

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
 Data File : VX045827.D
 Acq On : 17 Apr 2025 14:46
 Operator : JC/MD
 Sample : Q1818-05 100X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 3828

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\82X040225W.M
 Title : SW846 8260

Signal : TIC: VX045827.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.563	69	78	79	rBV4	3508	7160	1.44%	0.165%
2	1.605	80	85	89	rVB5	5295	10716	2.16%	0.247%
3	5.379	694	704	720	rBV	57148	171925	34.66%	3.962%
4	5.544	720	731	748	rVV	85039	243913	49.17%	5.622%
5	5.952	788	798	812	rBV	66749	179619	36.21%	4.140%
6	6.757	921	930	945	rBV	147106	358278	72.23%	8.257%
7	8.647	1234	1240	1250	rBV	305207	496026	100.00%	11.432%
8	10.049	1465	1470	1483	rBV	317672	452941	91.31%	10.439%
9	10.945	1611	1617	1620	rBV	4443	6243	1.26%	0.144%
10	10.988	1620	1624	1634	rVV	12302	22629	4.56%	0.522%
11	11.079	1634	1639	1650	rVB	279477	351724	70.91%	8.106%
12	11.488	1701	1706	1709	rBV4	6580	9051	1.82%	0.209%
13	11.591	1718	1723	1727	rBV2	10087	14142	2.85%	0.326%
14	11.841	1756	1764	1768	rBV3	6492	10189	2.05%	0.235%
15	11.933	1775	1779	1781	rBV2	6498	8737	1.76%	0.201%
16	11.969	1781	1785	1788	rVV	72989	89074	17.96%	2.053%
17	12.018	1788	1793	1801	rVV	353851	447802	90.28%	10.321%
18	12.097	1801	1806	1818	rVB	52434	78155	15.76%	1.801%
19	12.219	1822	1826	1836	rBV9	3118	7612	1.53%	0.175%
20	12.305	1836	1840	1848	rBV8	2921	5153	1.04%	0.119%
21	12.579	1880	1885	1908	rVV	219921	359300	72.44%	8.281%
22	12.768	1911	1916	1920	rVV2	17618	26579	5.36%	0.613%
23	12.817	1920	1924	1928	rVV	104525	128583	25.92%	2.963%
24	12.853	1928	1930	1943	rVB4	12216	19680	3.97%	0.454%
25	13.176	1978	1983	1986	rBV6	4720	8343	1.68%	0.192%
26	13.487	2029	2034	2035	rVV5	3525	5764	1.16%	0.133%
27	13.506	2035	2037	2042	rVB4	4878	6424	1.30%	0.148%
28	13.560	2042	2046	2049	rBV3	16369	25957	5.23%	0.598%
29	13.585	2049	2050	2058	rVB3	11641	13029	2.63%	0.300%
30	13.658	2058	2062	2066	rBV5	6559	10086	2.03%	0.232%
31	13.731	2069	2074	2078	rVV	87170	116595	23.51%	2.687%
32	13.774	2078	2081	2088	rVB2	13683	19621	3.96%	0.452%
33	13.841	2088	2092	2097	rVB5	5658	8561	1.73%	0.197%
34	13.902	2099	2102	2105	rBV3	4030	5331	1.07%	0.123%
35	13.981	2112	2115	2121	rVB6	5594	8398	1.69%	0.194%
36	14.103	2131	2135	2142	rVB2	11826	18520	3.73%	0.427%

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37	14.188	2145	2149	2159	rBV	68089	119365	24.06%	2.751%
38	14.451	2187	2192	2200	rBV	127335	171179	34.51%	3.945%
39	14.591	2211	2215	2222	rBV3	15608	29606	5.97%	0.682%
40	14.676	2226	2229	2231	rBV3	5129	6413	1.29%	0.148%
41	14.755	2238	2242	2244	rBV5	9190	11419	2.30%	0.263%
42	14.786	2244	2247	2252	rVV7	7983	11614	2.34%	0.268%
43	15.322	2330	2335	2340	rBV	58898	83031	16.74%	1.914%
44	15.414	2345	2350	2358	rVB2	89273	137040	27.63%	3.158%
45	15.987	2442	2444	2449	rBV5	13737	17378	3.50%	0.401%

