

Data Path : Z:\VOASRV\HPCHEM1\MSVOA D\DATA\VD081919\
 Data File : VD063661.D
 Acq On : 19 Aug 2019 16:51
 Operator : JC/SY
 Sample : K4385-17
 Misc : 5.62g/5ml/MSVOA D/SOIL
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 T8-D-(0)

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_D\METHOD\82D080919S.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	1.475	3	5	24	rVB	1204804	2918422	98.05%	13.190%
2	3.208	177	181	188	rBV2	72670	186107	6.25%	0.841%
3	3.808	234	242	253	rBV	61434	175392	5.89%	0.793%
4	6.919	549	558	564	rBV2	642849	1763518	59.25%	7.970%
5	7.037	564	570	587	rVB	973636	2687081	90.28%	12.144%
6	7.451	605	612	623	rBV	422335	1143949	38.43%	5.170%
7	8.209	683	689	707	rBV	1125083	2976472	100.00%	13.452%
8	10.404	905	912	920	rBV	1168236	2622220	88.10%	11.851%
9	12.363	1107	1111	1117	rBV	1608636	2482150	83.39%	11.218%
10	13.554	1228	1232	1239	rBV	1100372	1507765	50.66%	6.814%
11	13.712	1244	1248	1251	rVB	26591	46420	1.56%	0.210%
12	14.519	1326	1330	1334	rBV	1017678	1428085	47.98%	6.454%
13	15.110	1386	1390	1397	rBV4	18443	55880	1.88%	0.253%
14	15.287	1405	1408	1411	rBV2	37274	65230	2.19%	0.295%
15	15.385	1416	1418	1421	rBV	40180	68660	2.31%	0.310%
16	15.454	1422	1425	1430	rVV5	17681	44534	1.50%	0.201%
17	15.592	1435	1439	1442	rVB4	12700	33553	1.13%	0.152%
18	15.641	1442	1444	1446	rBV3	26137	40167	1.35%	0.182%
19	15.809	1458	1461	1464	rBV3	68151	94670	3.18%	0.428%
20	15.877	1465	1468	1470	rBV	50824	61359	2.06%	0.277%
21	15.927	1470	1473	1474	rBV3	50598	78725	2.64%	0.356%
22	16.045	1483	1485	1488	rVV4	20533	31271	1.05%	0.141%
23	16.143	1492	1495	1497	rBV2	81591	138974	4.67%	0.628%
24	16.202	1499	1501	1507	rVB3	90821	191052	6.42%	0.863%
25	16.301	1507	1511	1514	rBV6	37043	111271	3.74%	0.503%
26	16.380	1515	1519	1525	rVB7	63315	213580	7.18%	0.965%
27	16.478	1527	1529	1532	rBV3	47158	77478	2.60%	0.350%
28	16.586	1537	1540	1541	rVV3	45602	86567	2.91%	0.391%
29	16.655	1545	1547	1549	rVV2	64754	104292	3.50%	0.471%
30	16.704	1550	1552	1557	rVB5	46907	89380	3.00%	0.404%
31	16.882	1568	1570	1574	rVB5	31418	61457	2.06%	0.278%
32	16.950	1574	1577	1578	rBV3	15651	32339	1.09%	0.146%
33	17.039	1583	1586	1589	rVV4	82356	170335	5.72%	0.770%
34	17.138	1593	1596	1601	rVV5	41240	101973	3.43%	0.461%

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Stop Thrs : 0 Peak Location: TOP

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Title : SW846 8260

35	17.256	1604	1608	1611	rVV5	51462	110137	3.70%	0.498%
36	17.315	1611	1614	1620	rVV7	27794	66829	2.25%	0.302%
37	17.384	1620	1621	1628	rVB6	23351	59241	1.99%	0.268%

