LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045828.D
Acq On : 17 Apr 2025 15:09
Operator : JC/MD
Sample : Q1818-06 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3829

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: VX045828.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.544	67	75	76	rBV4	4402	7242	1.49%	0.222%
2	5.379	691	704	721	rBV	55566	165047	33.93%	5.050%
3	5.544	721	731	749	rVV2	80752	236811	48.68%	7.245%
4	5.952	787	798	812	rBV	64619	174769	35.93%	5.347%
5	6.757	921	930	950	rBV2	141860	351072	72.17%	10.741%
6	8.647	1233	1240	1259	rBV	294267	486421	100.00%	14.882%
7	10.049	1465	1470	1487	rBV	329765	445295	91.55%	13.624%
8	10.994	1621	1625	1634	rBV2	11602	21523	4.42%	0.658%
9	11.079	1634	1639	1652	rVV	270882	353421	72.66%	10.813%
10	11.591	1719	1723	1728	rBV3	4656	5964	1.23%	0.182%
11	11.969	1781	1785	1788	rBV	25961	30662	6.30%	0.938%
12	12.018	1788	1793	1801	rVB	343372	423331	87.03%	12.952%
13	12.097	1802	1806	1810	rVV2	16352	21302	4.38%	0.652%
14	12.579	1881	1885	1898	rBV	78100	131408	27.02%	4.020%
15	12.768	1911	1916	1920	rBV2	9816	14121	2.90%	0.432%
16	12.817	1920	1924	1928	rVV2	36364	45372	9.33%	1.388%
17	12.853	1928	1930	1934	rVB5	4653	5521	1.14%	0.169%
18	13.561	2043	2046	2049	rBV4	5978	8288	1.70%	0.254%
19	13.731	2069	2074	2079	rVB	44153	57016	11.72%	1.744%
20	14.097	2132	2134	2142	rVB8	3297	5946	1.22%	0.182%
21	14.188	2146	2149	2161	rVV2	58897	102429	21.06%	3.134%
22	14.451	2188	2192	2202	rVB	64335	87239	17.93%	2.669%
23	15.322	2330	2335	2341	rBV	27072	40119	8.25%	1.227%
24	15.414	2346	2350	2358	rVB4	29541	48253	9.92%	1.476%

