LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN051820\
Data File : VN061466.D
Acq On : 19 May 2020 7:43
Operator : JC/MD
Sample : L2645-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4

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_N\METHODS\82N051820W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.770	297	310	325	rBV2	266885	539590	13.15%	2.483%
2	3.760	595	618	642	rBV4	36464	119027	2.90%	0.548%
3	4.018	678	698	716	rBV2	13403	41970	1.02%	0.193%
4	4.481	816	842	863	rBV	174560	639033	15.57%	2.940%
5	4.731	894	920	960	rBV	1181131	4104082	100.00%	18.884%
6	4.992	974	1001	1033	rVB2	595104	2213987	53.95%	10.187%
7	5.902	1260	1284	1306	rBV4	32938	113481	2.77%	0.522%
8	6.477	1443	1463	1476	rBV4	23068	78143	1.90%	0.360%
9	6.577	1481	1494	1512	rVV2	44044	142440	3.47%	0.655%
10	6.770	1537	1554	1576	rVB3	16613	52568	1.28%	0.242%
11	7.349	1718	1734	1750	rVB5	19734	55113	1.34%	0.254%
12	7.551	1776	1797	1808	rBV	191582	486160	11.85%	2.237%
13	7.625	1808	1820	1835	rVV	365454	891026	21.71%	4.100%
14	7.706	1835	1845	1863	rVB4	57778	150159	3.66%	0.691%
15	7.992	1916	1934	1951	rVV3	261336	661146	16.11%	3.042%
16	8.095	1951	1966	1981	rVV	454042	1119946	27.29%	5.153%
17	8.178	1982	1992	2011	rVV4	83083	280578	6.84%	1.291%
18	8.551	2089	2108	2130	rBV	561899	1195284	29.12%	5.500%
19	9.011	2238	2251	2259	rBV6	23691	54934	1.34%	0.253%
20	9.487	2385	2399	2413	rVB3	55123	111140	2.71%	0.511%
21	9.622	2417	2441	2458	rBV3	100846	261530	6.37%	1.203%
22	9.825	2486	2504	2509	rBV	69455	136504	3.33%	0.628%
23	9.863	2509	2516	2539	rVV2	102410	202299	4.93%	0.931%
24	10.059	2563	2577	2597	rBV	915153	1676674	40.85%	7.715%
25	10.181	2604	2615	2626	rBV	95251	171900	4.19%	0.791%
26	10.275	2634	2644	2656	rVB2	68079	121996	2.97%	0.561%
27	10.352	2656	2668	2677	rVV	68802	117587	2.87%	0.541%
28	10.493	2697	2712	2728	rBV5	29755	68337	1.67%	0.314%
29	10.767	2789	2797	2812	rVB	75520	130563	3.18%	0.601%
30	11.268	2943	2953	2968	rVB3	19593	45275	1.10%	0.208%
31	11.381	2974	2988	3009	rBV	888642	1583591	38.59%	7.287%
32	11.487	3009	3021	3036	rVB	97214	189500	4.62%	0.872%
33	11.603	3047	3057	3073	rVB3	30192	61324	1.49%	0.282%
34	12.223	3240	3250	3264	rVB	42069	67285	1.64%	0.310%

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Title : SW846 8260

35	12.378	3284	3298	3321	rBV	686134	1163868	28.36%	5.355%
36	12.567	3344	3357	3369	rVB	78841	132378	3.23%	0.609%
37	12.866	3440	3450	3464	rBV	63526	103362	2.52%	0.476%
38	13.014	3486	3496	3508	rVB	51637	82683	2.01%	0.380%
39	13.320	3578	3591	3613	rBV	837700	1429242	34.82%	6.576%
40	13.487	3632	3643	3648	rBV	165730	268353	6.54%	1.235%
41	13.519	3648	3653	3661	rVV	166795	252508	6.15%	1.162%
42	13.567	3662	3668	3684	rVB3	57323	98018	2.39%	0.451%
43	13.648	3684	3693	3704	rBV2	29681	49034	1.19%	0.226%
44	13.921	3769	3778	3785	rVV	30631	48239	1.18%	0.222%
45	13.969	3785	3793	3804	rVB6	27676	47941	1.17%	0.221%
46	14.570	3966	3980	3990	rBV3	38281	74572	1.82%	0.343%
47	15.107	4135	4147	4158	rBV2	54586	98751	2.41%	0.454%