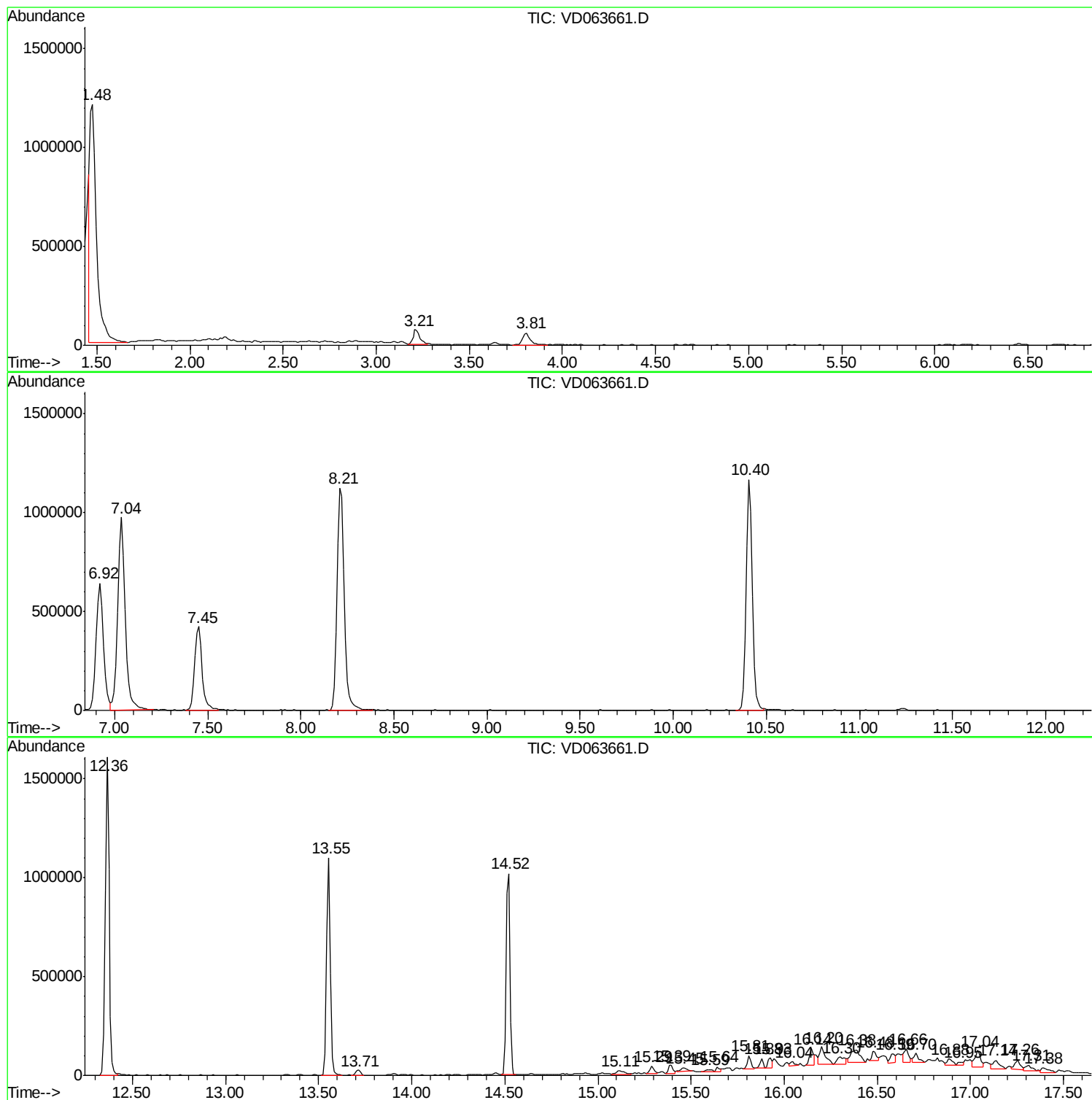
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Quant Title : SW846 8260