Sum of corrected areas: 3268572

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
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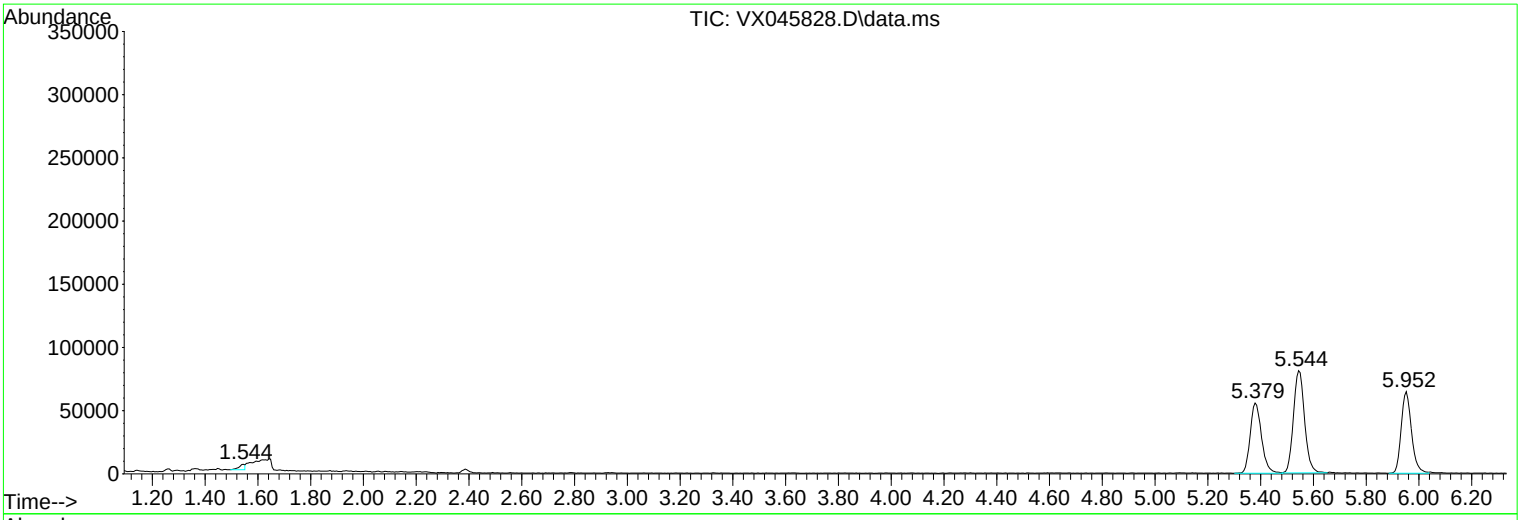
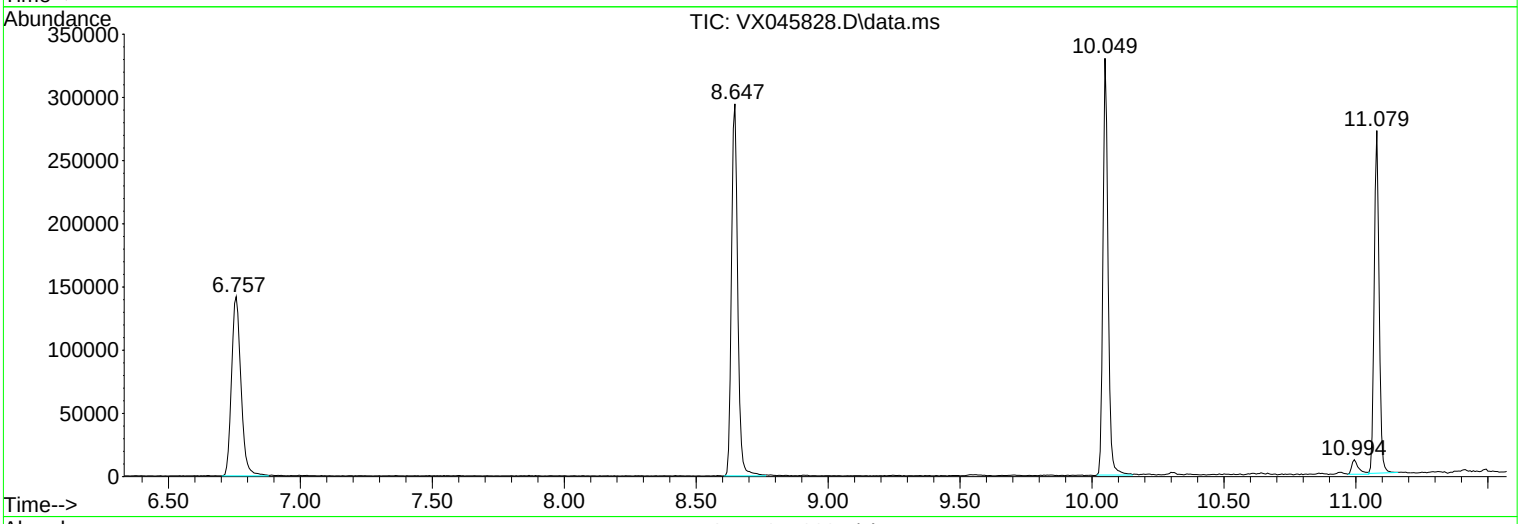
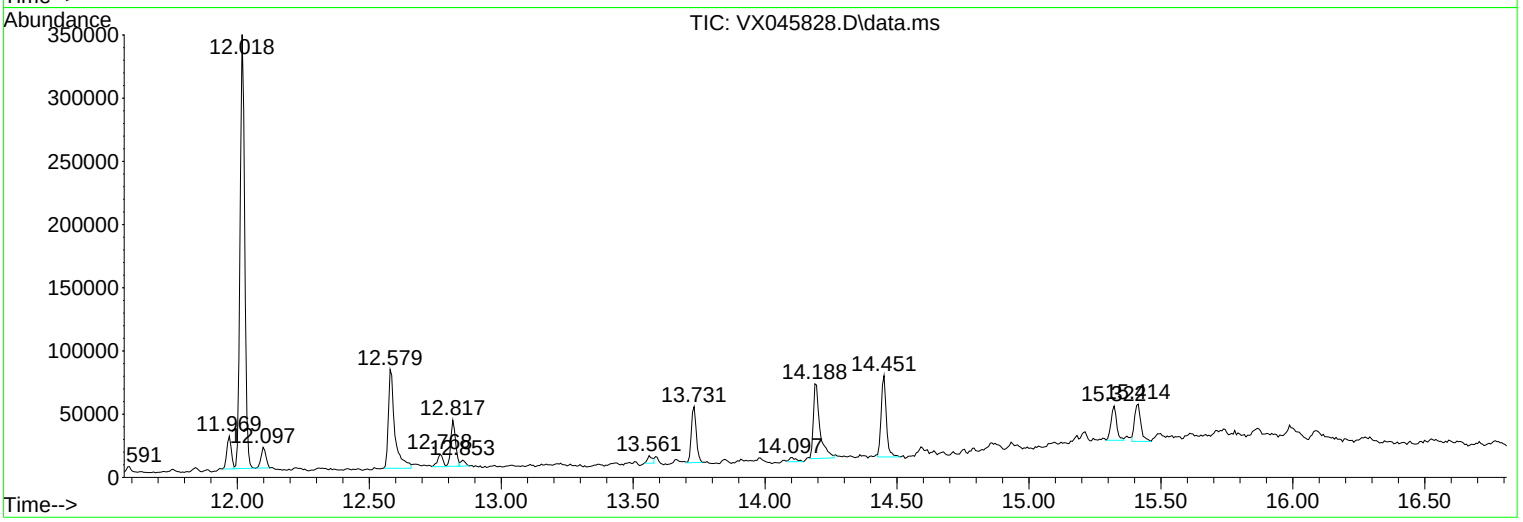
Instrument :
MSVOA_X
ClientSampleId :
3829

