

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050922\
 Data File : VX028569.D
 Acq On : 09 May 2022 14:03
 Operator : JC/MD
 Sample : N2650-03
 Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 ETGI-362

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\82X041922W.M
 Title : SW846 8260

Signal : TIC: VX028569.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.953	298	306	323	rBV	11573	36150	1.59%	0.132%
2	4.593	565	575	582	rBV2	10008	33726	1.49%	0.123%
3	5.391	694	706	721	rBV2	262186	777253	34.28%	2.830%
4	5.550	721	732	749	rVB	465447	1331556	58.73%	4.847%
5	5.958	788	799	816	rBV	259531	726852	32.06%	2.646%
6	6.361	857	865	886	rBV3	9715	33921	1.50%	0.123%
7	6.763	919	931	944	rBV	688474	1674717	73.87%	6.097%
8	8.647	1233	1240	1250	rBV	1415258	2267169	100.00%	8.253%
9	10.055	1465	1471	1483	rBV	1422589	1983254	87.48%	7.220%
10	11.085	1634	1640	1653	rBV	1151025	1531736	67.56%	5.576%
11	12.024	1789	1794	1802	rBV	1611616	1990793	87.81%	7.247%
12	12.262	1826	1833	1838	rBV10	10258	28283	1.25%	0.103%
13	12.311	1838	1841	1851	rVV5	23243	60793	2.68%	0.221%
14	12.561	1876	1882	1886	rBV5	14497	31718	1.40%	0.115%
15	12.658	1895	1898	1903	rBV2	31745	48527	2.14%	0.177%
16	12.731	1905	1910	1913	rVV5	13651	28209	1.24%	0.103%
17	12.817	1919	1924	1931	rBV2	129334	192054	8.47%	0.699%
18	12.927	1936	1942	1946	rVV	94485	142452	6.28%	0.519%
19	13.000	1949	1954	1957	rVV3	41756	83999	3.71%	0.306%
20	13.042	1957	1961	1964	rVB4	35138	48604	2.14%	0.177%
21	13.189	1981	1985	1987	rBV3	20605	26245	1.16%	0.096%
22	13.244	1990	1994	1997	rVV5	25173	51338	2.26%	0.187%
23	13.292	1998	2002	2008	rVB3	104961	159291	7.03%	0.580%
24	13.408	2016	2021	2028	rBV5	193067	445894	19.67%	1.623%
25	13.469	2028	2031	2034	rVV	89703	111251	4.91%	0.405%
26	13.518	2034	2039	2042	rVV2	96523	158004	6.97%	0.575%
27	13.554	2042	2045	2048	rVB	61620	70229	3.10%	0.256%
28	13.591	2048	2051	2054	rBV5	50221	64922	2.86%	0.236%
29	13.676	2061	2065	2072	rBV5	51222	100667	4.44%	0.366%
30	13.768	2077	2080	2083	rVV	156659	178809	7.89%	0.651%
31	13.804	2083	2086	2089	rVB	182026	204326	9.01%	0.744%
32	13.847	2089	2093	2097	rBV2	264192	363348	16.03%	1.323%
33	13.957	2109	2111	2114	rBV	46703	63901	2.82%	0.233%
34	14.018	2118	2121	2125	rVV2	116987	182362	8.04%	0.664%
35	14.067	2125	2129	2133	rVV2	308293	470908	20.77%	1.714%
36	14.176	2140	2147	2150	rBV4	259438	584647	25.79%	2.128%

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37	14.219	2150	2154	2159	rVB4	262243	438938	19.36%	1.598%
38	14.274	2160	2163	2166	rBV3	134024	182858	8.07%	0.666%
39	14.487	2194	2198	2205	rBV7	252169	569065	25.10%	2.072%
40	14.548	2206	2208	2210	rBV2	130773	144586	6.38%	0.526%
41	14.585	2211	2214	2216	rBV2	167133	177810	7.84%	0.647%
42	14.621	2216	2220	2226	rBV2	579124	911075	40.19%	3.317%
43	14.676	2226	2229	2232	rBV3	386478	571260	25.20%	2.080%
44	14.755	2239	2242	2246	rBV5	322686	429230	18.93%	1.563%
45	14.847	2255	2257	2266	rVB5	375305	526050	23.20%	1.915%
46	14.963	2273	2276	2284	rVB5	542298	935683	41.27%	3.406%
47	15.182	2307	2312	2315	rBV4	647366	1146587	50.57%	4.174%
48	15.420	2347	2351	2356	rVB2	900483	1258668	55.52%	4.582%
49	15.493	2359	2363	2368	rBV6	357818	927571	40.91%	3.377%
50	15.743	2400	2404	2410	rVB2	861829	1541282	67.98%	5.611%
51	16.267	2486	2490	2503	rVB5	350173	1009320	44.52%	3.674%
52	16.609	2542	2546	2556	rVB3	163363	411385	18.15%	1.498%

