

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
 Data File : VN073113.D
 Acq On : 25 Jun 2022 16:18
 Operator : JC\MD
 Sample : N3454-03
 Misc : 5.12g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 WC-16-1A-5-GR

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: VN073113.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.752	138	147	148	rBV7	9411	22186	1.12%	0.098%
2	2.810	153	157	161	rVV	17422	25623	1.30%	0.113%
3	2.957	180	182	190	rVB4	20109	45276	2.29%	0.200%
4	3.340	241	247	256	rVB2	14229	36312	1.84%	0.160%
5	4.993	520	528	543	rVB7	4929	20414	1.03%	0.090%
6	5.210	553	565	576	rBV2	16625	61055	3.09%	0.269%
7	5.481	601	611	617	rBV4	10878	33476	1.69%	0.148%
8	5.993	690	698	707	rVB3	14774	41616	2.10%	0.183%
9	7.287	908	918	927	rBV2	28784	87490	4.42%	0.386%
10	7.757	989	998	1004	rBV3	15497	40741	2.06%	0.180%
11	7.945	1019	1030	1035	rBV	227956	566922	28.66%	2.499%
12	8.010	1035	1041	1049	rVV	455016	1051053	53.13%	4.634%
13	8.092	1049	1055	1061	rVB5	18347	50645	2.56%	0.223%
14	8.363	1093	1101	1113	rVB	232412	546994	27.65%	2.412%
15	8.487	1113	1122	1129	rBV6	24939	72189	3.65%	0.318%
16	8.563	1129	1135	1139	rVV7	18263	44629	2.26%	0.197%
17	8.622	1140	1145	1155	rVB2	32743	87004	4.40%	0.384%
18	8.745	1163	1166	1175	rVB4	24598	49163	2.49%	0.217%
19	8.898	1184	1192	1205	rBV	632586	1349180	68.20%	5.948%
20	9.386	1264	1275	1282	rBV2	104131	264025	13.35%	1.164%
21	9.569	1300	1306	1312	rVB4	27401	59973	3.03%	0.264%
22	9.663	1318	1322	1326	rVB4	26143	44231	2.24%	0.195%
23	9.798	1341	1345	1353	rBV3	34237	60096	3.04%	0.265%
24	9.904	1359	1363	1368	rBV5	17222	33593	1.70%	0.148%
25	10.251	1419	1422	1427	rBV6	22614	34229	1.73%	0.151%
26	10.375	1435	1443	1456	rBV	923459	1823166	92.16%	8.038%
27	10.492	1461	1463	1467	rVV5	26834	44883	2.27%	0.198%
28	10.557	1467	1474	1483	rVB6	73415	208924	10.56%	0.921%
29	10.716	1496	1501	1507	rVB	78958	128702	6.51%	0.567%
30	10.798	1509	1515	1522	rBV4	96627	240769	12.17%	1.061%
31	11.228	1585	1588	1592	rVB2	67887	94843	4.79%	0.418%
32	11.280	1593	1597	1603	rVB2	145368	243927	12.33%	1.075%
33	11.333	1604	1606	1611	rBV5	32448	51897	2.62%	0.229%
34	11.386	1611	1615	1620	rVB4	59039	95227	4.81%	0.420%
35	11.486	1628	1632	1636	rBV4	66751	119868	6.06%	0.528%
36	11.680	1659	1665	1676	rBV	995016	1763439	89.14%	7.775%

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37	11.922	1703	1706	1711	rBV3	69469	131123	6.63%	0.578%
38	12.192	1747	1752	1759	rBV4	112964	233924	11.82%	1.031%
39	12.669	1827	1833	1841	rBV	1125680	1896591	95.87%	8.362%
40	12.839	1857	1862	1868	rBV7	237497	666406	33.69%	2.938%
41	12.986	1883	1887	1893	rBV6	94141	203542	10.29%	0.897%
42	13.221	1923	1927	1934	rVB	236661	376808	19.05%	1.661%
43	13.610	1988	1993	2003	rVB	1113179	1978265	100.00%	8.722%
44	13.933	2044	2048	2053	rVB3	464524	794005	40.14%	3.501%
45	14.439	2130	2134	2139	rVB4	492062	807448	40.82%	3.560%
46	14.604	2158	2162	2167	rVB4	382477	583026	29.47%	2.570%
47	14.763	2185	2189	2192	rBV2	250336	378127	19.11%	1.667%
48	15.127	2248	2251	2255	rVB3	309749	401484	20.29%	1.770%
49	15.398	2292	2297	2305	rVB3	536540	1017868	51.45%	4.488%
50	16.245	2434	2441	2447	rBV3	678806	1686840	85.27%	7.437%
51	16.515	2483	2487	2493	rBV	369258	762141	38.53%	3.360%
52	16.715	2516	2521	2533	rBV6	438993	1220717	61.71%	5.382%