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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Data File : VX045828.D
Acq On : 17 Apr 2025 15:09
Operator : JC/MD
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MSVOA_X
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Quant Title : SW846 8260

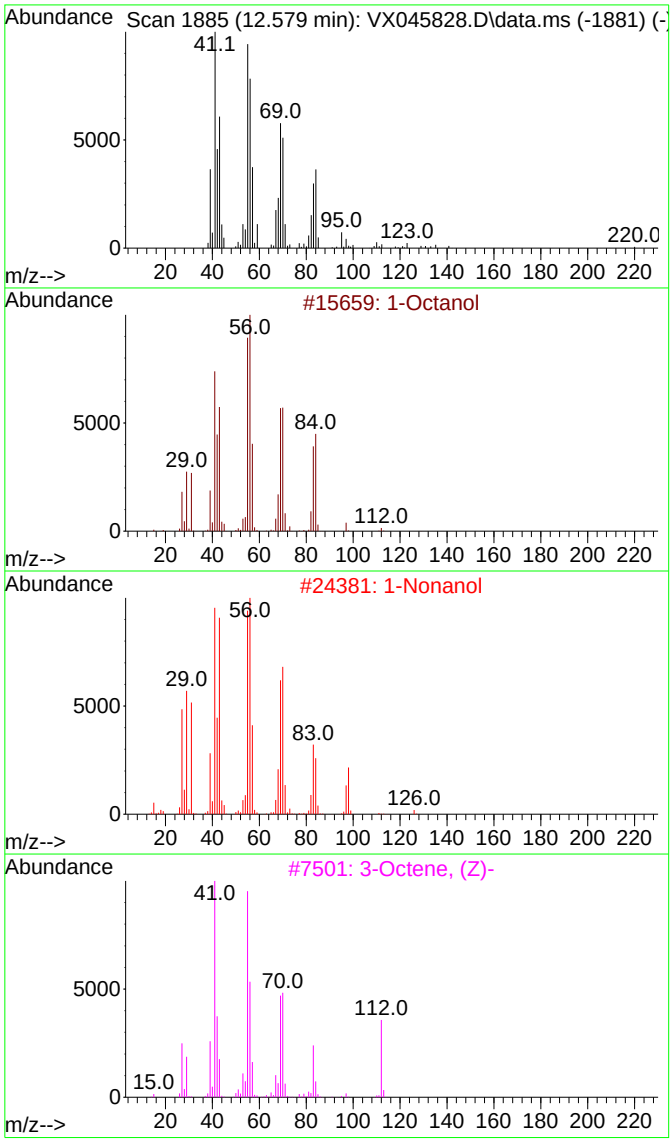
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

