LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN061818\
Data File : VN049345.D
Acq On : 18 Jun 2018 16:04
Operator : MD\SY
Sample : J3435-07 5X
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NW3

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\82N061618W.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	1.658	10	21	42	rBV	2072160	3049067	13.82%	1.944%
2	2.802	364	377	397	rVB	540292	1105348	5.01%	0.705%
3	3.130	468	479	496	rVB	272374	570721	2.59%	0.364%
4	5.050	1047	1076	1104	rBV	154411	563098	2.55%	0.359%
5	6.629	1544	1567	1595	rBV3	755483	2407040	10.91%	1.535%
6	7.593	1845	1867	1877	rBV	1309114	3335162	15.12%	2.127%
7	7.667	1878	1890	1911	rVB2	2401503	5968481	27.05%	3.806%
8	8.030	1986	2003	2029	rBV	1321106	3165108	14.35%	2.018%
9	8.178	2031	2049	2055	rBV6	136961	383577	1.74%	0.245%
10	8.587	2160	2176	2225	rVB	2870429	6267705	28.41%	3.997%
11	9.082	2306	2330	2346	rBV5	294720	821831	3.73%	0.524%
12	9.616	2483	2496	2520	rBV2	120578	292732	1.33%	0.187%
13	10.091	2628	2644	2657	rBV	5095350	9686937	43.91%	6.177%
14	10.156	2658	2664	2677	rVB	433943	796559	3.61%	0.508%
15	11.410	3038	3054	3073	rBV	3797379	6862097	31.10%	4.376%
16	11.513	3074	3086	3105	rVV	5629233	9523483	43.17%	6.073%
17	11.625	3105	3121	3145	rVB	11360429	22061891	100.00%	14.068%
18	11.950	3203	3222	3243	rBV	3689996	6142530	27.84%	3.917%
19	12.252	3304	3316	3331	rVB	641557	1052589	4.77%	0.671%
20	12.403	3349	3363	3389	rBV	3464254	5968844	27.05%	3.806%
21	12.593	3410	3422	3431	rBV	1489847	2370264	10.74%	1.511%
22	12.657	3431	3442	3449	rBV	5825187	9664576	43.81%	6.163%
23	12.734	3459	3466	3487	rVB	3203431	5076866	23.01%	3.237%
24	12.895	3501	3516	3535	rBV	3344841	5479326	24.84%	3.494%
25	13.043	3548	3562	3576	rBV	12816999	19643813	89.04%	12.526%
26	13.236	3613	3622	3631	rBV	149557	227246	1.03%	0.145%
27	13.345	3645	3656	3661	rBV	3591949	5945013	26.95%	3.791%
28	13.545	3698	3718	3727	rBV	3448281	6309658	28.60%	4.024%
29	13.741	3768	3779	3789	rBV2	217068	354532	1.61%	0.226%
30	13.805	3789	3799	3804	rBV	543548	848294	3.85%	0.541%
31	13.892	3817	3826	3836	rVB	778561	1164657	5.28%	0.743%
32	13.950	3836	3844	3850	rVV	228035	344426	1.56%	0.220%
33	13.998	3850	3859	3873	rVB2	893661	1458737	6.61%	0.930%
34	14.133	3890	3901	3911	rVB	218528	351555	1.59%	0.224%

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Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061618W.M
Title : SW846 8260

35	14.213	3914	3926	3931	rBV	448184	684130	3.10%	0.436%
36	14.252	3931	3938	3948	rVB	675372	1046161	4.74%	0.667%
37	14.480	3999	4009	4019	rBV	615355	954409	4.33%	0.609%
38	14.599	4031	4046	4057	rBV3	1300181	2442270	11.07%	1.557%
39	14.744	4081	4091	4106	rBV2	184354	324185	1.47%	0.207%
40	14.853	4109	4125	4132	rBV5	117791	282917	1.28%	0.180%
41	14.959	4150	4158	4169	rVB4	124018	253257	1.15%	0.161%
42	15.139	4202	4214	4227	rVB	908808	1568139	7.11%	1.000%

