LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD090424\
Data File : VD079778.D
Acq On : 04 Sep 2024 17:20
Operator : RP/MD
Sample : P3820-01
Misc : 5.02G/5.0ml/MSVOA_D/SOIL/A
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
STONE-1

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\82D083024S.M
Title : SW846 8260

Signal : TIC: VD079778.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.740	19	26	38	rVB	455628	747014	100.00%	32.574%
2	4.028	405	415	418	rBV4	3970	9935	1.33%	0.433%
3	4.799	535	546	560	rVB2	22240	70049	9.38%	3.055%
4	7.805	1047	1057	1063	rBV2	56048	138501	18.54%	6.039%
5	7.875	1063	1069	1081	rVB	55995	126782	16.97%	5.528%
6	8.228	1119	1129	1140	rBV2	71782	156772	20.99%	6.836%
7	8.775	1214	1222	1229	rBV	110534	224189	30.01%	9.776%
8	10.269	1469	1476	1484	rBV	139581	248771	33.30%	10.848%
9	10.663	1536	1543	1550	rBV4	4134	8844	1.18%	0.386%
10	11.581	1691	1699	1707	rBV	117672	200973	26.90%	8.764%
11	12.569	1859	1867	1874	rBV	65469	108157	14.48%	4.716%
12	13.516	2021	2028	2034	rVB	67773	111636	14.94%	4.868%
13	14.045	2113	2118	2125	rVB5	6480	10767	1.44%	0.470%
14	14.934	2264	2269	2271	rBV4	5879	8165	1.09%	0.356%
15	14.969	2271	2275	2278	rVB6	6188	8556	1.15%	0.373%
16	15.098	2291	2297	2300	rBV7	3524	8086	1.08%	0.353%
17	15.210	2312	2316	2320	rBV7	4303	8821	1.18%	0.385%
18	15.298	2326	2331	2335	rBV8	4115	9209	1.23%	0.402%
19	15.363	2338	2342	2346	rBV7	7159	15978	2.14%	0.697%
20	15.481	2360	2362	2366	rVB5	8975	11389	1.52%	0.497%
21	15.704	2396	2400	2407	rVB10	10747	21433	2.87%	0.935%
22	16.581	2544	2549	2558	rVB10	18024	39243	5.25%	1.711%

