

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY022725\
 Data File : VY021364.D
 Acq On : 27 Feb 2025 17:32
 Operator : SY/MD
 Sample : Q1411-01
 Misc : 5.02g/5.0mL/MSVOA_Y/SOIL/B
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 HR-02-02212025

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_Y\methods\82Y022525S.M
 Title : SW846 8260

Signal : TIC: VY021364.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.093	55	61	62	rBV3	780	1485	5.87%	0.713%
2	2.160	71	72	74	rBV2	1239	827	3.27%	0.397%
3	2.324	96	99	100	rBV3	891	912	3.60%	0.438%
4	2.641	150	151	155	rVB	866	653	2.58%	0.313%
5	3.105	224	227	231	rVB3	323	618	2.44%	0.297%
6	3.537	295	298	302	rBV2	430	658	2.60%	0.316%
7	3.580	302	305	308	rVB2	341	558	2.21%	0.268%
8	4.586	465	470	471	rBV	570	591	2.34%	0.284%
9	4.610	471	474	479	rVB3	468	894	3.53%	0.429%
10	6.226	735	739	741	rVB2	460	540	2.13%	0.259%
11	6.262	741	745	748	rBV2	406	648	2.56%	0.311%
12	7.634	962	970	976	rBV4	4296	10352	40.91%	4.968%
13	7.707	976	982	990	rVB2	8630	18279	72.24%	8.771%
14	8.061	1033	1040	1047	rBV4	3502	8097	32.00%	3.885%
15	8.610	1125	1130	1139	rBV	9694	19114	75.54%	9.172%
16	9.731	1311	1314	1318	rBV3	433	645	2.55%	0.310%
17	10.109	1370	1376	1384	rVB	13758	25303	100.00%	12.142%
18	10.445	1428	1431	1435	rVB4	480	833	3.29%	0.400%
19	10.737	1472	1479	1484	rBV4	963	1897	7.50%	0.910%
20	10.957	1513	1515	1516	rBV2	533	541	2.14%	0.260%
21	11.018	1519	1525	1529	rVV4	1907	3257	12.87%	1.563%
22	11.134	1541	1544	1548	rVB5	975	1098	4.34%	0.527%
23	11.420	1585	1591	1597	rBV	10427	17203	67.99%	8.255%
24	11.554	1608	1613	1615	rVB3	458	615	2.43%	0.295%
25	11.591	1615	1619	1621	rVV3	883	1259	4.98%	0.604%
26	11.609	1621	1622	1626	rVB2	1013	823	3.25%	0.395%
27	11.664	1626	1631	1634	rBV4	1355	2423	9.58%	1.163%
28	11.701	1634	1637	1643	rVB4	1236	2330	9.21%	1.118%
29	11.932	1668	1675	1681	rVB4	1950	3631	14.35%	1.742%
30	12.048	1690	1694	1699	rBV3	2357	3306	13.07%	1.586%
31	12.121	1703	1706	1710	rVV3	1917	3102	12.26%	1.489%
32	12.176	1710	1715	1718	rVB4	1897	3512	13.88%	1.685%
33	12.292	1732	1734	1738	rBV5	893	1043	4.12%	0.500%
34	12.408	1748	1753	1758	rBV3	6019	9324	36.85%	4.474%
35	12.481	1762	1765	1770	rVB6	699	874	3.45%	0.419%
36	12.536	1770	1774	1775	rBV2	507	707	2.79%	0.339%