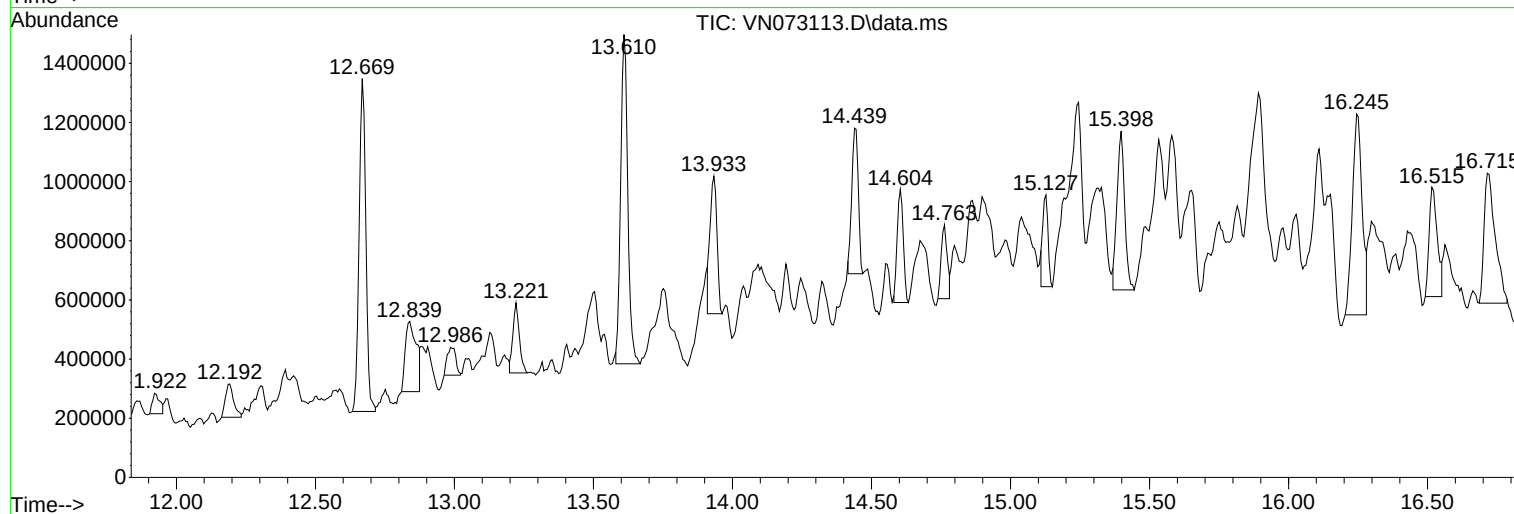
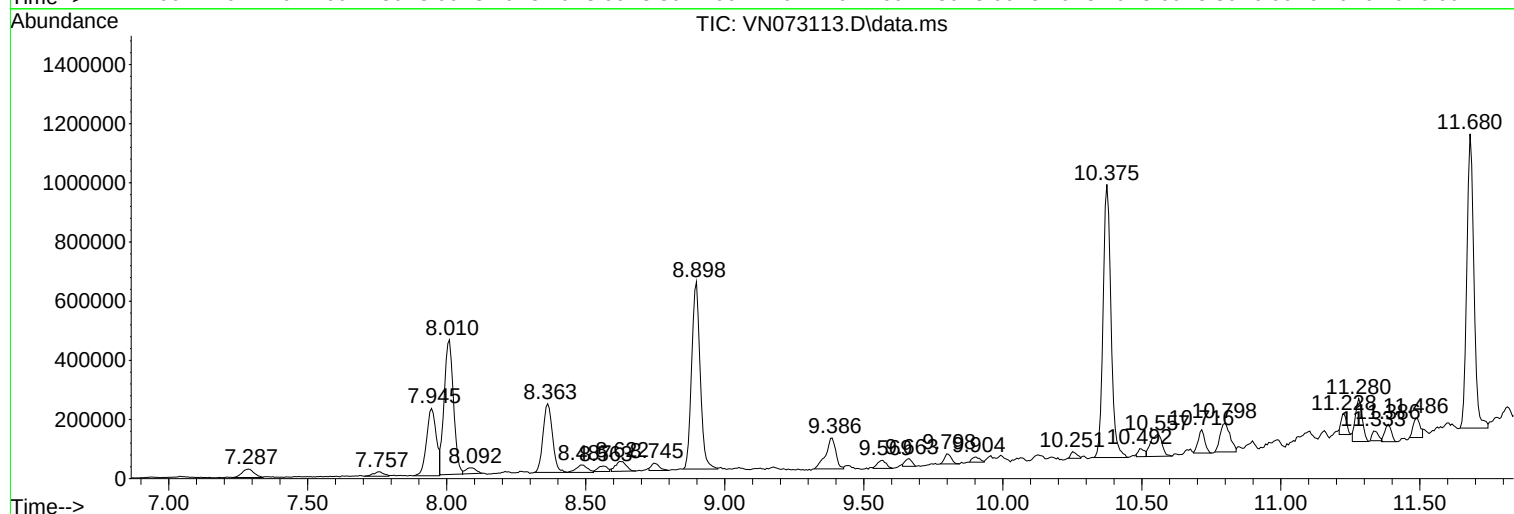
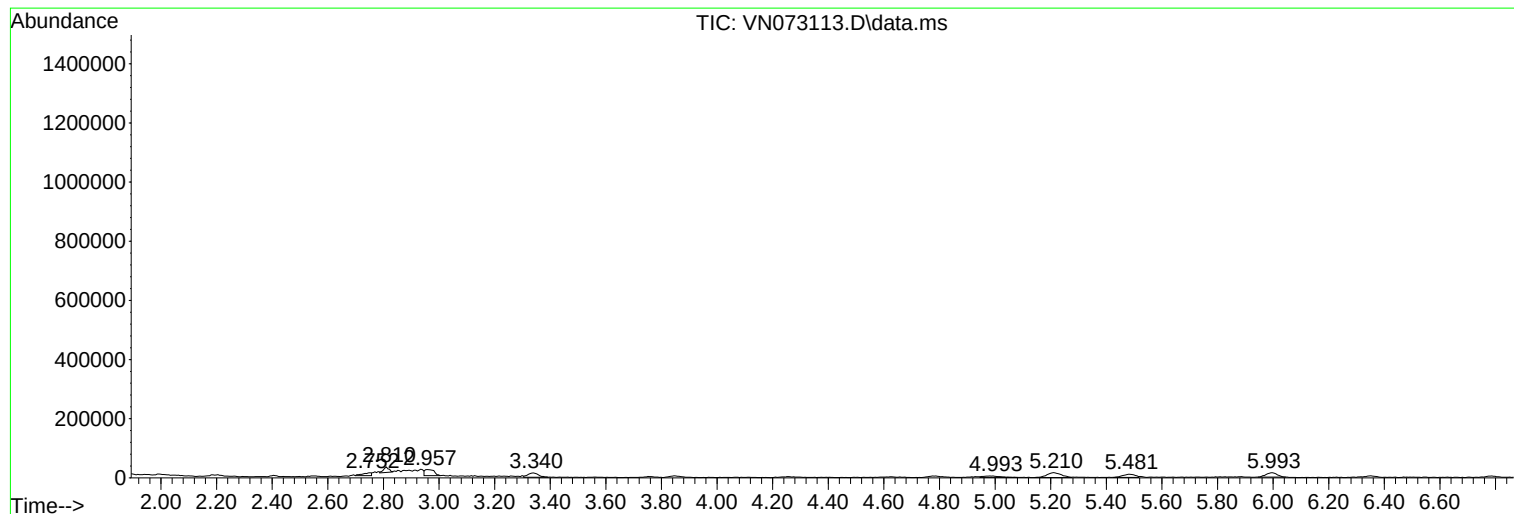
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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



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ClientSampleId :
WC-16-1A-5-GR

