

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD051322\
 Data File : VD073019.D
 Acq On : 14 May 2022 06:16
 Operator : VA/SY
 Sample : N2823-05
 Misc : 5.04G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 SC-5

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_D\Method\82D050222S.M
 Title : SW846 8260

Signal : TIC: VD073019.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.156	370	380	390	rBV2	40132	114961	1.32%	0.421%
2	7.191	885	896	912	rBV2	119787	362199	4.15%	1.328%
3	7.908	1008	1018	1023	rBV	235720	571940	6.56%	2.097%
4	7.973	1023	1029	1041	rVB	447853	1006108	11.54%	3.688%
5	8.326	1073	1089	1100	rBV3	225236	605407	6.94%	2.219%
6	8.861	1169	1180	1190	rBV	670042	1321166	15.15%	4.844%
7	9.044	1202	1211	1222	rBV2	61486	133005	1.52%	0.488%
8	10.220	1401	1411	1422	rBV	410802	731761	8.39%	2.683%
9	10.332	1422	1430	1437	rVV	1086060	1970751	22.60%	7.225%
10	11.638	1644	1652	1660	rBV	968233	1698394	19.47%	6.226%
11	11.714	1660	1665	1674	rVB	59328	102520	1.18%	0.376%
12	12.161	1734	1741	1749	rBV	648394	1028743	11.80%	3.771%
13	12.238	1749	1754	1765	rVB	78973	145468	1.67%	0.533%
14	12.620	1812	1819	1827	rVB	806054	1329499	15.24%	4.874%
15	12.896	1856	1866	1870	rBV5	62289	174888	2.01%	0.641%
16	12.938	1870	1873	1879	rVB	85314	128251	1.47%	0.470%
17	13.296	1924	1934	1941	rBV	113434	227799	2.61%	0.835%
18	13.561	1972	1979	1987	rBV	1021621	1665511	19.10%	6.106%
19	13.655	1987	1995	2011	rBV	5627059	8721806	100.00%	31.975%
20	14.020	2053	2057	2064	rVB2	78879	127506	1.46%	0.467%
21	14.232	2086	2093	2100	rBV	279081	468875	5.38%	1.719%
22	14.443	2122	2129	2135	rBV	345128	577285	6.62%	2.116%
23	14.879	2196	2203	2207	rBV5	96362	159005	1.82%	0.583%
24	15.085	2230	2238	2249	rBV2	389866	749049	8.59%	2.746%
25	15.379	2281	2288	2298	rBV	1223954	2286288	26.21%	8.382%
26	15.496	2298	2308	2317	rVB5	51200	154255	1.77%	0.566%
27	16.473	2466	2474	2486	rBV	253728	537034	6.16%	1.969%
28	16.679	2500	2509	2516	rBV3	75883	177419	2.03%	0.650%

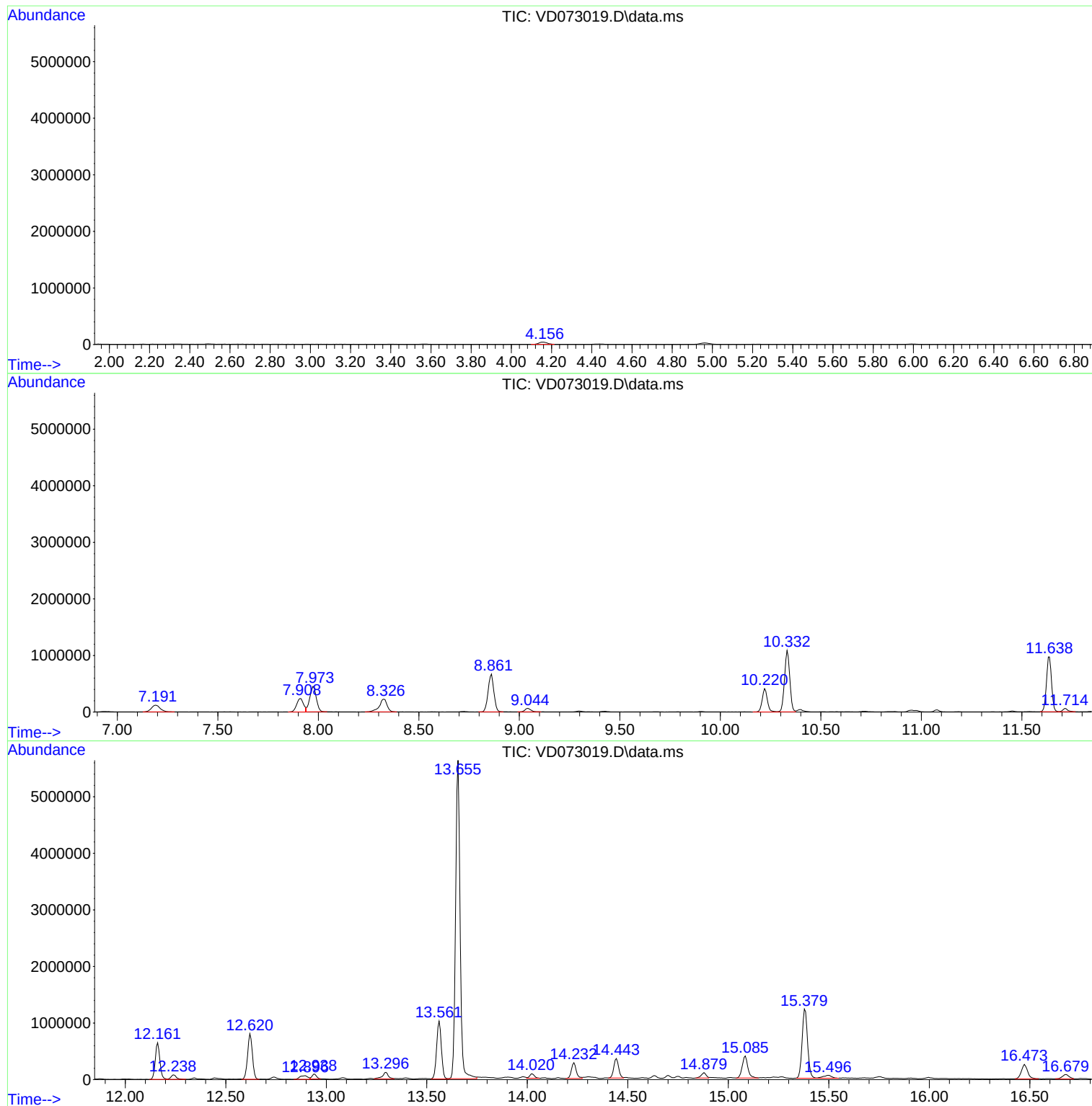
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ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
SC-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
SC-5