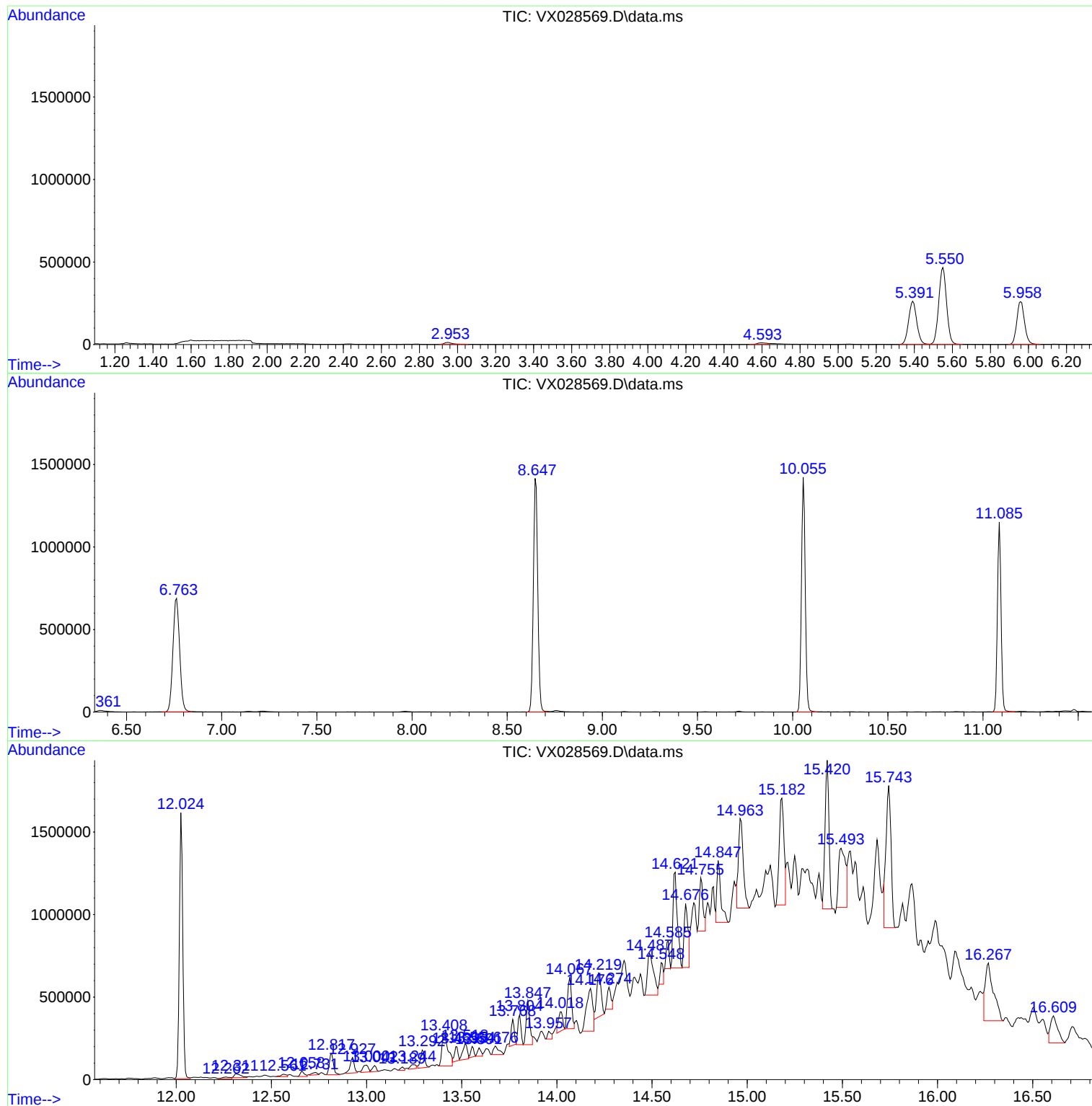
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Instrument :
MSVOA_X
ClientSampleId :
ETGI-362

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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