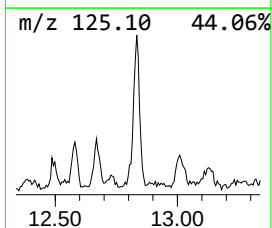
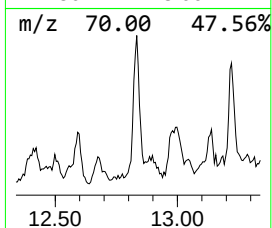
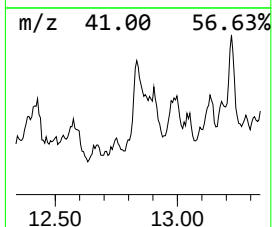
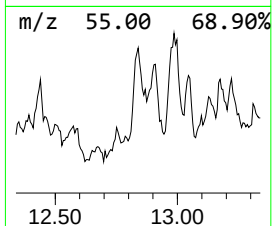
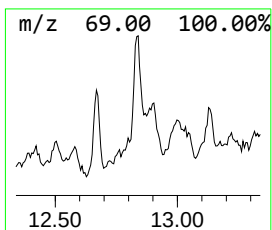
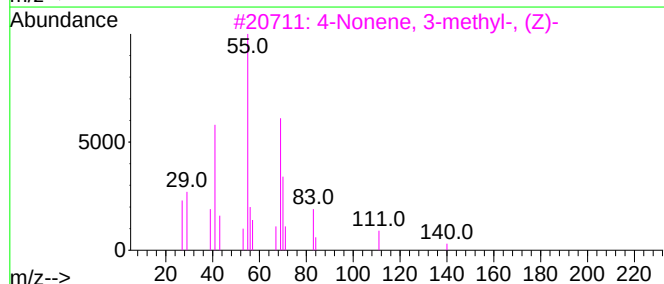
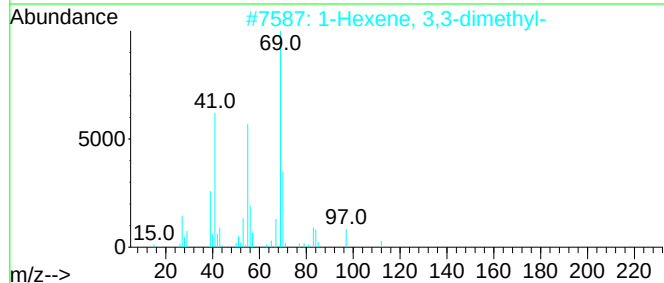
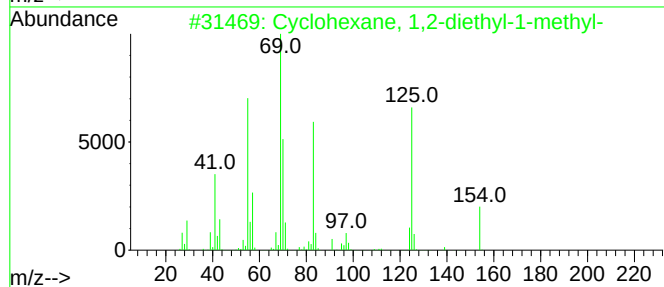
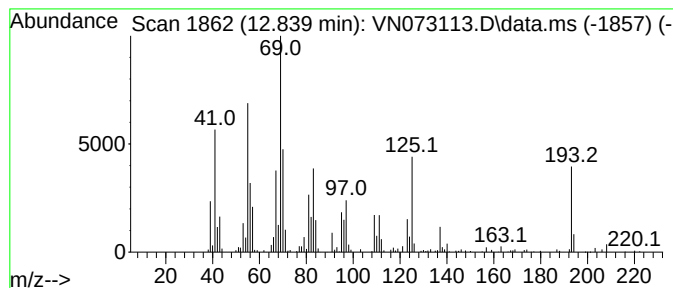
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown12.839 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.839	16.84 ug/l	666406	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2-diethyl-1-methyl-	154	C11H22	061141-79-5	47
2			1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	38
3			4-Nonene, 3-methyl-, (Z)-	140	C10H20	063830-69-3	38
4			2-Heptene, 4-methyl-, (E)-	112	C8H16	066225-17-0	27
5			8-Oxabicyclo[5.1.0]octane	112	C7H12O	000286-45-3	25



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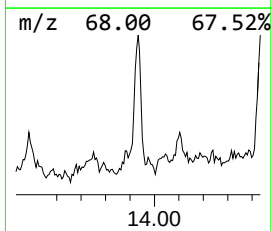
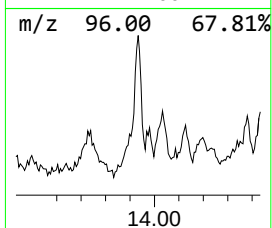
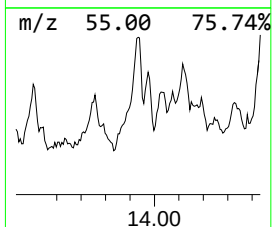
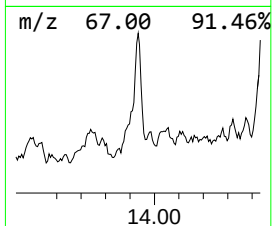
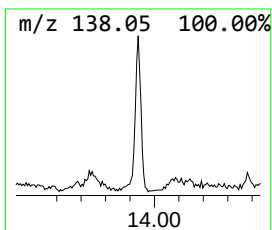
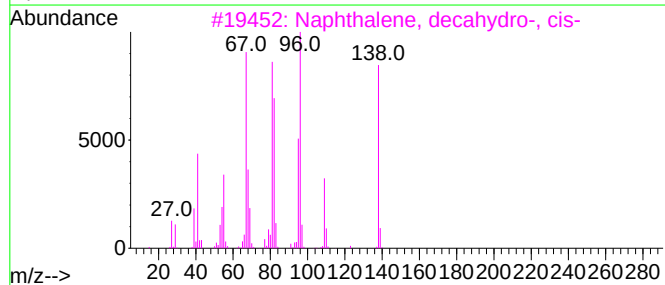
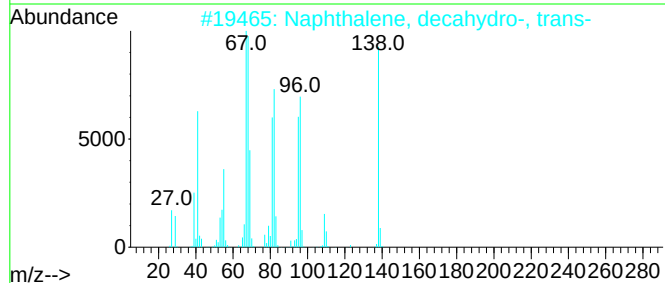
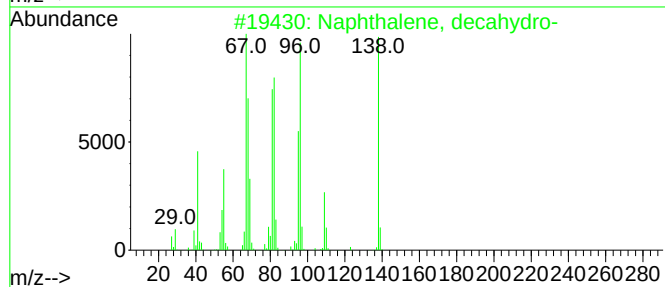
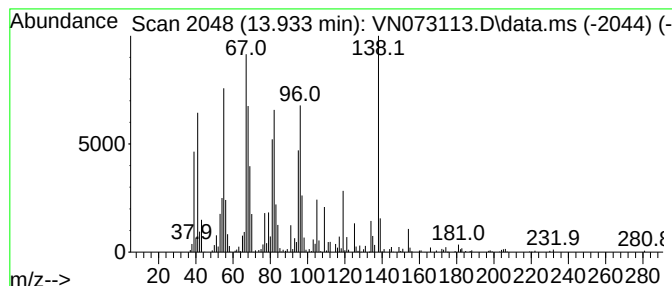
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 2 Naphthalene, decahydro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	20.07 ug/l	794005	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-	138	C10H18	000091-17-8	96
2			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	91
3			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	74
4			1,1'-Bicyclopentyl	138	C10H18	001636-39-1	64
5			Spiro[4.5]decane	138	C10H18	000176-63-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
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Misc : 5.12g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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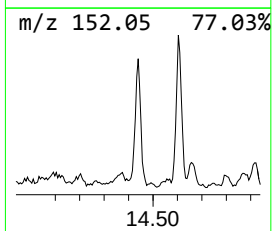
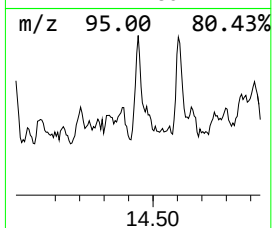
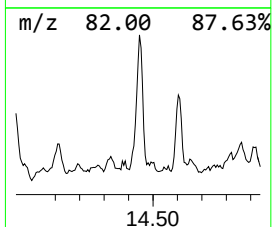
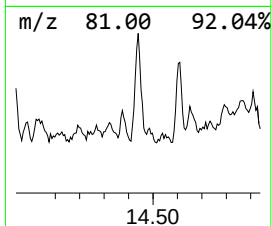
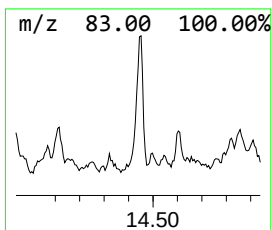
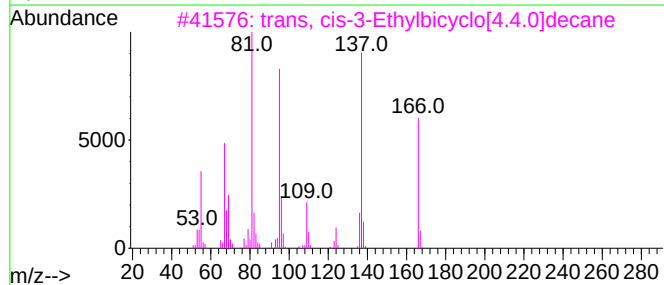
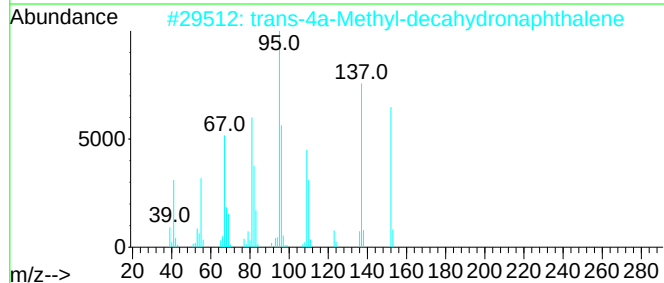
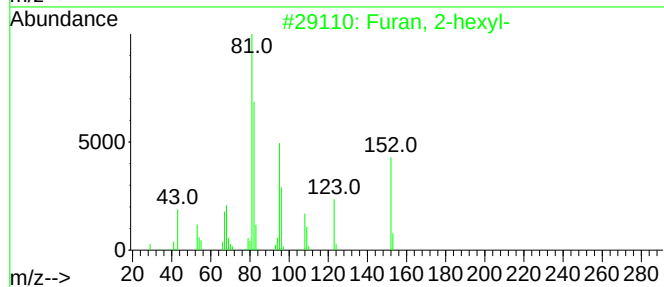
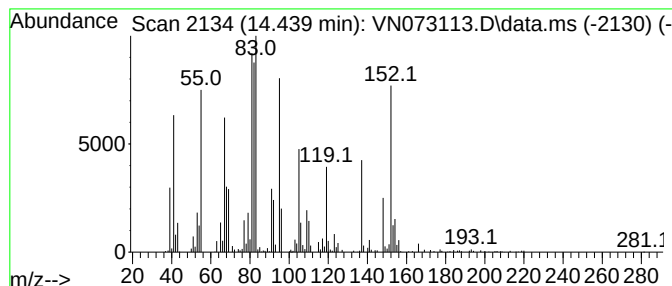
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Quant Title : SW846 8260

