

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY080421\
 Data File : VY005531.D
 Acq On : 04 Aug 2021 12:42
 Operator : SY/MD
 Sample : M3271-01
 Misc : 5.01G/5ML/MSVOA_Y/SOIL
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 TP-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_Y\methods\82Y080221S.M
 Title : SW846 8260

Signal : TIC: VY005531.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.046	32	37	44	rVB2	3373	6297	17.03%	2.500%
2	2.168	55	57	59	rBV2	478	579	1.57%	0.230%
3	2.363	87	89	92	rBV3	626	556	1.50%	0.221%
4	2.436	99	101	102	rBV	435	434	1.17%	0.172%
5	2.455	102	104	106	rVB2	793	738	2.00%	0.293%
6	2.516	112	114	118	rVB3	719	918	2.48%	0.364%
7	2.613	128	130	132	rVB	540	401	1.08%	0.159%
8	2.637	132	134	137	rBV3	571	584	1.58%	0.232%
9	2.765	153	155	158	rBV3	403	491	1.33%	0.195%
10	2.991	191	192	195	rVB3	524	474	1.28%	0.188%
11	3.223	227	230	235	rVB3	306	561	1.52%	0.223%
12	3.564	281	286	290	rBV3	230	426	1.15%	0.169%
13	4.113	370	376	377	rBV4	615	1204	3.26%	0.478%
14	4.716	470	475	476	rVV4	692	1109	3.00%	0.440%
15	4.735	476	478	483	rVB3	778	993	2.69%	0.394%
16	5.765	642	647	648	rBV2	390	403	1.09%	0.160%
17	5.899	667	669	671	rBV3	397	408	1.10%	0.162%
18	6.131	704	707	712	rBV3	278	459	1.24%	0.182%
19	6.186	712	716	717	rBV	314	406	1.10%	0.161%
20	6.753	805	809	811	rBV	463	604	1.63%	0.240%
21	7.100	865	866	869	rBV2	338	408	1.10%	0.162%
22	7.429	919	920	926	rVB2	398	485	1.31%	0.193%
23	7.576	942	944	947	rVB3	499	440	1.19%	0.175%
24	7.600	947	948	952	rBV2	384	409	1.11%	0.162%
25	7.722	961	968	975	rBV4	4411	10967	29.66%	4.355%
26	7.795	975	980	987	rVB2	8870	17485	47.29%	6.943%
27	7.960	1004	1007	1009	rVV2	389	448	1.21%	0.178%
28	8.002	1012	1014	1019	rVB3	304	370	1.00%	0.147%
29	8.094	1026	1029	1031	rBV2	417	452	1.22%	0.179%
30	8.149	1031	1038	1046	rVV2	5360	11716	31.69%	4.652%
31	8.228	1050	1051	1059	rVB2	374	688	1.86%	0.273%
32	8.295	1059	1062	1065	rBV4	394	539	1.46%	0.214%
33	8.319	1065	1066	1069	rBV3	371	459	1.24%	0.182%
34	8.502	1094	1096	1101	rVB3	498	649	1.76%	0.258%
35	8.697	1121	1128	1135	rVB2	14002	26698	72.21%	10.601%
36	9.630	1277	1281	1283	rBV4	440	505	1.37%	0.201%