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ETGI-362

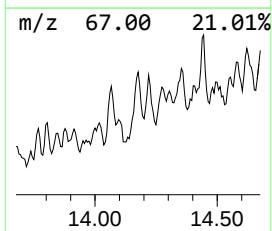
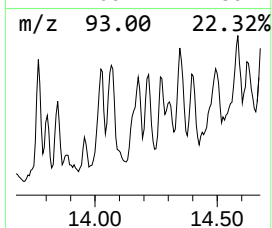
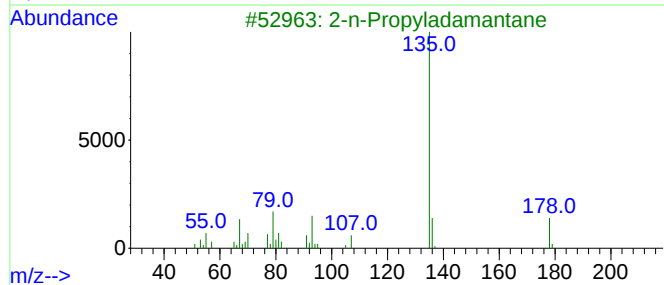
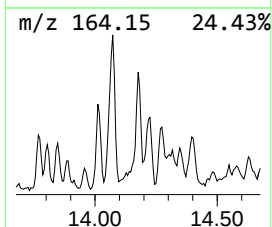
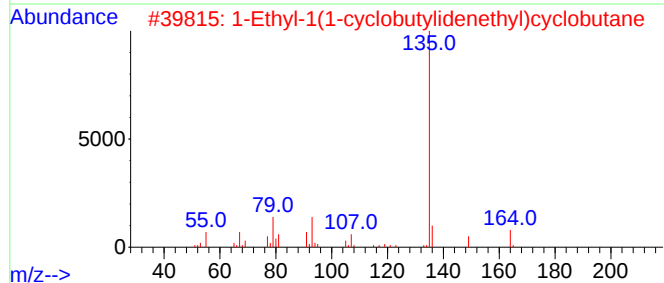
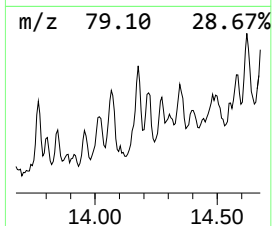
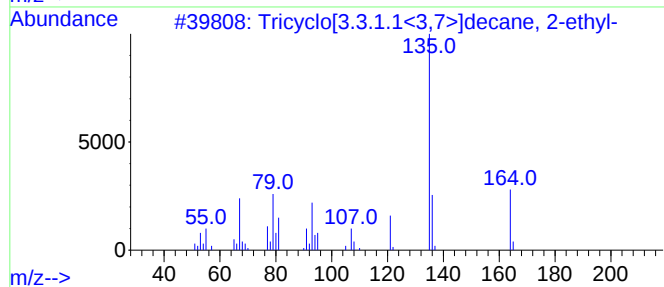
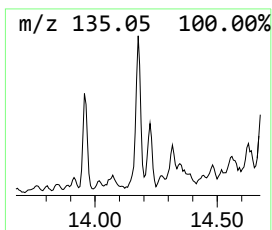
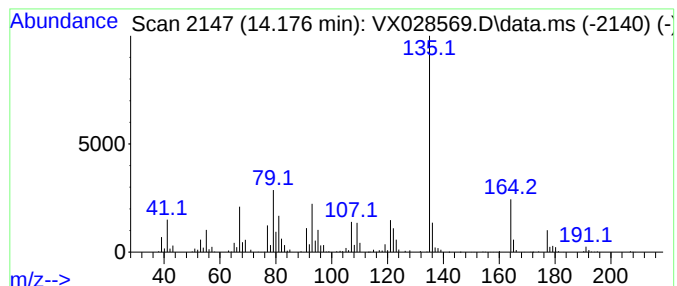
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 1 Tricyclo[3.3.1.1<3,7>]decan... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	14.68 ug/l	584647	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricyclo[3.3.1.1<3,7>]decane, 2-...	164	C12H20	014451-87-7	93
2			1-Ethyl-1(1-cyclobutylidenethyl)...	164	C12H20	1000215-13-7	70
3			2-n-Propyladamantane	178	C13H22	014451-88-8	64
4			N-[1-Adamantyl]aziridine	177	C12H19N	1000256-62-9	58
5			1-(2-Hydroxy-5-methylphenyl)prop...	164	C10H12O2	000938-45-4	53



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ETGI-362

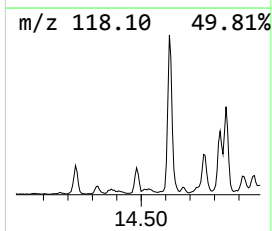
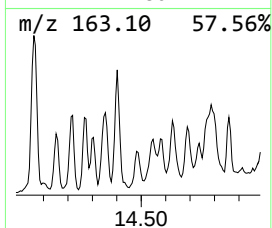
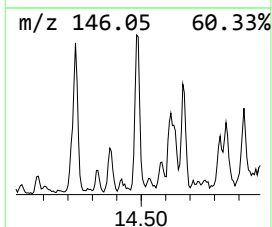
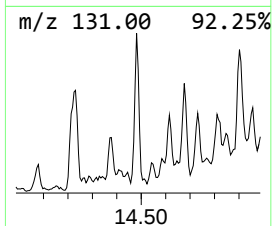
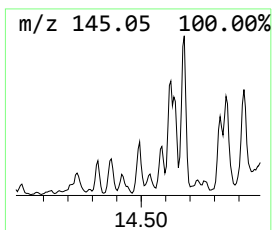
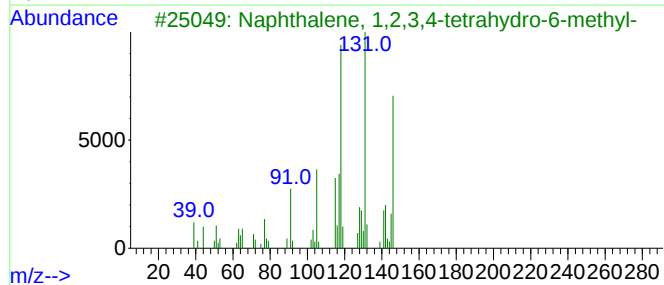
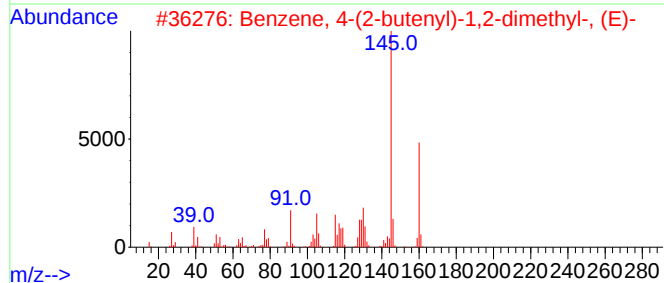
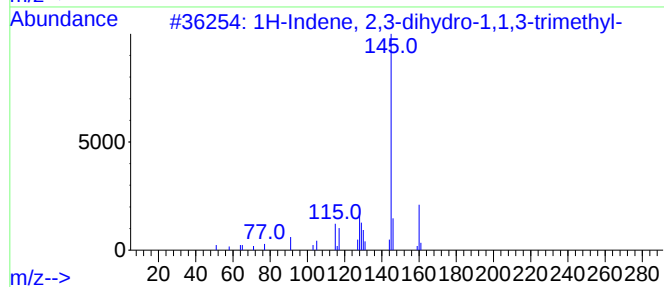
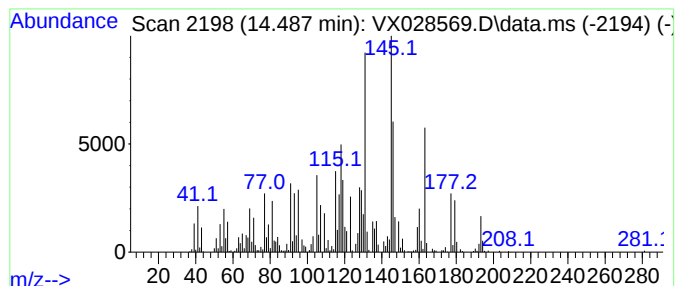
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown14.487 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.487	14.29 ug/l	569065	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	49
2			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	46
3			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	45
4			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	43
5			Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	42