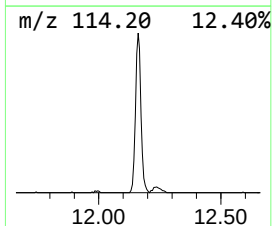
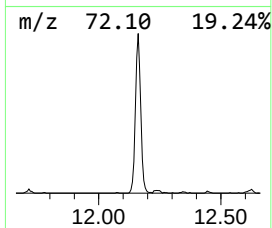
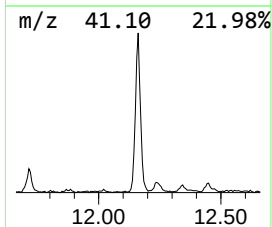
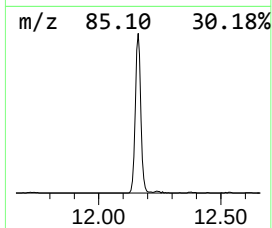
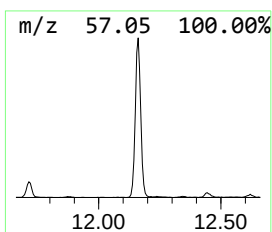
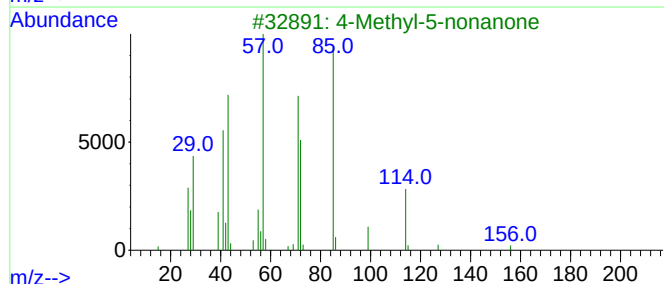
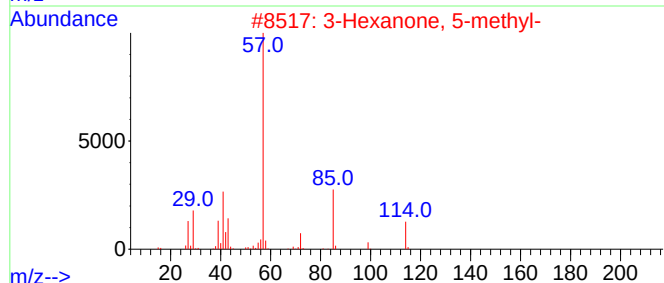
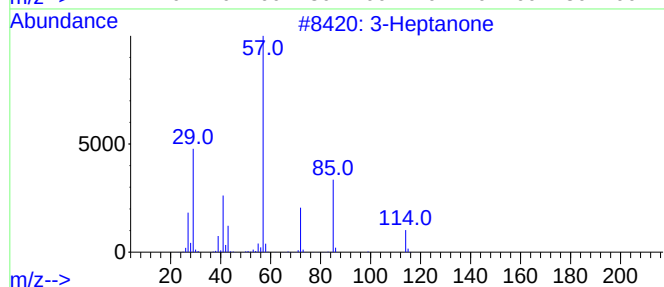
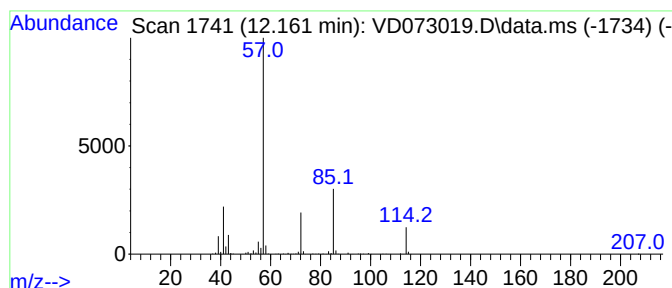
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
Quant Title : SW846 8260

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

Peak Number 1 3-Heptanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.161	30.29 ug/l	1028740	Chlorobenzene-d5	11.632

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptanone	114	C7H14O	000106-35-4	91
2			3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	53
3			4-Methyl-5-nonanone	156	C10H20O	035900-26-6	53
4			2-Butanone, 3,3-dimethyl-1-thioc...	157	C7H11NOS	057518-71-5	50
5			2-Butanone, 1-bromo-3,3-dimethyl-	178	C6H11BrO	005469-26-1	38



