

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011321\
 Data File : VX020591.D
 Acq On : 13 Jan 2021 14:02
 Operator : JC/MD
 Sample : M1056-01
 Misc : 5.96g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 CL-01-010821

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_X\METHOD\82X011121W.M
 Title : SW846 8260

Signal : TIC: VX020591.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.624	73	88	89	rBV	9125	31944	3.64%	0.466%
2	5.464	705	718	732	rBV	110397	318618	36.33%	4.650%
3	5.623	732	744	757	rBV	180653	510410	58.19%	7.449%
4	6.025	798	810	825	rBV	111131	293716	33.49%	4.286%
5	6.830	932	942	958	rBV	266076	640459	73.02%	9.346%
6	8.696	1241	1248	1257	rBV	570298	877110	100.00%	12.800%
7	10.098	1471	1478	1492	rBV	543793	767479	87.50%	11.200%
8	11.122	1640	1646	1655	rBV	447157	568932	64.86%	8.303%
9	11.512	1707	1710	1715	rVB3	8942	12249	1.40%	0.179%
10	11.793	1752	1756	1765	rVB	9062	13415	1.53%	0.196%
11	12.061	1795	1800	1806	rBV	584920	732477	83.51%	10.689%
12	12.134	1806	1812	1816	rVB4	6328	11872	1.35%	0.173%
13	12.207	1821	1824	1831	rVB4	6015	9103	1.04%	0.133%
14	12.353	1844	1848	1855	rVB3	16832	31358	3.58%	0.458%
15	12.457	1855	1865	1869	rBV	36898	53314	6.08%	0.778%
16	12.506	1869	1873	1879	rVB2	11133	18140	2.07%	0.265%
17	12.573	1879	1884	1885	rBV	8199	10442	1.19%	0.152%
18	12.738	1905	1911	1913	rBV4	8061	15171	1.73%	0.221%
19	12.762	1913	1915	1919	rVB3	9581	12986	1.48%	0.190%
20	12.859	1924	1931	1938	rBV7	19013	32444	3.70%	0.473%
21	12.927	1938	1942	1944	rBV3	14814	18838	2.15%	0.275%
22	13.006	1951	1955	1957	rBV	12377	19203	2.19%	0.280%
23	13.079	1961	1967	1970	rBV4	18245	30784	3.51%	0.449%
24	13.201	1981	1987	1992	rBV3	24668	47636	5.43%	0.695%
25	13.250	1992	1995	1998	rVV2	17118	19952	2.27%	0.291%
26	13.305	1998	2004	2005	rVV3	36365	52194	5.95%	0.762%
27	13.335	2005	2009	2013	rVV2	73132	108169	12.33%	1.579%
28	13.372	2013	2015	2019	rVB3	8086	9535	1.09%	0.139%
29	13.463	2025	2030	2038	rVB3	54633	104005	11.86%	1.518%
30	13.542	2038	2043	2046	rBV3	19367	30350	3.46%	0.443%
31	13.579	2046	2049	2052	rBV	15615	20414	2.33%	0.298%
32	13.628	2052	2057	2060	rVV3	25765	41866	4.77%	0.611%
33	13.664	2060	2063	2067	rVV6	6572	11910	1.36%	0.174%
34	13.707	2067	2070	2074	rVV2	17461	27304	3.11%	0.398%
35	13.835	2088	2091	2094	rBV2	12488	15179	1.73%	0.222%
36	13.890	2094	2100	2106	rVB3	40365	74683	8.51%	1.090%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011321\
 Data File : VX020591.D
 Acq On : 13 Jan 2021 14:02
 Operator : JC/MD
 Sample : M1056-01
 Misc : 5.96g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 CL-01-010821

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_X\METHOD\82X011121W.M
 Title : SW846 8260