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



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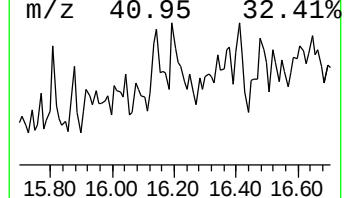
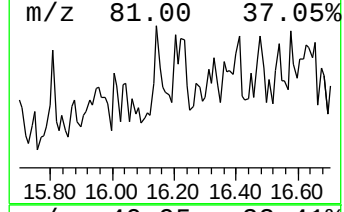
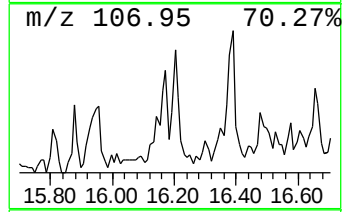
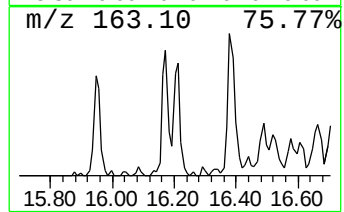
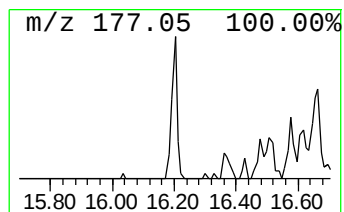
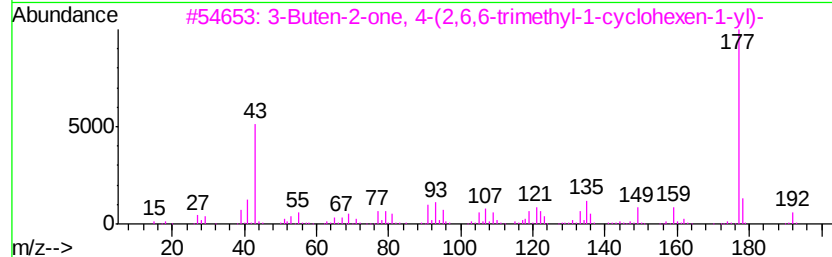
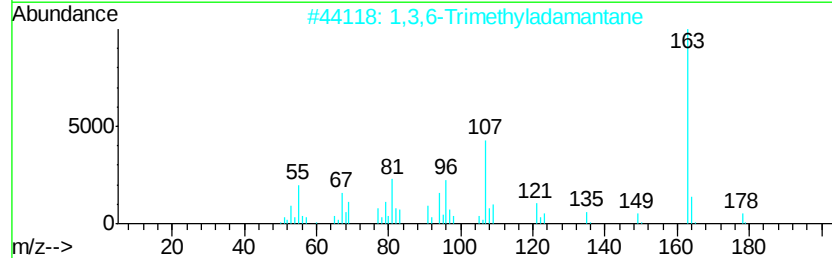
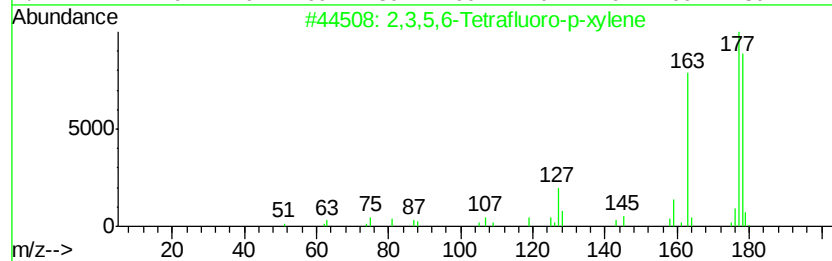
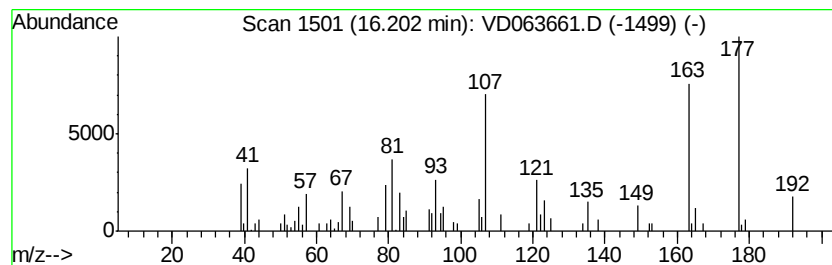
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_D\METHOD\82D080919S.M
 Quant Title : SW846 8260