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37	9.764	1300	1303	1307	rVB4	341	518	1.40%	0.206%
38	10.093	1353	1357	1360	rVB3	345	381	1.03%	0.151%
39	10.185	1365	1372	1380	rVV	21195	36972	100.00%	14.680%
40	10.252	1380	1383	1386	rVB3	384	470	1.27%	0.187%
41	10.362	1398	1401	1402	rBV2	413	460	1.24%	0.183%
42	10.587	1436	1438	1441	rVB3	447	382	1.03%	0.152%
43	10.630	1443	1445	1448	rVB3	401	404	1.09%	0.160%
44	10.679	1452	1453	1456	rBV2	472	448	1.21%	0.178%
45	10.715	1456	1459	1460	rBV2	647	616	1.67%	0.245%
46	11.099	1520	1522	1524	rBV3	407	458	1.24%	0.182%
47	11.124	1524	1526	1529	rVB3	408	422	1.14%	0.168%
48	11.227	1541	1543	1546	rVB3	524	521	1.41%	0.207%
49	11.264	1546	1549	1551	rBV4	305	494	1.34%	0.196%
50	11.307	1551	1556	1558	rVB3	461	695	1.88%	0.276%
51	11.343	1558	1562	1563	rBV3	558	397	1.07%	0.158%
52	11.496	1581	1587	1594	rBV	19955	33658	91.04%	13.364%
53	11.605	1602	1605	1607	rVV3	428	396	1.07%	0.157%
54	11.709	1618	1622	1626	rBV4	1007	1423	3.85%	0.565%
55	11.764	1626	1631	1634	rBV2	526	990	2.68%	0.393%
56	11.807	1634	1638	1639	rVB3	417	478	1.29%	0.190%
57	11.892	1650	1652	1656	rVB2	381	409	1.11%	0.162%
58	11.935	1656	1659	1660	rBV2	405	379	1.03%	0.150%
59	11.953	1660	1662	1665	rVB3	385	443	1.20%	0.176%
60	12.148	1692	1694	1696	rBV2	415	417	1.13%	0.166%
61	12.325	1721	1723	1727	rVV4	518	519	1.40%	0.206%
62	12.483	1744	1749	1755	rBV2	13509	20890	56.50%	8.294%
63	12.556	1758	1761	1762	rBV2	440	379	1.03%	0.150%
64	12.623	1768	1772	1773	rBV3	634	807	2.18%	0.320%
65	12.684	1778	1782	1784	rBV5	464	611	1.65%	0.243%
66	12.739	1788	1791	1795	rBV4	363	701	1.90%	0.278%
67	12.812	1801	1803	1806	rBV4	960	827	2.24%	0.328%
68	12.861	1808	1811	1815	rVB3	500	773	2.09%	0.307%
69	12.965	1826	1828	1831	rBV3	468	476	1.29%	0.189%
70	13.026	1836	1838	1841	rVB3	756	836	2.26%	0.332%
71	13.068	1843	1845	1847	rBV3	664	766	2.07%	0.304%
72	13.129	1852	1855	1859	rVB5	699	980	2.65%	0.389%
73	13.312	1884	1885	1887	rBV2	454	396	1.07%	0.157%
74	13.367	1891	1894	1899	rVV6	989	1743	4.71%	0.692%
75	13.428	1899	1904	1912	rVV2	13859	23757	64.26%	9.433%
76	13.495	1913	1915	1919	rVV5	485	490	1.33%	0.195%

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77	13.532	1919	1921	1924	rVV3	794	783	2.12%	0.311%
78	13.562	1924	1926	1929	rVB4	653	497	1.34%	0.197%
79	13.605	1932	1933	1934	rBV	670	375	1.01%	0.149%
80	13.623	1934	1936	1938	rVB3	568	640	1.73%	0.254%
81	13.703	1945	1949	1952	rVB5	1141	1700	4.60%	0.675%
82	13.739	1952	1955	1956	rBV3	1171	969	2.62%	0.385%
83	13.824	1965	1969	1971	rBV5	468	745	2.02%	0.296%
84	13.885	1977	1979	1982	rBV4	483	493	1.33%	0.196%
85	13.916	1982	1984	1987	rVB4	588	510	1.38%	0.202%
86	13.965	1990	1992	1993	rBV	885	433	1.17%	0.172%
87	14.111	2014	2016	2021	rBV5	658	917	2.48%	0.364%
88	14.154	2021	2023	2024	rBV2	734	571	1.54%	0.227%
89	14.227	2033	2035	2036	rBV	709	573	1.55%	0.228%
90	14.324	2050	2051	2052	rBV	802	464	1.26%	0.184%
91	14.367	2057	2058	2064	rVB6	1141	1200	3.25%	0.476%
92	14.483	2075	2077	2080	rVB4	1080	1142	3.09%	0.453%
93	14.800	2127	2129	2130	rBV2	1250	960	2.60%	0.381%
94	15.160	2186	2188	2189	rBV2	1179	991	2.68%	0.393%
95	15.233	2197	2200	2202	rBV3	1418	2249	6.08%	0.893%
96	15.336	2215	2217	2218	rBV2	1169	689	1.86%	0.274%
97	15.428	2229	2232	2238	rVB7	1936	3120	8.44%	1.239%
98	15.477	2238	2240	2241	rBV2	1175	864	2.34%	0.343%
99	15.580	2254	2257	2261	rBV4	1652	3024	8.18%	1.201%