37	13.963	2106	2112	2118	rBV4	41507	95991	10.94%	1.401%
38	14.012	2118	2120	2122	rVV	10854	10750	1.23%	0.157%
39	14.042	2122	2125	2127	rVV	14220	16304	1.86%	0.238%
40	14.073	2127	2130	2133	rVB3	24021	30086	3.43%	0.439%
41	14.115	2133	2137	2140	rBV2	35063	45338	5.17%	0.662%
42	14.146	2140	2142	2145	rVB2	10952	11605	1.32%	0.169%
43	14.201	2148	2151	2155	rVB	13337	14006	1.60%	0.204%
44	14.268	2155	2162	2168	rBV2	103780	185497	21.15%	2.707%
45	14.359	2174	2177	2182	rBV3	18972	26775	3.05%	0.391%
46	14.414	2182	2186	2190	rVV	34547	40222	4.59%	0.587%
47	14.457	2190	2193	2199	rVB5	13107	25857	2.95%	0.377%
48	14.524	2199	2204	2212	rBV3	63546	108776	12.40%	1.587%
49	14.597	2212	2216	2217	rBV4	13576	18367	2.09%	0.268%
50	14.652	2222	2225	2232	rVV2	75903	133166	15.18%	1.943%
51	14.713	2232	2235	2239	rVB3	43271	57507	6.56%	0.839%
52	14.768	2240	2244	2246	rBV3	20728	27324	3.12%	0.399%
53	14.792	2246	2248	2251	rVV2	12482	12402	1.41%	0.181%
54	14.829	2251	2254	2256	rVV3	16581	22542	2.57%	0.329%
55	14.859	2256	2259	2261	rVV2	19461	25490	2.91%	0.372%
56	14.890	2261	2264	2270	rVV2	27190	37555	4.28%	0.548%
57	14.944	2270	2273	2284	rVB3	21409	44947	5.12%	0.656%
58	15.091	2291	2297	2301	rBV4	15152	28270	3.22%	0.413%
59	15.225	2313	2319	2327	rBV	46365	93781	10.69%	1.369%
60	15.292	2327	2330	2332	rVV3	8631	12632	1.44%	0.184%
61	15.329	2333	2336	2338	rVV3	11803	13815	1.58%	0.202%
62	15.359	2338	2341	2346	rVB6	7899	14584	1.66%	0.213%
63	15.420	2347	2351	2359	rBV4	17543	32534	3.71%	0.475%
64	15.530	2365	2369	2373	rBV3	18313	24944	2.84%	0.364%
65	15.658	2386	2390	2394	rBV2	17289	26467	3.02%	0.386%
66	15.902	2426	2430	2433	rBV5	5951	9735	1.11%	0.142%
67	16.005	2443	2447	2451	rBV7	5973	11477	1.31%	0.167%

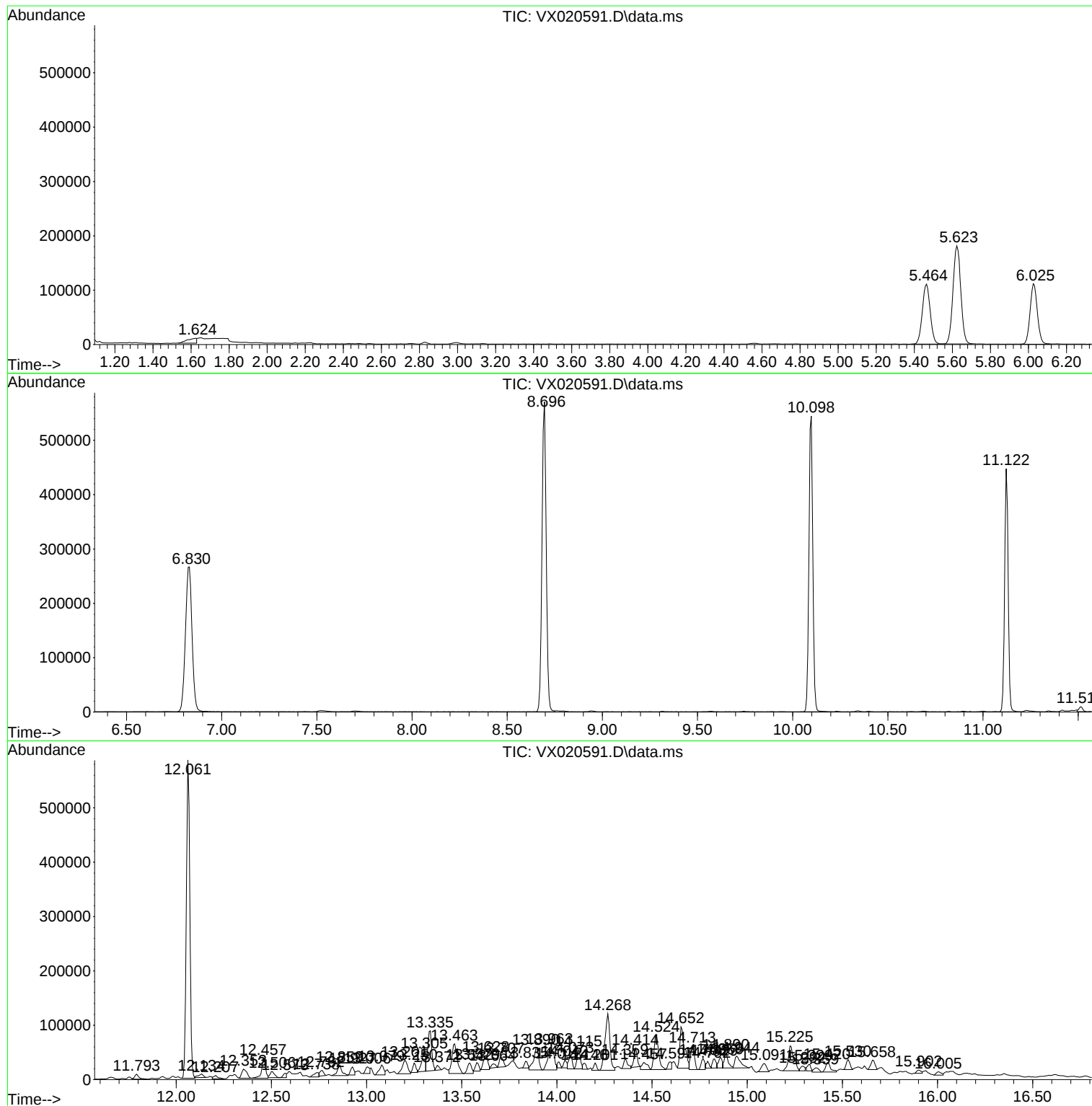
Sum of corrected areas: 6852407

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011321\
Data File : VX020591.D
Acq On : 13 Jan 2021 14:02
Operator : JC/MD
Sample : M1056-01
Misc : 5.96g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CL-01-010821