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SC-5

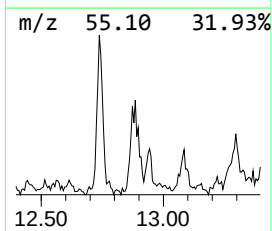
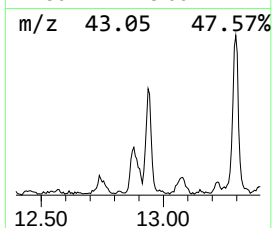
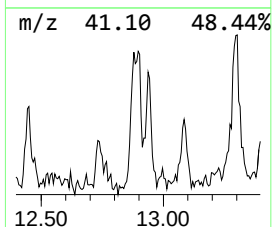
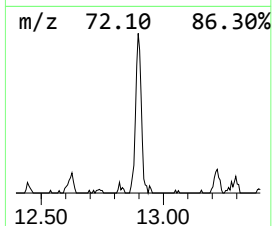
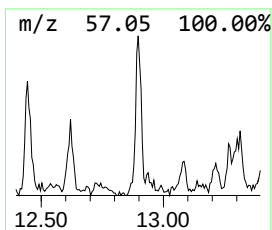
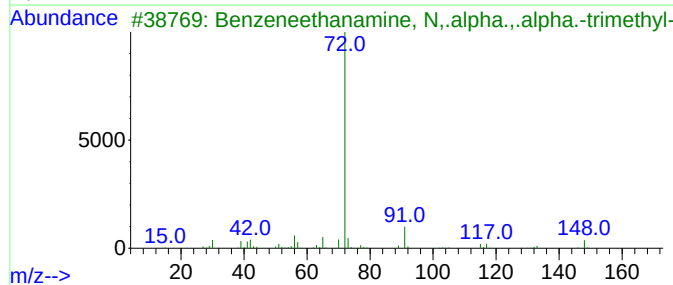
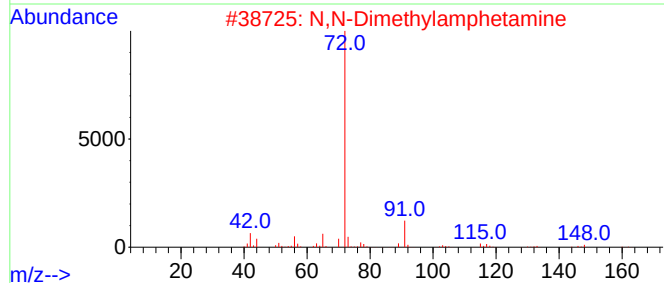
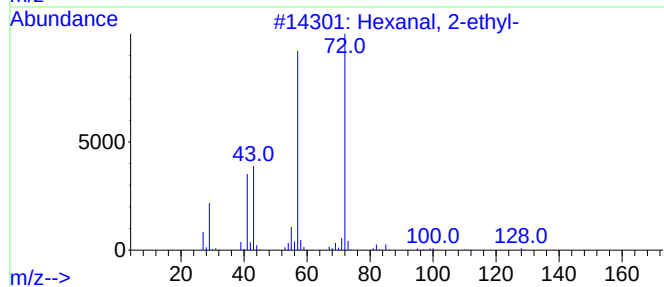
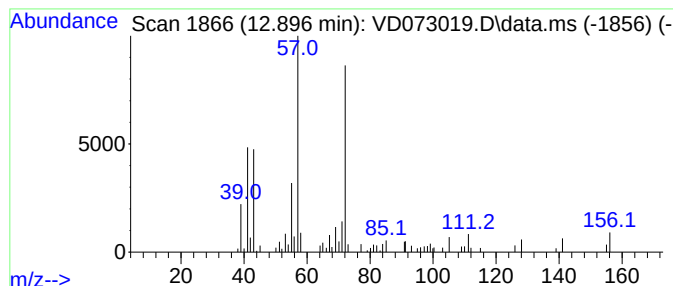
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
Quant Title : SW846 8260

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

Peak Number 2 Hexanal, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.896	5.25 ug/l	174888	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	50
2			N,N-Dimethylamphetamine	163	C11H17N	033286-27-0	47
3			Benzeneethanamine, N,.alpha.,.al...	163	C11H17N	000100-92-5	47
4			Boron, (N,2-dimethyl-2-propanami...	305	C8H13BF9N	128353-59-3	45
5			2-Methylpropanamide, N-(2-phenyl...	233	C15H23NO	1000490-77-7	38