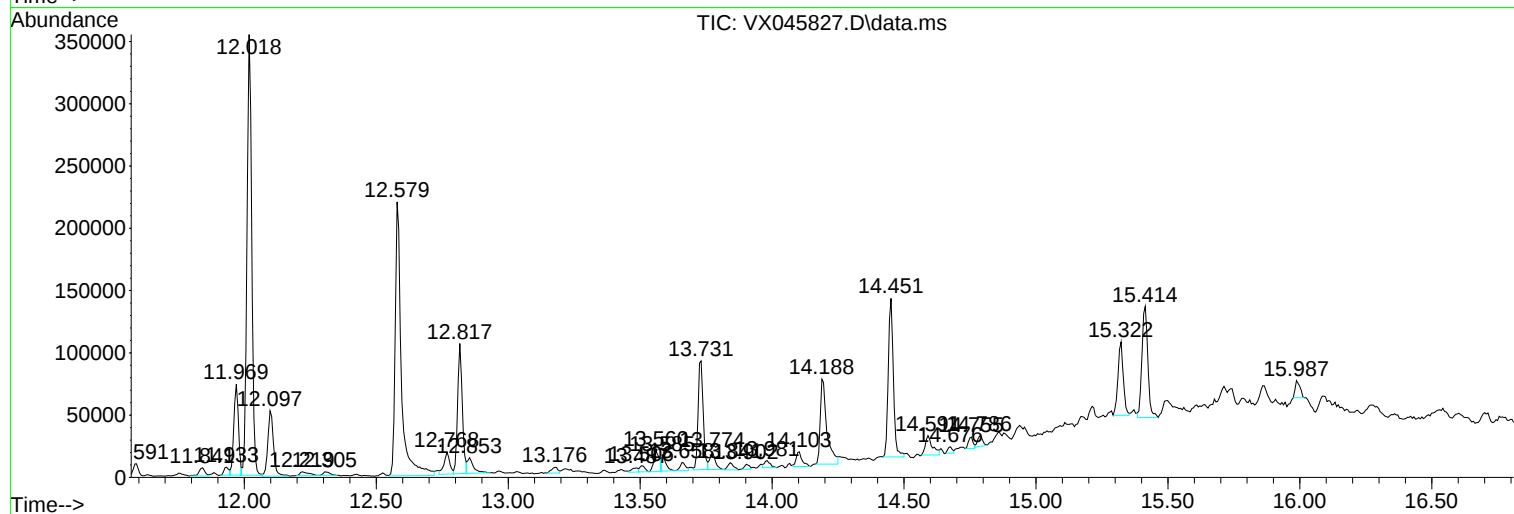
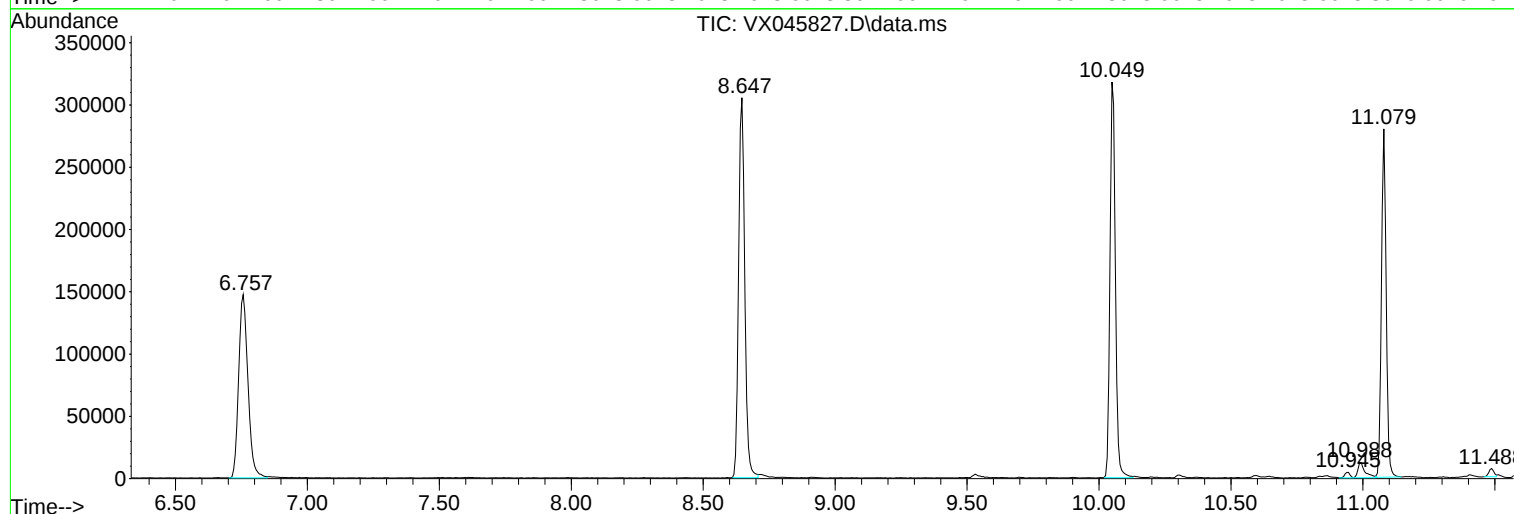
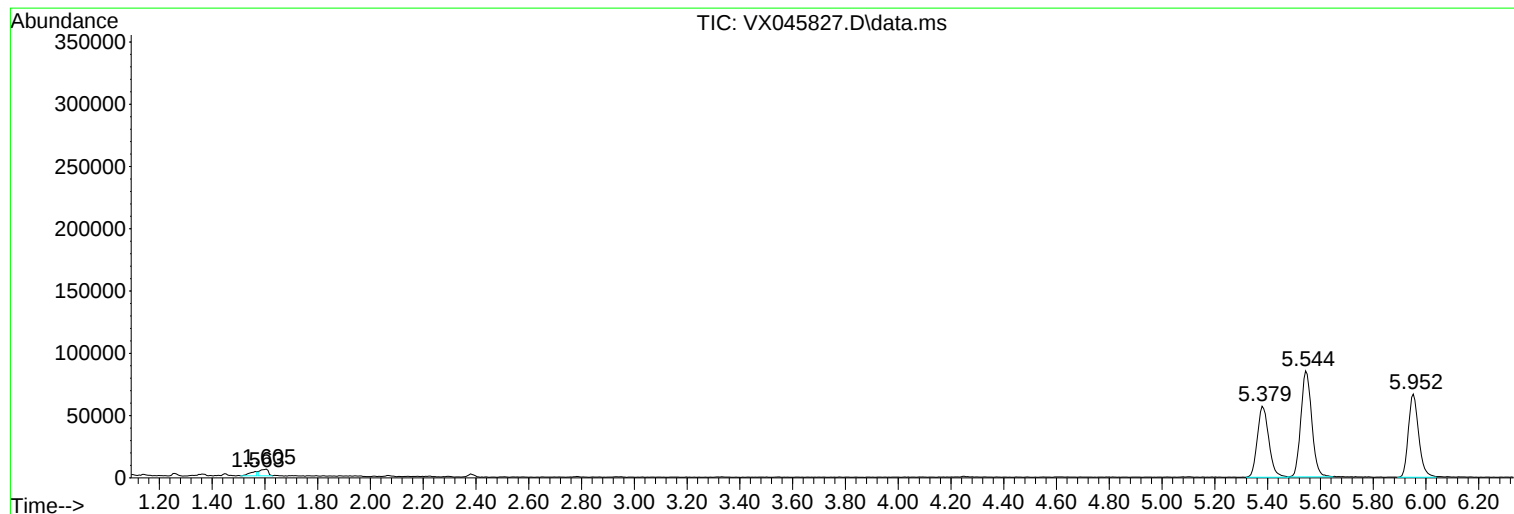
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