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011321\
Data File : VX020591.D
Acq On : 13 Jan 2021 14:02
Operator : JC/MD
Sample : M1056-01
Misc : 5.96g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CL-01-010821

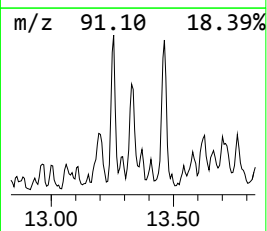
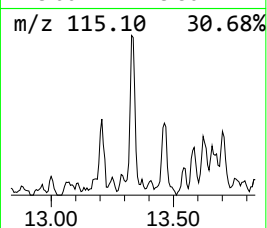
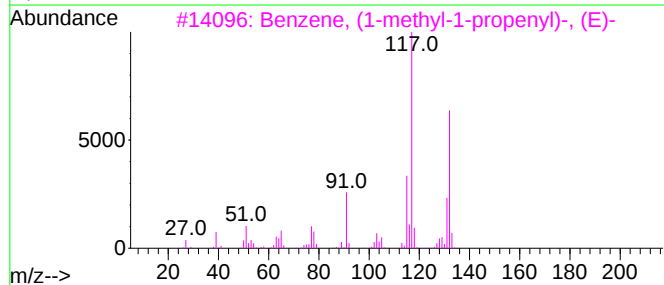
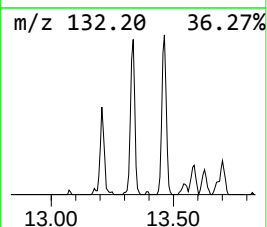
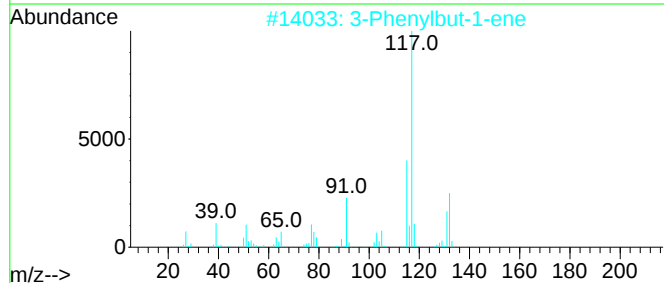
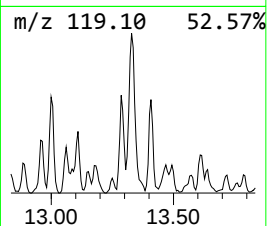
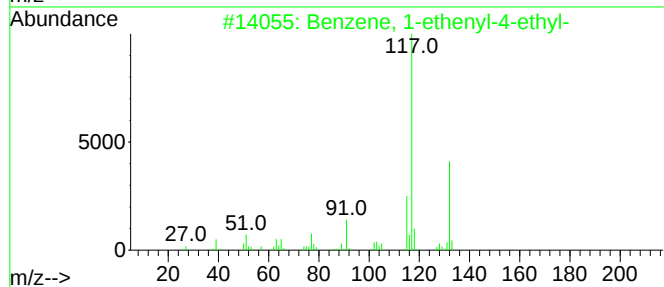
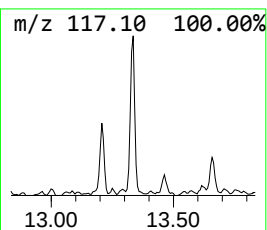
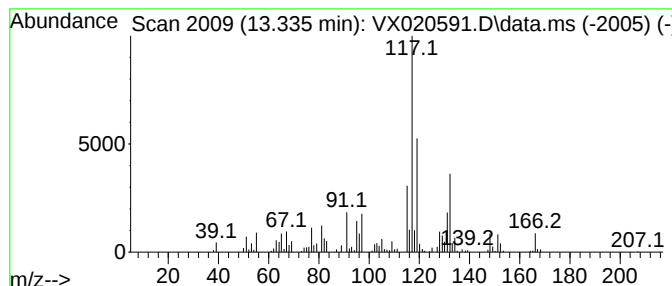
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	7.38 ug/l	108169	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	92
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	64
3			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	64
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	64
5			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011321\
Data File : VX020591.D
Acq On : 13 Jan 2021 14:02
Operator : JC/MD
Sample : M1056-01
Misc : 5.96g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CL-01-010821