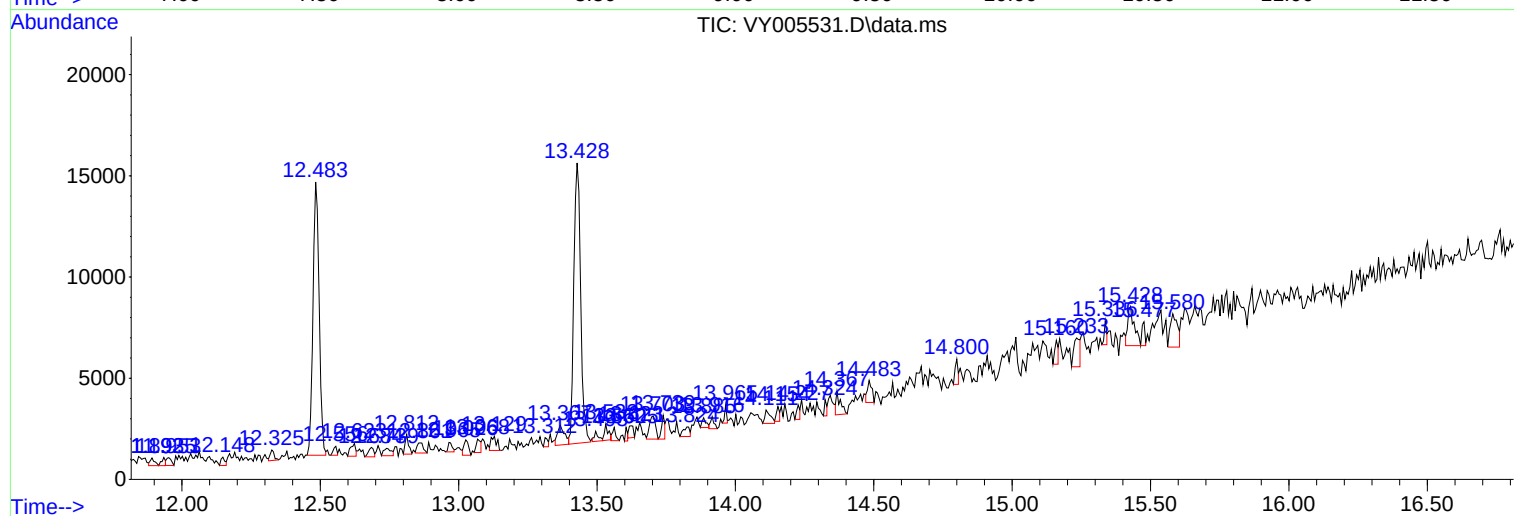
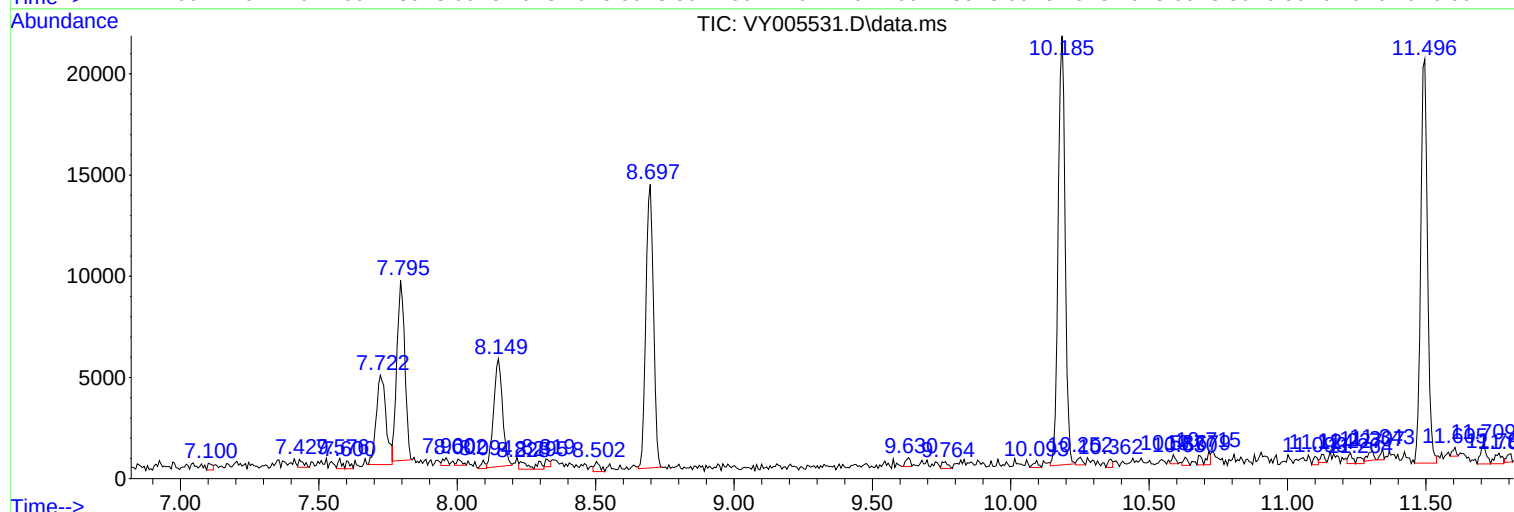
