

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041923\
 Data File : VY013355.D
 Acq On : 19 Apr 2023 19:02
 Operator : KP/MD
 Sample : 02366-05
 Misc : 4.35g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20230307-29-1

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\82Y041223S.M
 Title : SW846 8260

Signal : TIC: VY013355.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.863	3	7	20	rVB2	34602	68429	6.40%	0.689%
2	2.077	35	42	49	rBV2	23880	35538	3.32%	0.358%
3	2.223	60	66	67	rBV	33589	46240	4.32%	0.466%
4	2.247	67	70	81	rVB	61134	99776	9.33%	1.005%
5	2.388	89	93	101	rVB2	5845	10918	1.02%	0.110%
6	2.906	169	178	189	rBV2	39133	89986	8.41%	0.907%
7	3.253	227	235	247	rVB3	23962	60089	5.62%	0.605%
8	3.954	340	350	362	rBV	97805	350566	32.78%	3.532%
9	4.198	379	390	405	rVB2	56837	158782	14.85%	1.600%
10	4.716	461	475	495	rBV7	15962	78736	7.36%	0.793%
11	5.241	549	561	572	rVB5	4772	17780	1.66%	0.179%
12	5.747	635	644	658	rVB3	6663	21936	2.05%	0.221%
13	6.801	809	817	826	rVV8	5405	16972	1.59%	0.171%
14	6.990	838	848	865	rBV2	36962	117565	10.99%	1.184%
15	7.722	958	968	973	rBV	160000	383590	35.87%	3.865%
16	7.789	973	979	990	rVB	271697	614443	57.46%	6.191%
17	8.143	1028	1037	1049	rBV2	162666	364427	34.08%	3.672%
18	8.326	1061	1067	1076	rVB2	5956	16710	1.56%	0.168%
19	8.551	1097	1104	1111	rVB6	6393	13831	1.29%	0.139%
20	8.691	1118	1127	1139	rBV	393063	783671	73.28%	7.896%
21	8.923	1158	1165	1172	rBV2	7531	17729	1.66%	0.179%
22	9.185	1195	1208	1214	rBV8	10286	32107	3.00%	0.323%
23	9.618	1271	1279	1287	rBV2	7078	14357	1.34%	0.145%
24	9.746	1292	1300	1306	rBV4	5219	13468	1.26%	0.136%
25	10.179	1364	1371	1380	rBV	623625	1069385	100.00%	10.774%
26	10.368	1394	1402	1409	rVB5	6448	17634	1.65%	0.178%
27	10.520	1423	1427	1433	rVB4	7041	12519	1.17%	0.126%
28	10.612	1438	1442	1449	rVB9	5552	13871	1.30%	0.140%
29	11.087	1515	1520	1526	rVB2	15106	26525	2.48%	0.267%
30	11.301	1548	1555	1564	rVB6	13144	34924	3.27%	0.352%
31	11.490	1579	1586	1596	rBV2	562810	1055187	98.67%	10.631%
32	11.624	1605	1608	1613	rVB4	8943	13115	1.23%	0.132%
33	11.685	1613	1618	1621	rBV3	11757	23722	2.22%	0.239%
34	11.740	1624	1627	1632	rVB5	13430	20744	1.94%	0.209%
35	11.843	1639	1644	1647	rBV5	7709	13813	1.29%	0.139%
