

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX103122\
 Data File : VX032481.D
 Acq On : 31 Oct 2022 12:37
 Operator : JC/MD
 Sample : N5263-01
 Misc : 1.23g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31502

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\82X102622W.M
 Title : SW846 8260

Signal : TIC: VX032481.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.629	76	89	93	rBV10	4479	16150	2.46%	0.360%
2	1.940	138	140	146	rVB4	5706	6807	1.04%	0.152%
3	2.788	273	279	294	rVB	4208	10455	1.59%	0.233%
4	2.940	297	304	313	rBV2	3692	8723	1.33%	0.194%
5	4.867	614	620	633	rVB2	1715	6665	1.01%	0.148%
6	5.385	695	705	720	rVB	76353	221472	33.72%	4.933%
7	5.549	720	732	746	rBV	138465	391094	59.54%	8.711%
8	5.958	789	799	817	rBV	88089	227754	34.67%	5.073%
9	6.757	918	930	944	rBV	204932	491687	74.85%	10.952%
10	8.646	1233	1240	1250	rBV	423690	656862	100.00%	14.631%
11	10.055	1465	1471	1484	rBV	408601	551140	83.90%	12.276%
12	11.085	1634	1640	1650	rBV	301513	418667	63.74%	9.326%
13	12.024	1789	1794	1802	rBV	390561	489167	74.47%	10.896%
14	12.987	1944	1952	1958	rBV5	3489	6937	1.06%	0.155%
15	13.292	1997	2002	2007	rVB3	12840	18621	2.83%	0.415%
16	13.414	2017	2022	2025	rBV4	12443	21556	3.28%	0.480%
17	13.597	2048	2052	2054	rBV4	7274	11587	1.76%	0.258%
18	13.676	2061	2065	2067	rBV4	6454	10576	1.61%	0.236%
19	13.700	2067	2069	2073	rVB3	7103	8757	1.33%	0.195%
20	13.804	2082	2086	2089	rBV4	21142	30946	4.71%	0.689%
21	13.841	2089	2092	2096	rVV5	11538	18685	2.84%	0.416%
22	13.981	2111	2115	2118	rBV6	15157	31999	4.87%	0.713%
23	14.066	2126	2129	2132	rBV4	14565	24486	3.73%	0.545%
24	14.103	2132	2135	2139	rVB5	17575	23336	3.55%	0.520%
25	14.219	2151	2154	2160	rBV4	38856	68347	10.41%	1.522%
26	14.554	2206	2209	2211	rBV3	38949	55225	8.41%	1.230%
27	14.578	2211	2213	2216	rVV2	34717	39441	6.00%	0.879%
28	14.621	2217	2220	2221	rBV2	44660	52174	7.94%	1.162%
29	14.676	2226	2229	2232	rBV4	60651	96180	14.64%	2.142%
30	14.755	2239	2242	2245	rBV3	87878	113699	17.31%	2.533%
31	16.096	2458	2462	2479	rVB3	135418	360238	54.84%	8.024%