Sum of corrected areas: 2293270

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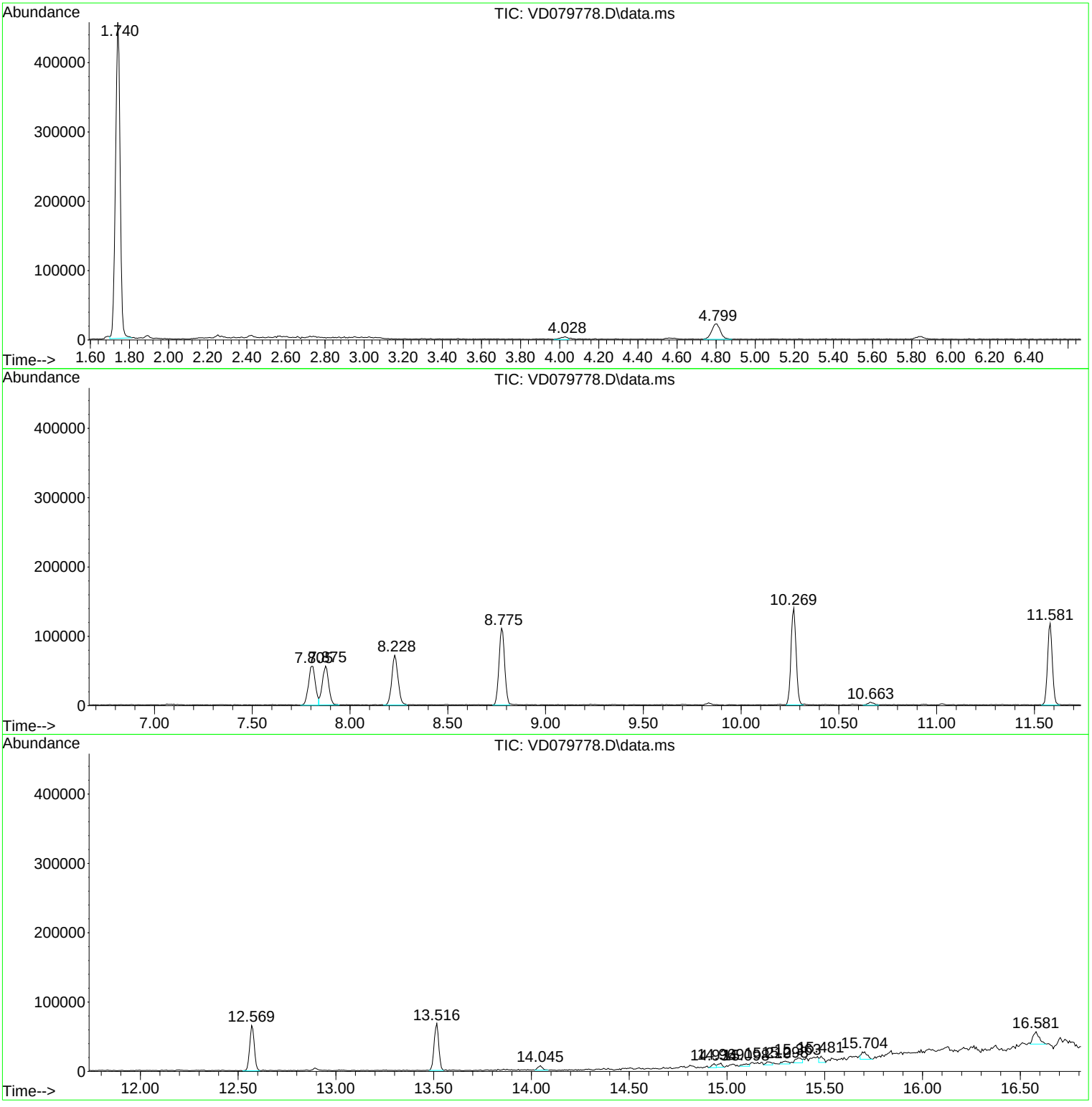
STONE-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D083024S.M
Quant Title : SW846 8260

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



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MSVOA_D
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D083024S.M
Quant Title : SW846 8260

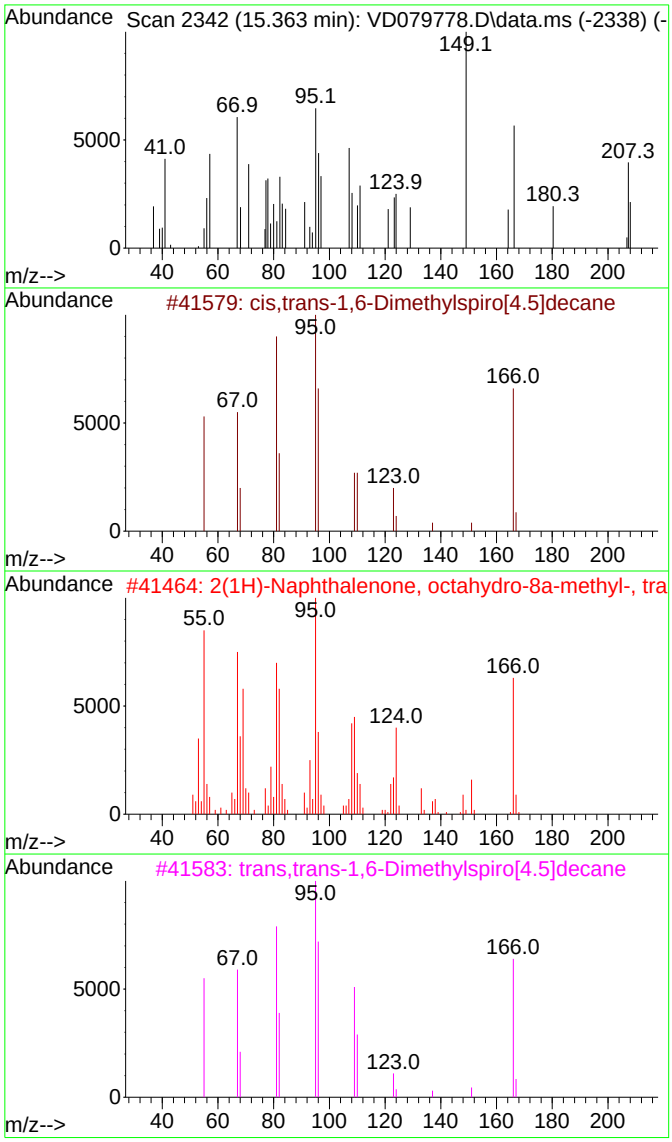
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