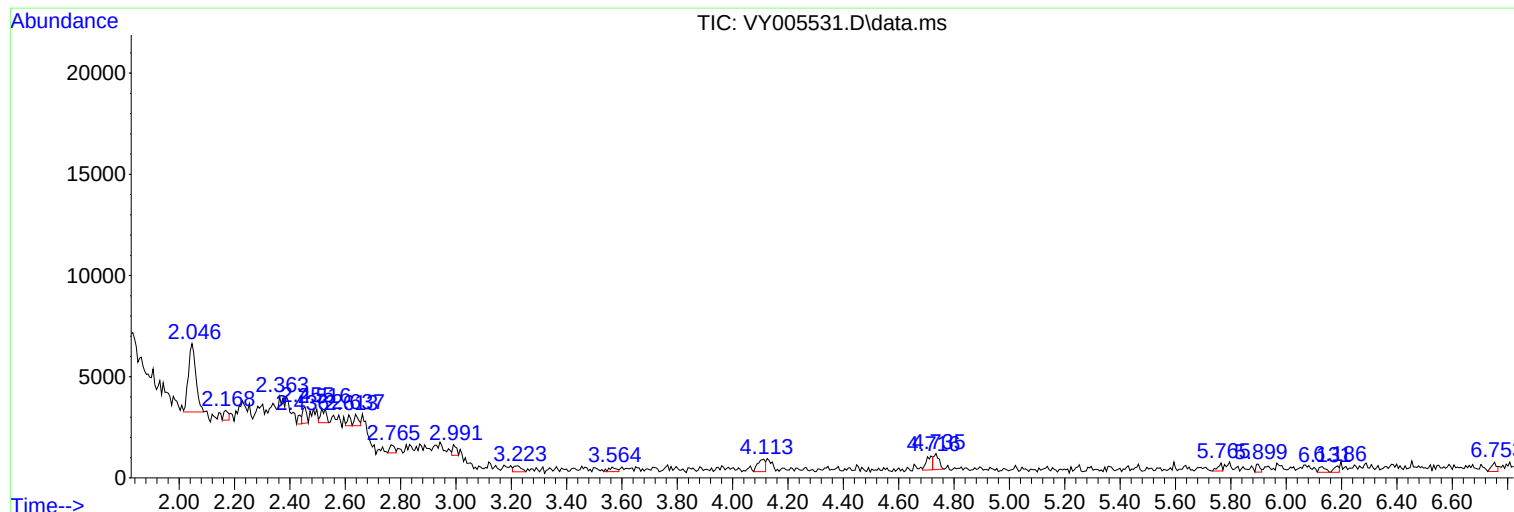
Sum of corrected areas: 251854