Sum of corrected areas: 156819231

LSC Report - Integrated Chromatogram

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MSVOA_N
ClientSampleId :
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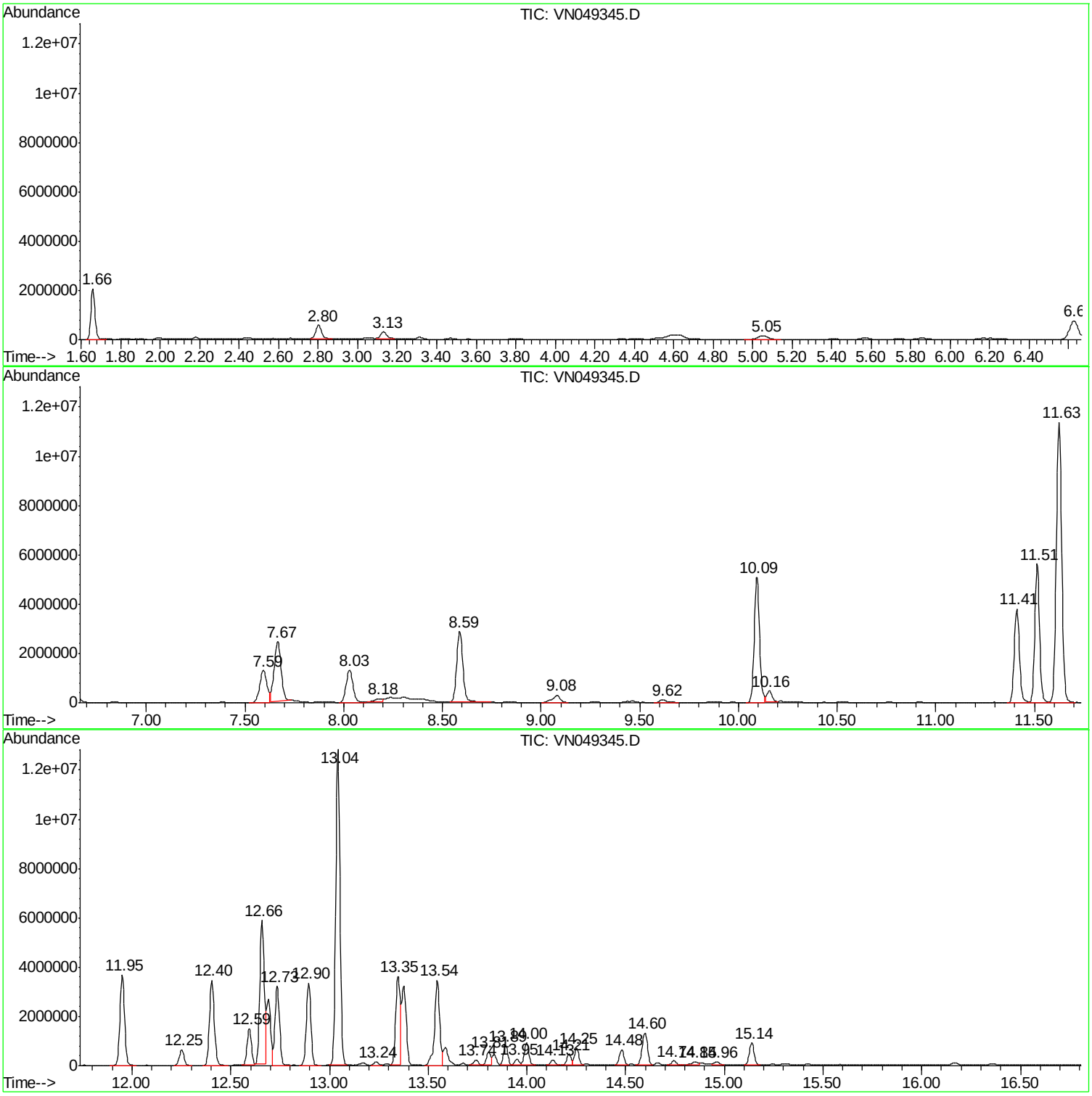
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061618W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061618W.M
Quant Title : SW846 8260

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

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.80	9.26 ug/l	1105350	Pentafluorobenzene	7.67

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	47
3	Pentane	72	C5H12	000109-66-0	33
4	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	12
5	1-Butene	56	C4H8	000106-98-9	11

****
Peak Number 2 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	20.16 ug/l	2407040	Pentafluorobenzene	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclohexane	84	C6H12	000110-82-7	87
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
5	Cyclobutane	56	C4H8	000287-23-0	47

****
Peak Number 3 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	81.28 ug/l	9664580	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91

****
Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

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

Library Search Compound Report

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NW3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061618W.M
Quant Title : SW846 8260

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

12.90	46.08 ug/l	5479330	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
3	Mesitylene	120	C9H12	000108-67-8	90
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90

****

Peak Number 5 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	53.07 ug/l	6309660	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	94
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	94
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	74
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72

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Peak Number 6 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	9.80 ug/l	1164660	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
3	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5	o-Cymene	134	C10H14	000527-84-4	95

****

Peak Number 7 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	12.27 ug/l	1458740	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual

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Instrument :
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Quant Title : SW846 8260

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

1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4 83
2	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9 83
3	Indan, 1-methyl-	132	C10H12	000767-58-8 81
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8 80
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1 80

****

Peak Number 8 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.25	8.80 ug/l	1046160	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94

****

Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	20.54 ug/l	2442270	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	86
5	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	83

Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Butane, 2-methyl-	2.80	9.3	ug/l	1105350	1	7.67	5968480	50.0
Cyclopentane, met...	6.63	20.2	ug/l	2407040	1	7.67	5968480	50.0
Benzene, 1-ethyl-...	12.66	81.3	ug/l	9664580	4	13.35	5945010	50.0
Benzene, 1-ethyl-...	12.90	46.1	ug/l	5479330	4	13.35	5945010	50.0
Indane	13.54	53.1	ug/l	6309660	4	13.35	5945010	50.0
Benzene, 1-ethyl-...	13.89	9.8	ug/l	1164660	4	13.35	5945010	50.0
Benzene, 1-etheny...	14.00	12.3	ug/l	1458740	4	13.35	5945010	50.0
Benzene, 1,2,3,4-...	14.25	8.8	ug/l	1046160	4	13.35	5945010	50.0
Benzene, 2-etheny...	14.60	20.5	ug/l	2442270	4	13.35	5945010	50.0