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ALS Vial : 42 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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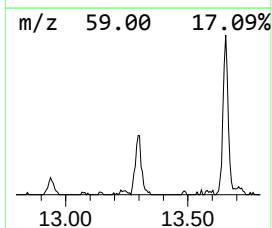
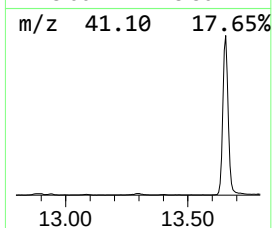
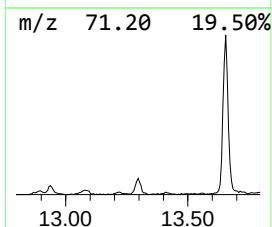
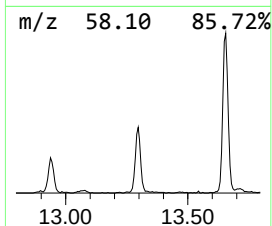
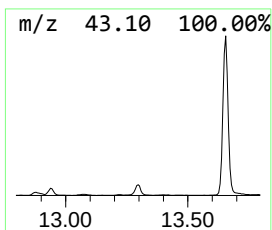
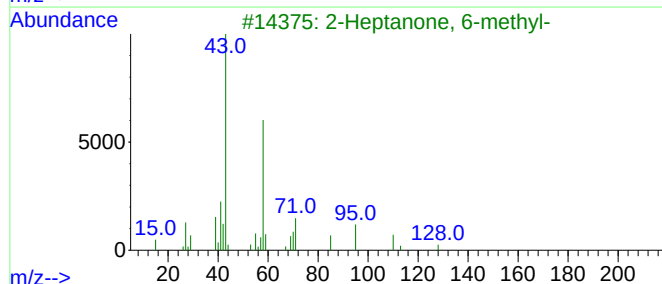
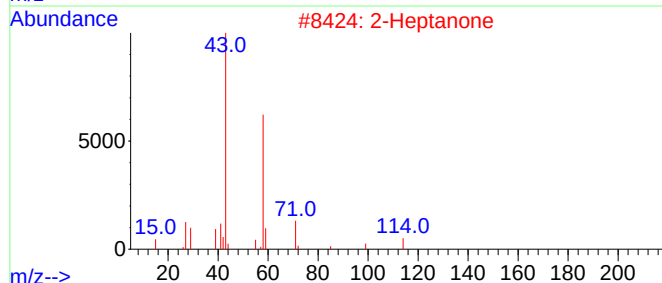
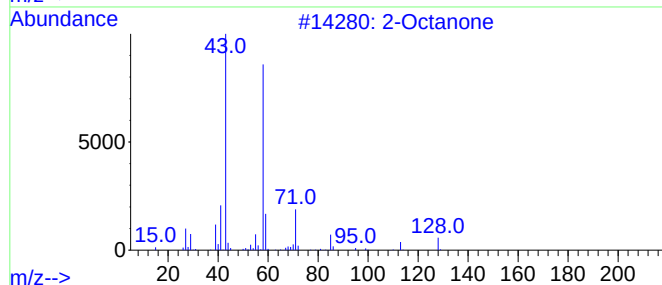
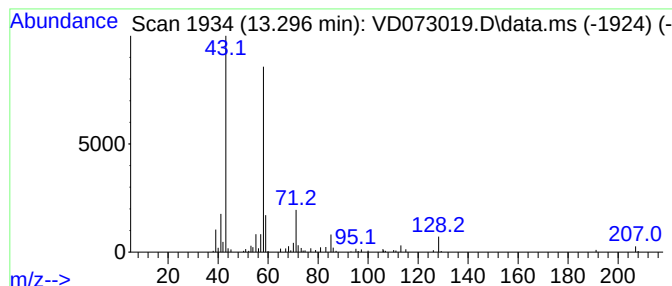
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
Quant Title : SW846 8260

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

Peak Number 3 2-Octanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.296	6.84 ug/l	227799	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octanone	128	C8H16O	000111-13-7	91
2			2-Heptanone	114	C7H14O	000110-43-0	72
3			2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	64
4			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	56
5			2-Nonanone	142	C9H18O	000821-55-6	56



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Misc : 5.04G/5.00ml/MSVOA_D/SOIL
ALS Vial : 42 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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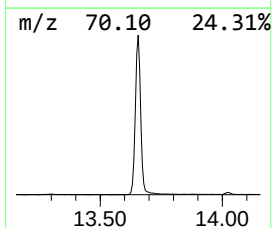
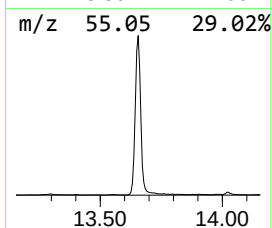
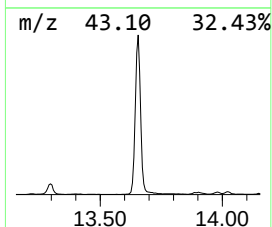
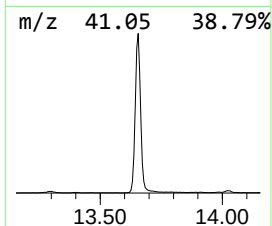
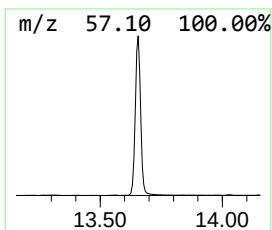
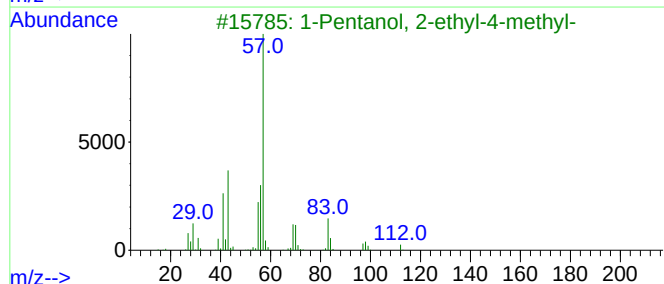
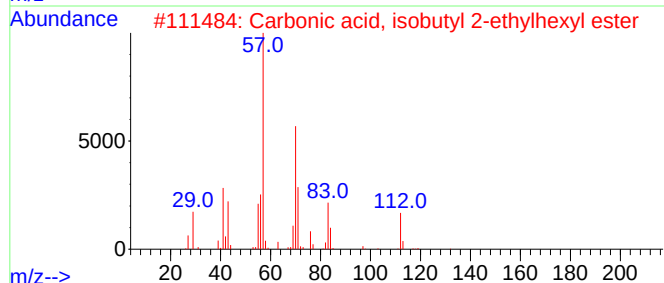
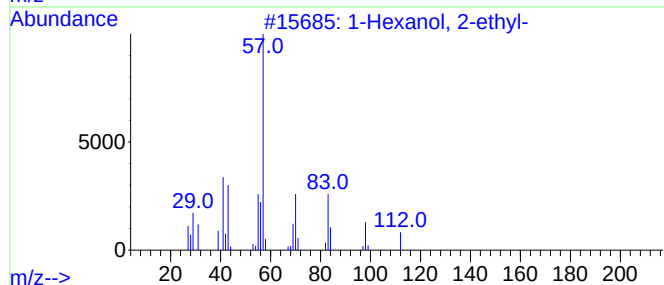
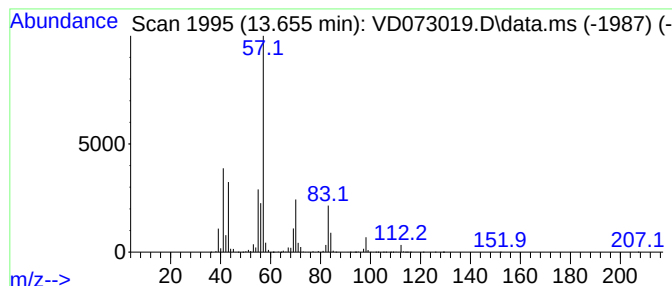
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Quant Title : SW846 8260