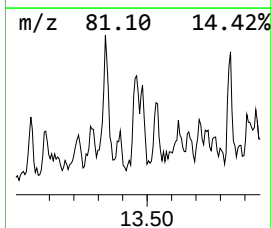
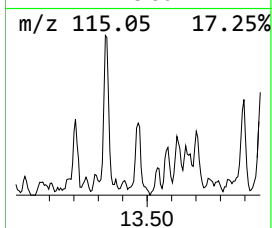
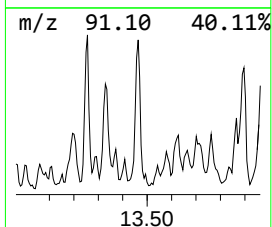
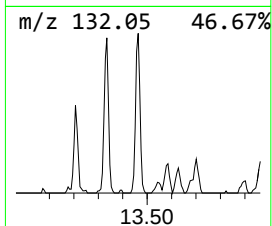
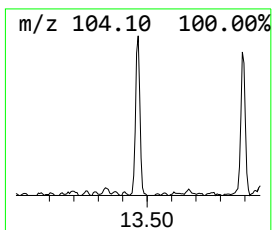
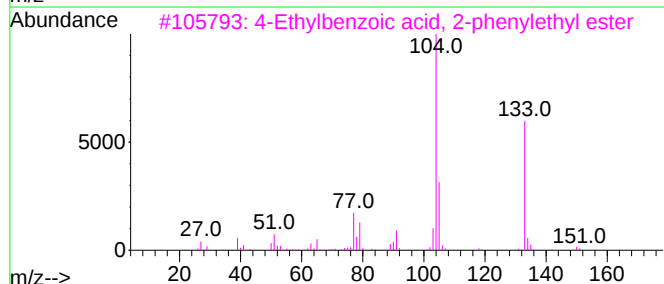
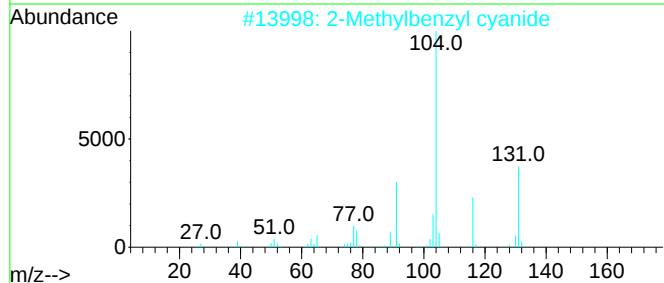
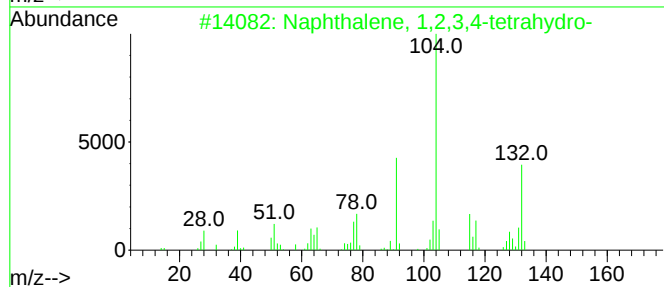
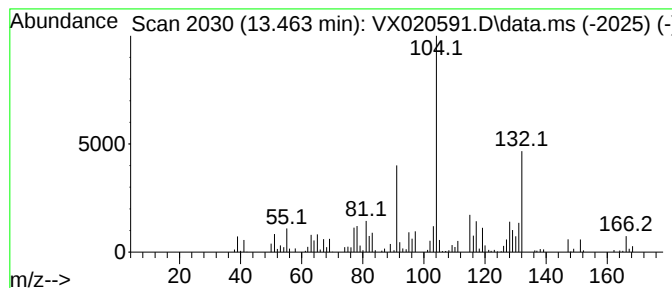
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Naphthalene, 1,2,3,4-tetrahydro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.463	7.10 ug/l	104005	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	89
2			2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	38
3			4-Ethylbenzoic acid, 2-phenyleth...	254	C17H18O2	1000293-50-1	35
4			Benzenemethanol, 2-methyl-, acetate	164	C10H12O2	017373-93-2	35
5			5-Phenylisoxazoline	147	C9H9NO	001006-66-2	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011321\
Data File : VX020591.D
Acq On : 13 Jan 2021 14:02
Operator : JC/MD
Sample : M1056-01
Misc : 5.96g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CL-01-010821