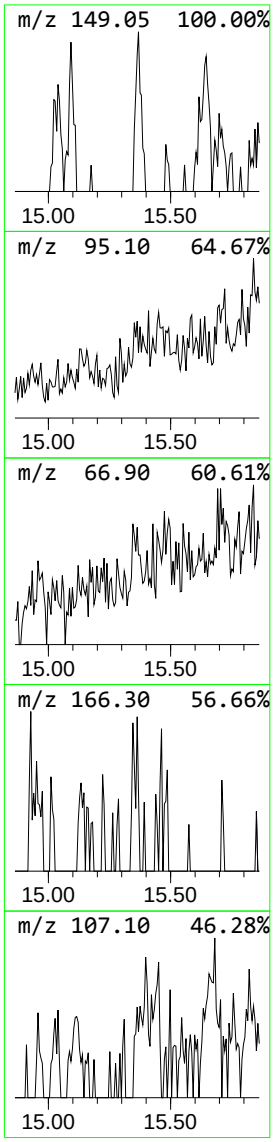
****

Peak Number 2 unknown15.363 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.363	7.16 ug/l	15978	1,4-Dichlorobenzene-d4	13.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis,trans-1,6-Dimethylspiro[4.5]...	166	C12H22	1000111-72-3	22
2	2(1H)-Naphthalenone, octahydro-8...	166	C11H18O	001197-95-1	22
3	trans,trans-1,6-Dimethylspiro[4....	166	C12H22	1000111-72-1	22
4	2-Amino-4-methoxybenzamide, Ac d...	208	C10H12N2O3	1000499-29-1	12
5	Naphthalene, decahydro-1,5-dimet...	166	C12H22	066552-62-3	11





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MSVOA_D
ClientSampleId :
STONE-1