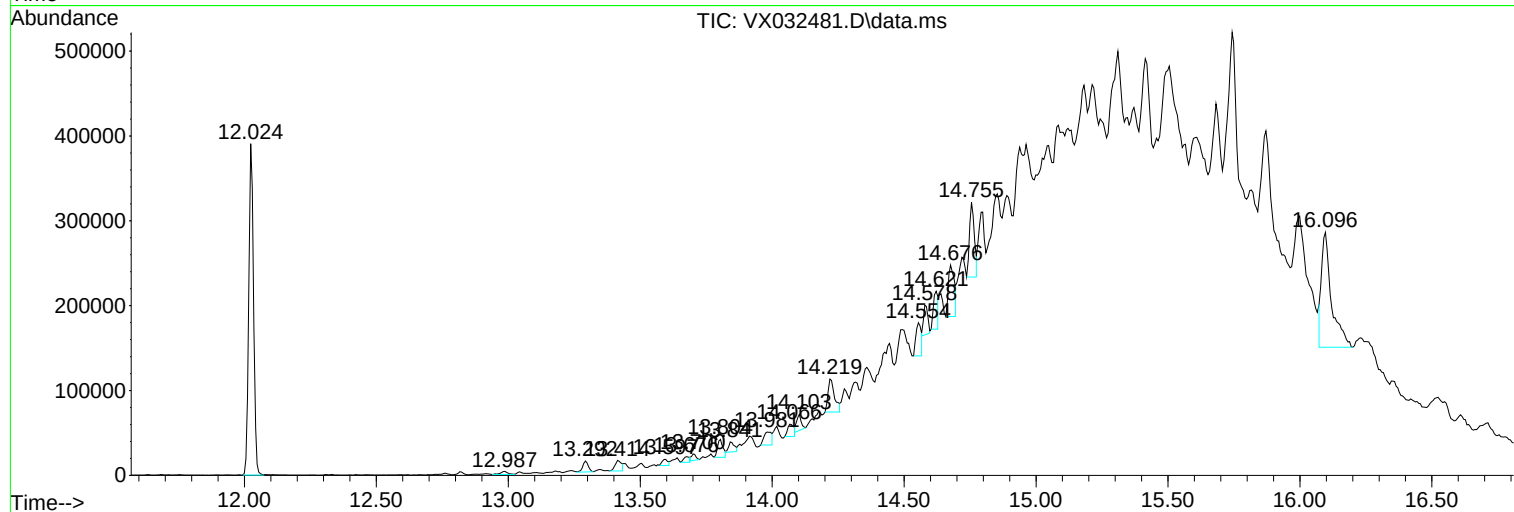
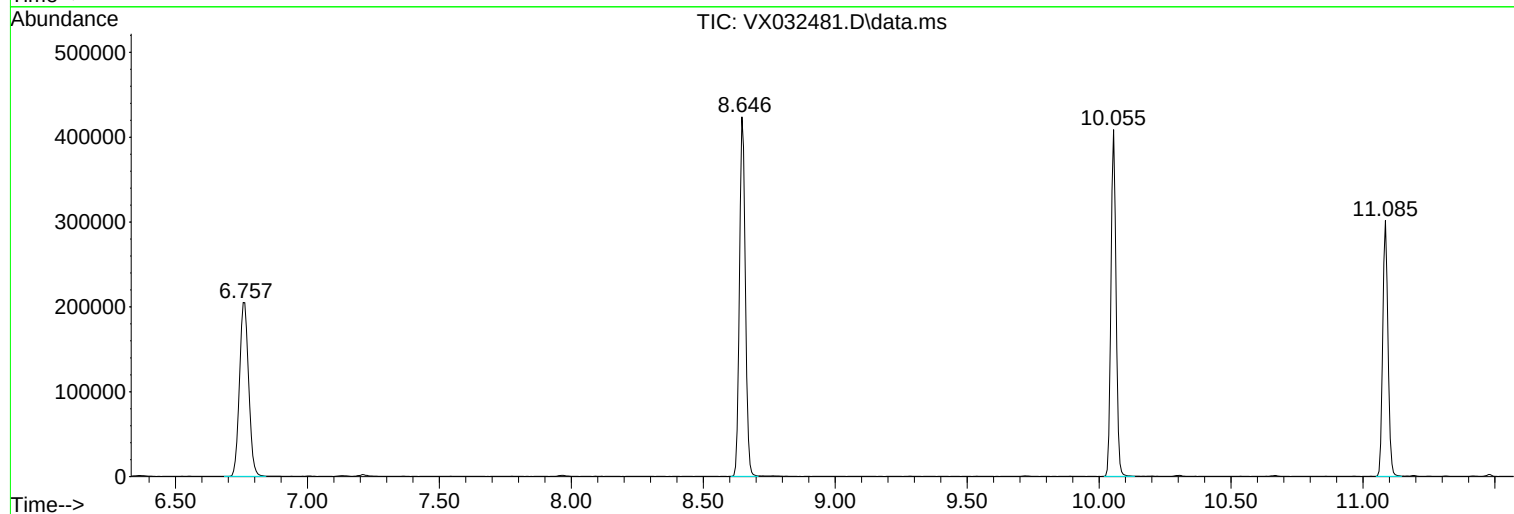
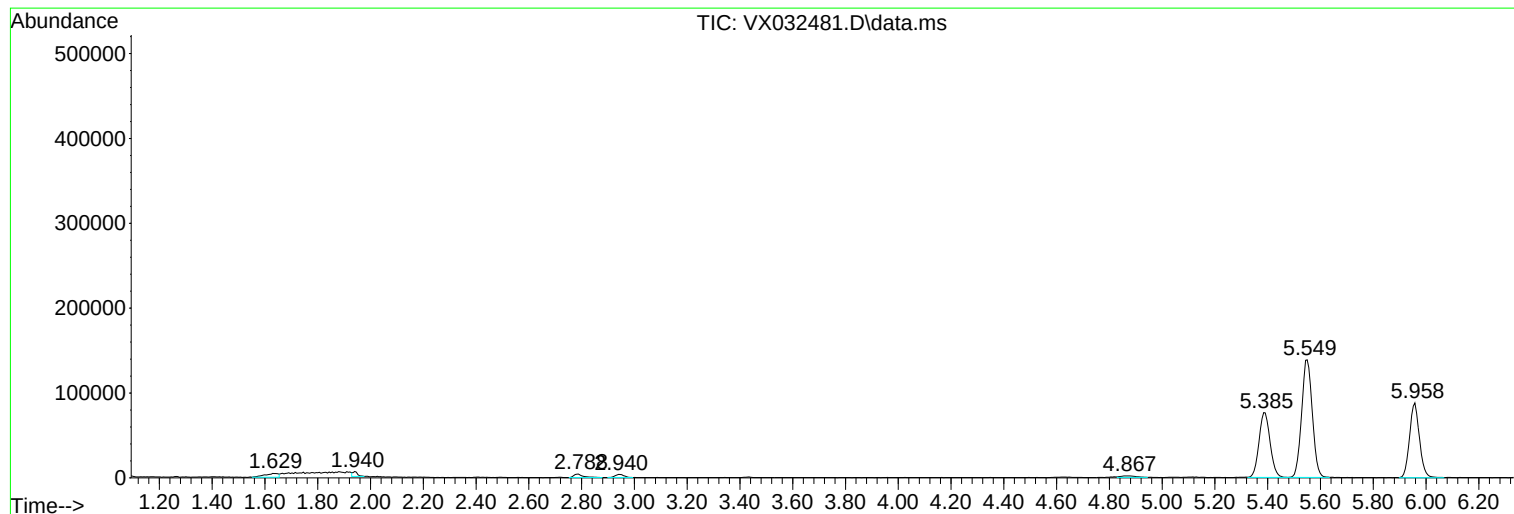
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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