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



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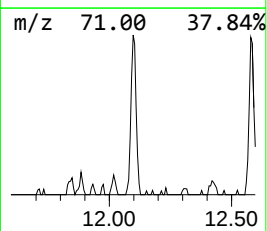
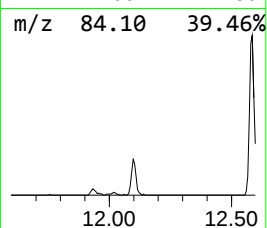
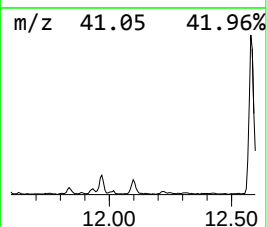
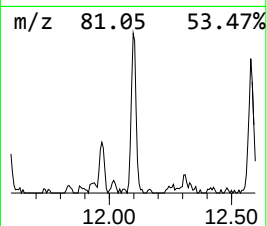
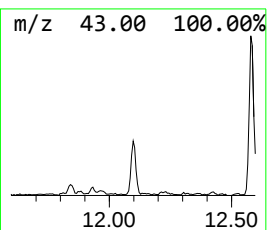
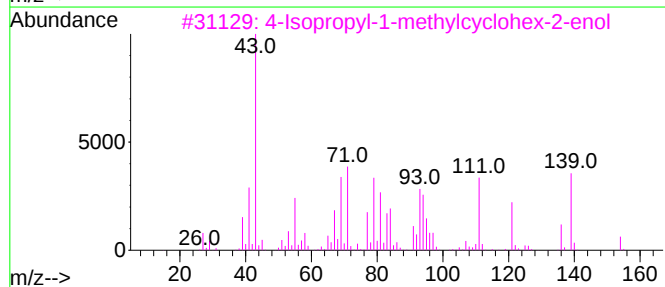
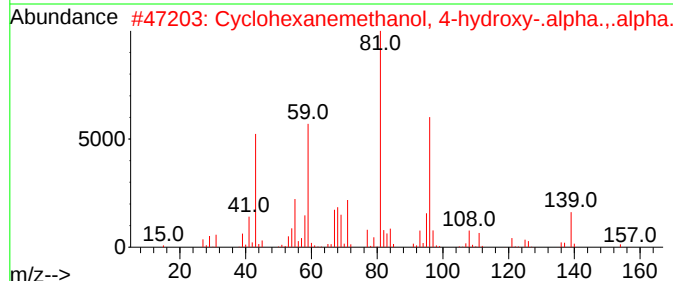
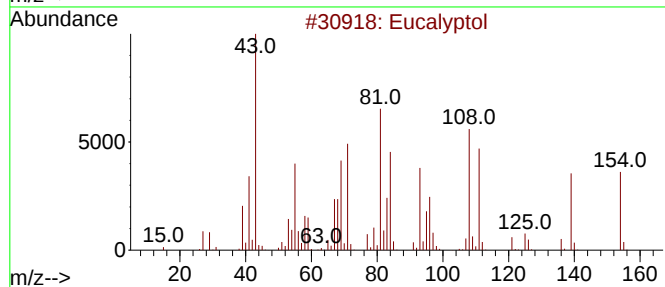
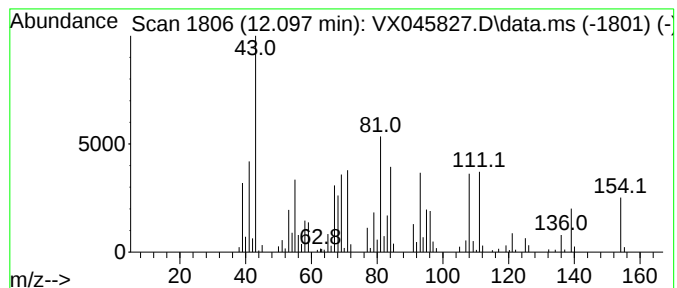
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

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

Peak Number 1 Eucalyptol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.097	8.73 ug/l	78155	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	97
2			Cyclohexanemethanol, 4-hydroxy-....	172	C10H20O2	000080-53-5	32
3			4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	25
4			7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	22
5			2-Cyclohexen-1-ol, 1-methyl-4-(1...	154	C10H18O	029803-81-4	22