Sum of corrected areas: 21733121

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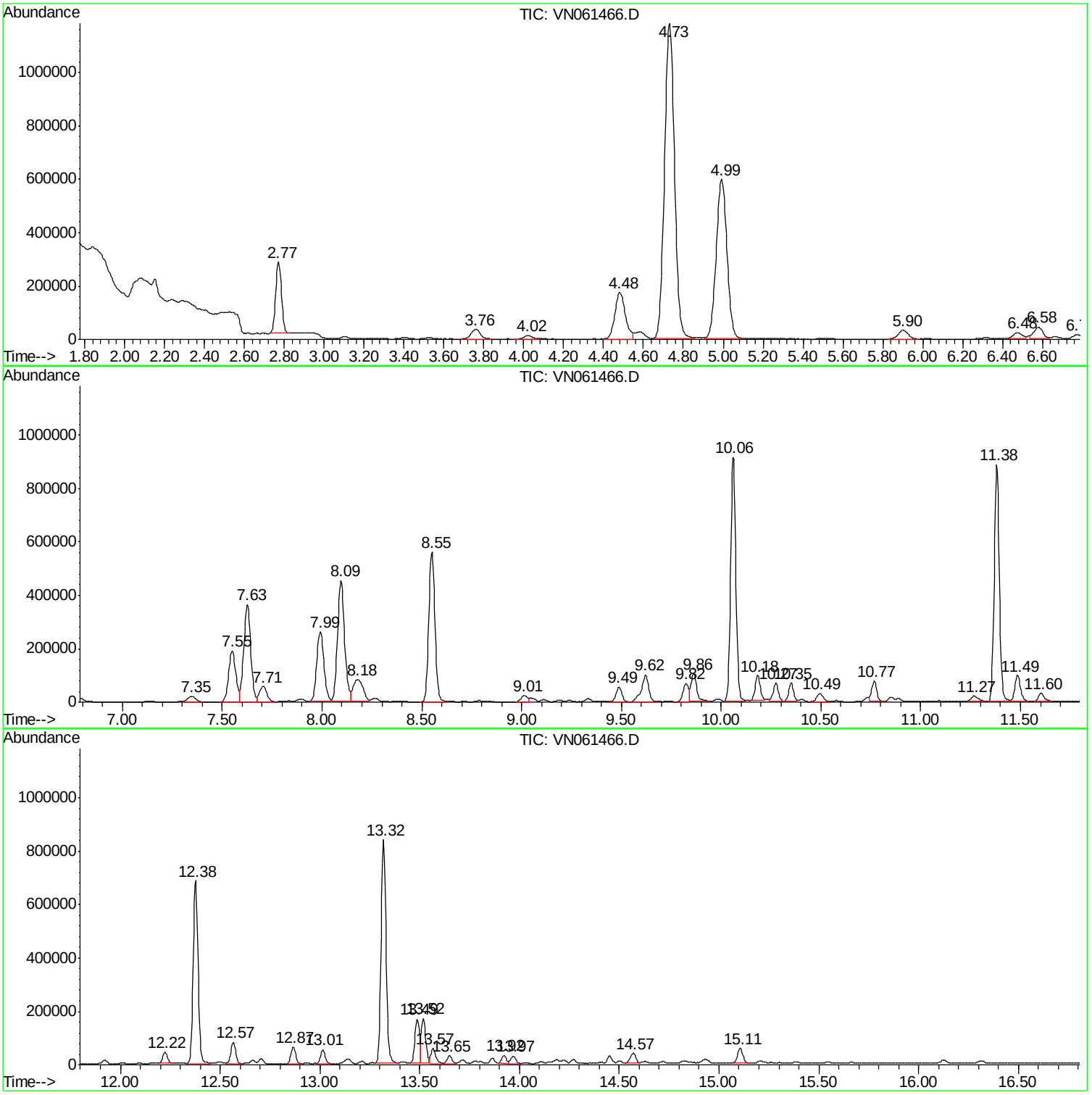
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N051820W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Peak Number 1 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.77	30.28 ug/l	539590	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2	3-Buten-1-ol	72	C4H8O	000627-27-0	43
3	Oxirane, trimethyl-	86	C5H10O	005076-19-7	33
4	Pentane	72	C5H12	000109-66-0	28
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	12