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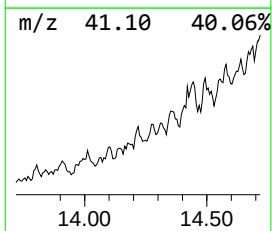
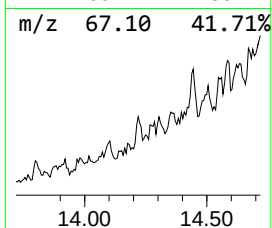
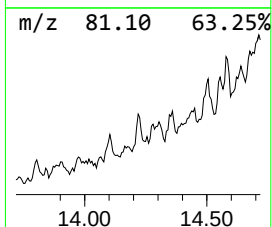
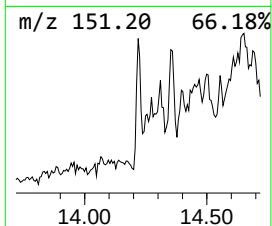
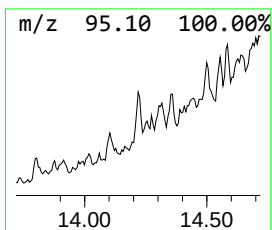
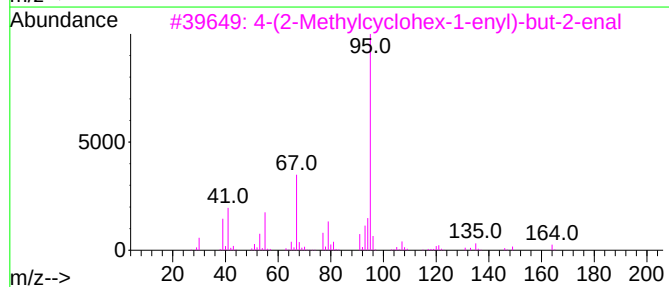
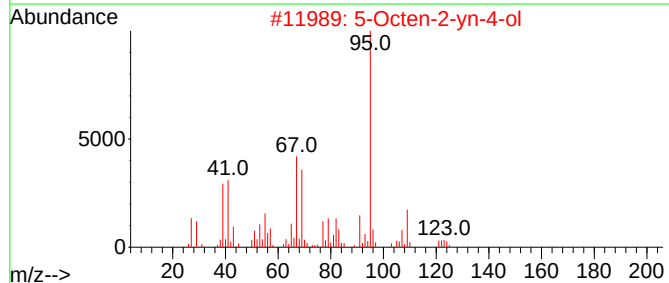
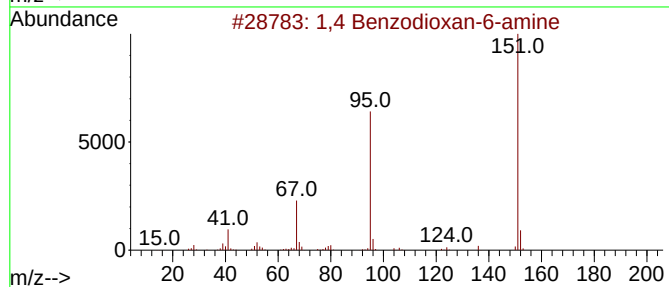
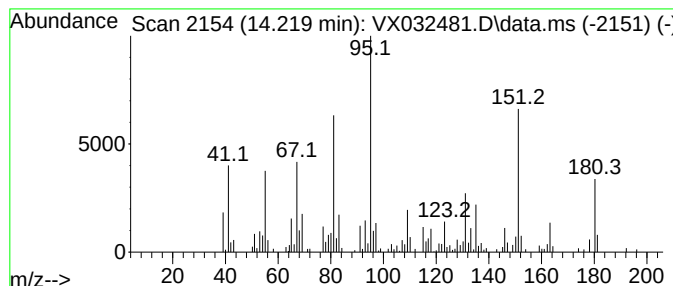
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown14.219 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.219	6.99 ug/l	68347	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4		Benzodioxan-6-amine	151	C8H9NO2	022013-33-8	49
2	5-Octen-2-yn-4-ol			124	C8H12O	1010196-87-1	45
3	4-(2-Methylcyclohex-1-enyl)-but-...			164	C11H16O	1000188-10-0	38
4	1,4-Pentadiene, 2,3,3-trimethyl-			110	C8H14	000756-02-5	38
5	2-Norbornyl bromide			174	C7H11Br	029342-65-2	35