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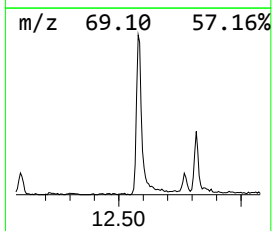
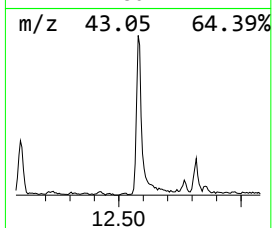
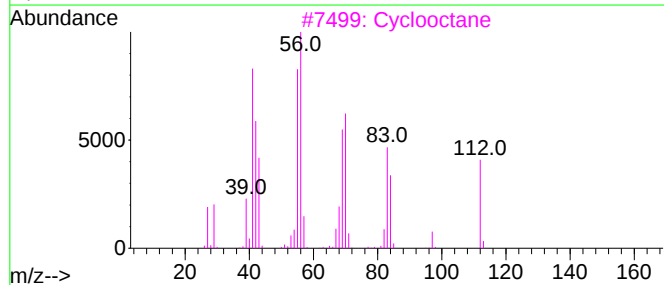
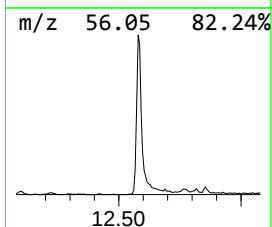
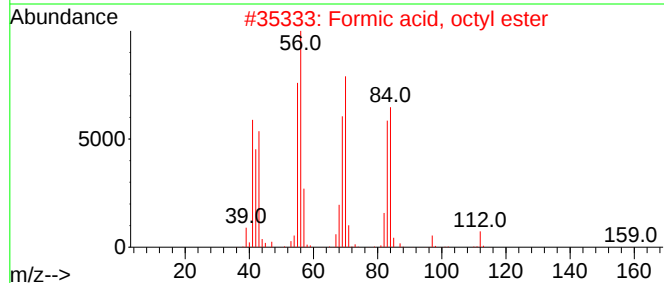
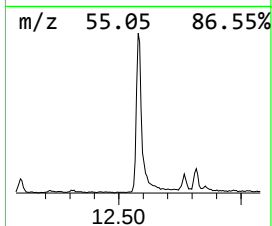
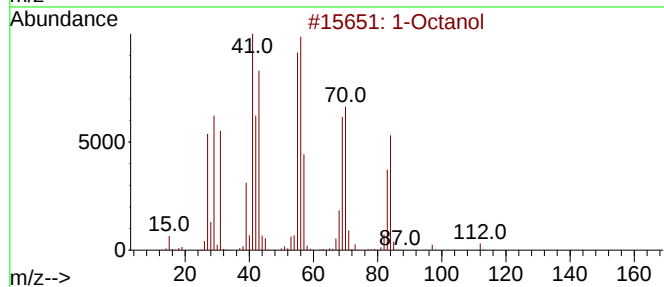
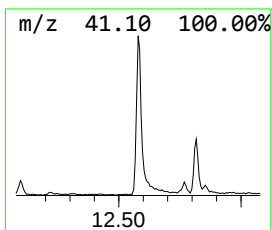
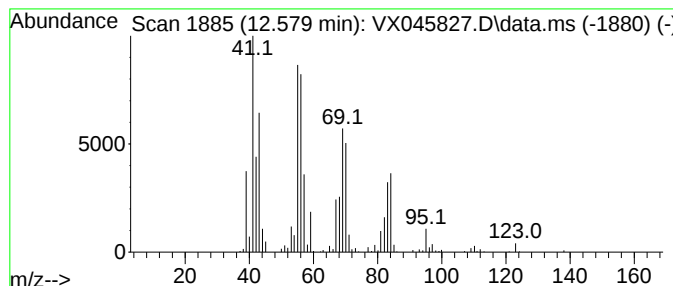
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Octanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.579	40.12 ug/l	359300	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol	130	C8H18O	000111-87-5	72
2			Formic acid, octyl ester	158	C9H18O2	000112-32-3	64
3			Cyclooctane	112	C8H16	000292-64-8	52
4			1-Pentene, 3,4-dimethyl-	98	C7H14	007385-78-6	43
5			Pentane, 2-cyclopropyl-	112	C8H16	005458-16-2	38



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ALS Vial : 12 Sample Multiplier: 1

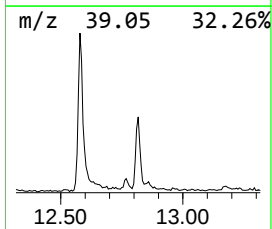
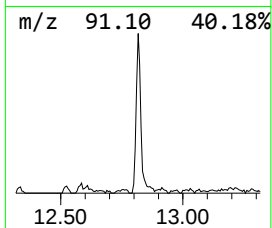
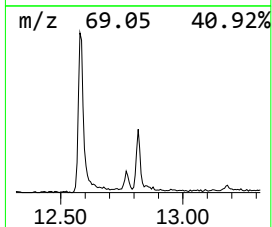
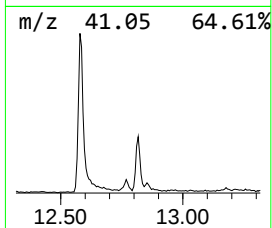
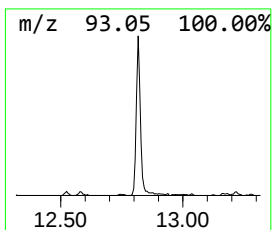
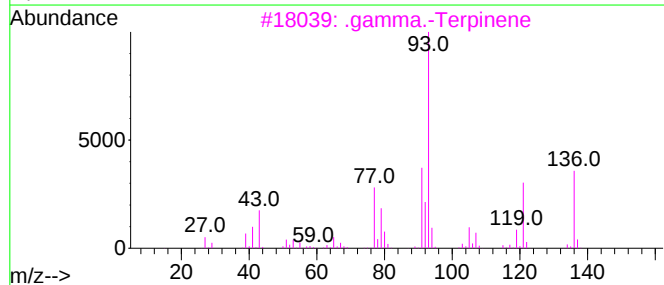
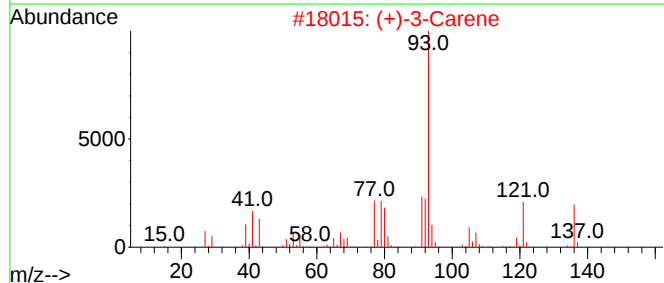
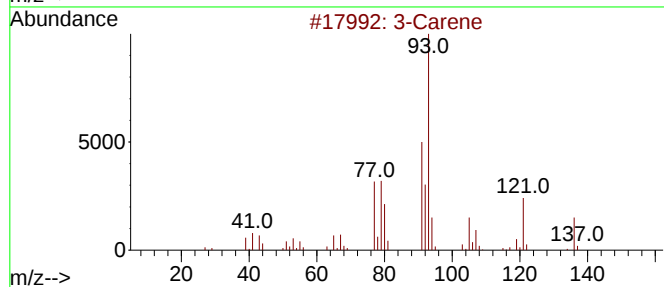
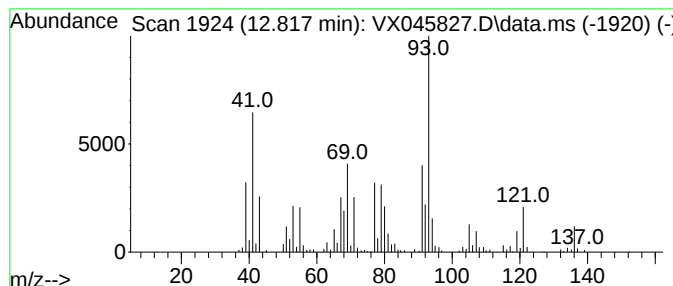
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Quant Title : SW846 8260