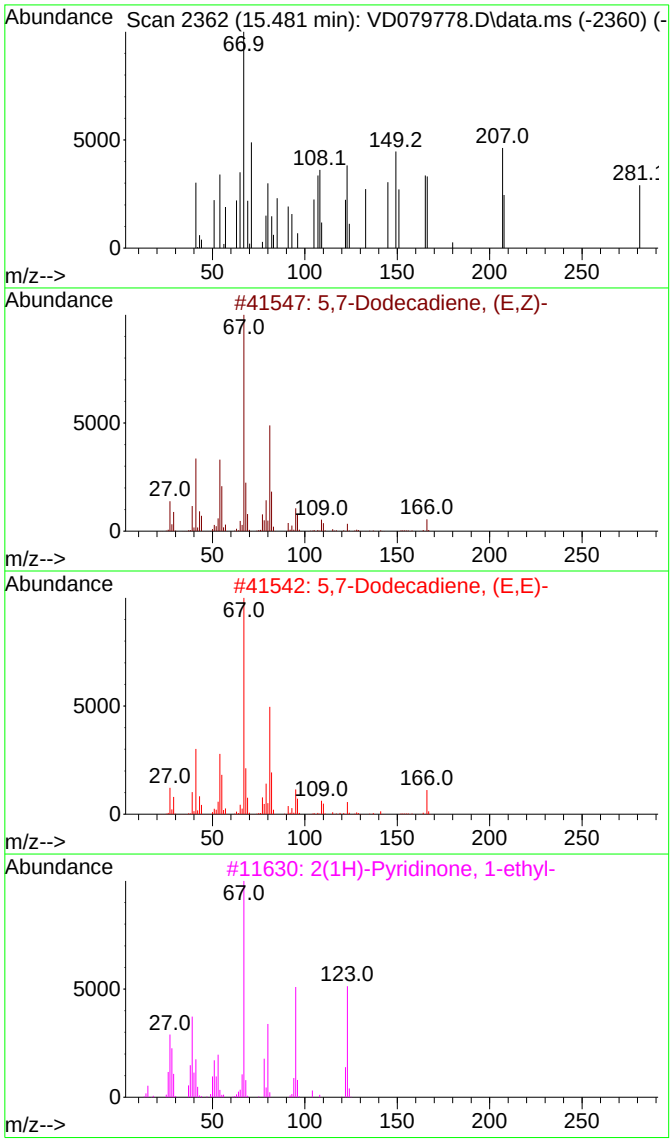
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D083024S.M
Quant Title : SW846 8260

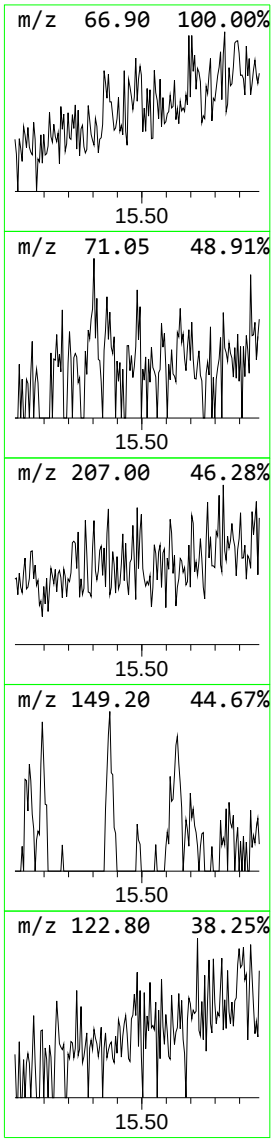
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 unknown15.481 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	5.10 ug/l	11389	1,4-Dichlorobenzene-d4	13.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,7-Dodecadiene, (E,Z)-	166	C12H22	021293-04-9	18
2	5,7-Dodecadiene, (E,E)-	166	C12H22	030651-68-4	18
3	2(1H)-Pyridinone, 1-ethyl-	123	C7H9NO	013337-79-6	12
4	4-Nonyne	124	C9H16	020184-91-2	11
5	1-Cyclopentylacetonitrile	107	C7H9N	022734-04-9	9