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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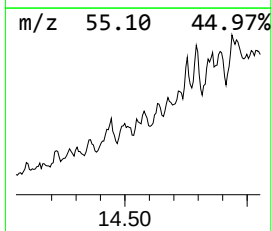
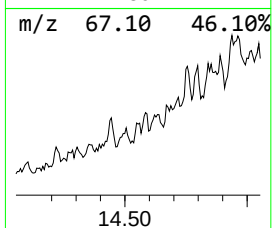
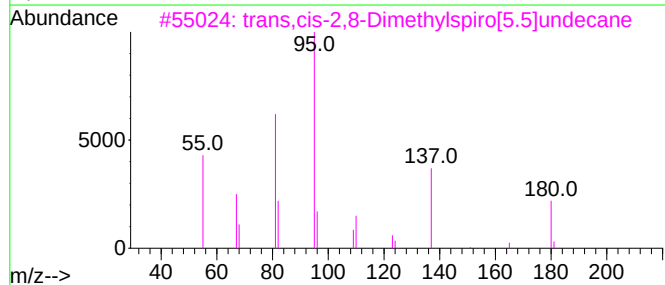
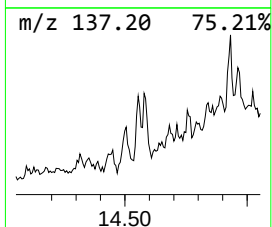
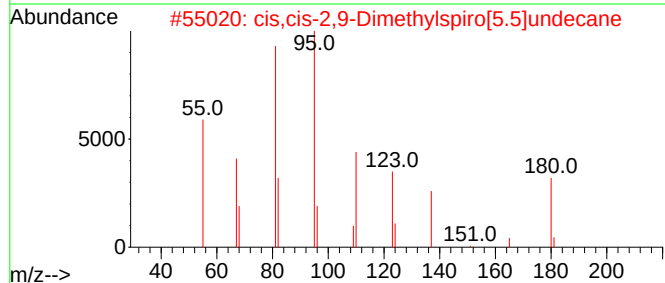
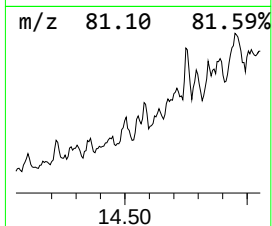
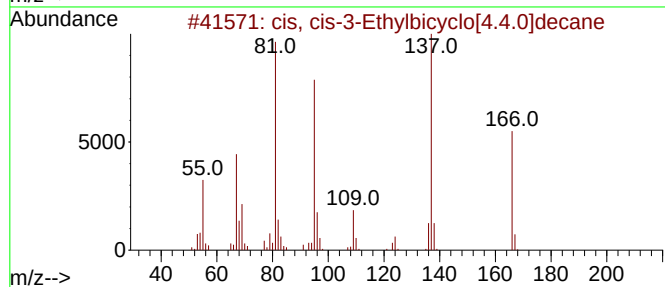
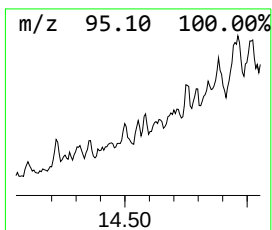
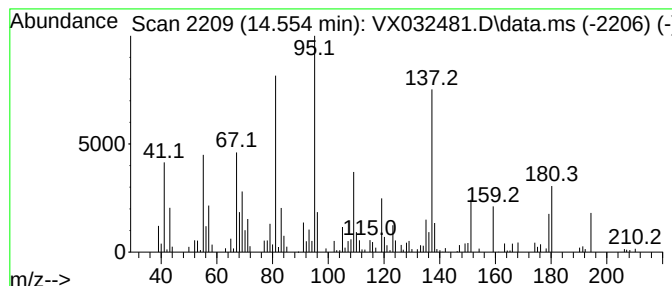
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 2 cis, cis-3-Ethylbicyclo[4.4... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.554	5.64 ug/l	55225	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis, cis-3-Ethylbicyclo[4.4.0]de...	166	C12H22	066660-42-2	62
2			cis,cis-2,9-Dimethylspiro[5.5]un...	180	C13H24	095472-51-8	49
3			trans,cis-2,8-Dimethylspiro[5.5]...	180	C13H24	095472-52-9	46
4			4,6-Heptadien-2-one, 3,6-dimethy...	180	C12H20O	077822-50-5	41
5			2-Ethenoxy-1,7,7-trimethylbicycl...	180	C12H20O	1000432-15-0	35