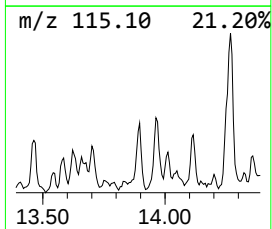
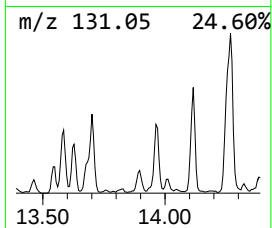
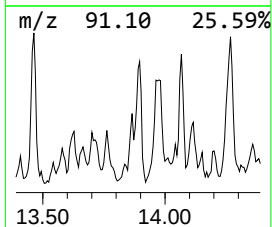
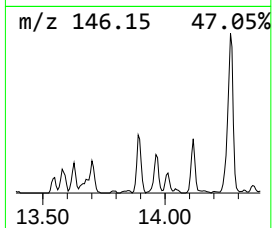
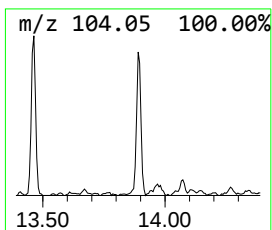
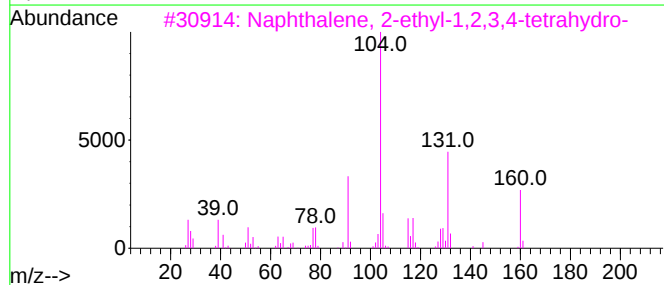
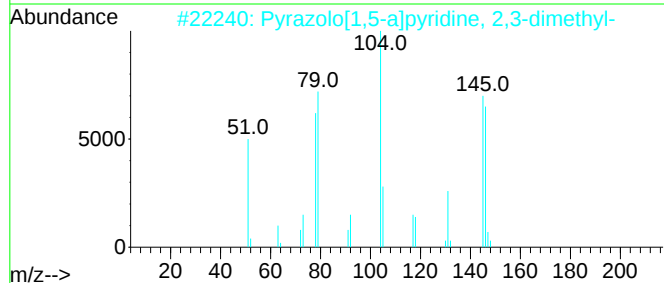
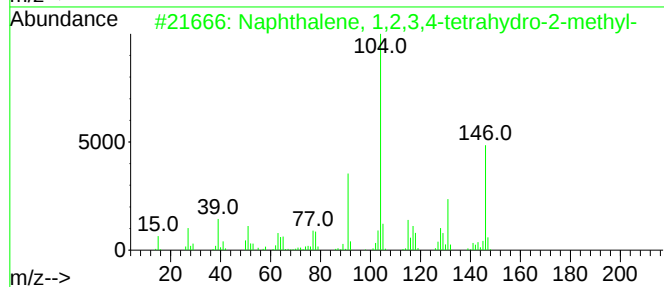
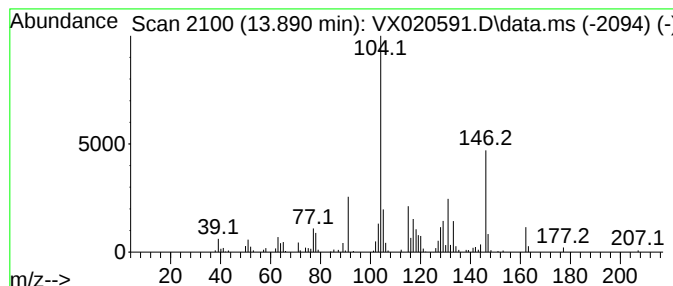
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.890	5.10 ug/l	74683	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	003877-19-8	87
2			Pyrazolo[1,5-a]pyridine, 2,3-dim...	146	C9H10N2	028537-56-6	58
3			Naphthalene, 2-ethyl-1,2,3,4-tet...	160	C12H16	032367-54-7	47
4			Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	47
5			2(1H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000530-93-8	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011321\
Data File : VX020591.D
Acq On : 13 Jan 2021 14:02
Operator : JC/MD
Sample : M1056-01
Misc : 5.96g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CL-01-010821