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
STONE-1

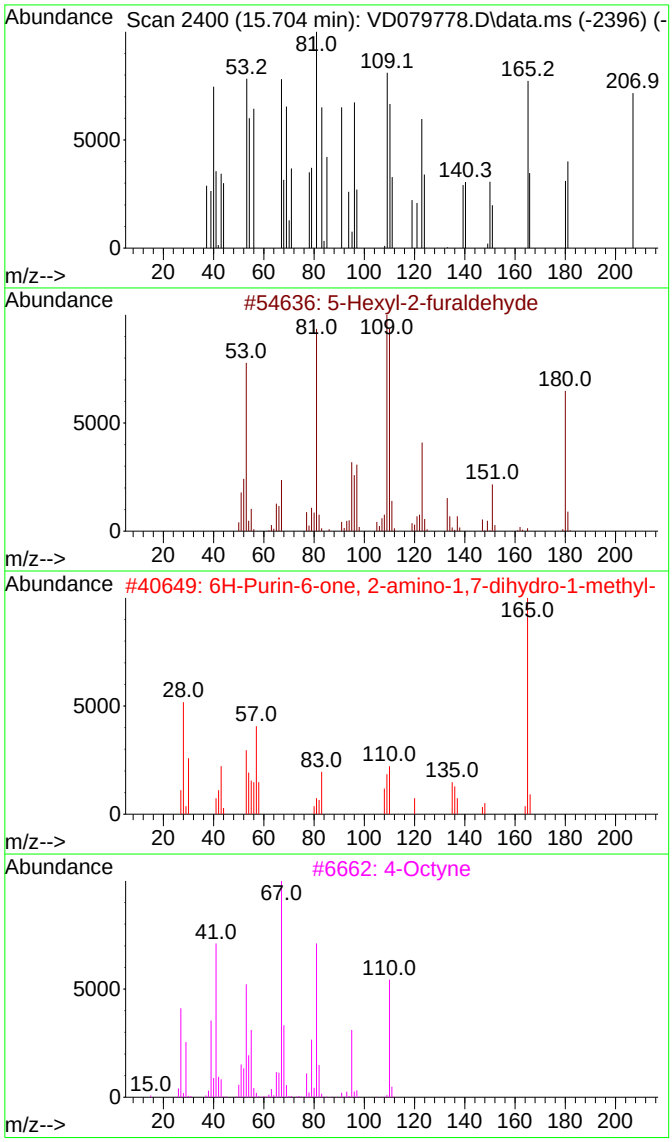
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D083024S.M
Quant Title : SW846 8260

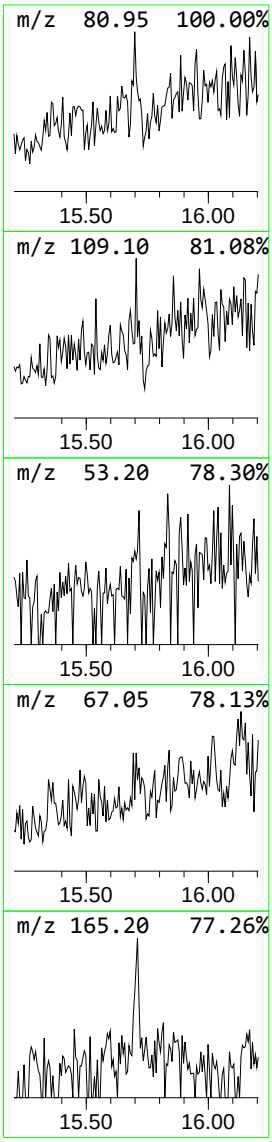
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 5-Hexyl-2-furaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.704	9.60 ug/l	21433	1,4-Dichlorobenzene-d4	13.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Hexyl-2-furaldehyde	180	C11H16O2	007011-80-5	52
2	6H-Purin-6-one, 2-amino-1,7-dihy...	165	C6H7N5O	000938-85-2	50
3	4-Octyne	110	C8H14	001942-45-6	35
4	2-Cyclopenten-1-one, 3-ethyl-	110	C7H10O	005682-69-9	35
5	Pinocarvone	150	C10H14O	030460-92-5	27