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

Peak Number 3 3-Carene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.817	14.36 ug/l	128583	1,4-Dichlorobenzene-d4	12.018	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Carene	136	C10H16	013466-78-9	96
2	(+)-3-Carene	136	C10H16	000498-15-7	87
3	.gamma.-Terpinene	136	C10H16	000099-85-4	87
4	.beta.-Pinene	136	C10H16	000127-91-3	81
5	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	81



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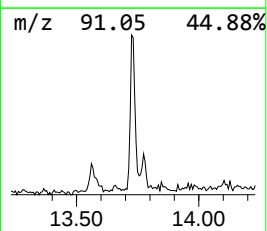
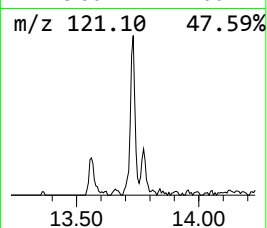
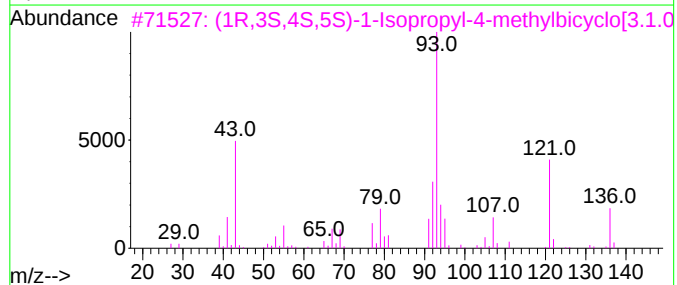
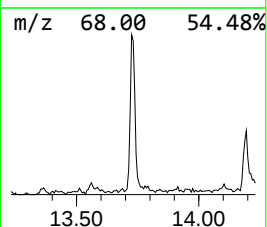
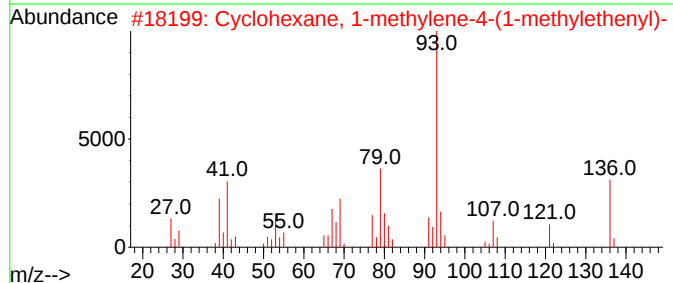
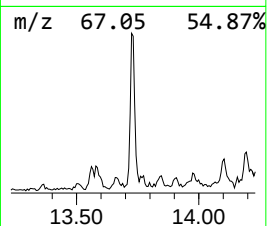
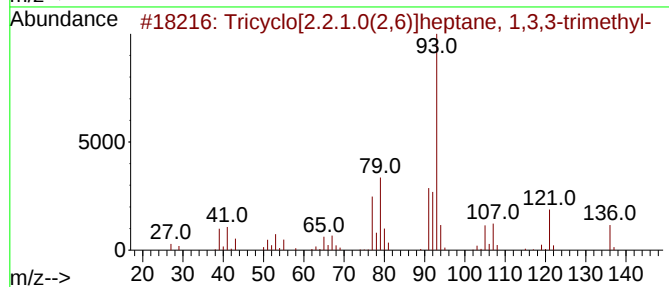
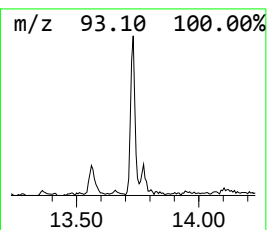
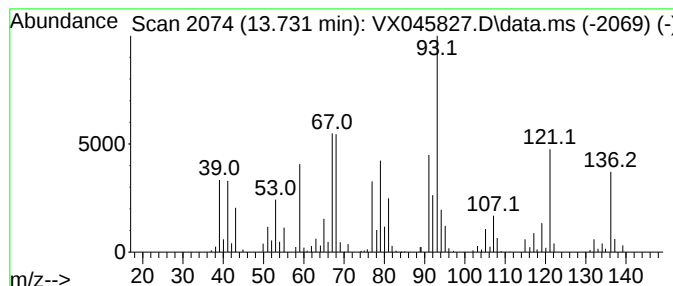
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Quant Title : SW846 8260

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

Peak Number 4 unknown13.731 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.731	13.02 ug/l	116595	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	49
2			Cyclohexane, 1-methylene-4-(1-me...	136	C10H16	000499-97-8	49
3			(1R,3S,4S,5S)-1-Isopropyl-4-meth...	196	C12H20O2	370557-87-2	49
4			3-Carene	136	C10H16	013466-78-9	49
5			.gamma.-Terpinene	136	C10H16	000099-85-4	46