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y080221S.M
Quant Title : SW846 8260

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



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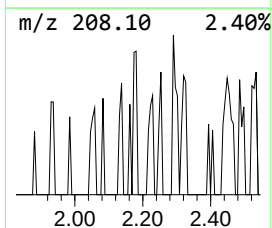
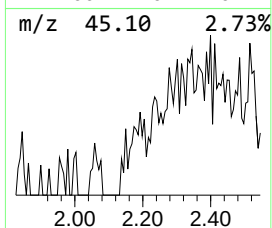
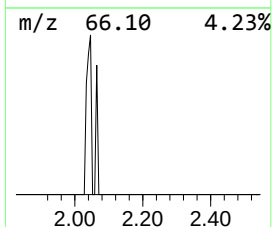
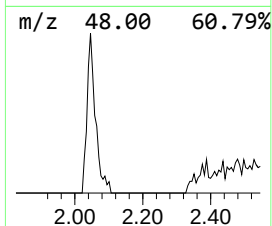
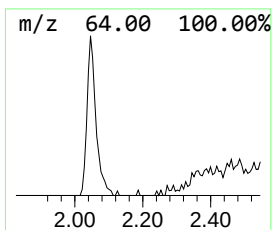
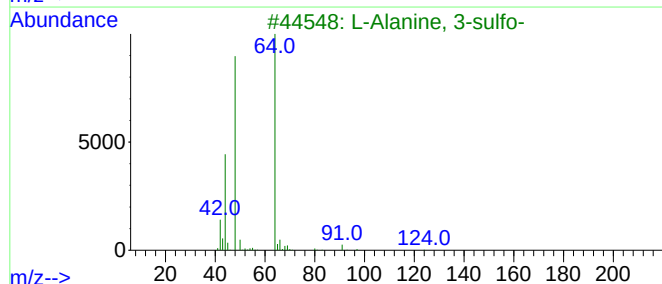
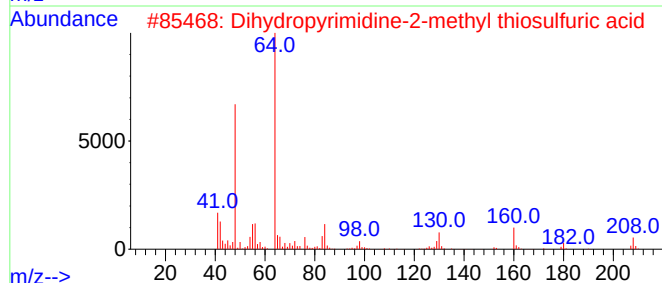
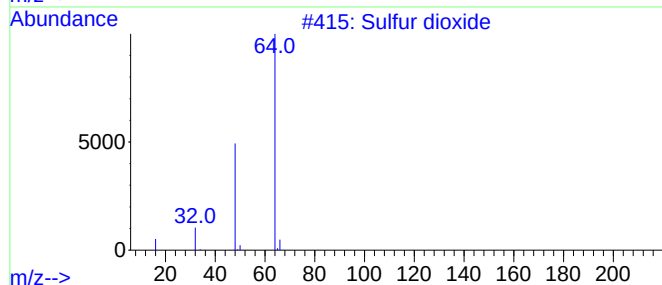
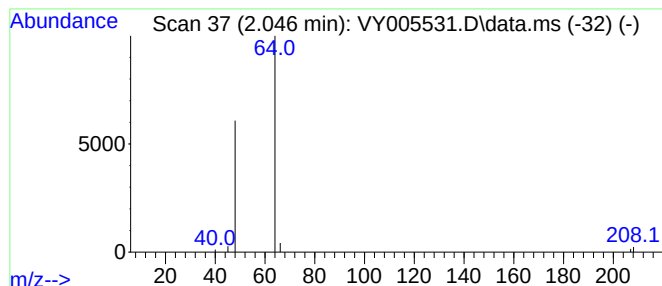
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y080221S.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.046	18.01 ug/l	6297	Pentafluorobenzene	7.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	64
4			1,1,1,2,2,3,3,4,4,5,5-Undecaflu...	602	C10F22O2S	1000486-78-5	9
5			Thiosulfuric acid (H2S2O3), S-(2...	320	C11H16N2O3S3	040284-00-2	9