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

Peak Number 3 unknown14.439 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.439	20.41 ug/l	807448	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2-hexyl-	152	C10H16O	003777-70-6	43
2			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	38
3			trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	38
4			Dodeca-1,6-dien-12-ol, 6,10-dime...	210	C14H26O	1000156-13-8	38
5			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	35



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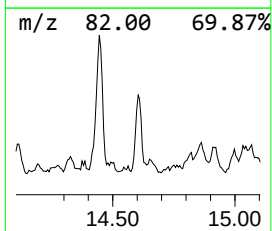
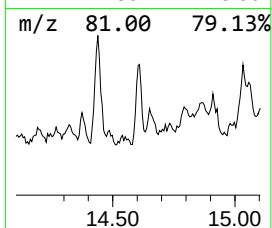
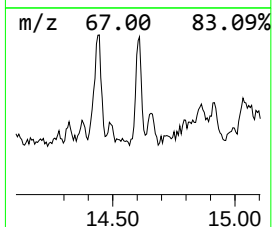
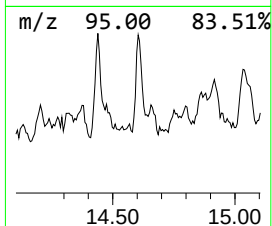
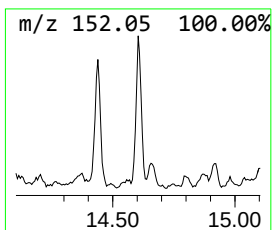
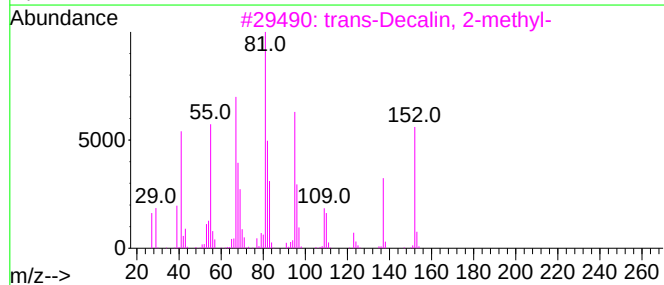
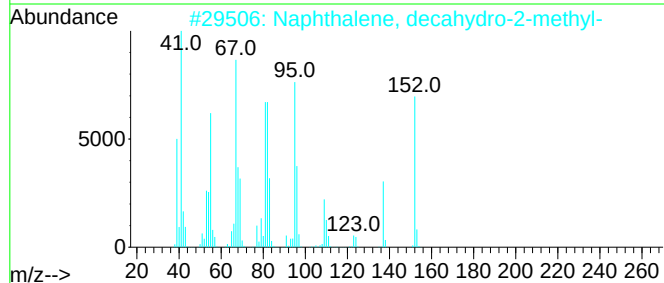
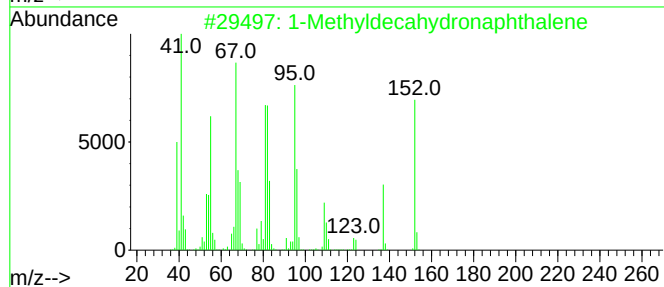
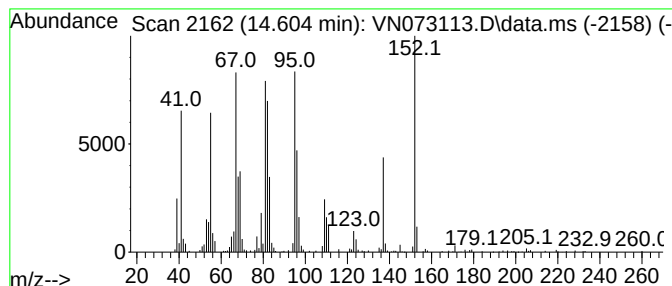
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 4 1-Methyldecahydronaphthalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.604	14.74 ug/l	583026	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	95
2			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	95
3			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	94
4			cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	87
5			Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	005948-04-9	58