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.655	261.84 ug/l	8721810	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	59
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
5			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	53



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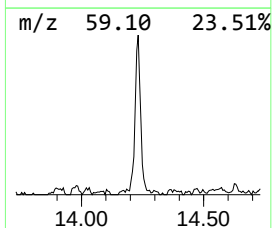
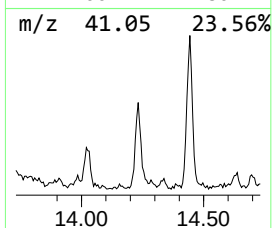
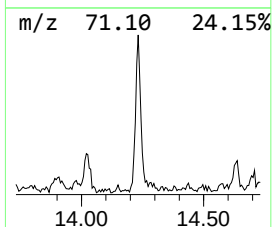
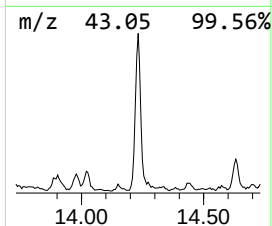
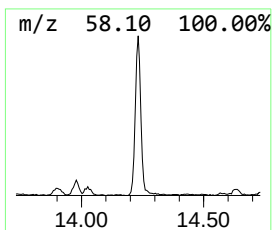
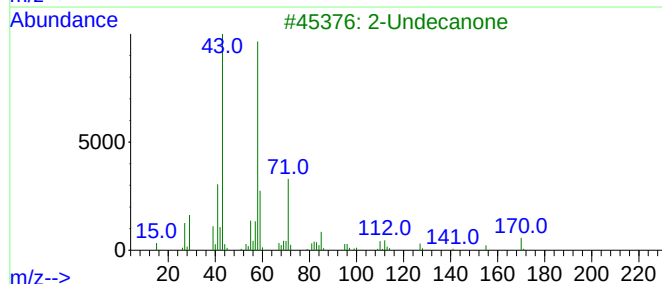
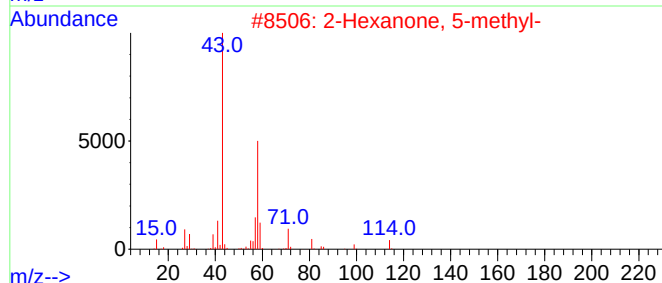
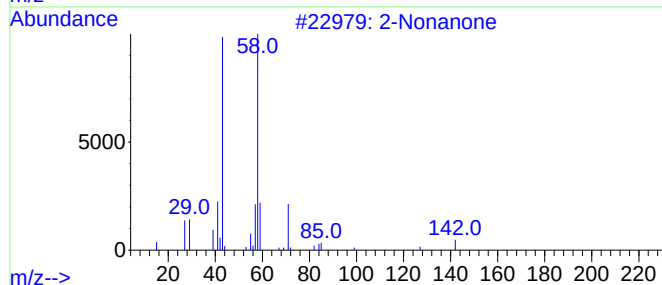
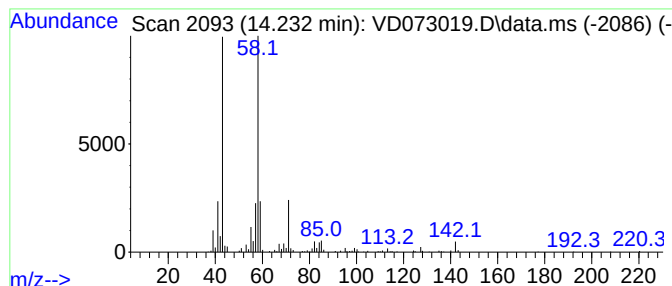
Instrument :
MSVOA_D
ClientSampleId :
SC-5

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Quant Title : SW846 8260

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

Peak Number 5 2-Nonanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.232	14.08 ug/l	468875	1,4-Dichlorobenzene-d4		13.561	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Nonanone		142	C9H18O	000821-55-6	94
2	2-Hexanone, 5-methyl-		114	C7H14O	000110-12-3	78
3	2-Undecanone		170	C11H22O	000112-12-9	78
4	2-Dodecanone		184	C12H24O	006175-49-1	78
5	2-Heptanone		114	C7H14O	000110-43-0	64