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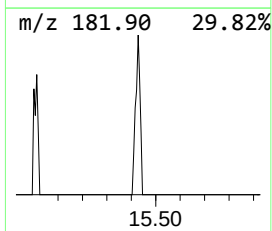
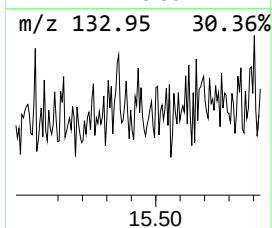
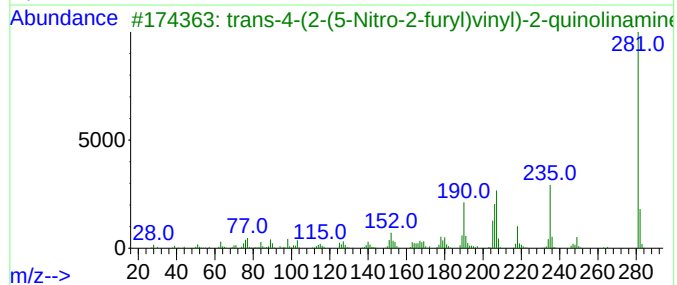
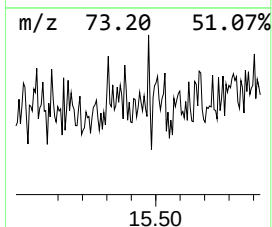
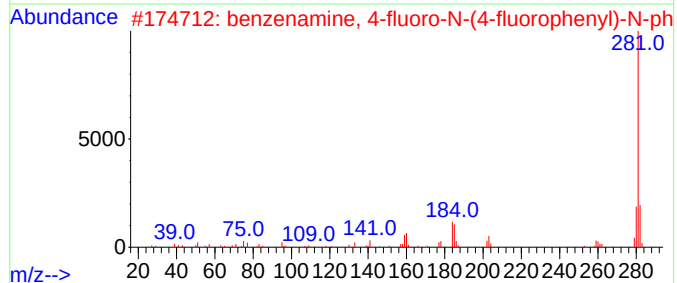
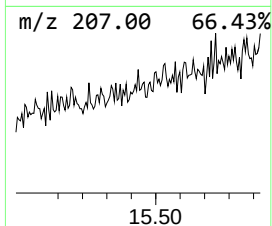
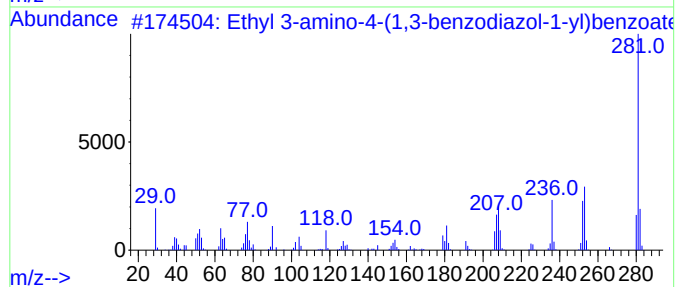
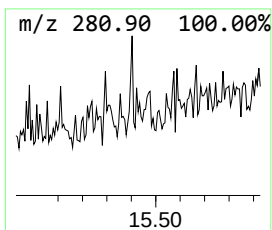
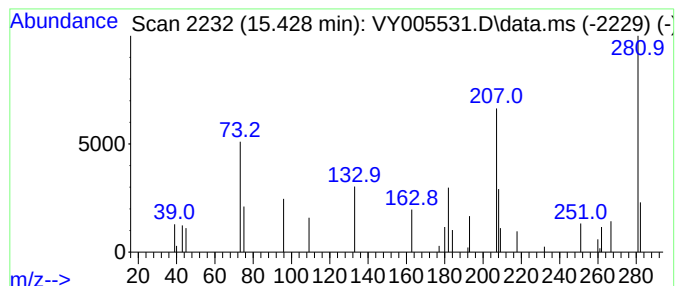
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown15.428 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.428	6.57 ug/l	3120	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl 3-amino-4-(1,3-benzodiazol...	281	C16H15N3O2	1000444-00-5	43
2			benzenamine, 4-fluoro-N-(4-fluor...	281	C18H13F2N	1000397-18-4	35
3			trans-4-(2-(5-Nitro-2-furyl)viny...	281	C15H11N3O3	000847-10-9	32
4			1,6-Dihydropyridine-3-carboxylic...	282	C16H14N2O3	1010270-81-4	27
5			6-Methoxy-4-methylamino-2-triflu...	281	C13H10F3N3O	1000311-86-1	9