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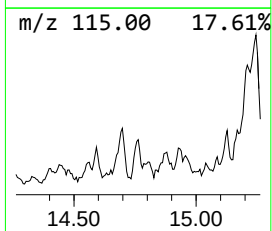
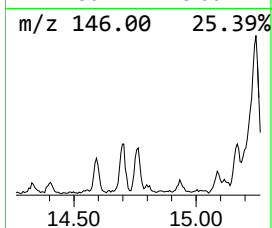
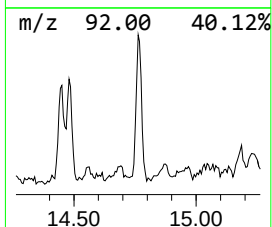
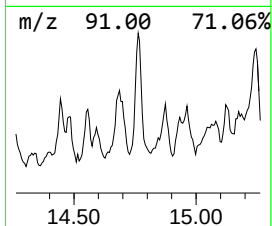
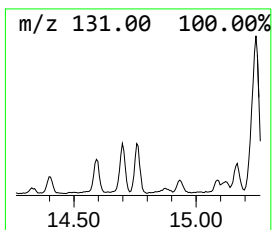
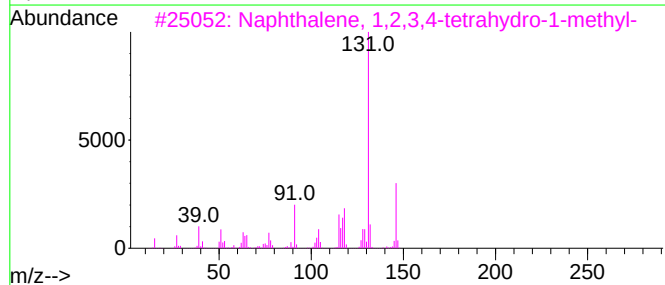
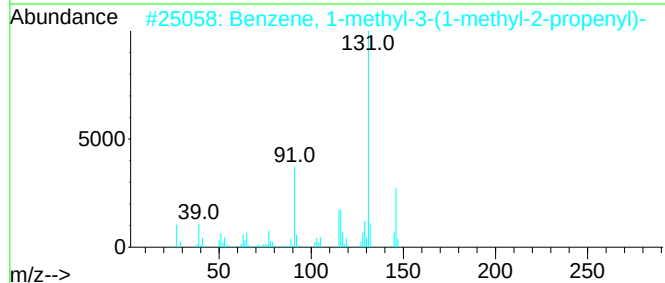
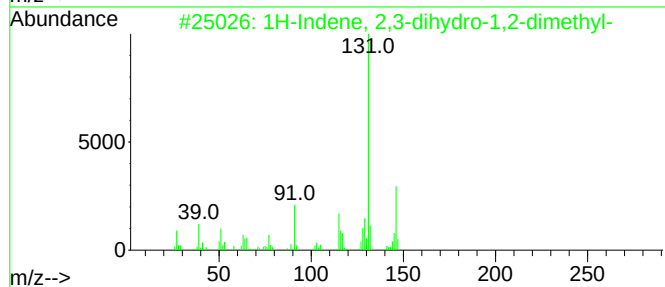
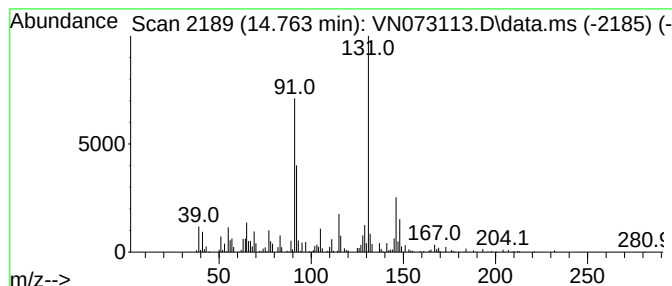
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Quant Title : SW846 8260

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

Peak Number 5 1H-Indene, 2,3-dihydro-1,2-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.763	9.56 ug/l	378127	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	83
2			Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	64
3			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	64
4			Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	64
5			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073113.D
Acq On : 25 Jun 2022 16:18
Operator : JC\MD
Sample : N3454-03
Misc : 5.12g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-1A-5-GR