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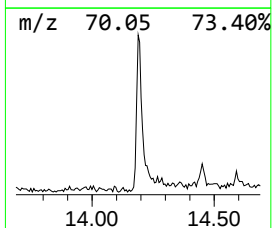
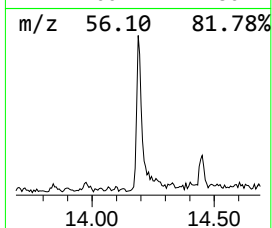
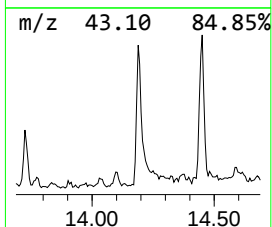
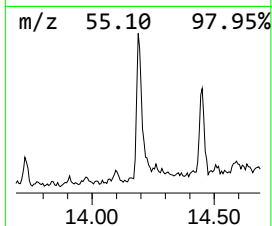
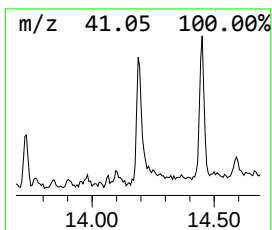
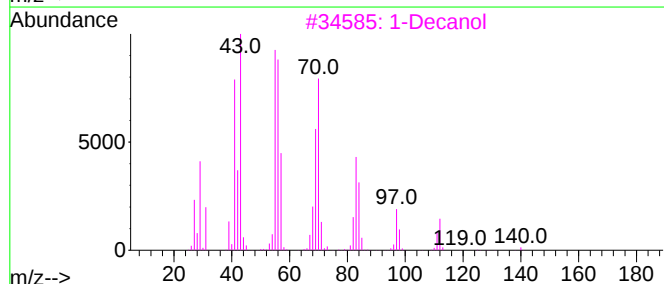
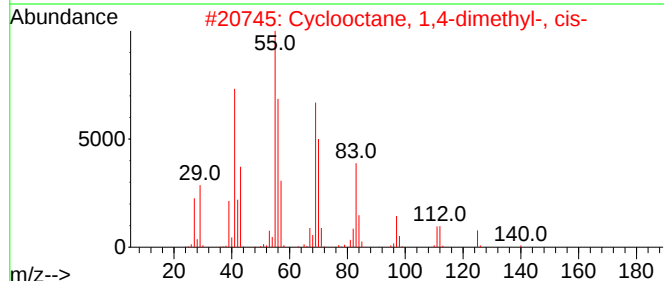
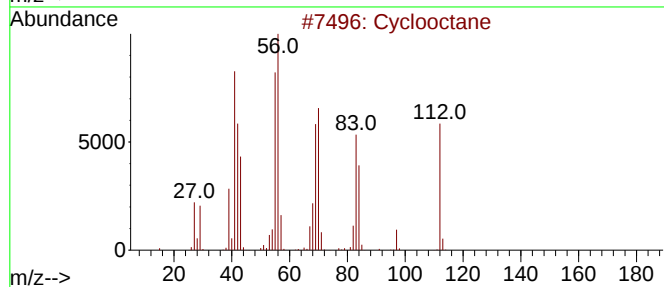
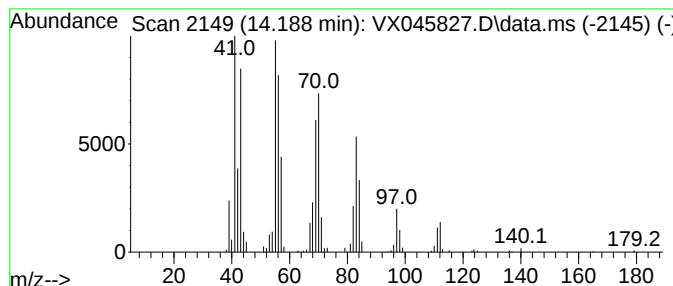
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Quant Title : SW846 8260

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

Peak Number 5 Cyclooctane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.188	13.33 ug/l	119365	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooctane	112	C8H16	000292-64-8	91
2			Cyclooctane, 1,4-dimethyl-, cis-	140	C10H20	013151-99-0	90
3			1-Decanol	158	C10H22O	000112-30-1	87
4			Cyclooctane, 1,4-dimethyl-, trans-	140	C10H20	013151-98-9	80
5			Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045827.D
Acq On : 17 Apr 2025 14:46
Operator : JC/MD
Sample : Q1818-05 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3828

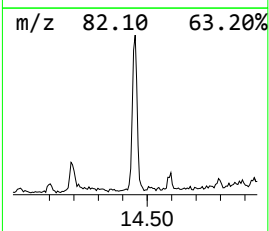
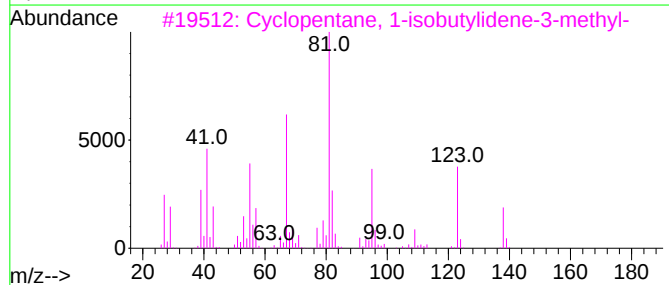
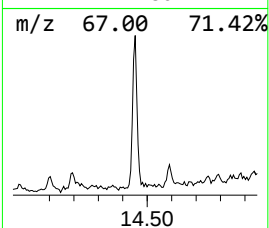
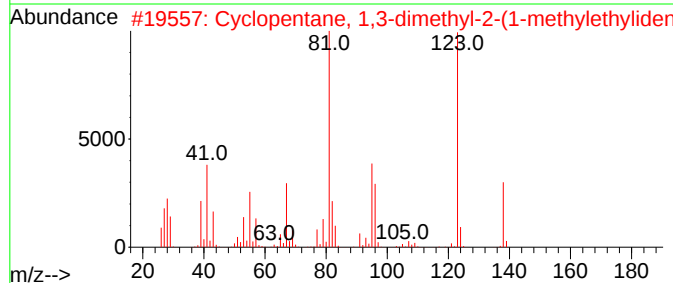
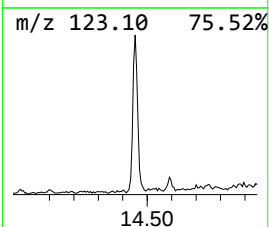
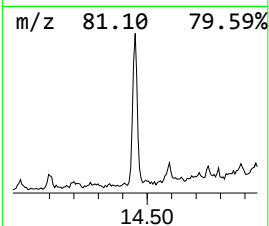
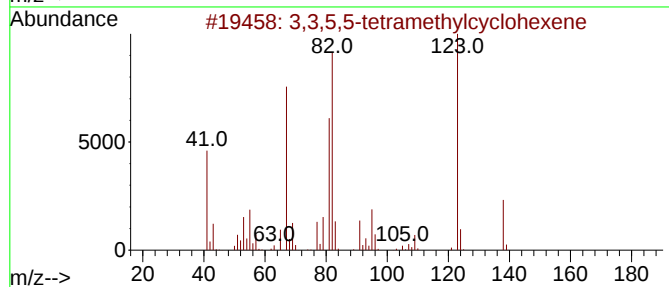
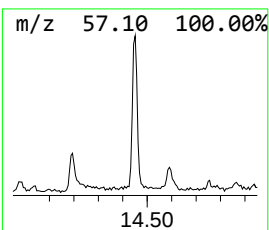
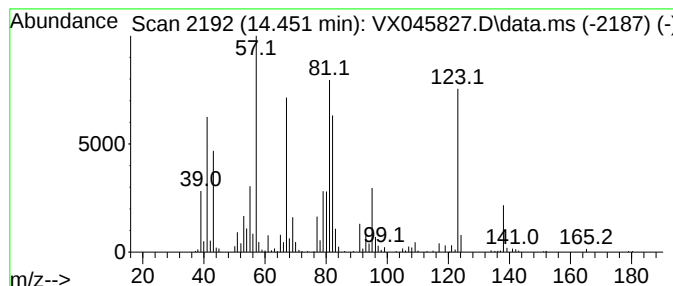
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Quant Title : SW846 8260