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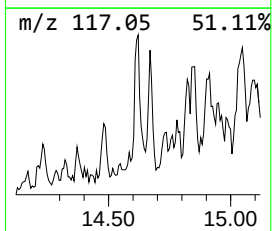
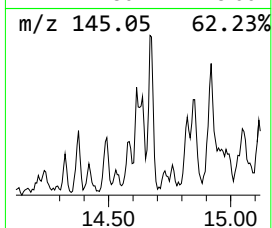
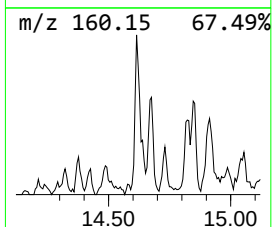
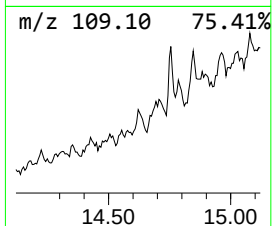
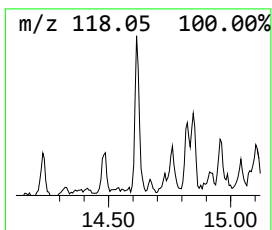
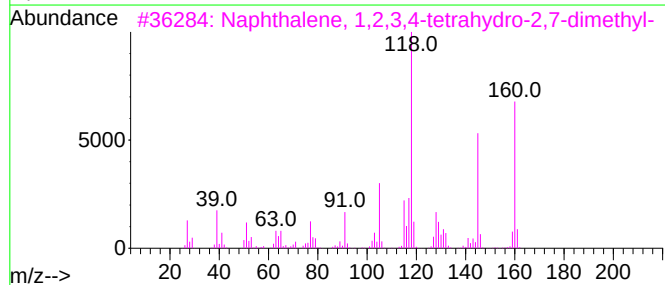
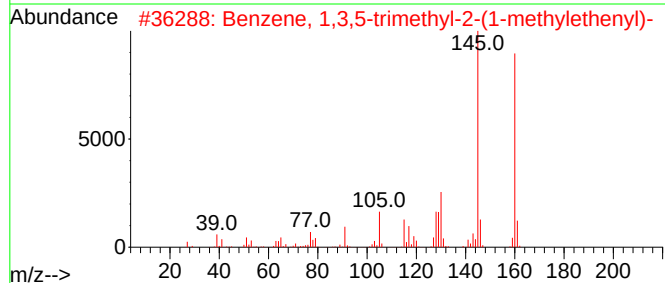
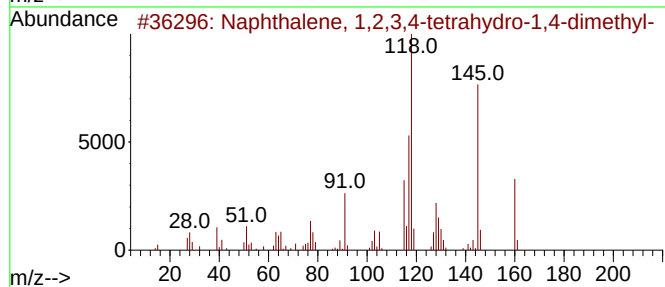
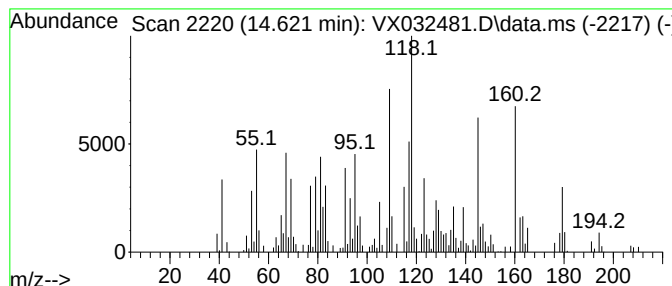
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	5.33 ug/l	52174	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	50
2			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	45
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	41
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	38
5			1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	014944-23-1	30