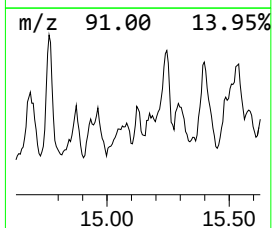
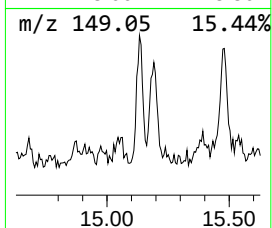
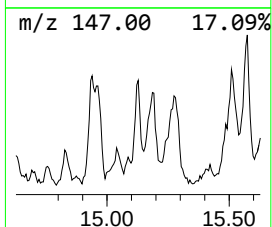
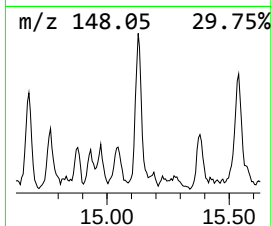
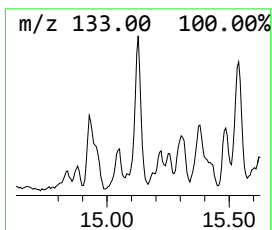
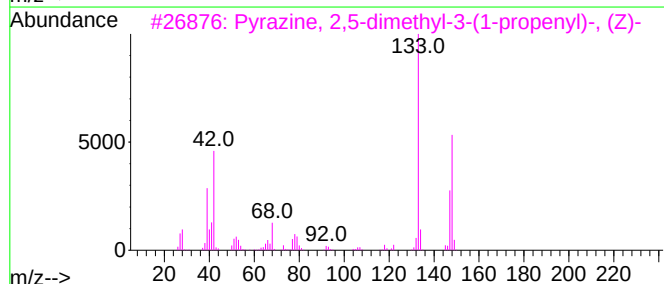
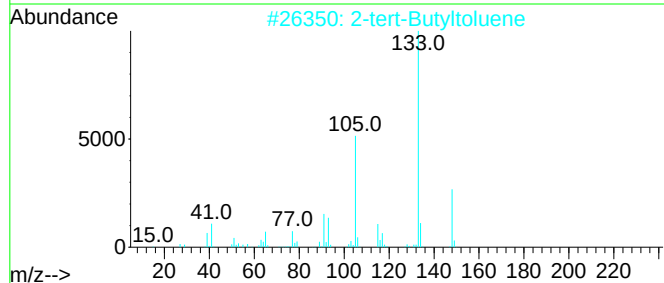
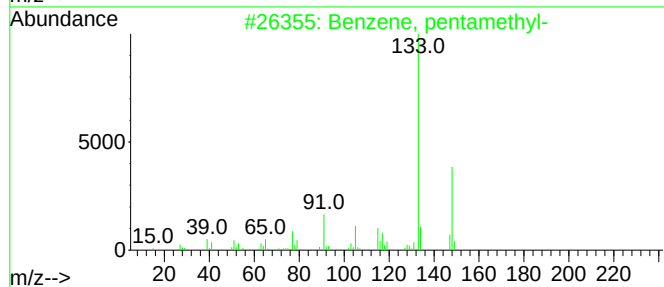
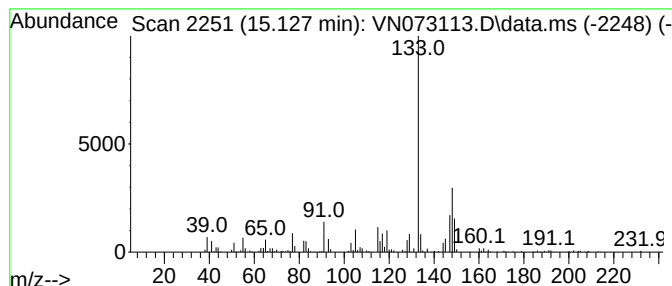
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, pentamethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	10.15 ug/l	401484	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			2-tert-Butyltoluene	148	C11H16	001074-92-6	62
3			Pyrazine, 2,5-dimethyl-3-(1-prop...	148	C9H12N2	055138-73-3	59
4			3,4-Dimethylcumene	148	C11H16	1000370-34-1	58
5			Benzene, 1,3-dimethyl-5-(1-methy...	148	C11H16	004706-90-5	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073113.D
Acq On : 25 Jun 2022 16:18
Operator : JC\MD
Sample : N3454-03
Misc : 5.12g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-1A-5-GR

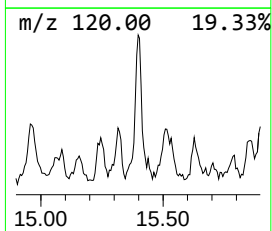
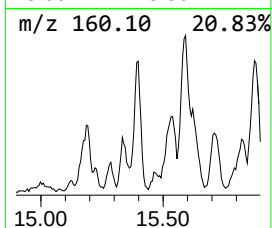
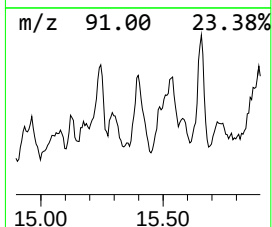
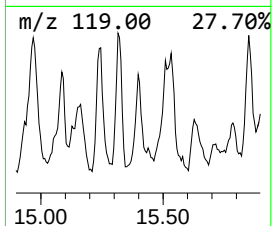
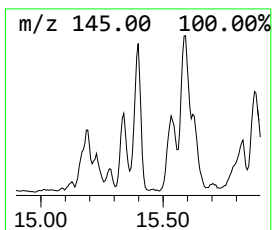
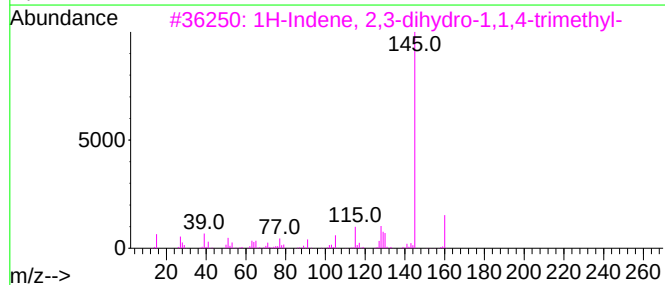
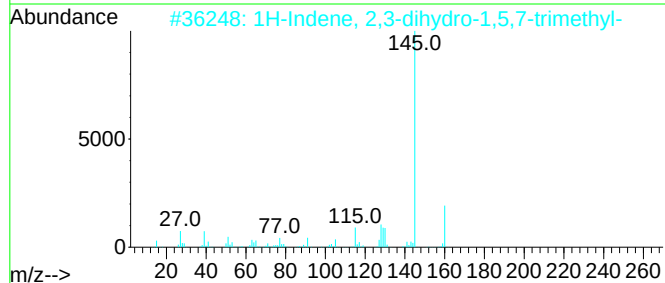
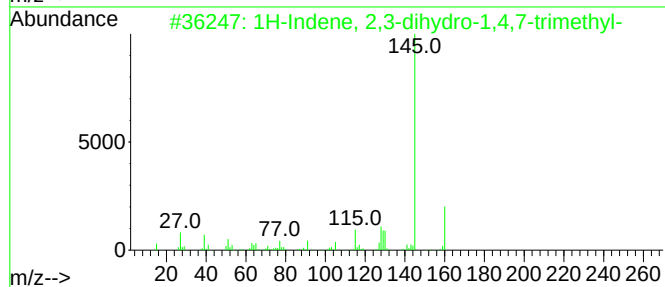
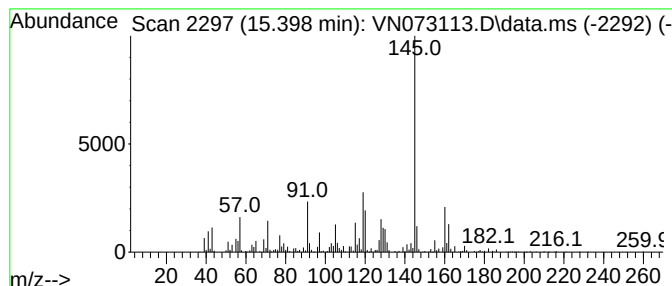
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Quant Title : SW846 8260

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

Peak Number 7 1H-Indene, 2,3-dihydro-1,4,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	25.73 ug/l	1017870	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,4,7-tri...	160	C12H16	054340-87-3	93		
2	1H-Indene, 2,3-dihydro-1,5,7-tri...	160	C12H16	054340-88-4	92		
3	1H-Indene, 2,3-dihydro-1,1,4-tri...	160	C12H16	016204-72-1	83		
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	70		
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	025419-33-4	70		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073113.D
Acq On : 25 Jun 2022 16:18
Operator : JC\MD
Sample : N3454-03
Misc : 5.12g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-1A-5-GR