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

 Peak Number 2 unknown16.20 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	6.69 ug/l	191052	1,4-Dichlorobenzene-d4	14.52

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3,5,6-Tetrafluoro-p-xylene			178	C8H6F4	000703-87-7	47
2	1,3,6-Trimethyladamantane			178	C13H22	024139-37-5	37
3	3-Buten-2-one, 4-(2,6,6-trimethy...			192	C13H20O	014901-07-6	35
4	1,4-Methanophthalazine, 1,4,4a,5...			206	C13H22N2	109746-14-7	32
5	2,3'-Bipyridine, 1',3,4,4',5,5',...			164	C10H16N2	018017-50-0	27



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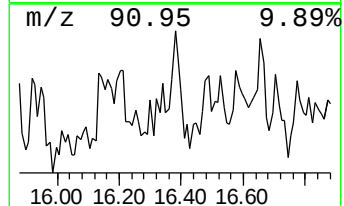
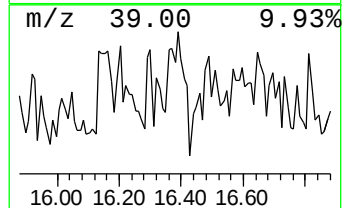
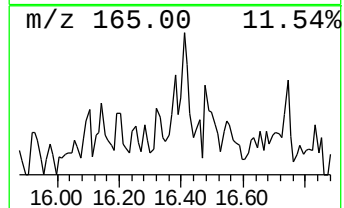
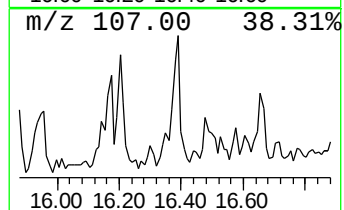