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Instrument :
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ClientSampleId :
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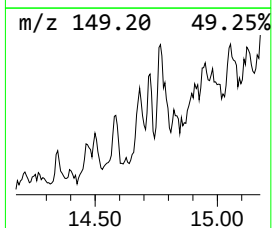
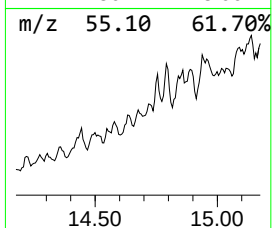
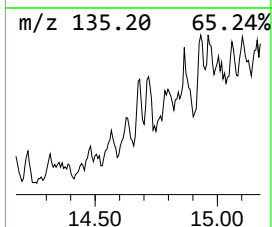
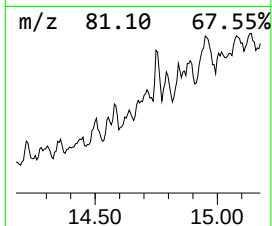
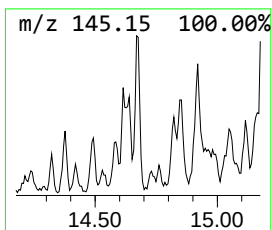
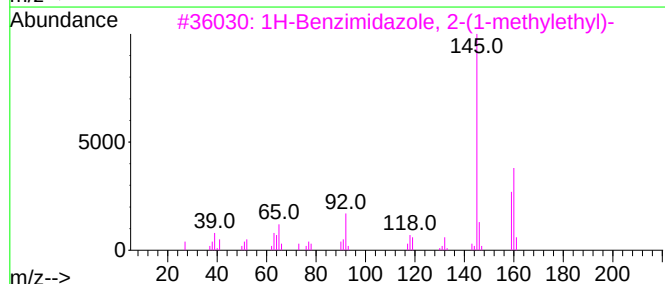
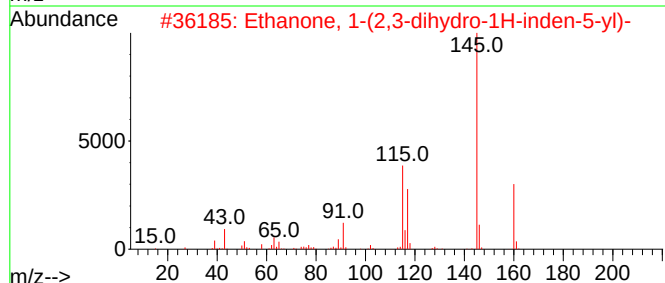
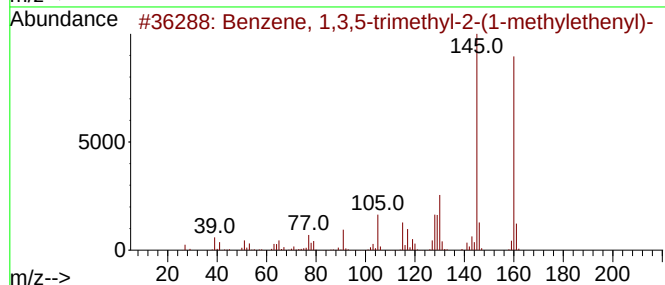
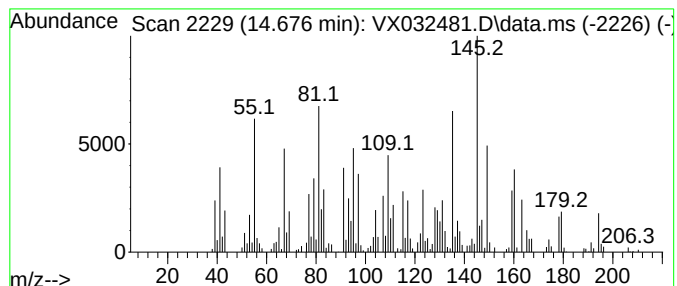
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Quant Title : SW846 8260

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

Peak Number 4 unknown14.676 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.676	9.83 ug/l	96180	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	38
2			Ethanone, 1-(2,3-dihydro-1H-inde...	160	C11H12O	004228-10-8	38
3			1H-Benzimidazole, 2-(1-methyleth...	160	C10H12N2	005851-43-4	38
4			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	38
5			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	30