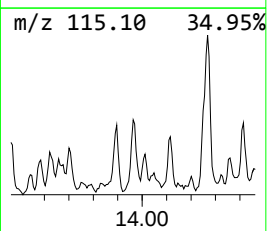
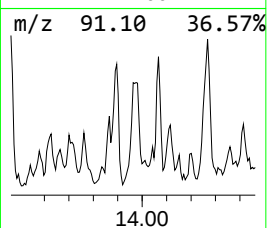
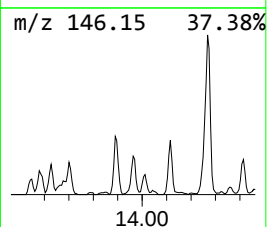
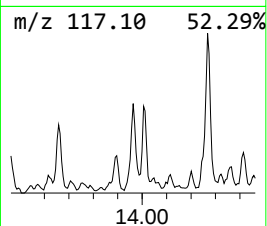
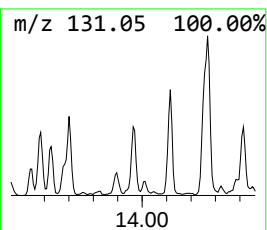
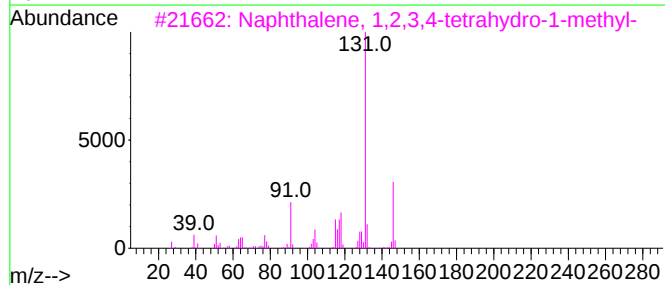
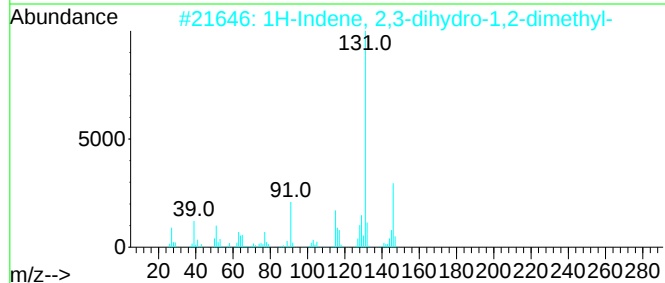
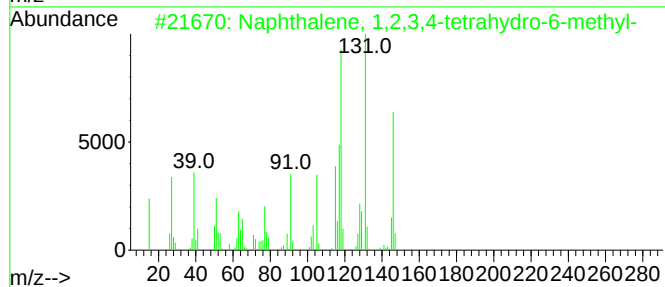
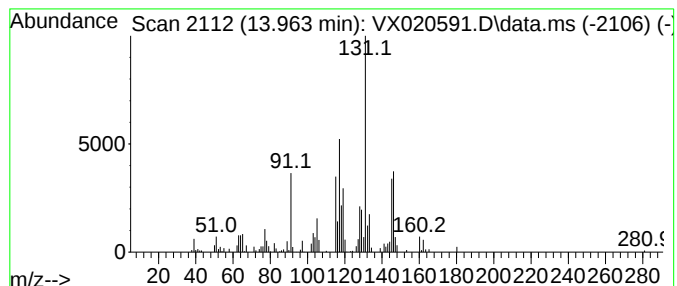
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.963	6.55 ug/l	95991	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	62
2			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	55
3			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	55
4			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	55
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	160	C12H16	078920-29-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011321\
Data File : VX020591.D
Acq On : 13 Jan 2021 14:02
Operator : JC/MD
Sample : M1056-01
Misc : 5.96g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CL-01-010821

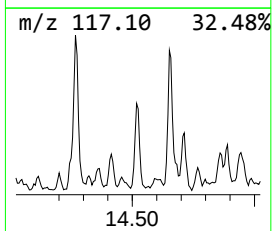
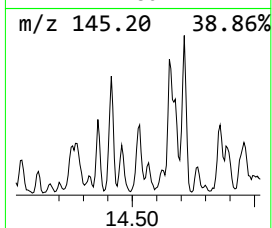
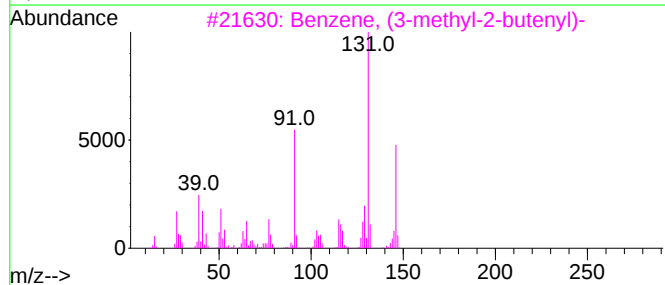
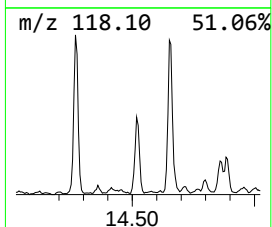
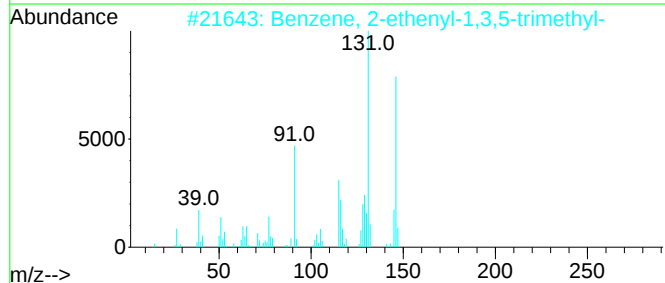
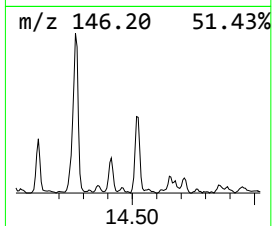
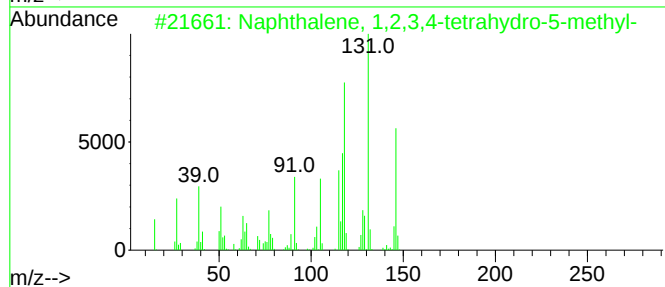
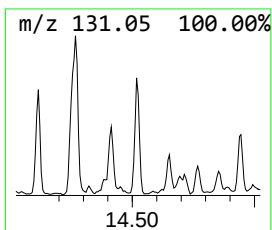
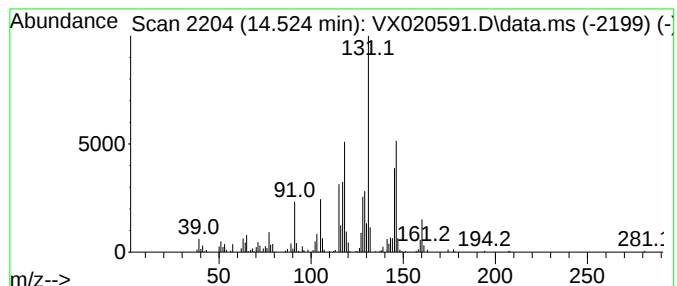
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Naphthalene, 1,2,3,4-tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.524	7.43 ug/l	108776	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	76
2			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	64
3			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	60
4			2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	58
5			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011321\
Data File : VX020591.D
Acq On : 13 Jan 2021 14:02
Operator : JC/MD
Sample : M1056-01
Misc : 5.96g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CL-01-010821