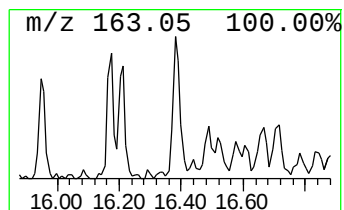
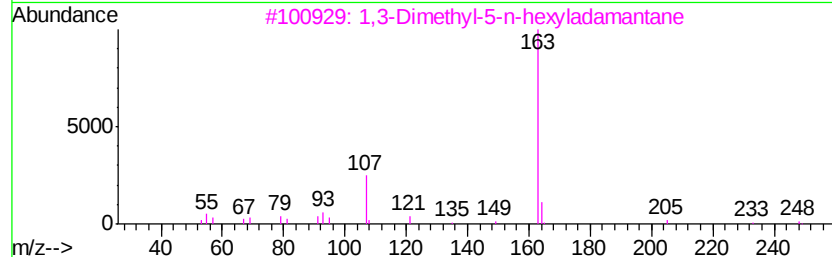
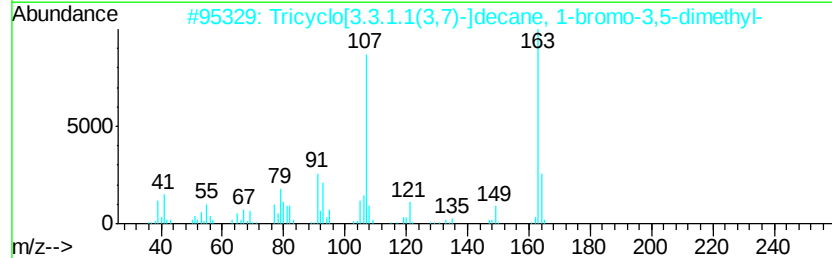
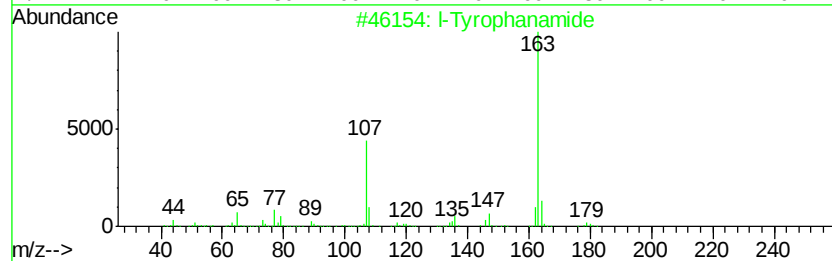
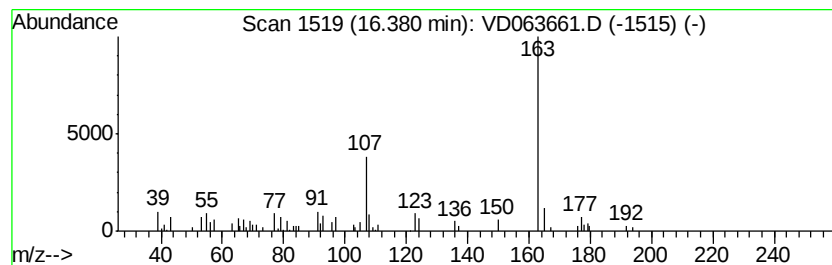
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Peak Number 3 l-Tyrophanamide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.38	7.48 ug/l	213580	1,4-Dichlorobenzene-d4	14.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		l-Tyrophanamide	180 C9H12N2O2	1000131-25-3 64
2		Tricyclo[3.3.1.1(3,7)]decane, 1...	242 C12H19Br	000941-37-7 59
3		1,3-Dimethyl-5-n-hexyladamantane	248 C18H32	052873-50-4 59
4		1,3,6-Trimethyladamantane	178 C13H22	024139-37-5 45
5		9H-Purin-6-amine, N,9-dimethyl-	163 C7H9N5	002009-52-1 45



