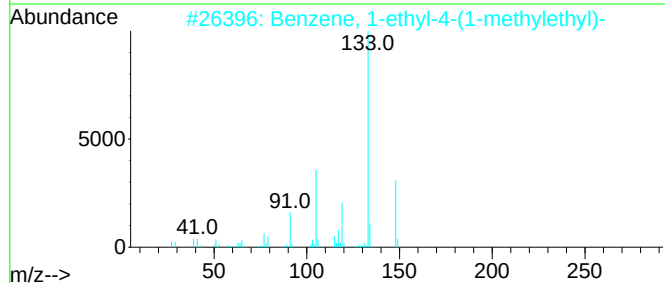
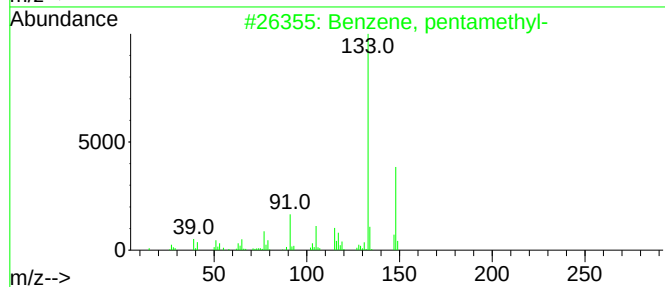
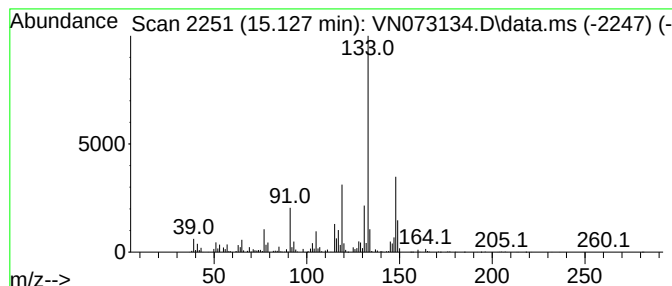
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, pentamethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	32.59 ug/l	1727190	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, pentamethyl-	148	C11H16	000700-12-9	76
2			Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	72
3			1,3-Diisopropoxy-1,3-dimethyl-1,...	232	C10H24O2Si2	198066-66-9	68
4			Benzene, 1,3-dimethyl-5-(1-methy...	148	C11H16	004706-90-5	62
5			Benzene, 1,4-dimethyl-2-(1-methy...	148	C11H16	004132-72-3	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073134.D
Acq On : 26 Jun 2022 02:54
Operator : JC\MD
Sample : N3494-16
Misc : 5.66g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-6

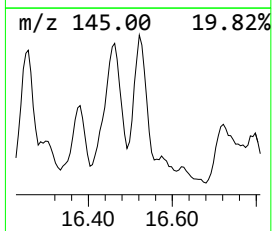
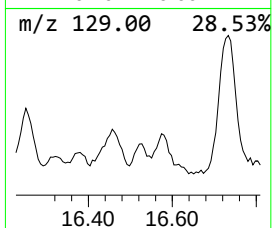
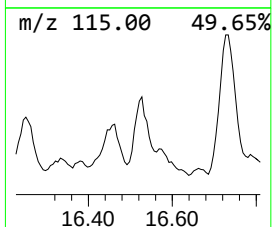
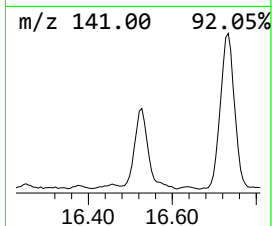
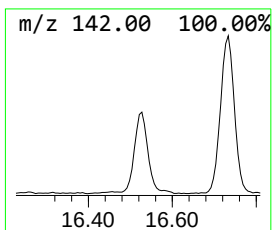
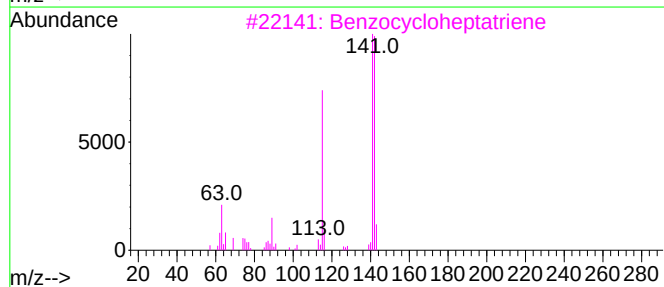
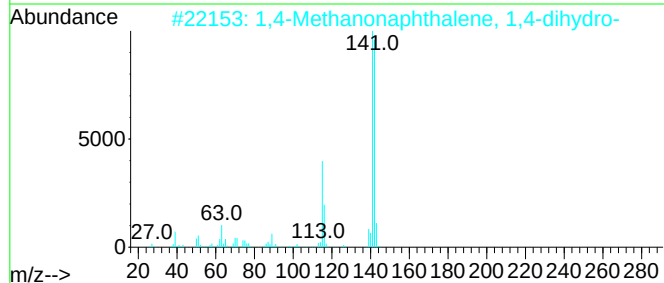
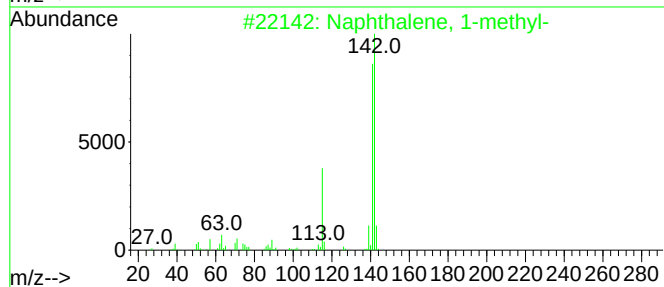
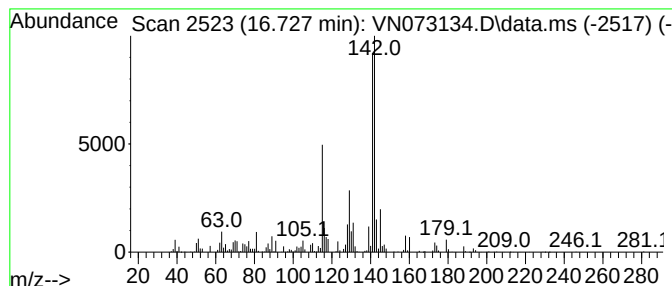
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Quant Title : SW846 8260

