

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091025\
 Data File : VY023331.D
 Acq On : 10 Sep 2025 14:26
 Operator : SY/MD
 Sample : Q3066-03
 Misc : 5.10g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 VNJ-242

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\82Y090825S.M

Title : SW846 8260

Signal : TIC: VY023331.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.616	465	475	489	rBV2	30581	97681	2.95%	0.545%
2	5.652	632	645	655	rBV2	42583	135190	4.09%	0.755%
3	7.634	960	970	977	rBV	485005	1189094	35.95%	6.639%
4	7.713	977	983	1002	rVB	675246	1561220	47.20%	8.716%
5	8.060	1031	1040	1056	rBV	380761	865517	26.16%	4.832%
6	8.615	1122	1131	1150	rBV	1214566	2370444	71.66%	13.234%
7	10.109	1367	1376	1394	rBV	1957020	3307923	100.00%	18.468%
8	11.414	1582	1590	1603	rBV	1798599	2911862	88.03%	16.257%
9	12.407	1745	1753	1763	rBV	1305371	2021397	61.11%	11.286%
10	13.346	1899	1907	1916	rBV	1555389	2363044	71.44%	13.193%
11	15.169	2195	2206	2211	rBV	151008	255507	7.72%	1.427%
12	15.236	2211	2217	2224	rVV	212000	361098	10.92%	2.016%
13	15.321	2224	2231	2240	rVB	264214	471287	14.25%	2.631%