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37	12.566	1775	1779	1788	rVB9	2540	4820	19.05%	2.313%
38	12.645	1788	1792	1797	rBV7	1486	2545	10.06%	1.221%
39	12.725	1797	1805	1811	rBV10	2800	6864	27.13%	3.294%
40	12.828	1819	1822	1824	rBV4	378	551	2.18%	0.264%
41	12.865	1826	1828	1832	rVV3	1417	1722	6.81%	0.826%
42	12.914	1832	1836	1839	rVV4	852	1655	6.54%	0.794%
43	12.963	1841	1844	1852	rVB5	3239	5129	20.27%	2.461%
44	13.036	1852	1856	1857	rBV3	487	652	2.58%	0.313%
45	13.054	1857	1859	1861	rVB3	686	555	2.19%	0.266%
46	13.091	1861	1865	1866	rBV3	531	587	2.32%	0.282%
47	13.145	1871	1874	1877	rBV5	490	795	3.14%	0.381%
48	13.176	1877	1879	1883	rVB4	1003	996	3.94%	0.478%
49	13.243	1883	1890	1895	rBV6	2312	5804	22.94%	2.785%
50	13.347	1901	1907	1914	rVB2	4386	7883	31.15%	3.783%
51	13.462	1922	1926	1927	rBV3	592	690	2.73%	0.331%
52	13.664	1955	1959	1965	rBV5	2785	5098	20.15%	2.446%
53	13.718	1965	1968	1971	rVB3	1258	1100	4.35%	0.528%
54	13.761	1971	1975	1977	rBV3	591	746	2.95%	0.358%
55	13.846	1985	1989	1991	rBV3	763	1233	4.87%	0.592%
56	13.895	1995	1997	2002	rVB4	951	1103	4.36%	0.529%
57	13.987	2008	2012	2014	rBV2	553	699	2.76%	0.335%
58	14.096	2028	2030	2036	rBV3	683	1155	4.56%	0.554%
59	14.170	2039	2042	2043	rBV3	1425	1545	6.11%	0.741%
60	14.224	2048	2051	2057	rVB4	556	778	3.07%	0.373%
61	14.340	2066	2070	2075	rVB5	1460	2422	9.57%	1.162%
62	14.816	2143	2148	2150	rBV2	529	703	2.78%	0.337%
63	15.541	2265	2267	2271	rBV2	472	559	2.21%	0.268%
64	16.060	2350	2352	2357	rVB3	440	610	2.41%	0.293%
65	16.316	2389	2394	2395	rBV2	525	683	2.70%	0.328%
66	16.742	2461	2464	2466	rVB4	625	760	3.00%	0.365%