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
STONE-1

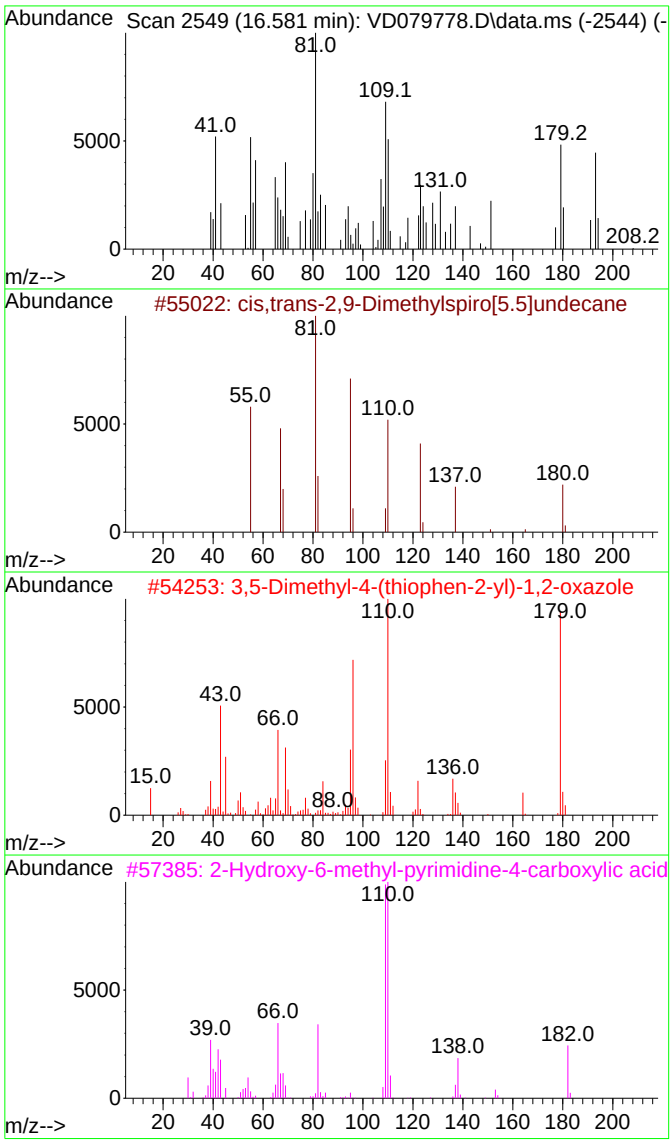
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D083024S.M
Quant Title : SW846 8260

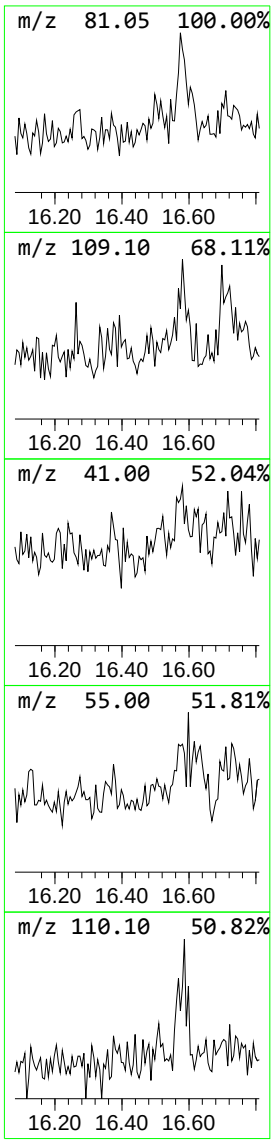
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 unknown16.581 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.581	17.58 ug/l	39243	1,4-Dichlorobenzene-d4	13.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis,trans-2,9-Dimethylspiro[5.5]...	180	C13H24	095530-74-8	42
2	3,5-Dimethyl-4-(thiophen-2-yl)-1...	179	C9H9NOS	1000411-47-9	35
3	2-Hydroxy-6-methyl-pyrimidine-4-...	182	C8H10N2O3	1000317-77-7	27
4	3-(Furan-2-ylmethyl-methyl-sulfa...	295	C13H13NO5S	1000300-37-8	27
5	2-Bromo-N-(furan-2-ylmethyl)benz...	329	C12H12BrNO3S	1003082-00-5	27





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown15.363	15.363	7.2	ug/l	15978	4	13.516	111636	50.0
unknown15.481	15.481	5.1	ug/l	11389	4	13.516	111636	50.0
5-Hexyl-2-fural...	15.704	9.6	ug/l	21433	4	13.516	111636	50.0
unknown16.581	16.581	17.6	ug/l	39243	4	13.516	111636	50.0