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Operator : JC/MD
Sample : N2650-03
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ETGI-362

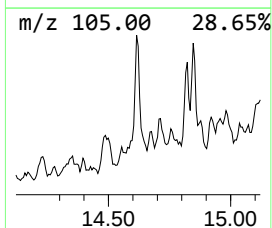
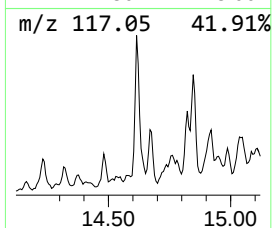
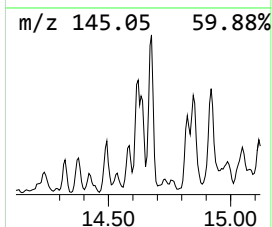
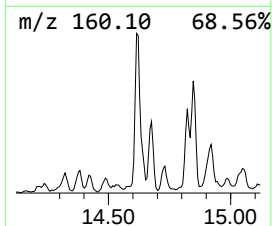
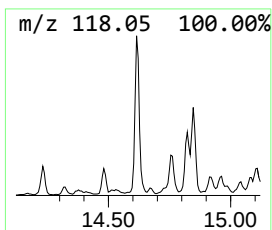
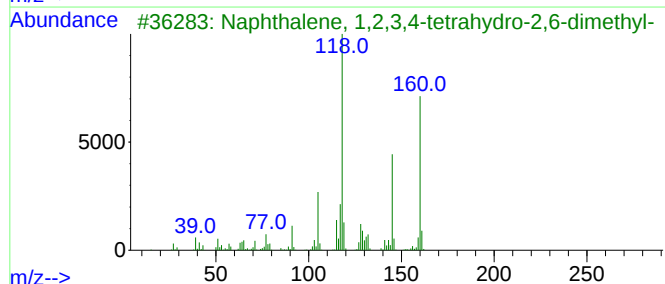
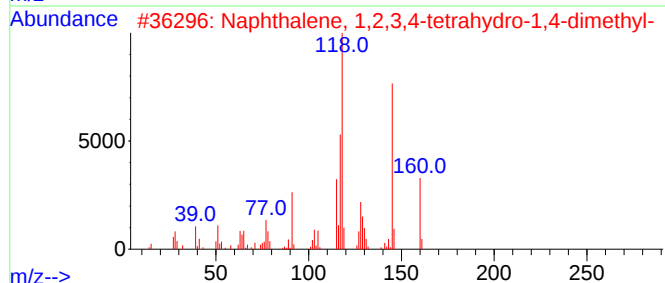
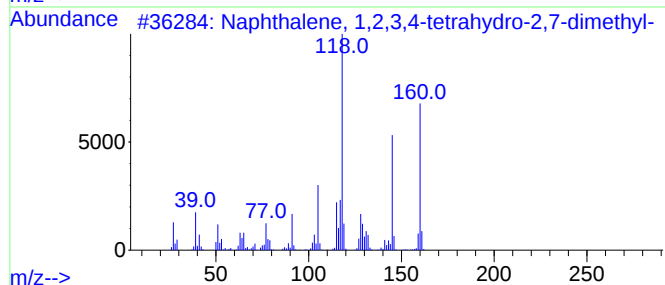
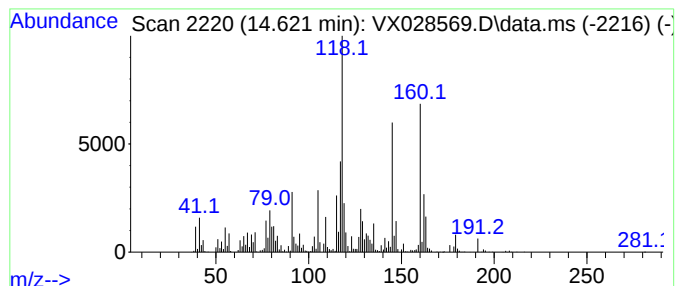
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	22.88 ug/l	911075	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	86
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	68
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	52
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	001076-61-5	50
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	50