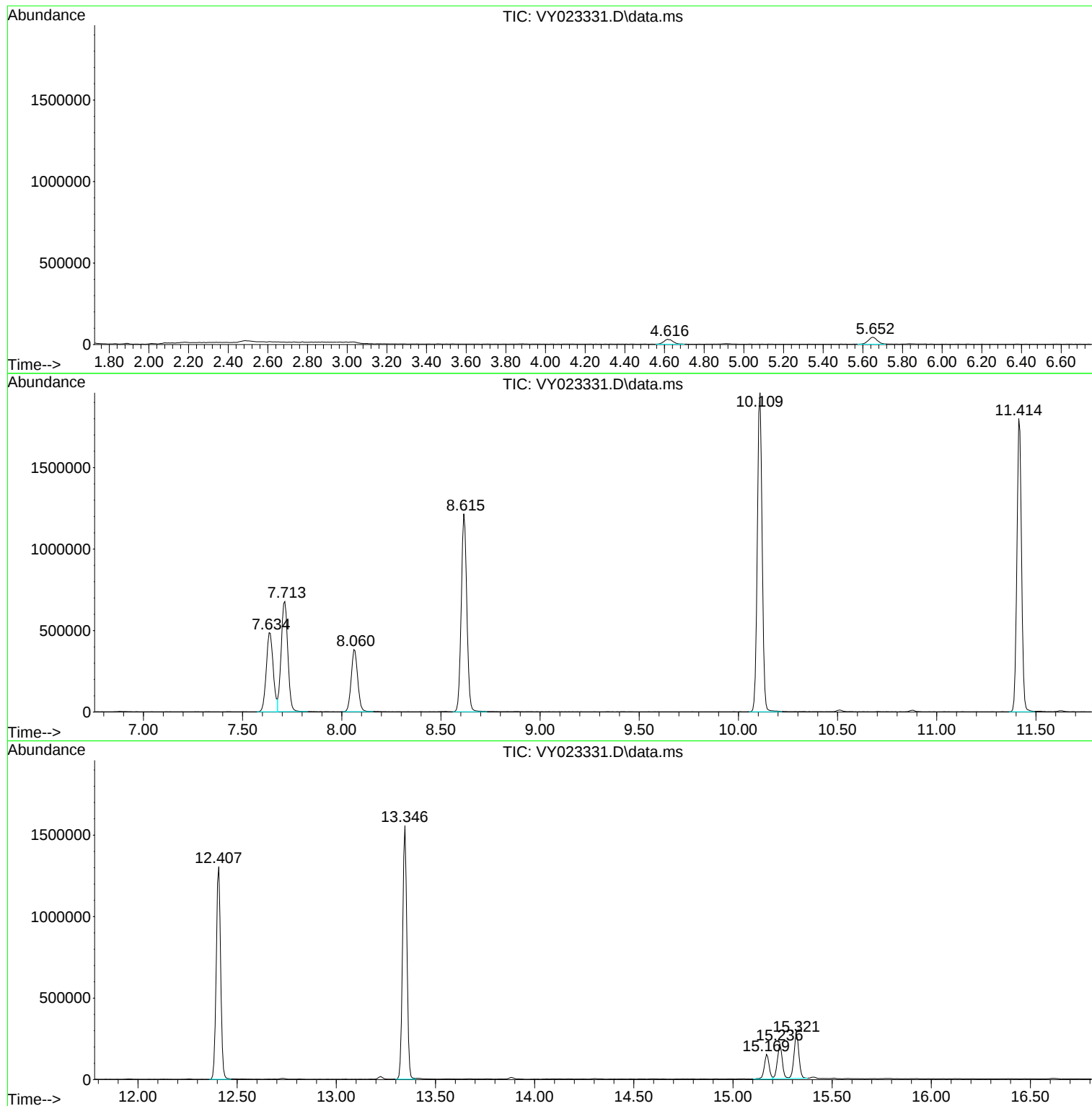
Sum of corrected areas: 17911264

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Quant Title : SW846 8260

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



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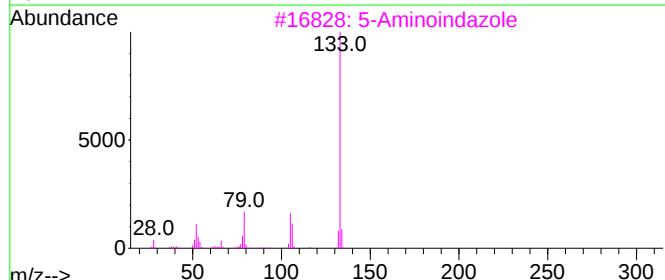
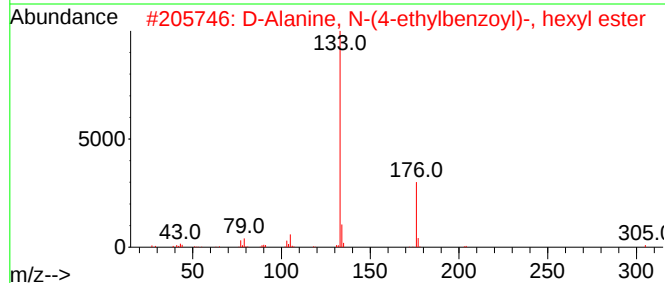
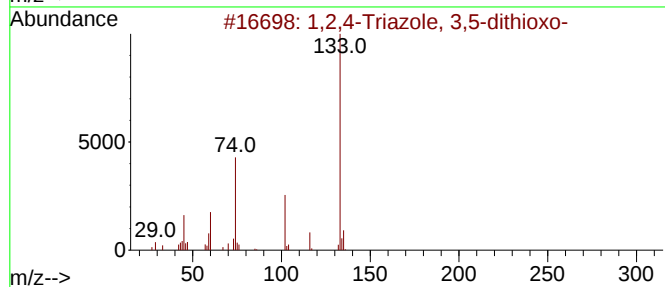
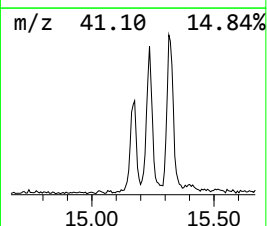
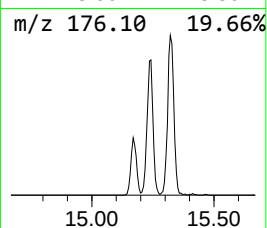
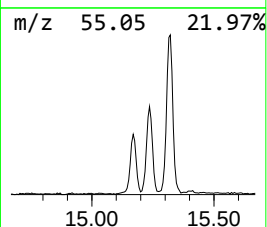
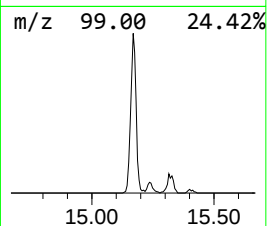
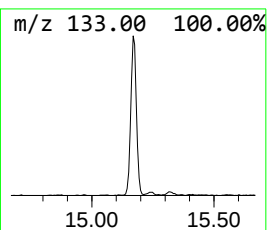
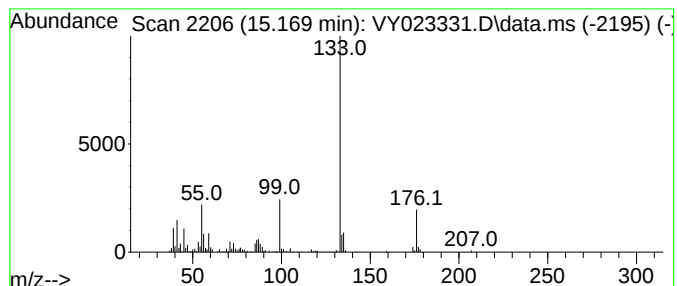
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090825S.M
Quant Title : SW846 8260