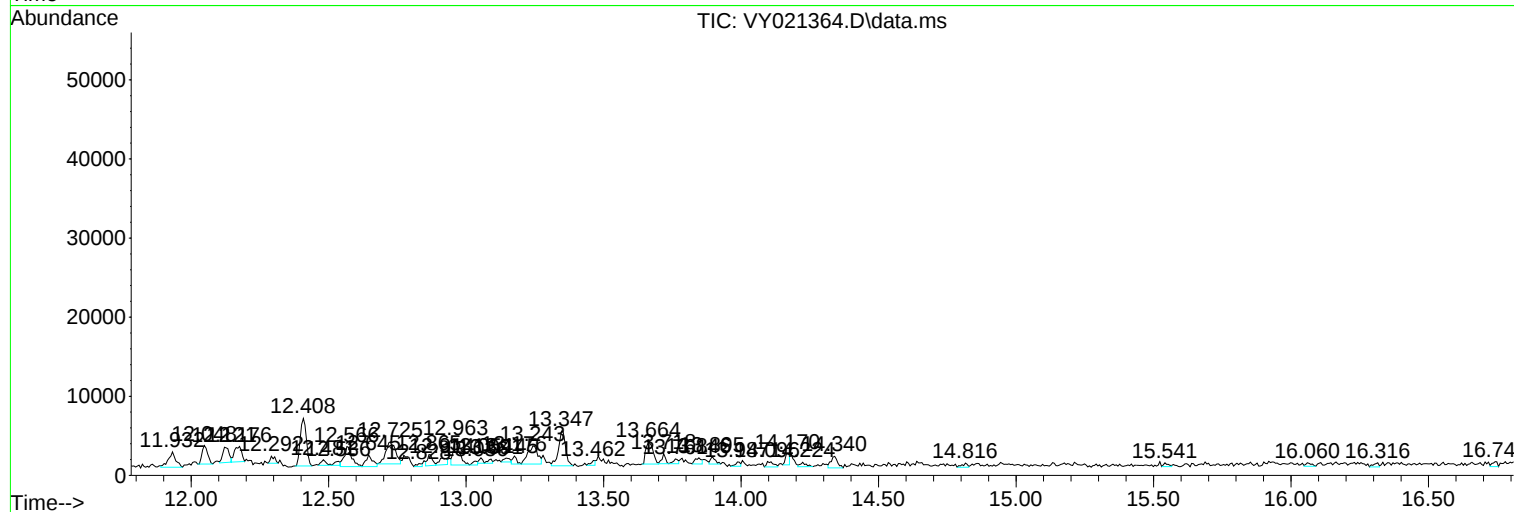
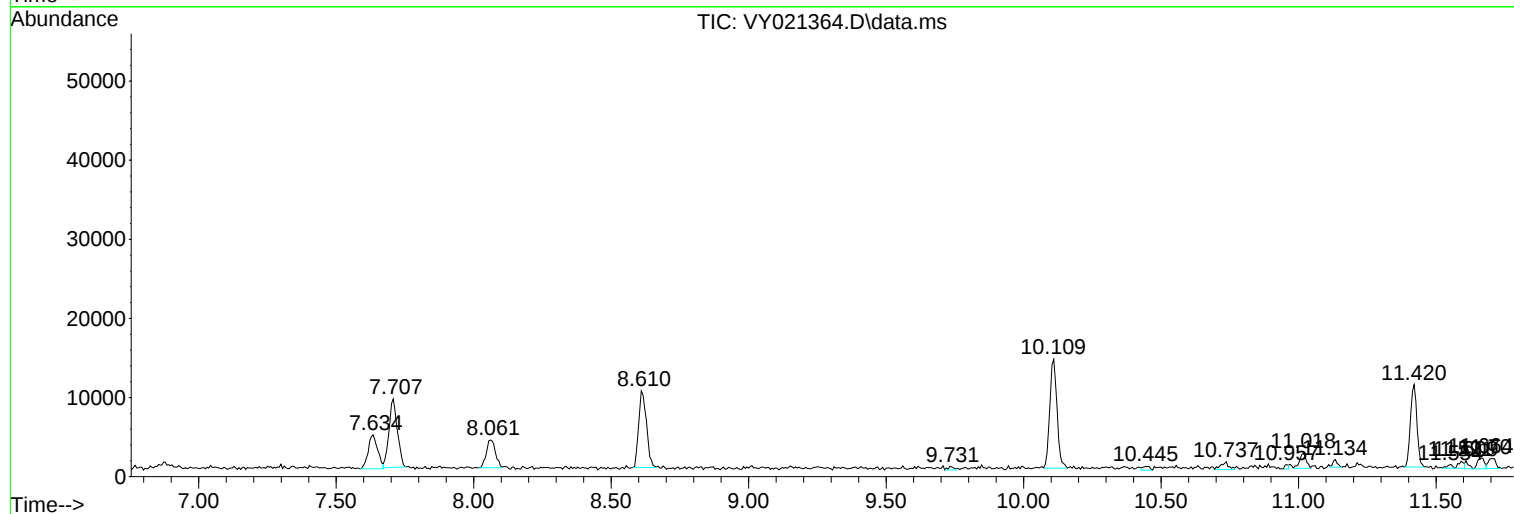
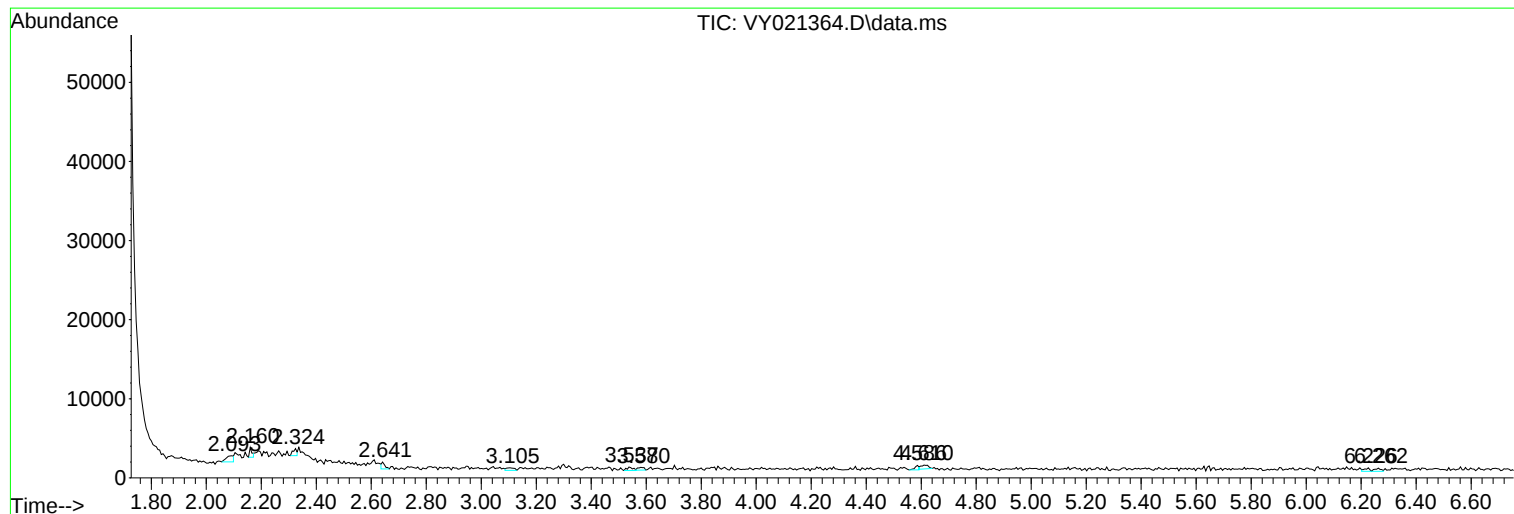
Sum of corrected areas: 208394