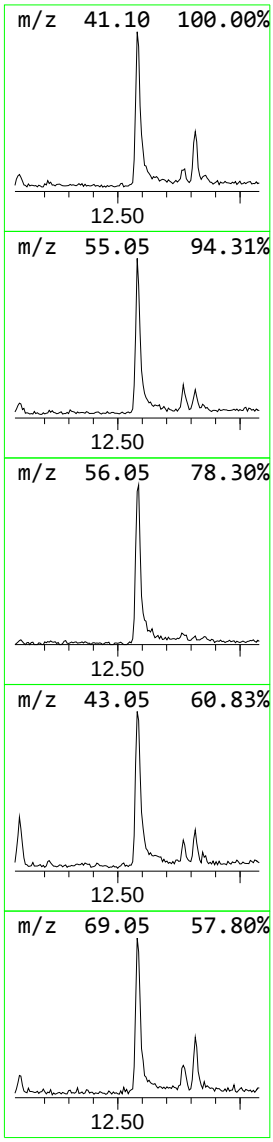
****

Peak Number 1 1-Octanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.579	15.52 ug/l	131408	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol	130	C8H18O	000111-87-5	86
2	1-Nonanol	144	C9H20O	000143-08-8	78
3	3-Octene, (Z)-	112	C8H16	014850-22-7	64
4	1-Heptene, 3-methyl-	112	C8H16	004810-09-7	52
5	1-Octene	112	C8H16	000111-66-0	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045828.D
Acq On : 17 Apr 2025 15:09
Operator : JC/MD
Sample : Q1818-06 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3829

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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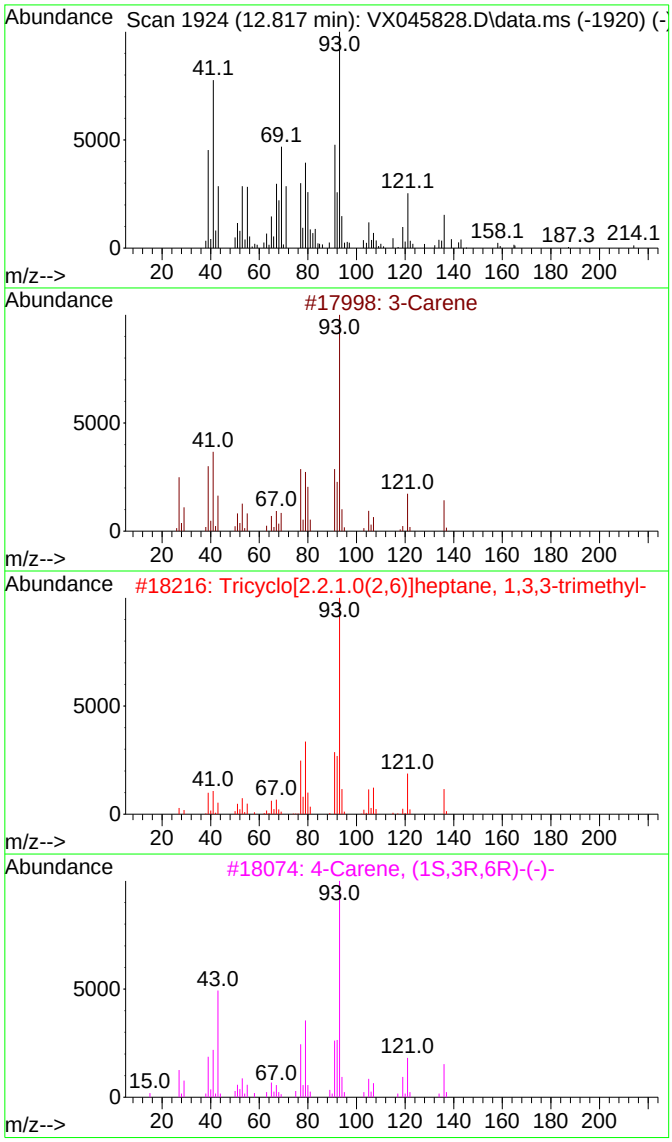
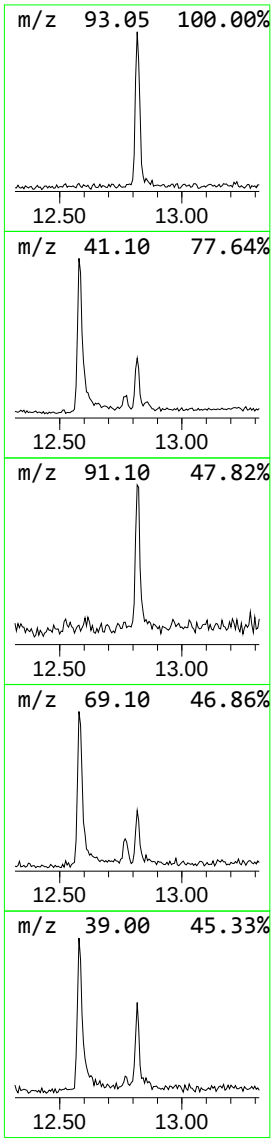
Peak Number 2 3-Carene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.817	5.36 ug/l	45372	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Carene	136	C10H16	013466-78-9	94
2	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	89
3	4-Carene, (1S,3R,6R)-(-)-	136	C10H16	005208-49-1	76
4	Camphene	136	C10H16	000079-92-5	74
5	(+)-4-Carene	136	C10H16	029050-33-7	68