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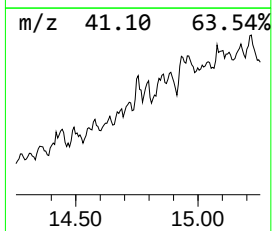
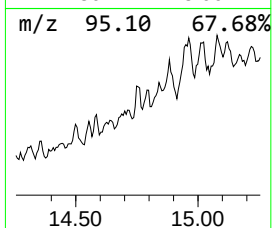
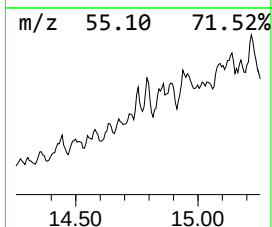
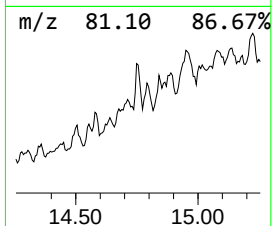
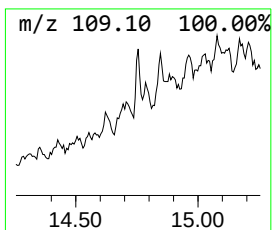
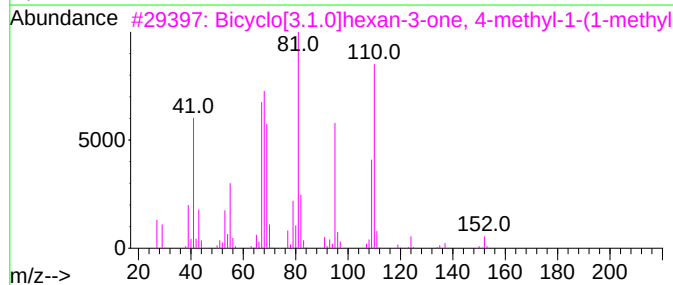
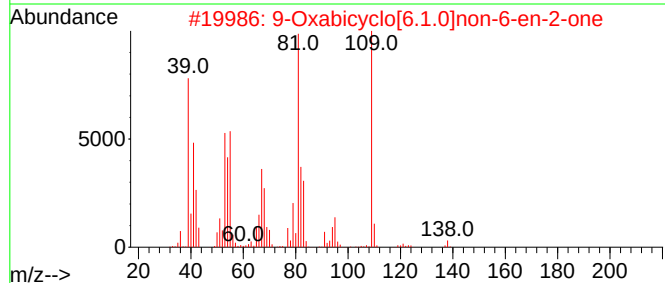
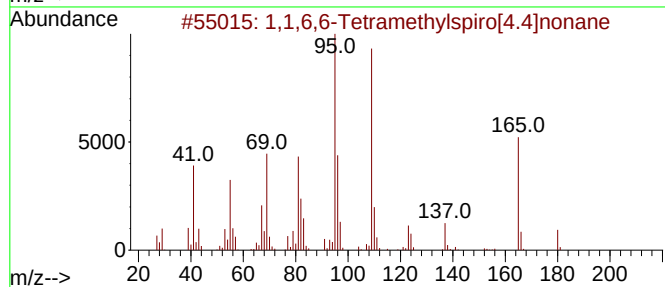
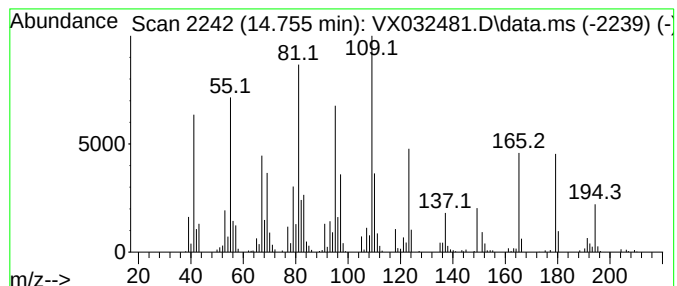
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown14.755 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.755	11.62 ug/l	113699	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1,6,6-Tetramethylspiro[4.4]nonane	180	C13H24	074054-92-5	30
2			9-Oxabicyclo[6.1.0]non-6-en-2-one	138	C8H10O2	1000211-01-6	30
3			Bicyclo[3.1.0]hexan-3-one, 4-met...	152	C10H16O	001125-12-8	25
4			1-(1-Butynyl)cyclopentanol	138	C9H14O	1000342-86-5	25
5			2,3-DI-T-BUTYLCYCLOPROP-2-ENONE	166	C11H18O	019985-79-6	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX103122\
Data File : VX032481.D
Acq On : 31 Oct 2022 12:37
Operator : JC/MD
Sample : N5263-01
Misc : 1.23g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