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Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	35.86 ug/l	639033	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3	Butane, 2-methyl-	72	C5H12	000078-78-4	36
4	Cyclobutane, methyl-	70	C5H10	000598-61-8	33
5	Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	16

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Peak Number 3 Cyclopentane, methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	7.99 ug/l	142440	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	45
5	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	36

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Peak Number 4 Pentane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.

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ALS Vial : 46 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N051820W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.71	8.43 ug/l	150159	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	56
3	5,5-Dimethyl-1,3-dioxan-2-one	130	C6H10O3	003592-12-9	50
4	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	50
5	Heptane	100	C7H16	000142-82-5	47

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Peak Number 5 Amylene hydrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.09	46.85 ug/l	1119950	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	83
2	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	40
3	3-Hexanol	102	C6H14O	000623-37-0	39
4	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	33
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	10

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Peak Number 6 Pentane, 2,2,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.18	11.74 ug/l	280578	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	53
2	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	50
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	50
4	2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	40
5	1-Propanol, 2,2-dimethyl-	88	C5H12O	000075-84-3	38

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Peak Number 7 Pentane, 2,3,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.62	10.94 ug/l	261530	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual

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TIC Integration Parameters: LSCINT.P

1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4 90
2	Undecane, 2,8-dimethyl-	184	C13H28	017301-25-6 72
3	Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3 59
4	Hexane, 3-methyl-	100	C7H16	000589-34-4 59
5	Heptane, 4-methyl-	114	C8H18	000589-53-7 59

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Peak Number 8 2-Pentanol, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.86	8.46 ug/l	202299	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	78
2	3-Methyl-oxirane-2-carboxylic ac...	116	C5H8O3	1000194-20-4	64
3	1,2-Butanediol	90	C4H10O2	000584-03-2	45
4	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	40
5	2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	39

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Peak Number 9 Benzene, 1,2-diethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	9.39 ug/l	268353	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
2	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	96
3	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	96
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91

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Peak Number 10 Deltacyclene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	8.83 ug/l	252508	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Deltacyclene	118	C9H10	007785-10-6	59
2	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	53
3	Indole	117	C8H7N	000120-72-9	50

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4	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	42
5	Benzyl nitrile	117	C8H7N	000140-29-4	37

Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methyl-	2.77	30.3	ug/l	539590	1	7.63	891026	50.0
Butane, 2,3-dimet...	4.48	35.9	ug/l	639033	1	7.63	891026	50.0
Cyclopentane, met...	6.58	8.0	ug/l	142440	1	7.63	891026	50.0
Pentane, 2,3-dime...	7.71	8.4	ug/l	150159	1	7.63	891026	50.0
Amylene hydrate	8.09	46.9	ug/l	1119950	2	8.55	1195280	50.0
Pentane, 2,2,4-tr...	8.18	11.7	ug/l	280578	2	8.55	1195280	50.0
Pentane, 2,3,3-tr...	9.62	10.9	ug/l	261530	2	8.55	1195280	50.0
2-Pentanol, 2-met...	9.86	8.5	ug/l	202299	2	8.55	1195280	50.0
Benzene, 1,2-diet...	13.49	9.4	ug/l	268353	4	13.32	1429240	50.0
Deltacyclene	13.52	8.8	ug/l	252508	4	13.32	1429240	50.0