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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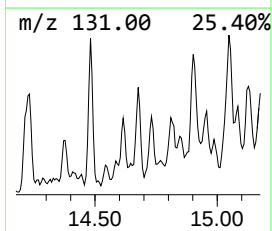
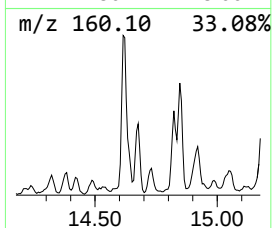
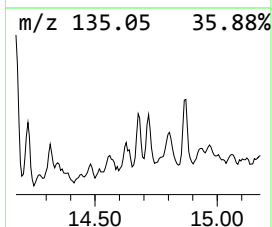
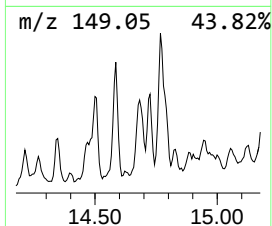
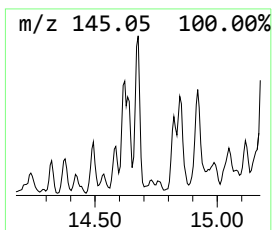
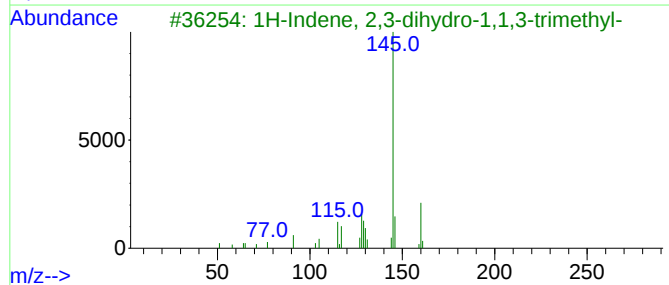
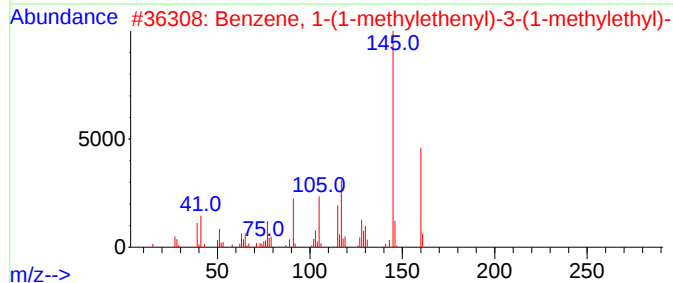
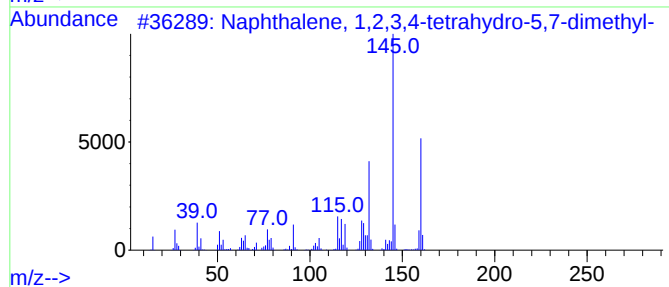
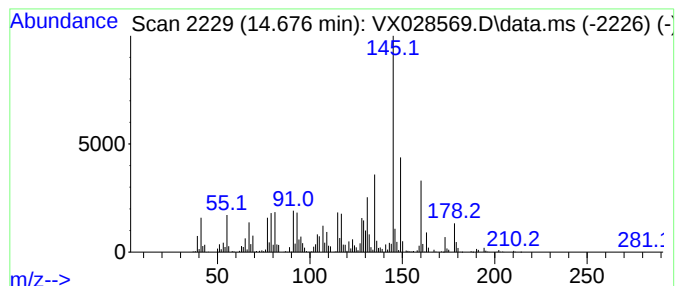
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.676	14.35 ug/l	571260	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	55
2			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	55
3			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	55
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	55
5			1H-Indene, 2,3-dihydro-1,5,7-tri...	160	C12H16	054340-88-4	50