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Data File : VX045828.D
Acq On : 17 Apr 2025 15:09
Operator : JC/MD
Sample : Q1818-06 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3829

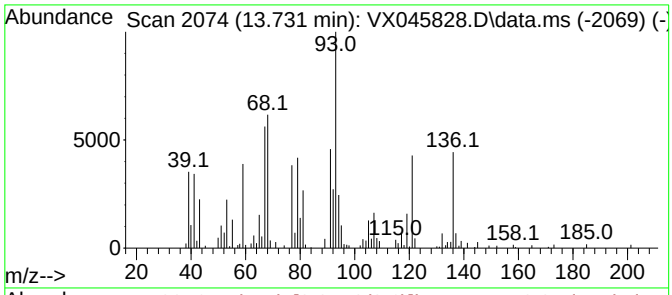
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

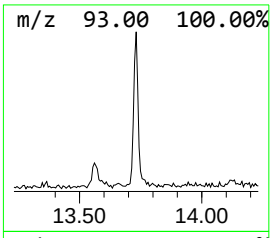
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

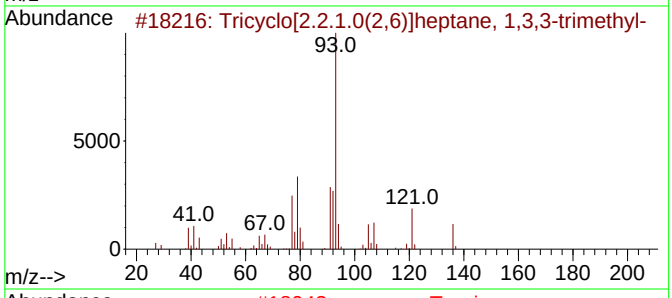
****
Peak Number 3 Tricyclo[2.2.1.0(2,6)]hepta... Concentration Rank 4

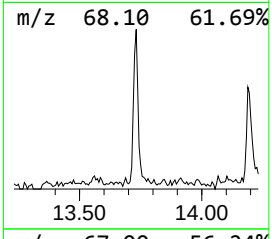
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.731	6.73 ug/l	57016	1,4-Dichlorobenzene-d4	12.018

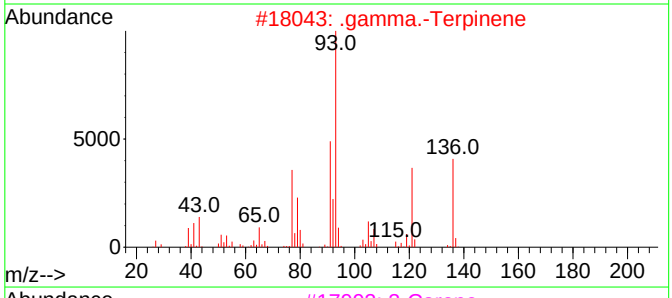
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	93
2	.gamma.-Terpinene	136	C10H16	000099-85-4	90
3	3-Carene	136	C10H16	013466-78-9	83
4	(+)-4-Carene	136	C10H16	029050-33-7	60
5	(+)-3-Carene	136	C10H16	000498-15-7	60

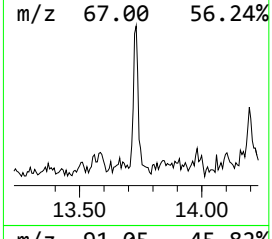


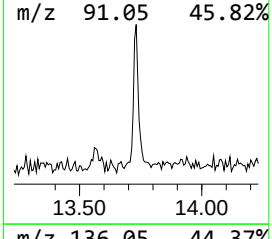


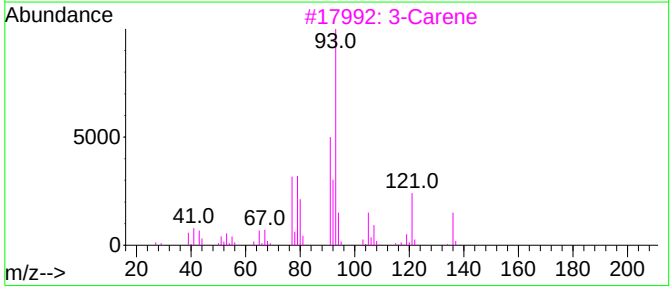


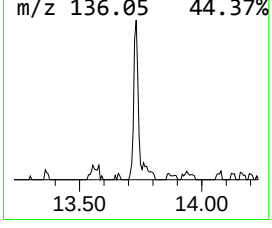












Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
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Sample : Q1818-06 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3829