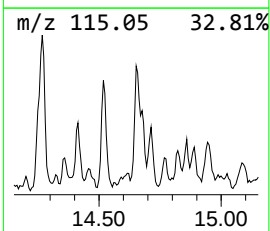
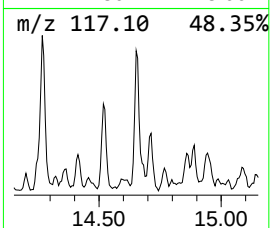
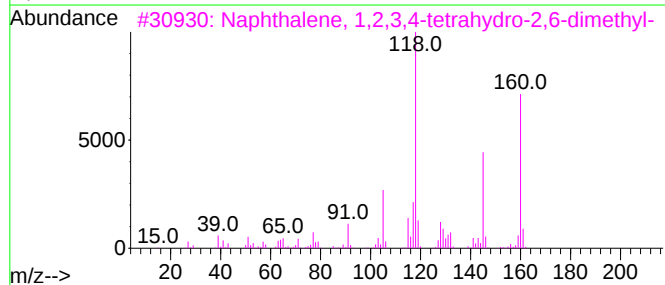
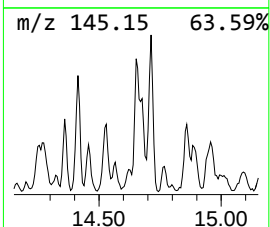
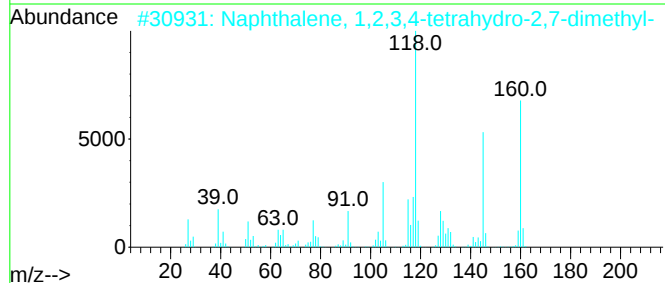
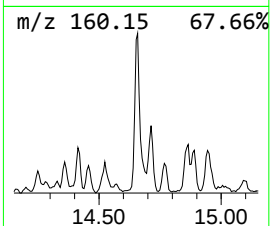
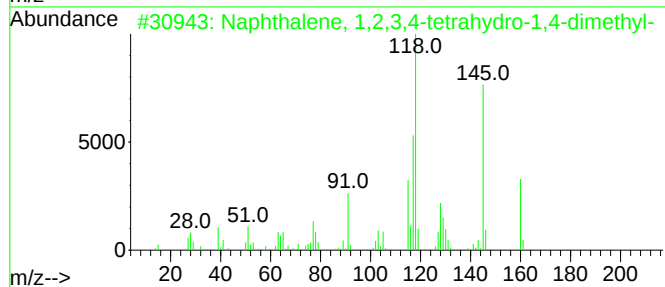
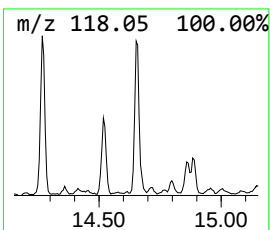
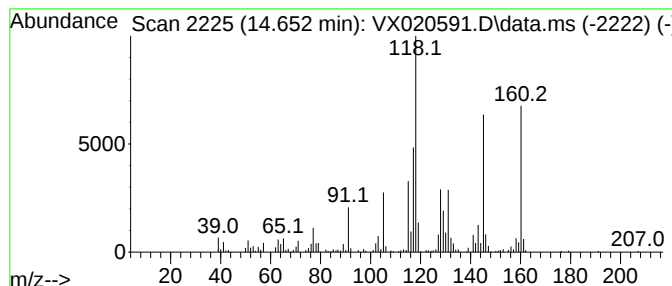
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.652	9.09 ug/l	133166	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	83
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	68
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	62
4			1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	014944-23-1	52
5			1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	001590-08-5	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011321\
Data File : VX020591.D
Acq On : 13 Jan 2021 14:02
Operator : JC/MD
Sample : M1056-01
Misc : 5.96g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CL-01-010821