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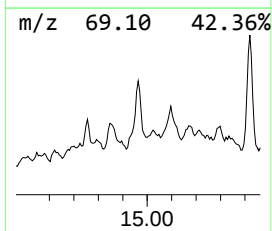
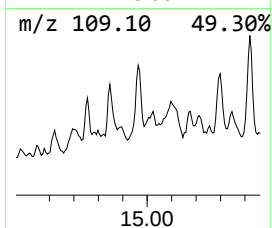
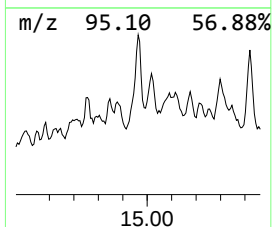
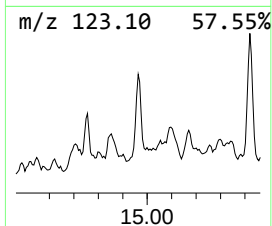
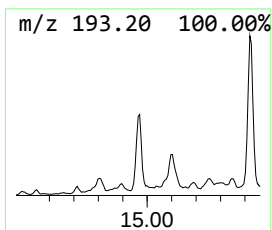
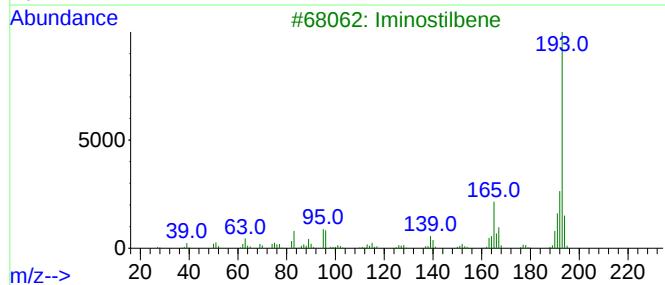
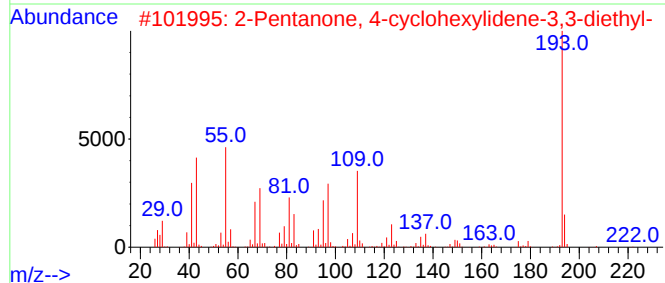
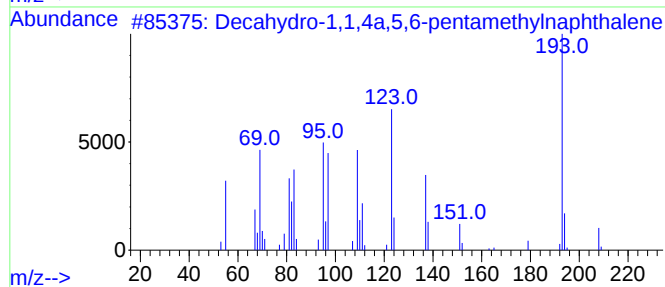
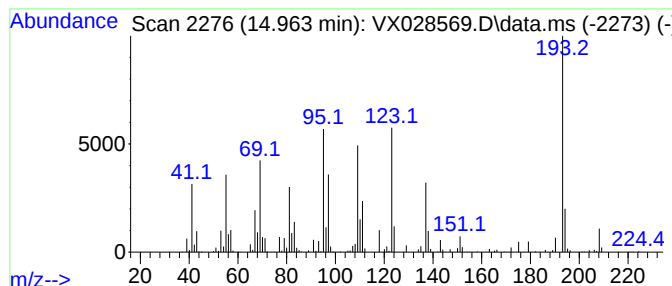
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 5 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.963	23.50 ug/l	935683	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	58
2			2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	49
3			Iminostilbene	193	C14H11N	000256-96-2	30
4			1-Anthracenamine	193	C14H11N	000610-49-1	27
5			Vinyltris(cyclopropyl)silane	178	C11H18Si	1000109-97-3	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050922\
Data File : VX028569.D
Acq On : 09 May 2022 14:03
Operator : JC/MD
Sample : N2650-03
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ETGI-362

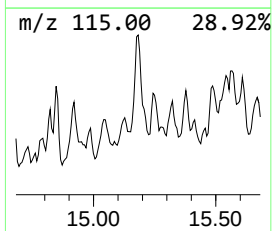
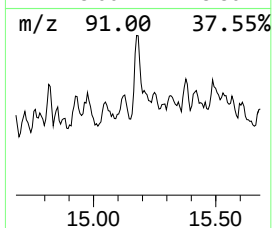
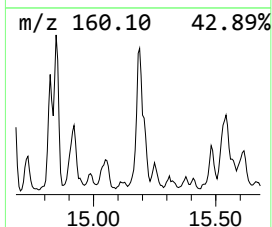
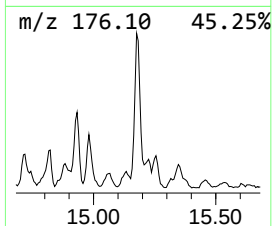
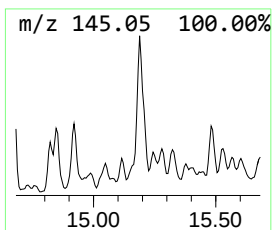
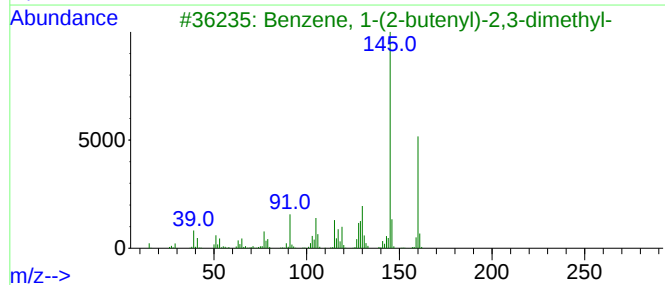
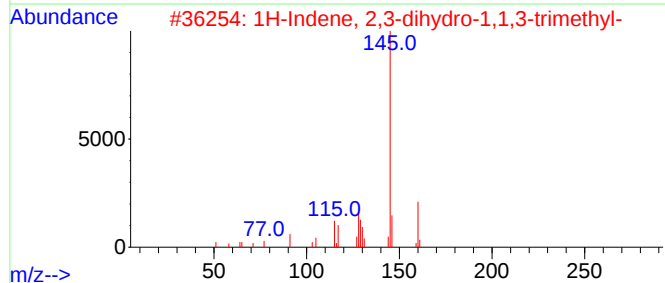
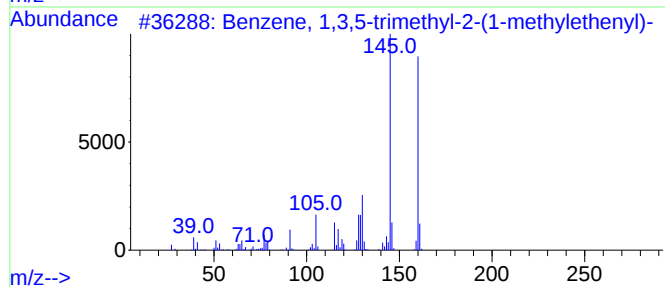
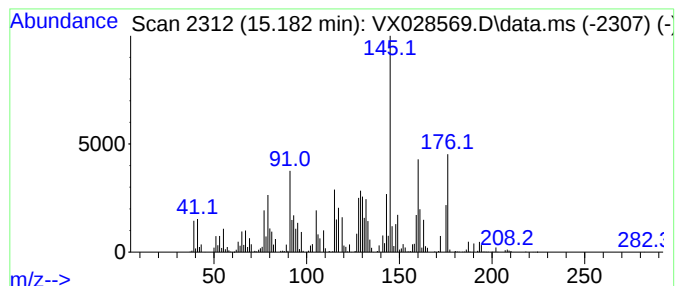
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,3,5-trimethyl-2-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.182	28.80 ug/l	1146590	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	55
2			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	55
3			Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	55
4			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	55
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050922\
Data File : VX028569.D
Acq On : 09 May 2022 14:03
Operator : JC/MD
Sample : N2650-03
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ETGI-362