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

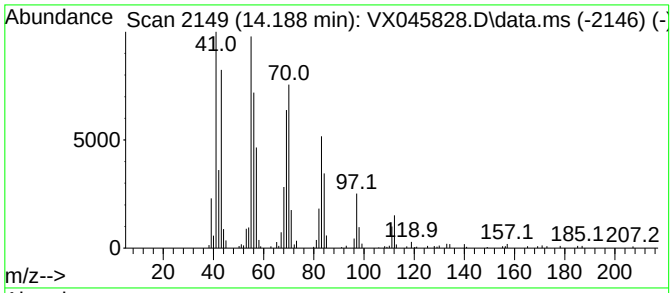
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

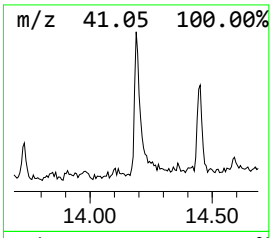
****

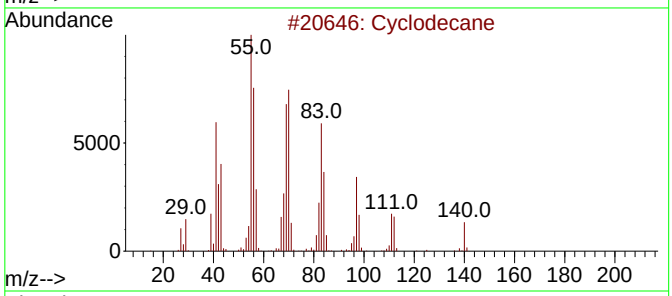
Peak Number 4 Cyclodecane Concentration Rank 2

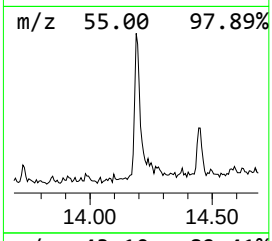
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.188	12.10 ug/l	102429	1,4-Dichlorobenzene-d4	12.018

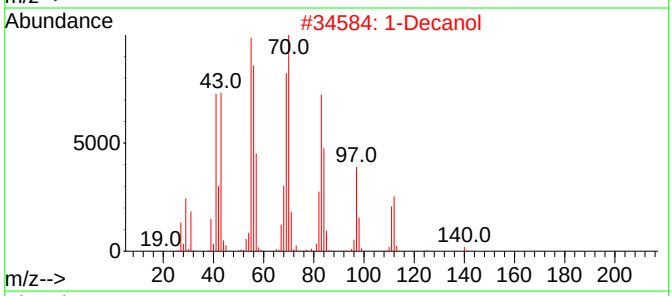
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclodecane	140	C10H20	000293-96-9	95
2	1-Decanol	158	C10H22O	000112-30-1	91
3	3-Dodecene, (Z)-	168	C12H24	007239-23-8	86
4	1-Undecene	154	C11H22	000821-95-4	80
5	Octane, 3-chloro-	148	C8H17Cl	001117-79-9	72

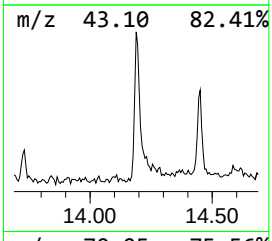


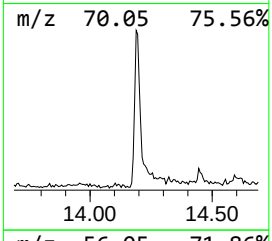


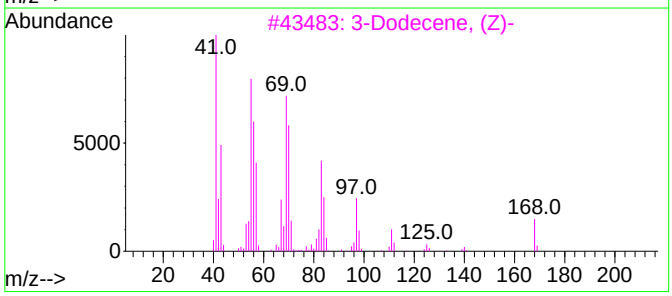


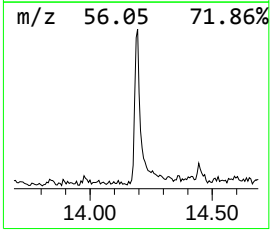












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Instrument :
MSVOA_X
ClientSampleId :
3829