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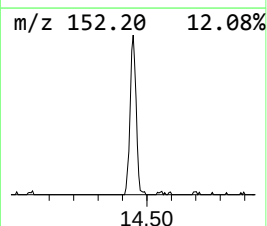
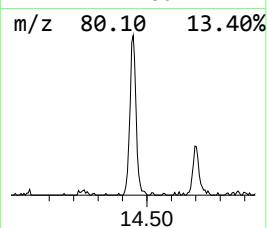
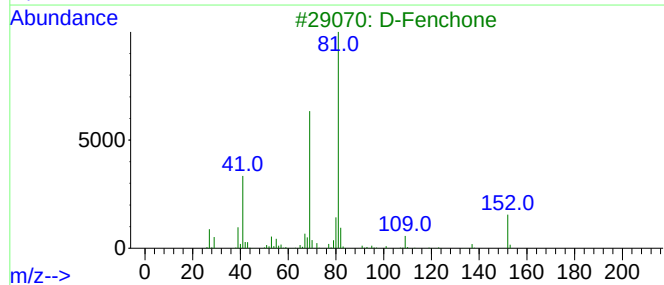
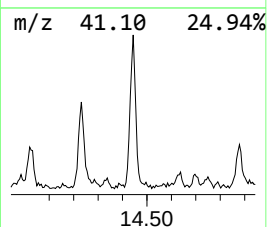
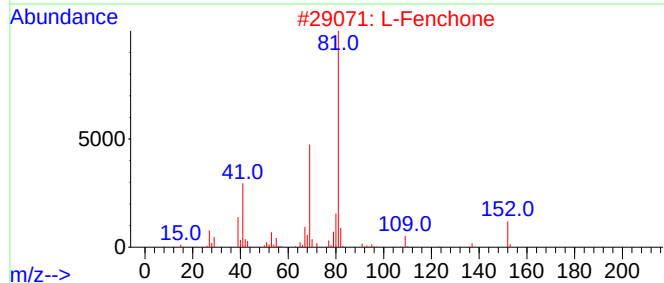
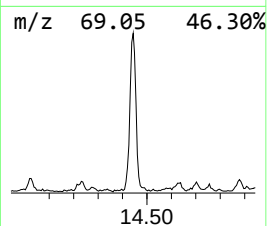
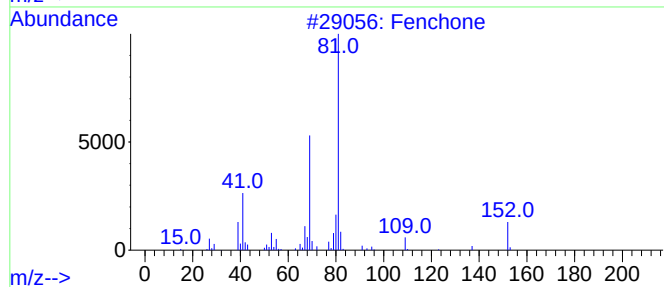
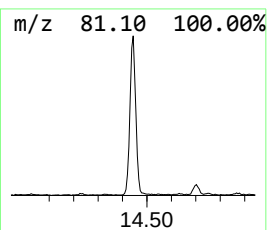
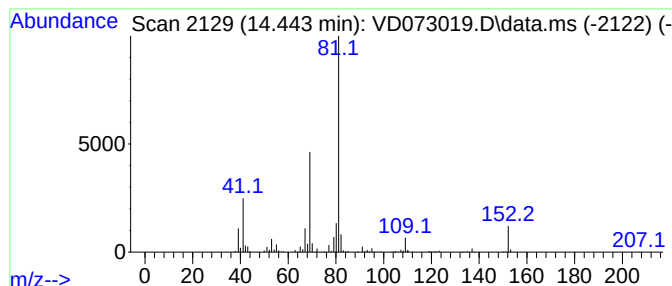
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Quant Title : SW846 8260

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

Peak Number 6 Fenchone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.443	17.33 ug/l	577285	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchone	152	C10H16O	001195-79-5	95
2			L-Fenchone	152	C10H16O	007787-20-4	94
3			D-Fenchone	152	C10H16O	004695-62-9	90
4			2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	50
5			Cyclohexane, 1,3-dichloro-, cis-	152	C6H10Cl2	024955-63-3	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD051322\
Data File : VD073019.D
Acq On : 14 May 2022 06:16
Operator : VA/SY
Sample : N2823-05
Misc : 5.04G/5.00ml/MSVOA_D/SOIL
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
SC-5

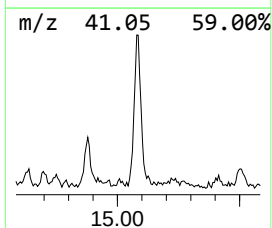
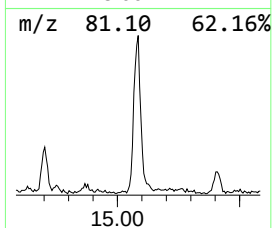
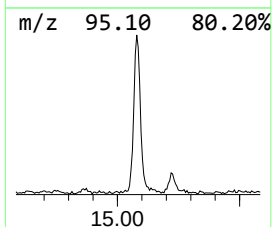
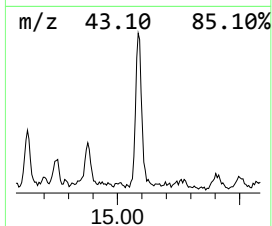
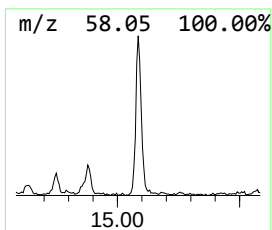
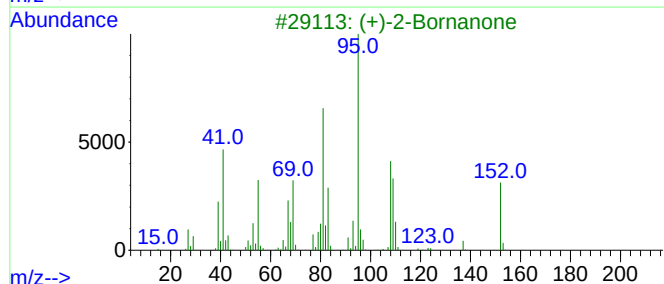
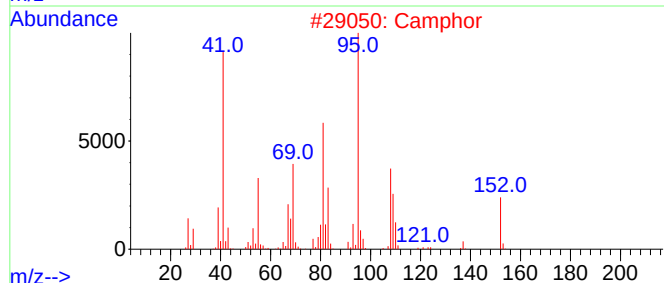
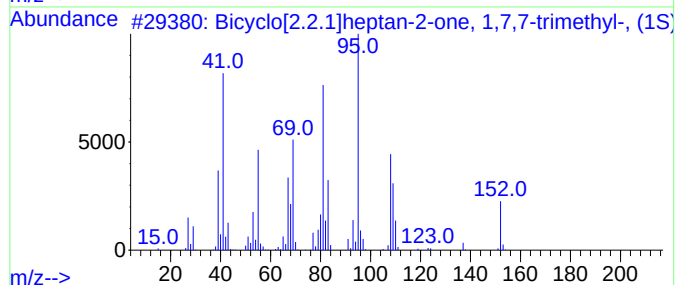
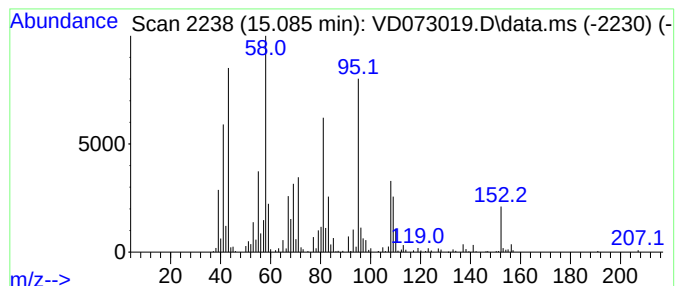
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Quant Title : SW846 8260