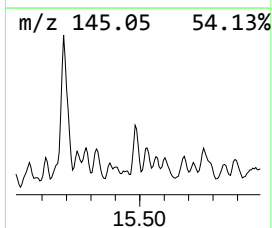
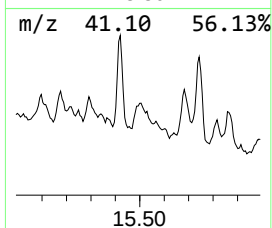
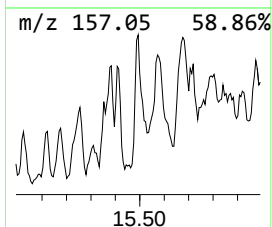
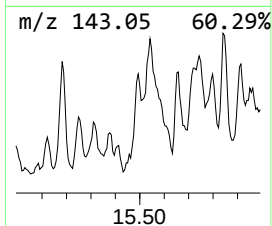
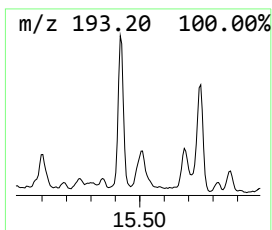
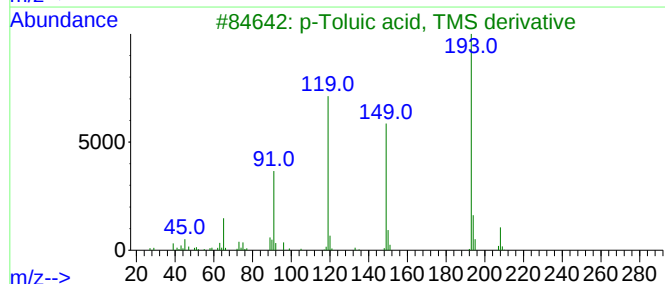
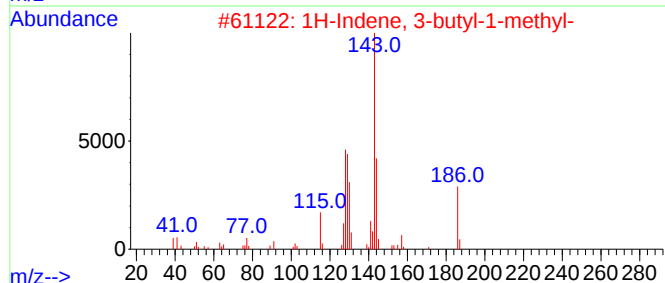
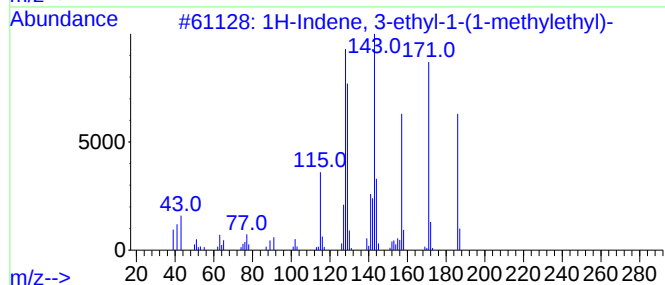
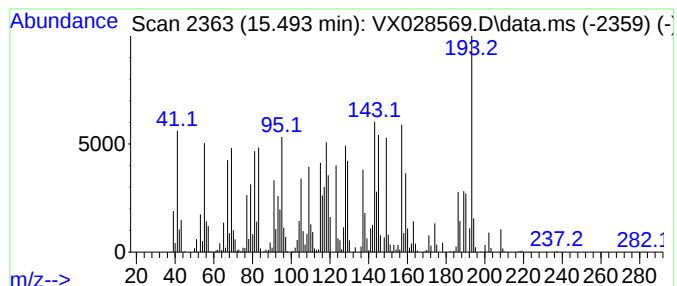
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Quant Title : SW846 8260

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

Peak Number 8 unknown15.493 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.493	23.30 ug/l	927571	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 3-ethyl-1-(1-methylet...	186	C14H18	111400-85-2	30		
2	1H-Indene, 3-butyl-1-methyl-	186	C14H18	111400-84-1	25		
3	p-Toluic acid, TMS derivative	208	C11H16O2Si	053358-36-4	15		
4	[1,1'-Biphenyl]-4-acetonitrile	193	C14H11N	031603-77-7	11		
5	1-Methyl-3-(trifluoromethyl)-1H-...	193	C7H10F3N3	1000511-73-1	11		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050922\
Data File : VX028569.D
Acq On : 09 May 2022 14:03
Operator : JC/MD
Sample : N2650-03
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ETGI-362