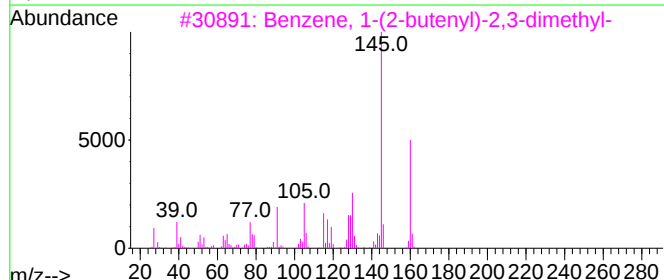
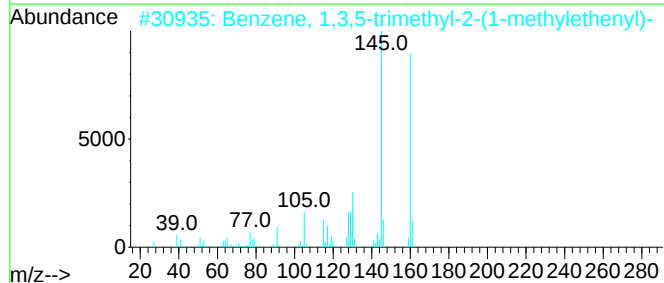
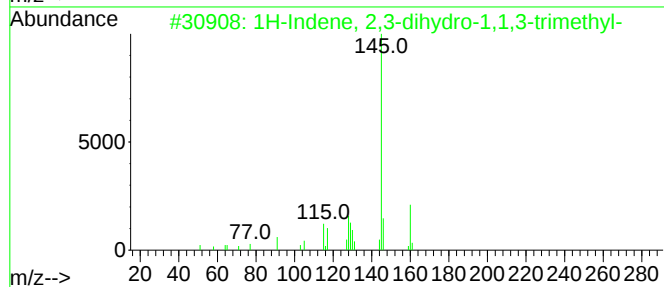
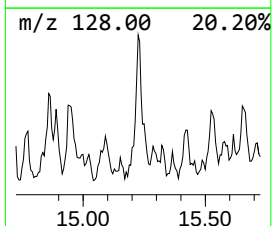
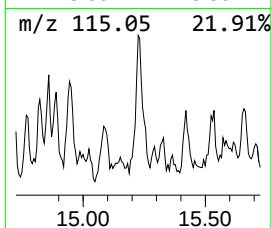
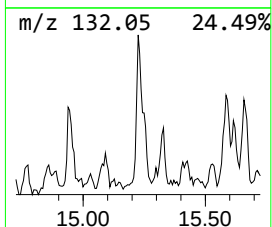
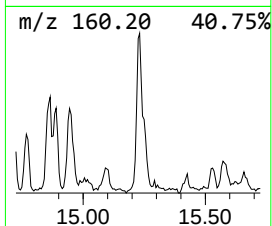
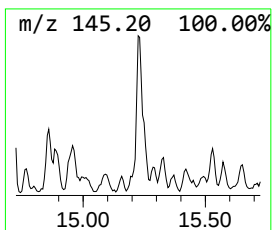
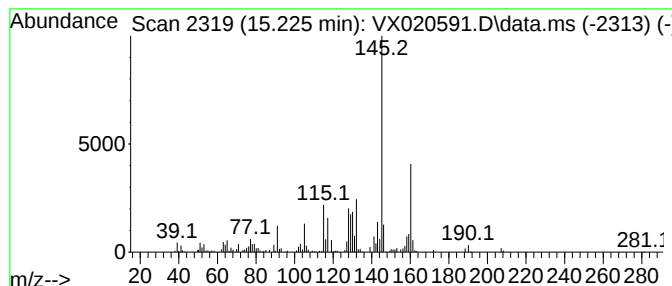
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.225	6.40 ug/l	93781	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	95
2			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	89
3			Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	89
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	020027-77-4	81
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011321\
Data File : VX020591.D
Acq On : 13 Jan 2021 14:02
Operator : JC/MD
Sample : M1056-01
Misc : 5.96g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CL-01-010821

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1-ethe...	13.335	7.4	ug/l	108169	4	12.061	732477	50.0
Naphthalene, 1,...	13.463	7.1	ug/l	104005	4	12.061	732477	50.0
Naphthalene, 1,...	13.890	5.1	ug/l	74683	4	12.061	732477	50.0
Naphthalene, 1,...	13.963	6.5	ug/l	95991	4	12.061	732477	50.0
Naphthalene, 1,...	14.524	7.4	ug/l	108776	4	12.061	732477	50.0
Naphthalene, 1,...	14.652	9.1	ug/l	133166	4	12.061	732477	50.0
1H-Indene, 2,3-...	15.225	6.4	ug/l	93781	4	12.061	732477	50.0