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

Peak Number 6 3,3,5,5-tetramethylcyclohexene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	19.11 ug/l	171179	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,3,5,5-tetramethylcyclohexene	138	C10H18	1000510-60-7	91
2			Cyclopentane, 1,3-dimethyl-2-(1-methylethylidene)-3-methyl-	138	C10H18	061142-30-1	58
3			Cyclopentane, 1-isobutylidene-3-methyl-	138	C10H18	1000150-62-1	49
4			Cyclohexene,1-(2-methylpropyl)-	138	C10H18	003983-03-7	46
5			Propylidencyclohexane	124	C9H16	002129-93-3	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045827.D
Acq On : 17 Apr 2025 14:46
Operator : JC/MD
Sample : Q1818-05 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3828

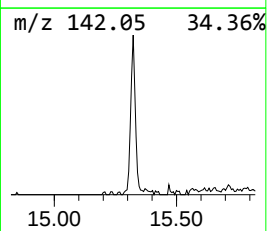
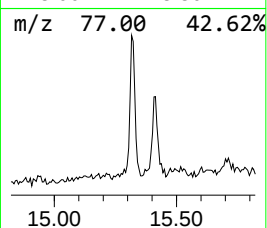
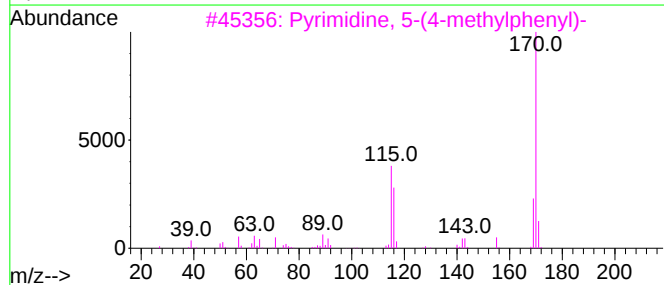
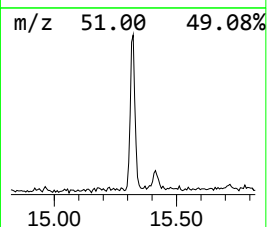
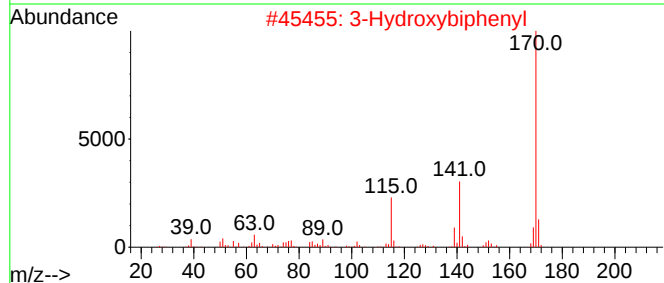
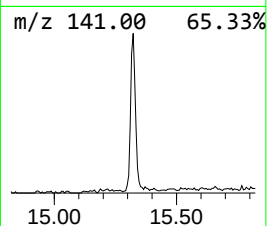
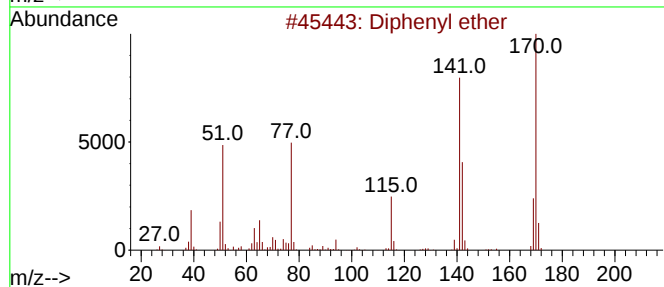
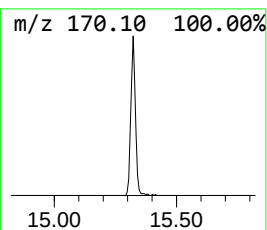
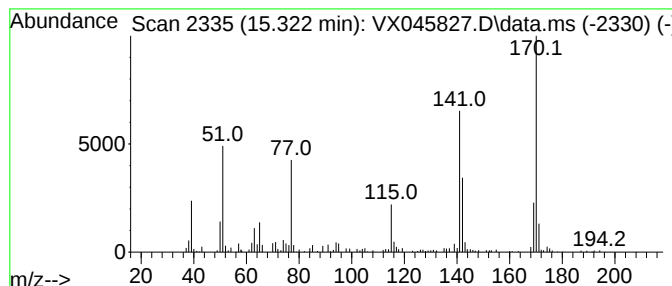
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Quant Title : SW846 8260