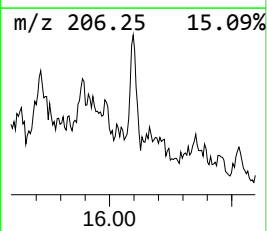
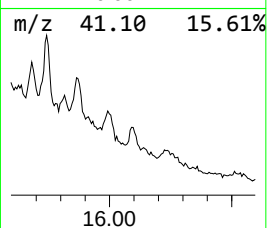
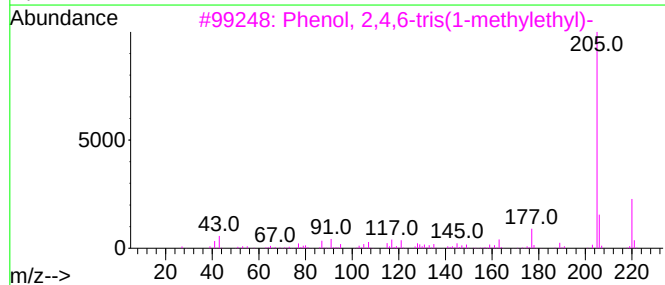
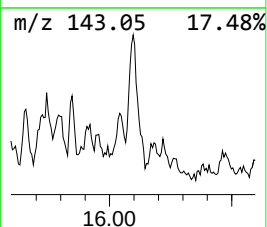
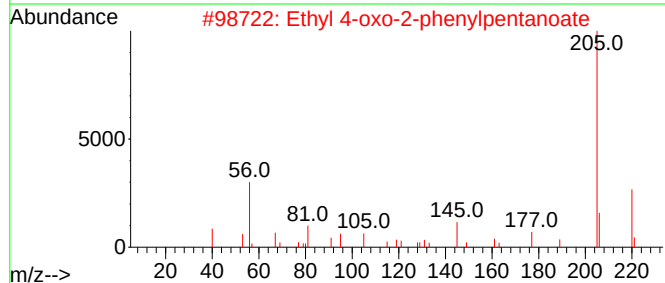
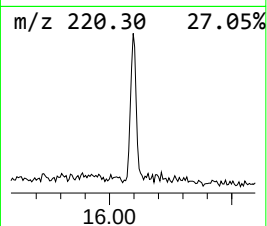
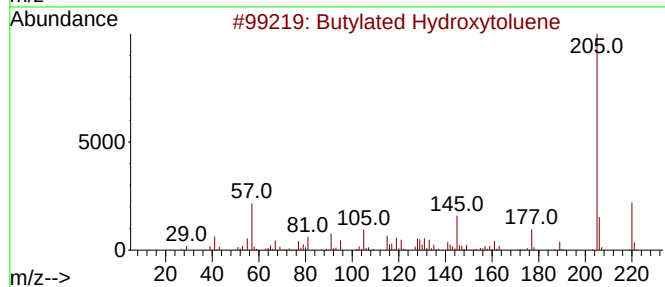
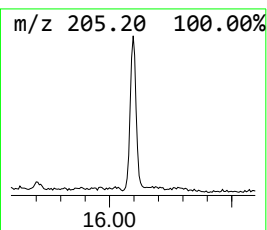
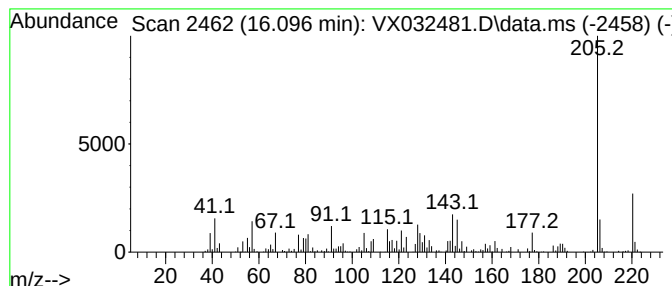
Instrument :
MSVOA_X
ClientSampleId :
31502

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 6 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.		
16.096	36.82 ug/l	360238	1,4-Dichlorobenzene-d4		12.024		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	93
2			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	81
3			Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	74
4			2H-1-Benzopyran, 6,7-dimethoxy-2...	220	C13H16O3	000644-06-4	70
5			2-Methyl-4,5-dimethoxycrotonophe...	220	C13H16O3	207233-94-1	64



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Misc : 1.23g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31502

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.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
unknown14.219	14.219	7.0	ug/l	68347	4	12.024	489167	50.0
cis, cis-3-Ethy...	14.554	5.6	ug/l	55225	4	12.024	489167	50.0
Naphthalene, 1,...	14.621	5.3	ug/l	52174	4	12.024	489167	50.0
unknown14.676	14.676	9.8	ug/l	96180	4	12.024	489167	50.0
unknown14.755	14.755	11.6	ug/l	113699	4	12.024	489167	50.0
Butylated Hydro...	16.096	36.8	ug/l	360238	4	12.024	489167	50.0