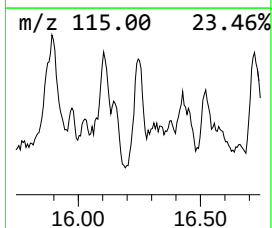
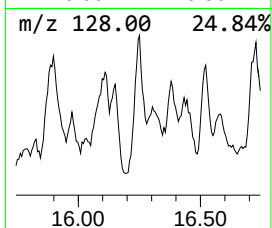
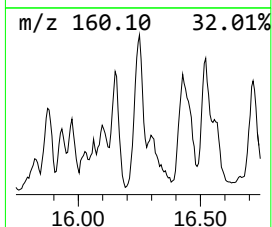
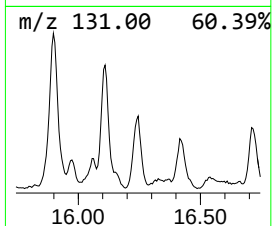
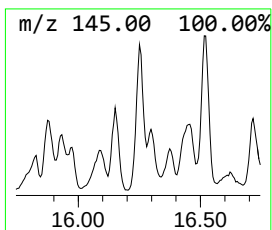
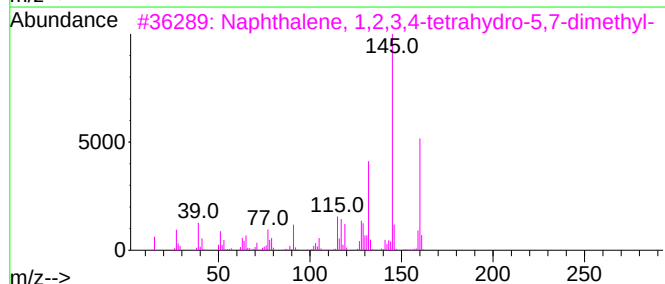
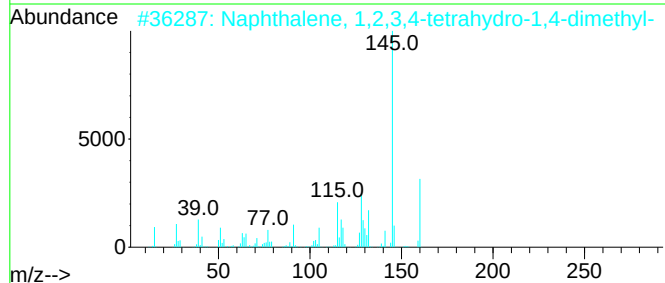
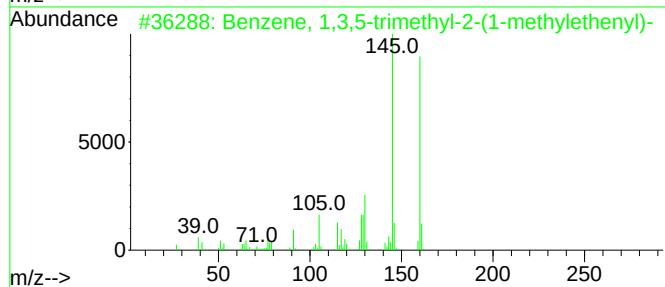
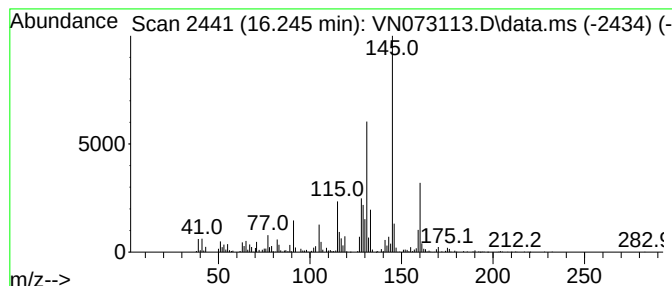
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,3,5-trimethyl-2-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.245	42.63 ug/l	1686840	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	83
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	64
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	60
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	001076-61-5	55
5			Benzene, 1-(1-methylethenyl)-2-(...	160	C12H16	005557-93-7	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073113.D
Acq On : 25 Jun 2022 16:18
Operator : JC\MD
Sample : N3454-03
Misc : 5.12g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-1A-5-GR

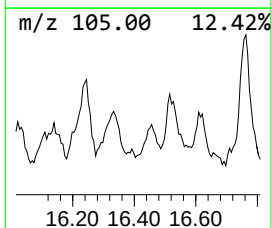
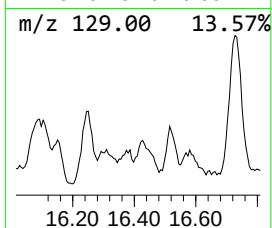
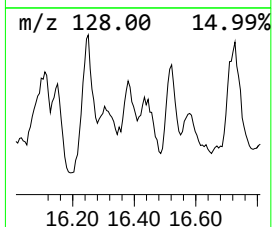
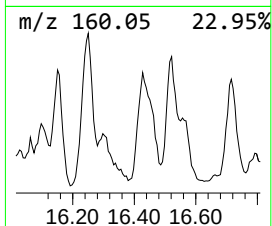
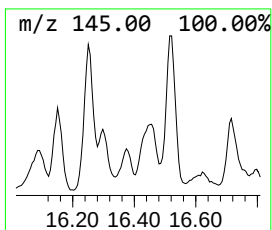
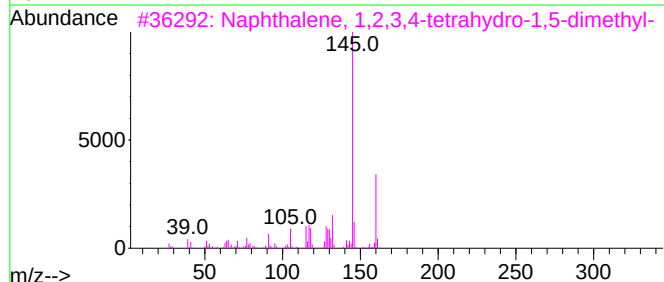
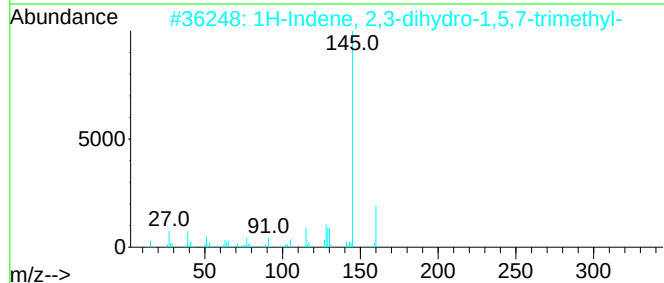
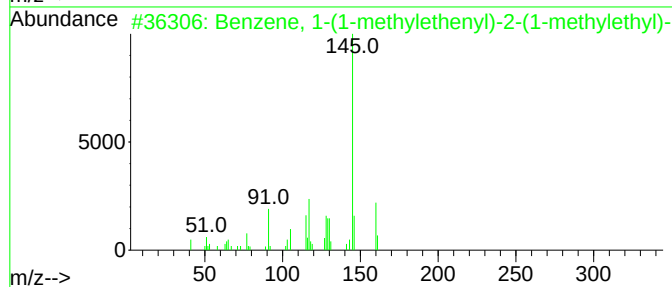
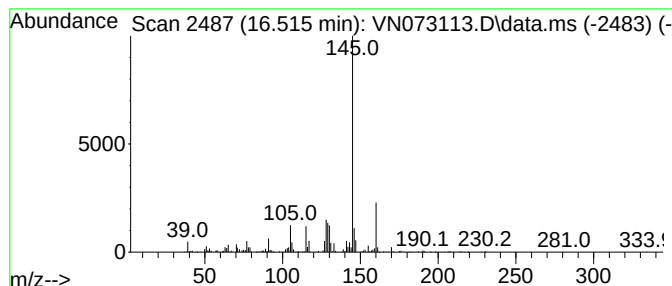
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Quant Title : SW846 8260