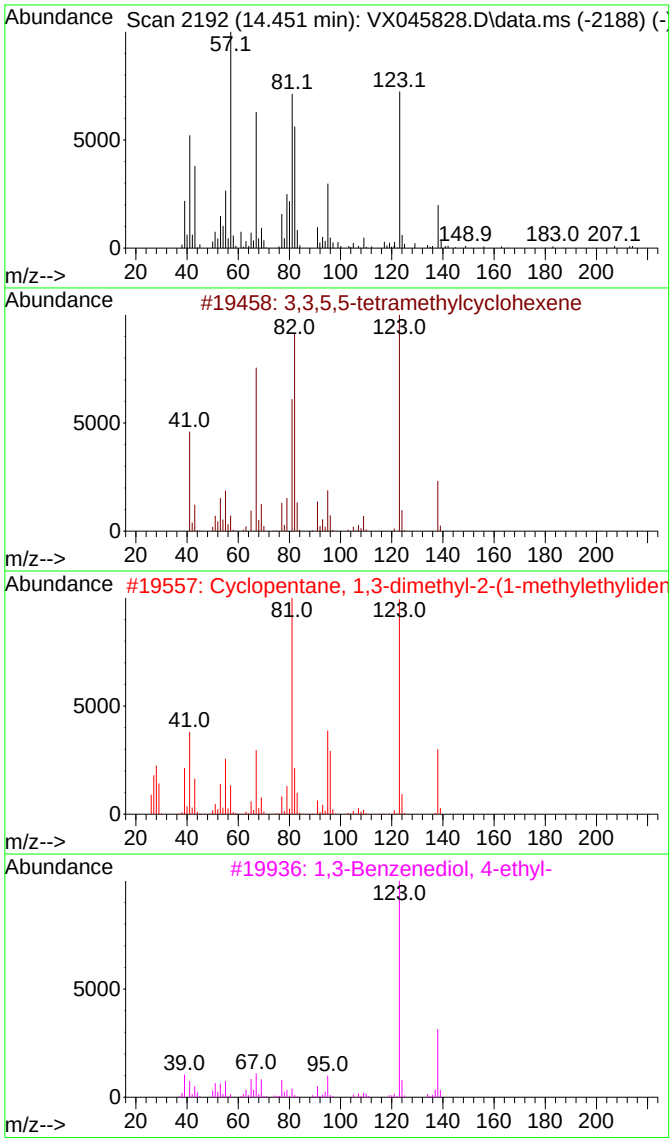
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

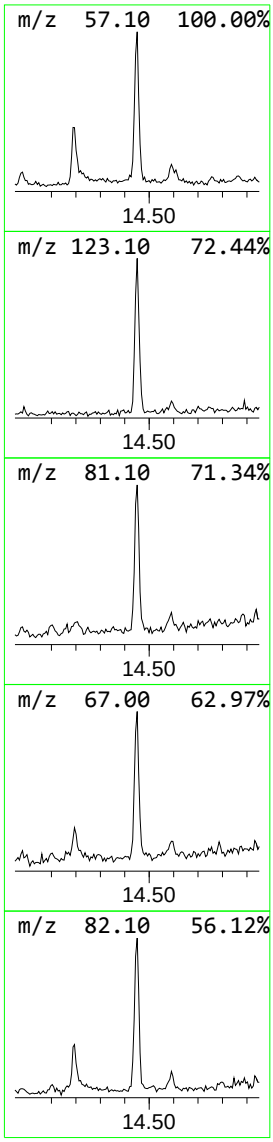
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3,3,5,5-tetramethylcyclohexene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	10.30 ug/l	87239	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	93
2	Cyclopentane, 1,3-dimethyl-2-(1-...	138	C10H18	061142-30-1	46
3	1,3-Benzenediol, 4-ethyl-	138	C8H10O2	002896-60-8	46
4	cis-3-Hexenyl heptine carbonate	222	C14H22O2	068698-58-8	43
5	Cyclopentene, 1,3-dimethyl-2-(1-...	138	C10H18	061142-32-3	43





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MSVOA_X
ClientSampleId :
3829