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

Peak Number 7 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.085	22.49 ug/l	749049	1,4-Dichlorobenzene-d4	13.561

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	96
2		Camphor	152	C10H16O	000076-22-2	95
3		(+)-2-Bornanone	152	C10H16O	000464-49-3	95
4		2-Decanone	156	C10H20O	000693-54-9	70
5		5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD051322\
Data File : VD073019.D
Acq On : 14 May 2022 06:16
Operator : VA/SY
Sample : N2823-05
Misc : 5.04G/5.00ml/MSVOA_D/SOIL
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
SC-5

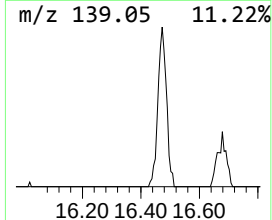
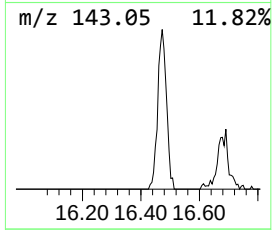
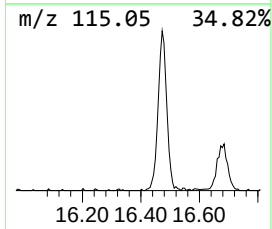
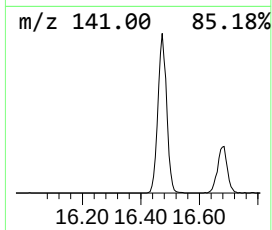
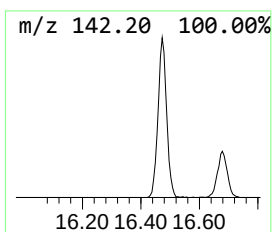
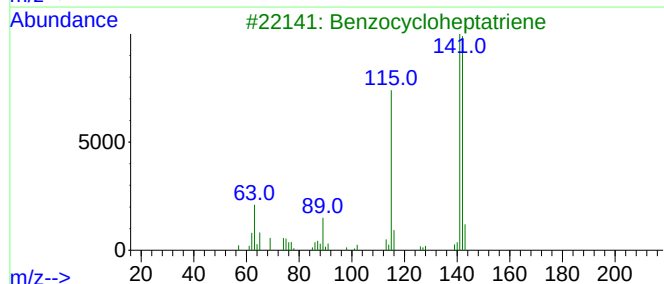
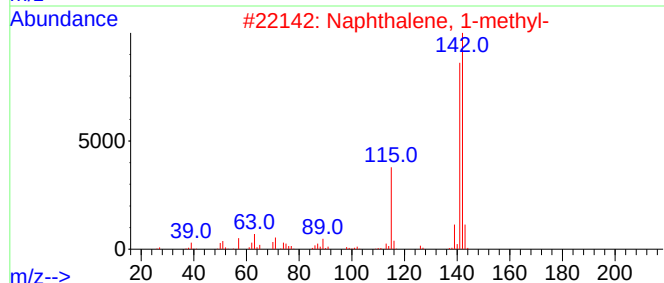
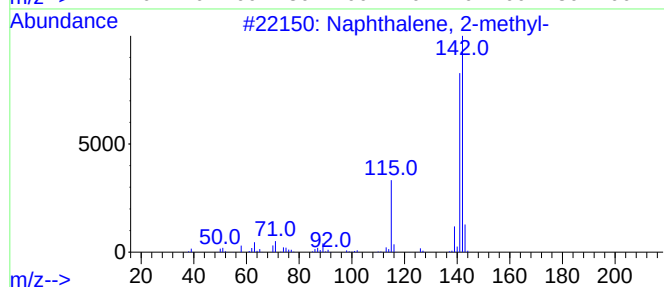
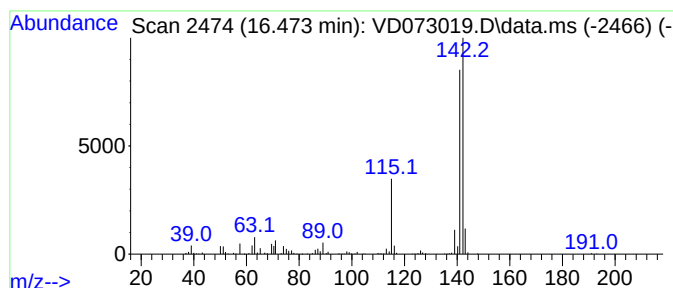
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.473	16.12 ug/l	537034	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	94
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1-Naphthaleneacetamide	185	C12H11NO	000086-86-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD051322\
Data File : VD073019.D
Acq On : 14 May 2022 06:16
Operator : VA/SY
Sample : N2823-05
Misc : 5.04G/5.00ml/MSVOA_D/SOIL
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
SC-5