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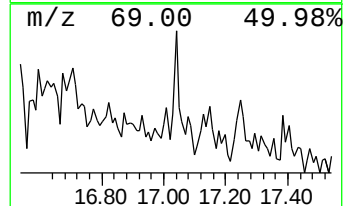
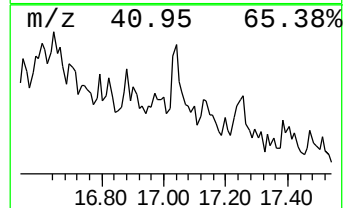
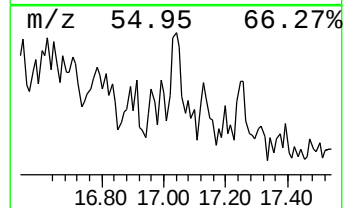
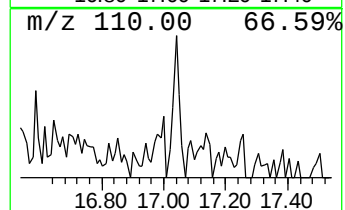
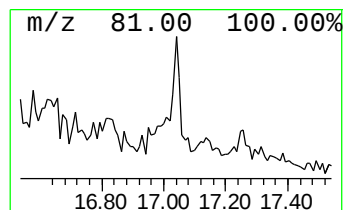
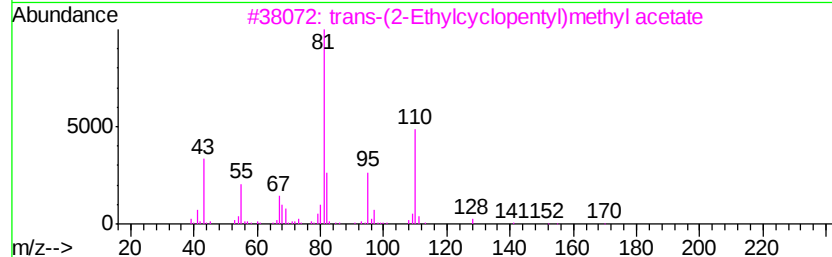
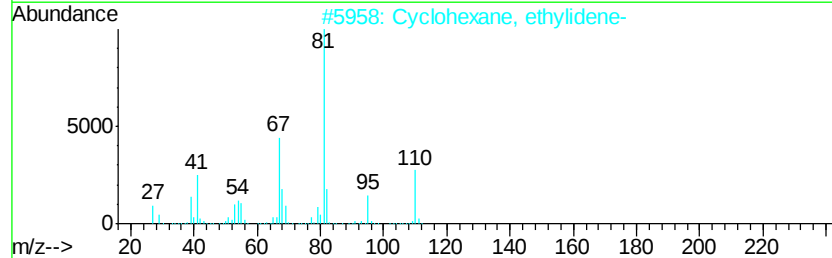
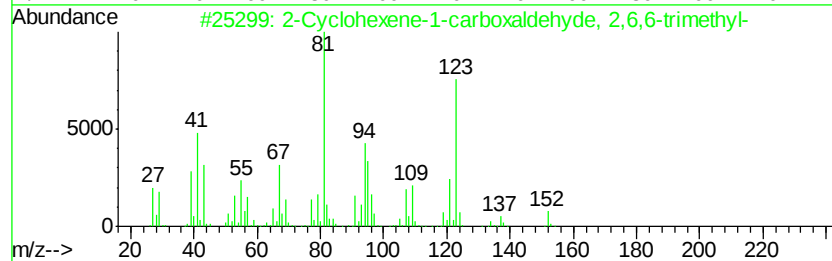
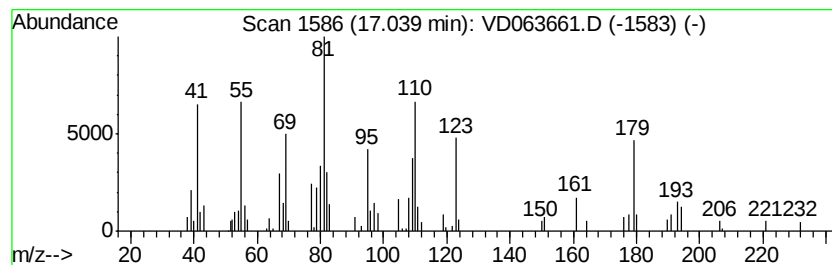
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Peak Number 4 unknown17.04 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.04	5.96 ug/l	170335	1,4-Dichlorobenzene-d4	14.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Cyclohexene-1-carboxaldehyde, ...	152 C10H16O	000432-24-6	43
2	Cyclohexane, ethylidene-	110 C8H14	001003-64-1	38
3	trans-(2-Ethylcyclopentyl)methyl...	170 C10H18O2	1000099-13-9	38
4	2-Ethylcyclohexanol, heptafluoro...	324 C12H15F7O2	959079-92-6	35
5	Methyl ethyl cyclopentene	110 C8H14	019780-56-4	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown16.20	16.20	6.7	ug/l	191052	4	14.52	1428090	50.0
l-Tyrophanamide	16.38	7.5	ug/l	213580	4	14.52	1428090	50.0
unknown17.04	17.04	6.0	ug/l	170335	4	14.52	1428090	50.0