36	11.886	1647	1651	1656	rVB8	8148	14548	1.36%	0.147%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	12.002	1663	1670	1677	rBV4	28741	69901	6.54%	0.704%
38	12.124	1681	1690	1694	rVB3	21566	41837	3.91%	0.422%
39	12.203	1694	1703	1705	rBV5	34671	69807	6.53%	0.703%
40	12.233	1705	1708	1713	rVB2	46860	72724	6.80%	0.733%
41	12.319	1713	1722	1727	rBV8	14530	40713	3.81%	0.410%
42	12.483	1741	1749	1755	rBV3	452199	754376	70.54%	7.601%
43	12.557	1755	1761	1762	rBV4	15769	27011	2.53%	0.272%
44	12.642	1768	1775	1783	rVB6	60274	141942	13.27%	1.430%
45	12.727	1783	1789	1795	rBV8	31285	87530	8.19%	0.882%
46	12.813	1795	1803	1816	rVB10	49350	219309	20.51%	2.210%
47	12.947	1822	1825	1829	rVB4	22277	25998	2.43%	0.262%
48	13.002	1829	1834	1837	rBV6	11552	23707	2.22%	0.239%
49	13.038	1837	1840	1842	rBV4	18256	24327	2.27%	0.245%
50	13.069	1842	1845	1852	rVB2	52932	74244	6.94%	0.748%
51	13.130	1852	1855	1857	rBV4	10377	13812	1.29%	0.139%
52	13.172	1858	1862	1869	rBV4	24997	45488	4.25%	0.458%
53	13.288	1872	1881	1885	rBV2	81692	175098	16.37%	1.764%
54	13.361	1890	1893	1897	rVV4	31879	57433	5.37%	0.579%
55	13.428	1898	1904	1909	rVV	469371	809964	75.74%	8.161%
56	13.477	1909	1912	1918	rVB2	65077	132105	12.35%	1.331%
57	13.569	1923	1927	1931	rVB3	20454	28632	2.68%	0.288%
58	13.629	1931	1937	1943	rBV	127827	236510	22.12%	2.383%
59	13.745	1950	1956	1961	rBV5	54461	107196	10.02%	1.080%
60	13.965	1987	1992	2003	rVB3	79686	171023	15.99%	1.723%
61	14.081	2006	2011	2015	rBV2	34346	58314	5.45%	0.588%
62	14.209	2027	2032	2035	rBV7	18320	29451	2.75%	0.297%
63	14.257	2035	2040	2044	rBV4	34595	64656	6.05%	0.651%
64	14.392	2055	2062	2063	rBV6	22622	43794	4.10%	0.441%
65	14.422	2064	2067	2070	rVB4	30354	41224	3.85%	0.415%
66	14.568	2085	2091	2096	rVB4	16985	37350	3.49%	0.376%
67	14.678	2104	2109	2114	rBV4	37391	84295	7.88%	0.849%
68	14.733	2114	2118	2128	rVB5	45817	108127	10.11%	1.089%
69	14.940	2148	2152	2159	rBV8	19932	39365	3.68%	0.397%
70	15.160	2185	2188	2190	rBV4	10977	13766	1.29%	0.139%
71	15.233	2196	2200	2206	rVB	51302	86281	8.07%	0.869%
72	15.525	2245	2248	2255	rVB3	17725	29355	2.75%	0.296%
73	15.605	2255	2261	2266	rVB7	24705	54783	5.12%	0.552%
74	16.489	2401	2406	2413	rVB7	17414	40215	3.76%	0.405%