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

Peak Number 9 1H-Indene, 2,3-dihydro-1,5,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.515	19.26 ug/l	762141	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-(1-methylethenyl)-2-(...	160	C12H16	005557-93-7	93
2			1H-Indene, 2,3-dihydro-1,5,7-tri...	160	C12H16	054340-88-4	91
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	91
4			Benzene, (2,2-dimethyl-1-methyle...	160	C12H16	005676-29-9	90
5			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073113.D
Acq On : 25 Jun 2022 16:18
Operator : JC\MD
Sample : N3454-03
Misc : 5.12g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-1A-5-GR

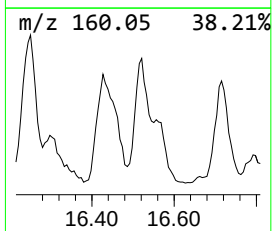
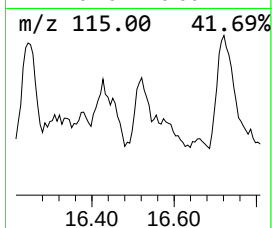
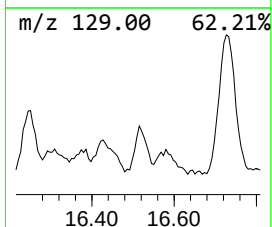
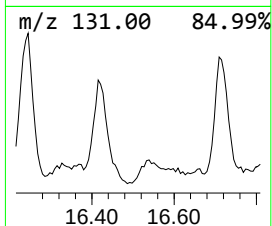
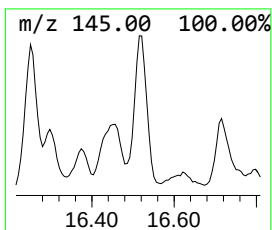
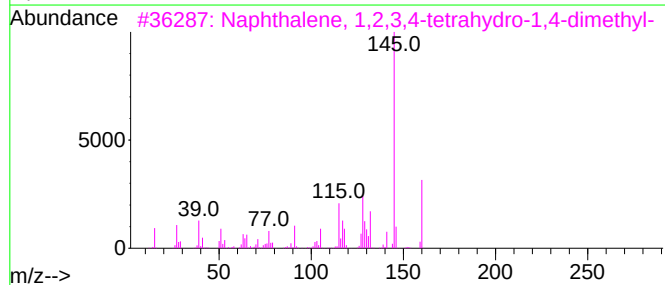
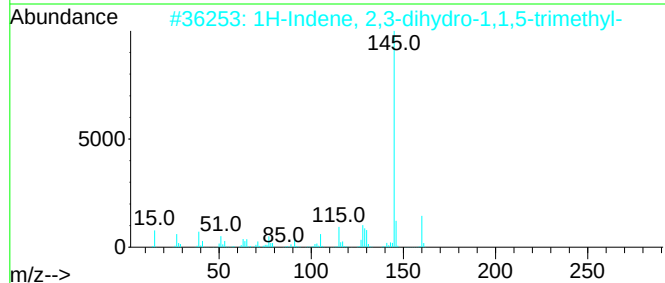
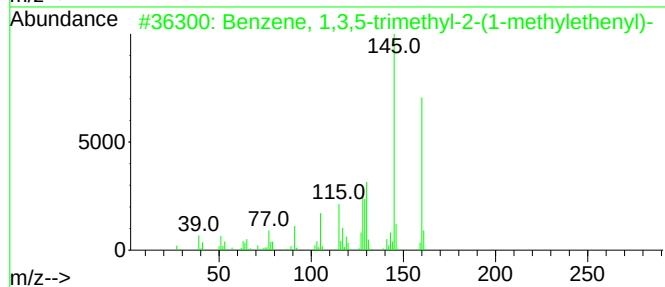
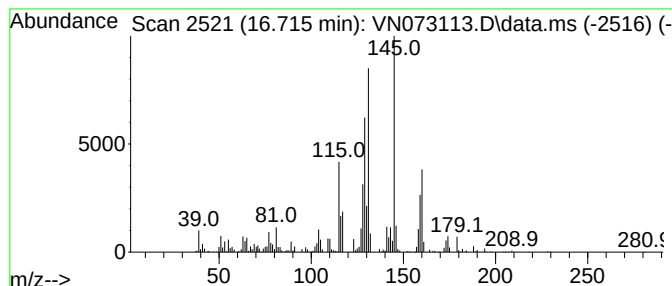
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Quant Title : SW846 8260

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

Peak Number 10 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.715	30.85 ug/l	1220720	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	60
2			1H-Indene, 2,3-dihydro-1,1,5-tri...	160	C12H16	040650-41-7	55
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	43
4			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	43
5			Ethanone, 1-(2,3-dihydro-1H-inde...	160	C11H12O	004228-10-8	41



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073113.D
Acq On : 25 Jun 2022 16:18
Operator : JC\MD
Sample : N3454-03
Misc : 5.12g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-1A-5-GR

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Naphthalene, de...	13.933	20.1	ug/l	794005	4	13.610	1978270	50.0
unknown14.439	14.439	20.4	ug/l	807448	4	13.610	1978270	50.0
1-Methyldecahyd...	14.604	14.7	ug/l	583026	4	13.610	1978270	50.0
1H-Indene, 2,3-...	14.763	9.6	ug/l	378127	4	13.610	1978270	50.0
Benzene, pentam...	15.127	10.2	ug/l	401484	4	13.610	1978270	50.0
1H-Indene, 2,3-...	15.398	25.7	ug/l	1017870	4	13.610	1978270	50.0
Benzene, 1,3,5-...	16.245	42.6	ug/l	1686840	4	13.610	1978270	50.0
1H-Indene, 2,3-...	16.515	19.3	ug/l	762141	4	13.610	1978270	50.0
1H-Indene, 2,3-...	16.715	30.9	ug/l	1220720	4	13.610	1978270	50.0