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Quant Title : SW846 8260

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



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Quant Title : SW846 8260

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

Peak Number 1 unknown12.566 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.566	30.57 ug/l	4820	1,4-Dichlorobenzene-d4	13.353

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (1,1-dimethylpropyl)-	154	C11H22	031797-64-5	12
2			Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	12
3			Isodecyl methacrylate	226	C14H26O2	029964-84-9	12
4			Cyclohexane, 1,2-diethyl-1-methyl-	154	C11H22	061141-79-5	12
5			Cyclohexane, 2,4-diethyl-1-methyl-	154	C11H22	061142-70-9	12

Peak Number 2 unknown12.646 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.646	16.14 ug/l	2545	1,4-Dichlorobenzene-d4	13.353

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Menth-8-ene	138	C10H18	015193-25-6	27
2			2-Cyclopenten-1-one, 2-pentyl-	152	C10H16O	025564-22-1	17
3			(3aR,4S,7R,7aS)-3a,7a-Dimethyloc...	164	C12H20	067152-02-7	17
4			1H-Indene, octahydro-	124	C9H16	000496-10-6	16
5			Disparlure	282	C19H38O	029804-22-6	12

Peak Number 3 unknown12.725 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.725	43.54 ug/l	6864	1,4-Dichlorobenzene-d4	13.353

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Tetradecenal, (Z)-	210	C14H26O	053939-27-8	43
2			1-Hexadecanol	242	C16H34O	036653-82-4	43
3			Cyclododecane	168	C12H24	000294-62-2	38
4			n-Tridecan-1-ol	200	C13H28O	000112-70-9	38
5			17-Octadecynoic acid	280	C18H32O2	034450-18-5	38

Peak Number 4 unknown12.865 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.865	10.92 ug/l	1722	1,4-Dichlorobenzene-d4	13.353

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TIC Library : C:\Database\NIST0.L
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Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane-1,3-dione, 2-allylam...	207	C12H17NO2	104926-37-6	38
2			2,4-Dimethyl-3-nitrobicyclo[3.2....	197	C10H15NO3	1000192-17-3	16
3			(-)-trans-Pinane	138	C10H18	033626-25-4	12
4			Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	9
5			Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	9

Peak Number 5 unknown12.963 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	32.53 ug/l	5129	1,4-Dichlorobenzene-d4	13.353

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Piperidine, 3,5-dimethyl-	113	C7H15N	035794-11-7	47
2			1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	35
3			Decanal	156	C10H20O	000112-31-2	32
4			trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	25
5			Heptanal	114	C7H14O	000111-71-7	25

Peak Number 6 unknown13.243 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.243	36.81 ug/l	5804	1,4-Dichlorobenzene-d4	13.353

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	47
2			Octane, 2-cyclohexyl-	196	C14H28	002883-05-8	47
3			Azeleoneitrile	150	C9H14N2	001675-69-0	43
4			Cyclohexane, (1,3-dimethylbutyl)-	168	C12H24	061142-19-6	40
5			Dodecane, 2-cyclohexyl-	252	C18H36	013151-82-1	40

Peak Number 7 Cyclohexane, 1-methyl-4-(1-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.664	32.34 ug/l	5098	1,4-Dichlorobenzene-d4	13.353

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-25-0	68
2			Naphthalene, decahydro-	138	C10H18	000091-17-8	64
3			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	64
4			1,1'-Bicyclopentyl	138	C10H18	001636-39-1	58
5			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	53

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TIC Library : C:\Database\NIST0.L
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Peak Number 8 Cyclohexanone, 2-methyl-5-(... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.340	15.36 ug/l	2422	1,4-Dichlorobenzene-d4	13.353

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	007764-50-3	59
2			Spiro[5.5]undecane	152	C11H20	000180-43-8	50
3			Spiropentane	68	C5H8	000157-40-4	43
4			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	42
5			1,3-Cyclohexanedione, 2-(2-prope...	152	C9H12O2	042738-68-1	40

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown12.566	12.566	30.6	ug/l	4820	4	13.353	7883	50.0
unknown12.646	12.646	16.1	ug/l	2545	4	13.353	7883	50.0
unknown12.725	12.725	43.5	ug/l	6864	4	13.353	7883	50.0
unknown12.865	12.865	10.9	ug/l	1722	4	13.353	7883	50.0
unknown12.963	12.963	32.5	ug/l	5129	4	13.353	7883	50.0
unknown13.243	13.243	36.8	ug/l	5804	4	13.353	7883	50.0
Cyclohexane, 1-...	13.664	32.3	ug/l	5098	4	13.353	7883	50.0
Cyclohexanone, ...	14.340	15.4	ug/l	2422	4	13.353	7883	50.0