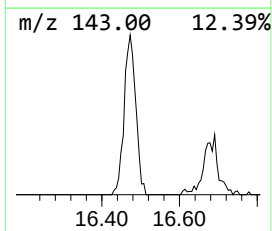
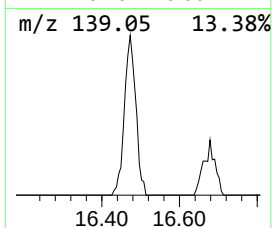
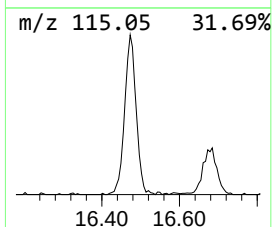
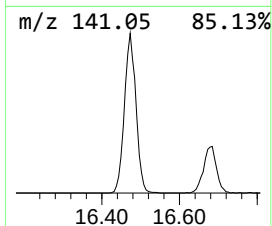
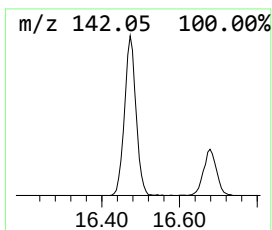
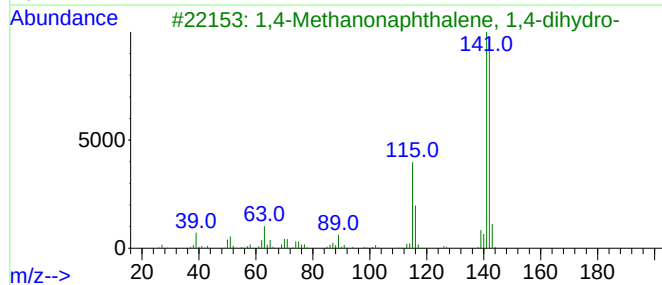
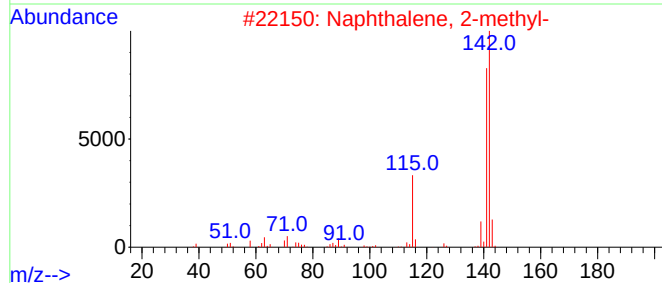
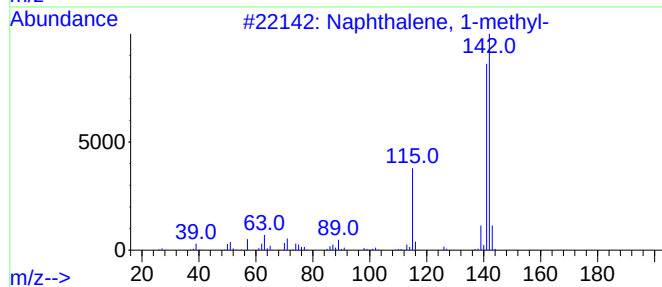
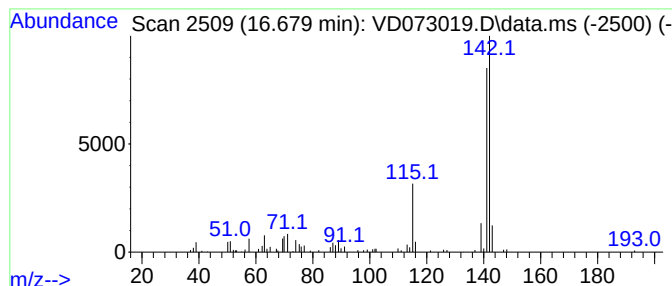
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
Quant Title : SW846 8260

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

Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.679	5.33 ug/l	177419	1,4-Dichlorobenzene-d4	13.561

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	91
3		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4		Benzocycloheptatriene	142	C11H10	000264-09-5	90
5		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD051322\
Data File : VD073019.D
Acq On : 14 May 2022 06:16
Operator : VA/SY
Sample : N2823-05
Misc : 5.04G/5.00ml/MSVOA_D/SOIL
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
SC-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.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
3-Heptanone	12.161	30.3	ug/l	1028740	3	11.632	1698390	50.0
Hexanal, 2-ethyl-	12.896	5.3	ug/l	174888	4	13.561	1665510	50.0
2-Octanone	13.296	6.8	ug/l	227799	4	13.561	1665510	50.0
1-Hexanol, 2-et...	13.655	261.8	ug/l	8721810	4	13.561	1665510	50.0
2-Nonanone	14.232	14.1	ug/l	468875	4	13.561	1665510	50.0
Fenchone	14.443	17.3	ug/l	577285	4	13.561	1665510	50.0
Bicyclo[2.2.1]h...	15.085	22.5	ug/l	749049	4	13.561	1665510	50.0
Naphthalene, 1-...	16.473	16.1	ug/l	537034	4	13.561	1665510	50.0
1,4-Methanonaph...	16.679	5.3	ug/l	177419	4	13.561	1665510	50.0