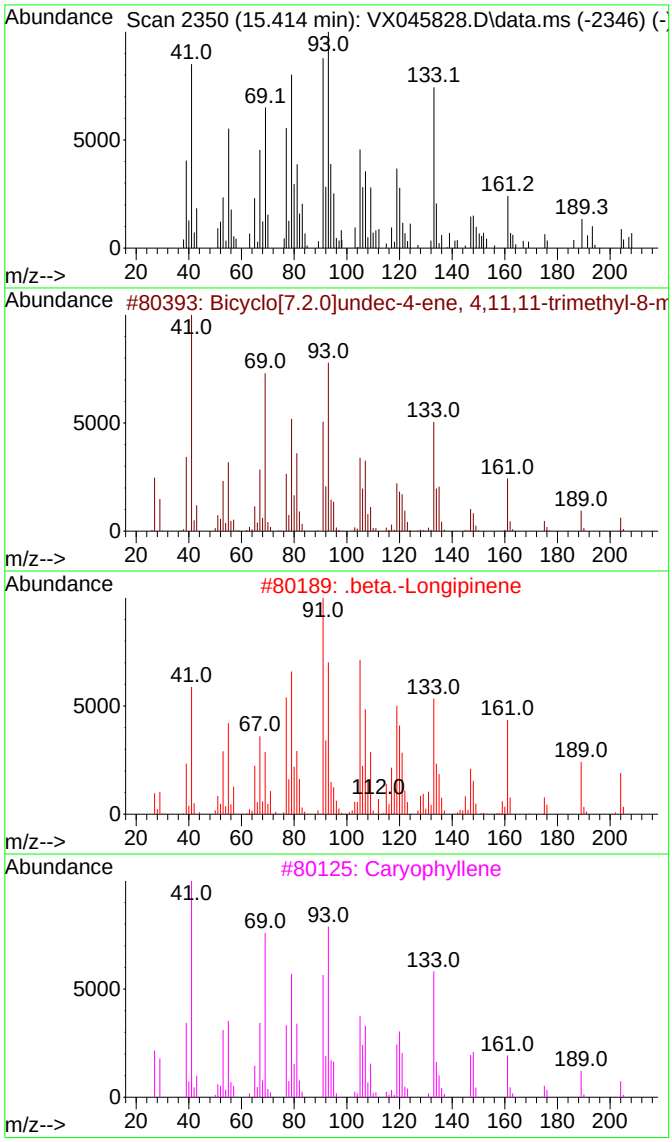
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

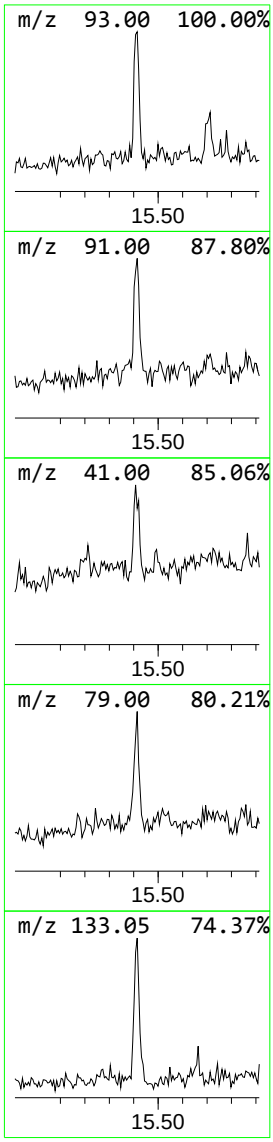
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Bicyclo[7.2.0]undec-4-ene, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.414	5.70 ug/l	48253	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	93
2	.beta.-Longipinene	204	C15H24	041432-70-6	91
3	Caryophyllene	204	C15H24	000087-44-5	90
4	(1S,5S,6R)-6-Methyl-2-methylene-...	204	C15H24	015438-94-5	70
5	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045828.D
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ClientSampleId :
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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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Octanol	12.579	15.5	ug/l	131408	4	12.018	423331	50.0
3-Carene	12.817	5.4	ug/l	45372	4	12.018	423331	50.0
Tricyclo[2.2.1....	13.731	6.7	ug/l	57016	4	12.018	423331	50.0
Cyclodecane	14.188	12.1	ug/l	102429	4	12.018	423331	50.0
3,3,5,5-tetrame...	14.451	10.3	ug/l	87239	4	12.018	423331	50.0
Bicyclo[7.2.0]u...	15.414	5.7	ug/l	48253	4	12.018	423331	50.0