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

Peak Number 1 Unknown15.169 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.169	5.41 ug/l	255507	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,4-Triazole, 3,5-dithioxo-	133	C2H3N3S2	005650-03-3	43
2			D-Alanine, N-(4-ethylbenzoyl)-, ...	305	C18H27NO3	1000354-08-8	42
3			5-Aminoindazole	133	C7H7N3	019335-11-6	37
4			3-Methylthiazolidine-2-thione	133	C4H7NS2	001908-87-8	37
5			Benzamide, 4-ethyl-N-methyl-N-pe...	233	C15H23NO	1000420-69-5	33



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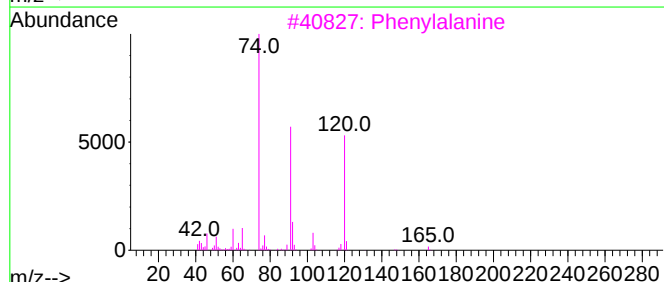
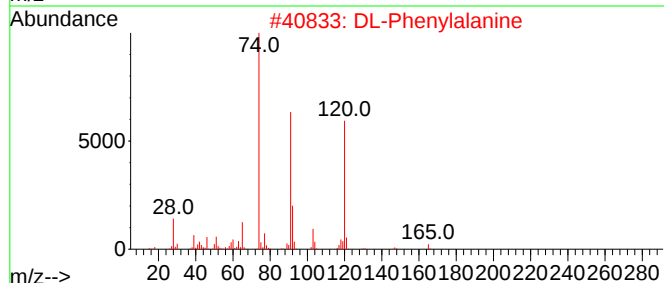
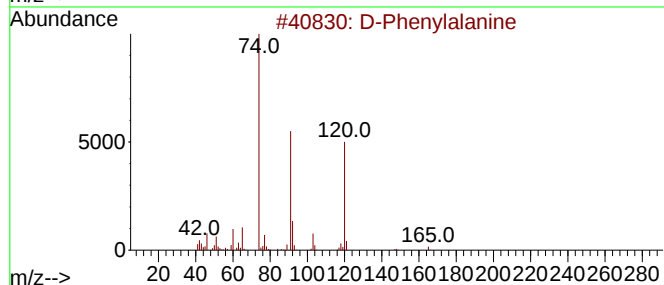
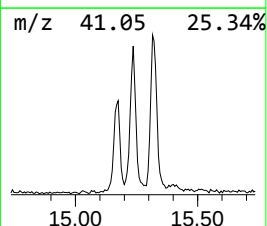
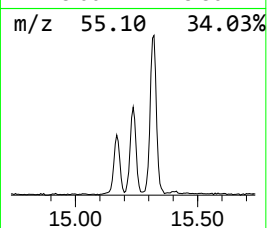
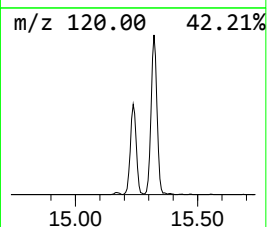
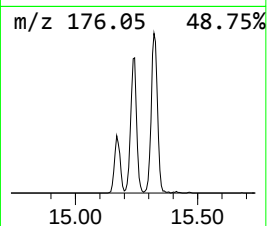
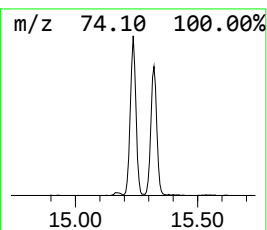
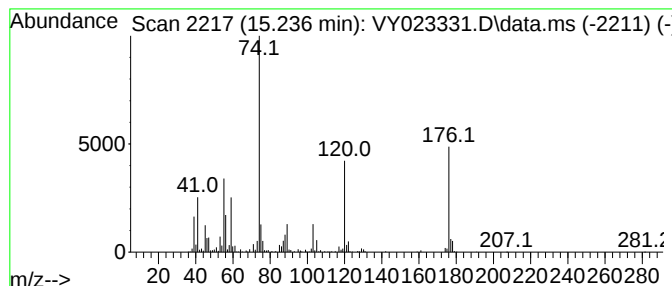
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Peak Number 2 unknown15.236 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.236	7.64 ug/l	361098	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Phenylalanine	165	C9H11NO2	000673-06-3	28
2			DL-Phenylalanine	165	C9H11NO2	000150-30-1	28
3			Phenylalanine	165	C9H11NO2	000063-91-2	28
4			1,3,4-Thiadiazol-2-amine, 5-methyl-	115	C3H5N3S	000108-33-8	25
5			Pentanoic acid, 3-hydroxy-2-meth...	174	C9H18O3	1000151-17-3	25