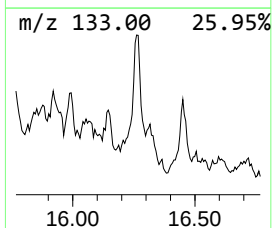
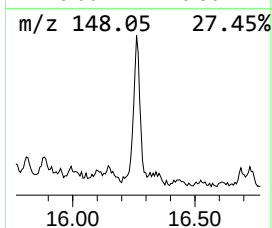
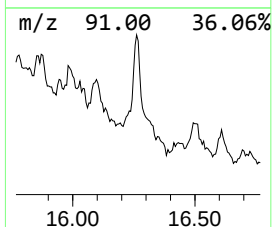
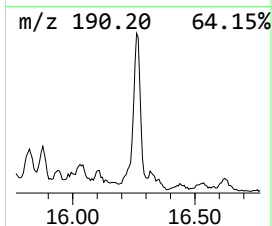
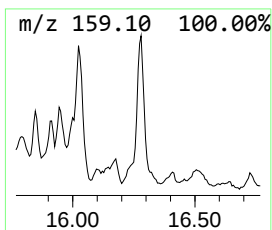
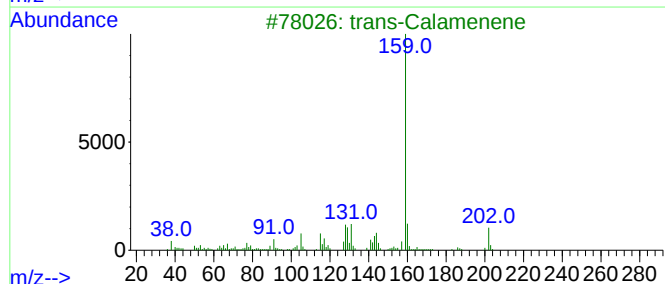
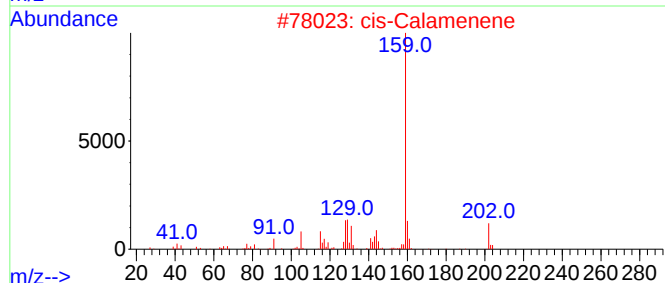
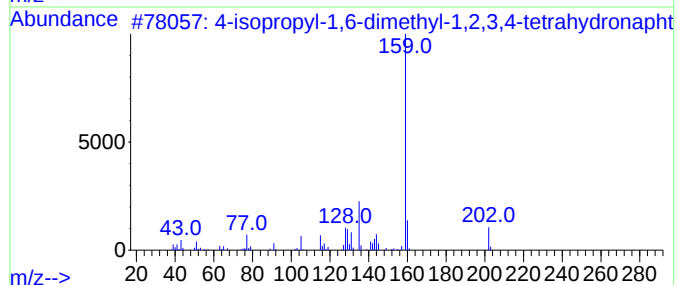
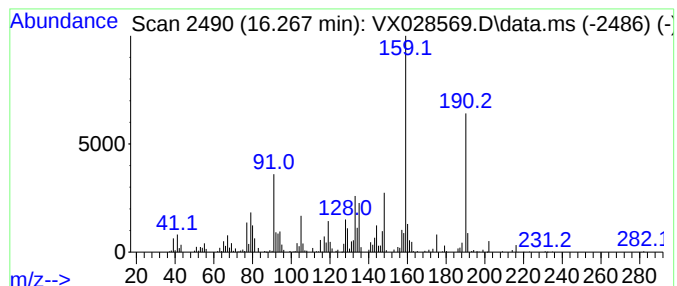
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 10 4-isopropyl-1,6-dimethyl-1,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.267	25.35 ug/l	1009320	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-isopropyl-1,6-dimethyl-1,2,3,4...	202	C15H22	1000378-99-6	55
2			cis-Calamenene	202	C15H22	072937-55-4	46
3			trans-Calamenene	202	C15H22	073209-42-4	46
4			Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	38
5			Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	021693-51-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050922\
Data File : VX028569.D
Acq On : 09 May 2022 14:03
Operator : JC/MD
Sample : N2650-03
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ETGI-362

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.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
Tricyclo[3.3.1....	14.176	14.7	ug/l	584647	4	12.024	1990790	50.0
unknown14.487	14.487	14.3	ug/l	569065	4	12.024	1990790	50.0
Naphthalene, 1,...	14.621	22.9	ug/l	911075	4	12.024	1990790	50.0
Naphthalene, 1,...	14.676	14.4	ug/l	571260	4	12.024	1990790	50.0
Decahydro-1,1,4...	14.963	23.5	ug/l	935683	4	12.024	1990790	50.0
Benzene, 1,3,5-...	15.182	28.8	ug/l	1146590	4	12.024	1990790	50.0
unknown15.493	15.493	23.3	ug/l	927571	4	12.024	1990790	50.0
4-isopropyl-1,6...	16.267	25.4	ug/l	1009320	4	12.024	1990790	50.0