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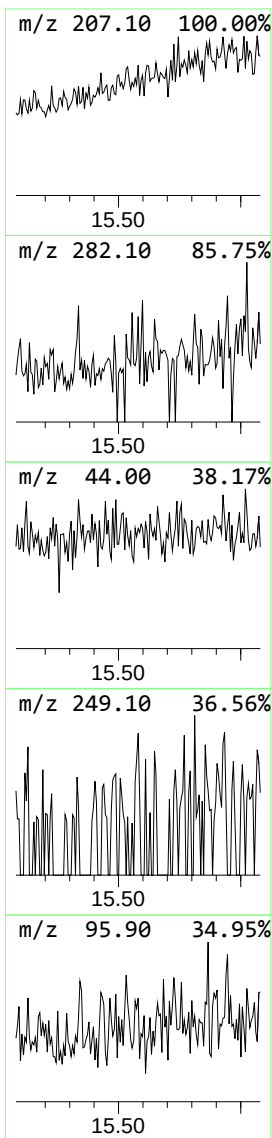
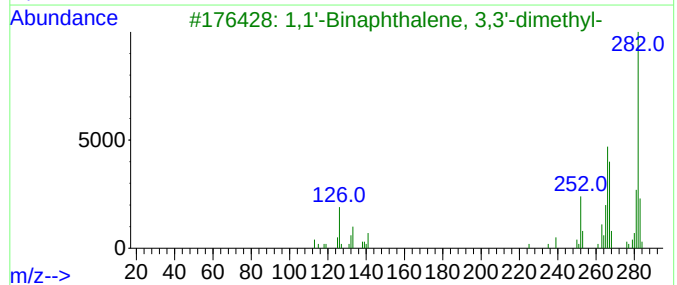
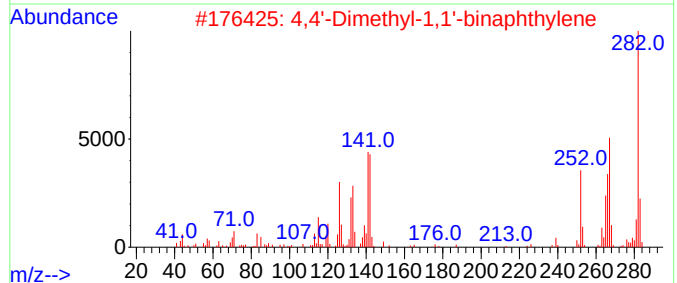
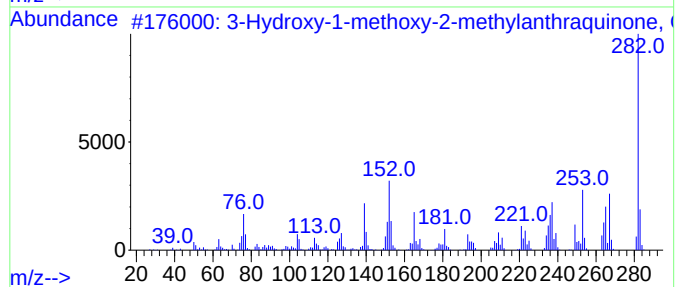
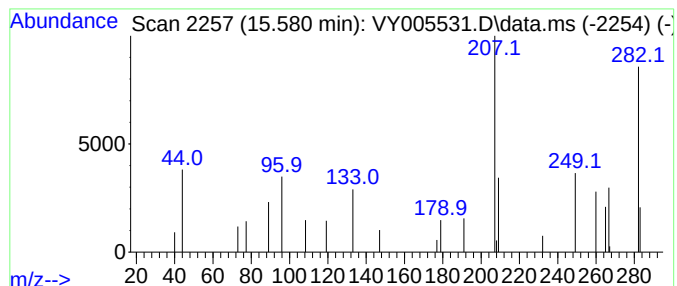
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Quant Title : SW846 8260

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

Peak Number 3 unknown15.580 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.580	6.36 ug/l	3024	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hydroxy-1-methoxy-2-methylantr...	282	C17H14O4	022170-88-3	35
2			4,4'-Dimethyl-1,1'-binaphthylene	282	C22H18	019224-41-0	35
3			1,1'-Binaphthalene, 3,3'-dimethyl-	282	C22H18	034042-82-5	35
4			1,1'-Binaphthalene, 8,8'-dimethyl-	282	C22H18	032693-05-3	35
5			Dibenz[c,E]cycloheptene, 3,4,7-t...	282	C18H18O3	145068-70-8	27



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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
Sulfur dioxide	2.046	18.0	ug/l	6297	1	7.801	17485	50.0
unknown15.428	15.428	6.6	ug/l	3120	4	13.428	23757	50.0
unknown15.580	15.580	6.4	ug/l	3024	4	13.428	23757	50.0