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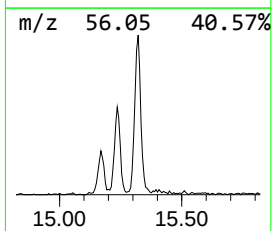
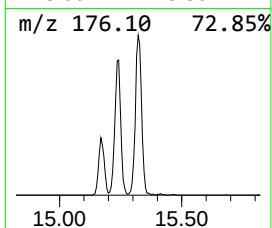
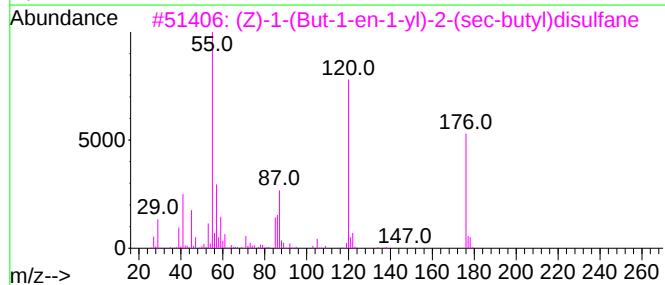
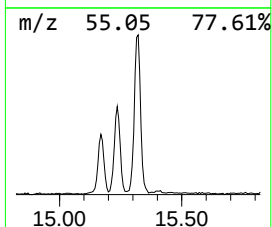
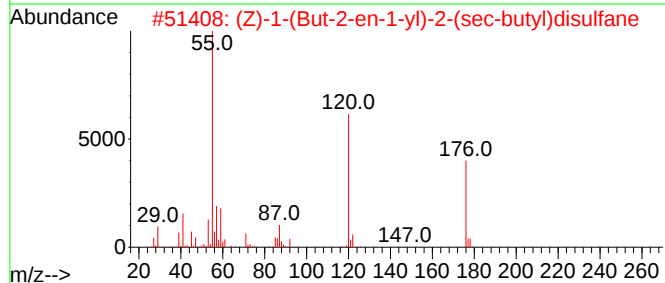
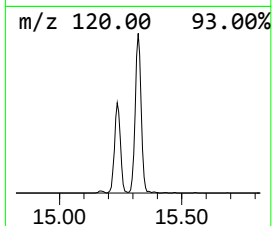
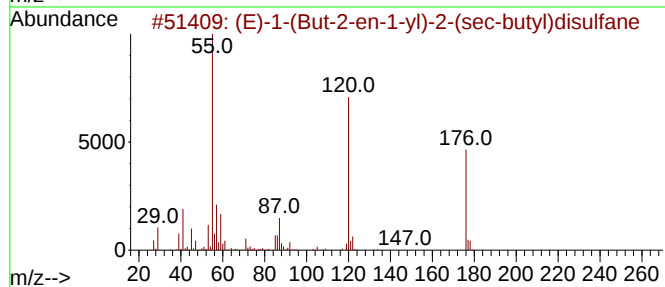
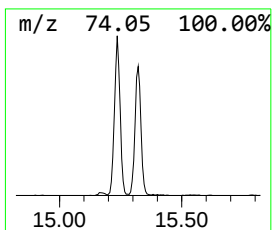
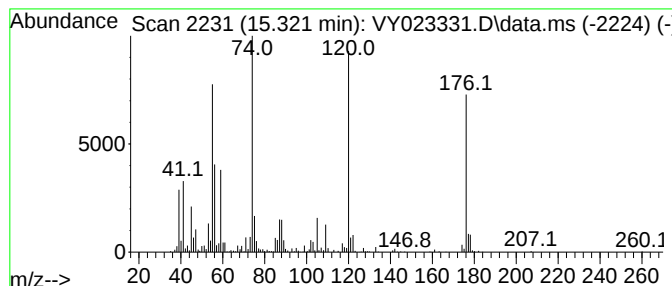
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Peak Number 3 Unknown15.321 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.321	9.97 ug/l	471287	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-1-(But-2-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-24-9	46		
2	(Z)-1-(But-2-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-23-8	46		
3	(Z)-1-(But-1-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-21-6	35		
4	(E)-1-(But-1-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-22-7	27		
5	dl-Homoserine	119	C4H9NO3	001927-25-9	22		



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ClientSampleId :
VNJ-242

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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Unknown15.169	15.169	5.4	ug/l	255507	4	13.346	2363040	50.0
unknown15.236	15.236	7.6	ug/l	361098	4	13.346	2363040	50.0
Unknown15.321	15.321	10.0	ug/l	471287	4	13.346	2363040	50.0