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.
16.727	52.56 ug/l	2785630	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
2			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	76
3			Benzocycloheptatriene	142	C11H10	000264-09-5	70
4			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	64
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073134.D
Acq On : 26 Jun 2022 02:54
Operator : JC\MD
Sample : N3494-16
Misc : 5.66g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.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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1-Ethyl-2,2,6-t...	13.757	31.7	ug/l	1681290	4	13.610	2650150	50.0
Benzene, 2-ethy...	14.151	33.5	ug/l	1773360	4	13.610	2650150	50.0
Naphthalene, de...	14.445	36.5	ug/l	1936660	4	13.610	2650150	50.0
Benzene, 1,2,4,...	14.474	40.3	ug/l	2136310	4	13.610	2650150	50.0
1-Methyldecahyd...	14.610	32.5	ug/l	1724200	4	13.610	2650150	50.0
Benzene, 1-meth...	14.851	62.6	ug/l	3317980	4	13.610	2650150	50.0
m-Toluic acid, ...	14.910	55.3	ug/l	2931710	4	13.610	2650150	50.0
Benzene, pentam...	15.127	32.6	ug/l	1727190	4	13.610	2650150	50.0
Naphthalene, 1-...	16.727	52.6	ug/l	2785630	4	13.610	2650150	50.0