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

Peak Number 7 Diphenyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.322	9.27 ug/l	83031	1,4-Dichlorobenzene-d4	12.018

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Diphenyl ether	170	C12H10O	000101-84-8	98
2		3-Hydroxybiphenyl	170	C12H10O	000580-51-8	43
3		Pyrimidine, 5-(4-methylphenyl)-	170	C11H10N2	1000380-55-0	38
4		2-Troponyl difluoroborate	170	C7H5BF2O2	022502-10-9	38
5		Pyrazine, 2-(4-methylphenyl)-	170	C11H10N2	1000380-54-6	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045827.D
Acq On : 17 Apr 2025 14:46
Operator : JC/MD
Sample : Q1818-05 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3828

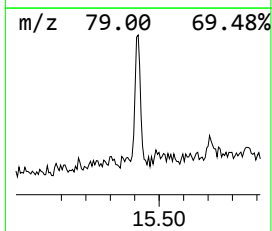
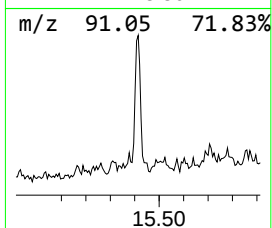
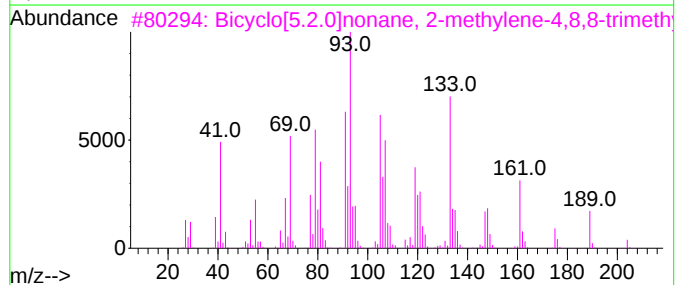
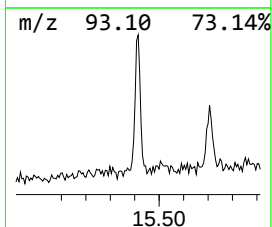
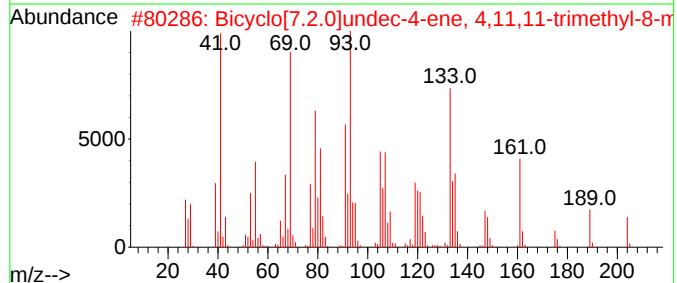
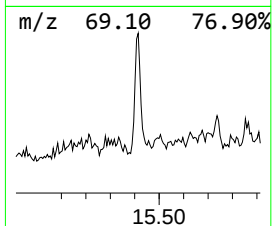
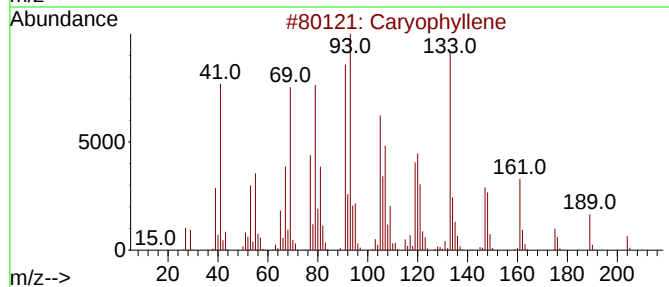
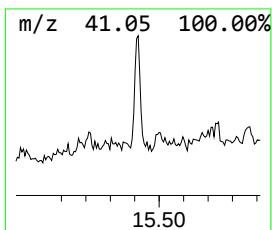
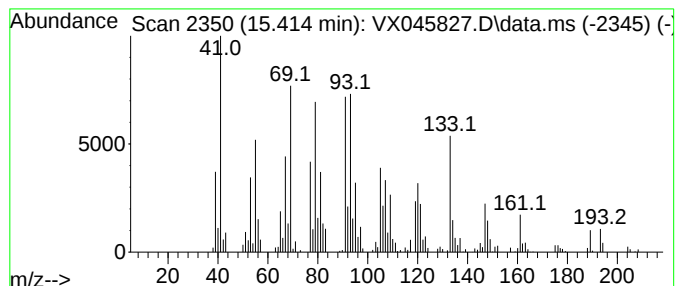
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Quant Title : SW846 8260

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

Peak Number 8 Caryophyllene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.414	15.30 ug/l	137040	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Caryophyllene	204	C15H24	000087-44-5	98
2			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	93
3			Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	90
4			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	87
5			Caryophyllene oxide	220	C15H24O	001139-30-6	41



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045827.D
Acq On : 17 Apr 2025 14:46
Operator : JC/MD
Sample : Q1818-05 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3828

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.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
Eucalyptol	12.097	8.7	ug/l	78155	4	12.018	447802	50.0
1-Octanol	12.579	40.1	ug/l	359300	4	12.018	447802	50.0
3-Carene	12.817	14.4	ug/l	128583	4	12.018	447802	50.0
unknown13.731	13.731	13.0	ug/l	116595	4	12.018	447802	50.0
Cyclooctane	14.188	13.3	ug/l	119365	4	12.018	447802	50.0
3,3,5,5-tetrame...	14.451	19.1	ug/l	171179	4	12.018	447802	50.0
Diphenyl ether	15.322	9.3	ug/l	83031	4	12.018	447802	50.0
Caryophyllene	15.414	15.3	ug/l	137040	4	12.018	447802	50.0