Sum of corrected areas: 9925296

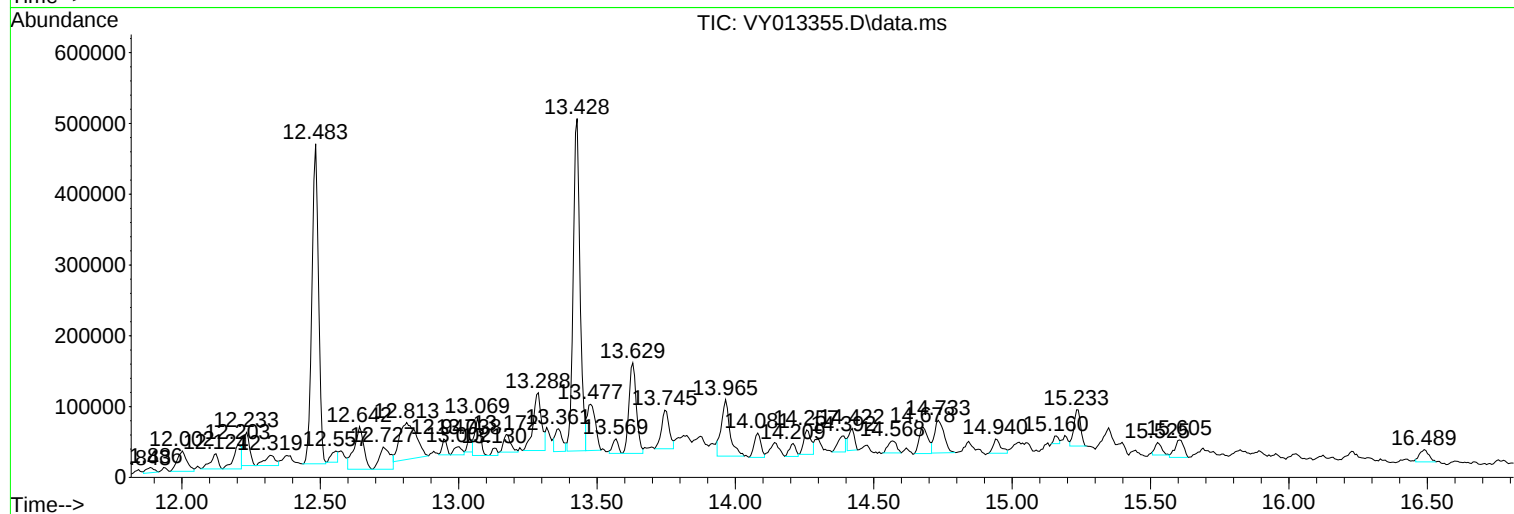
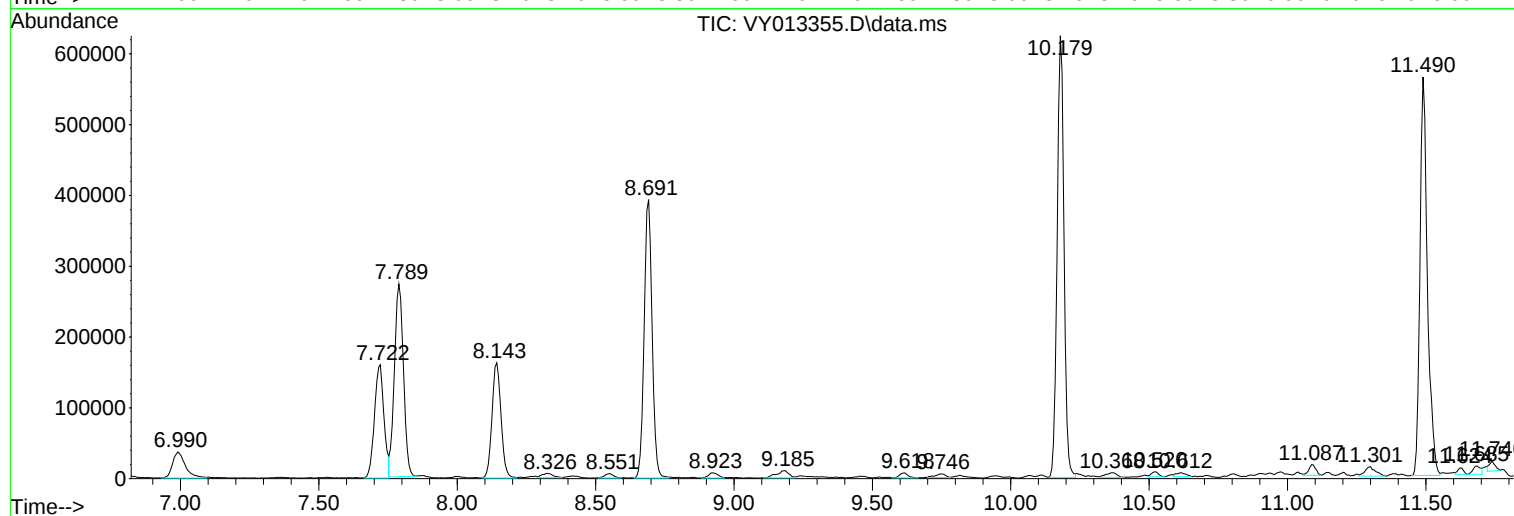
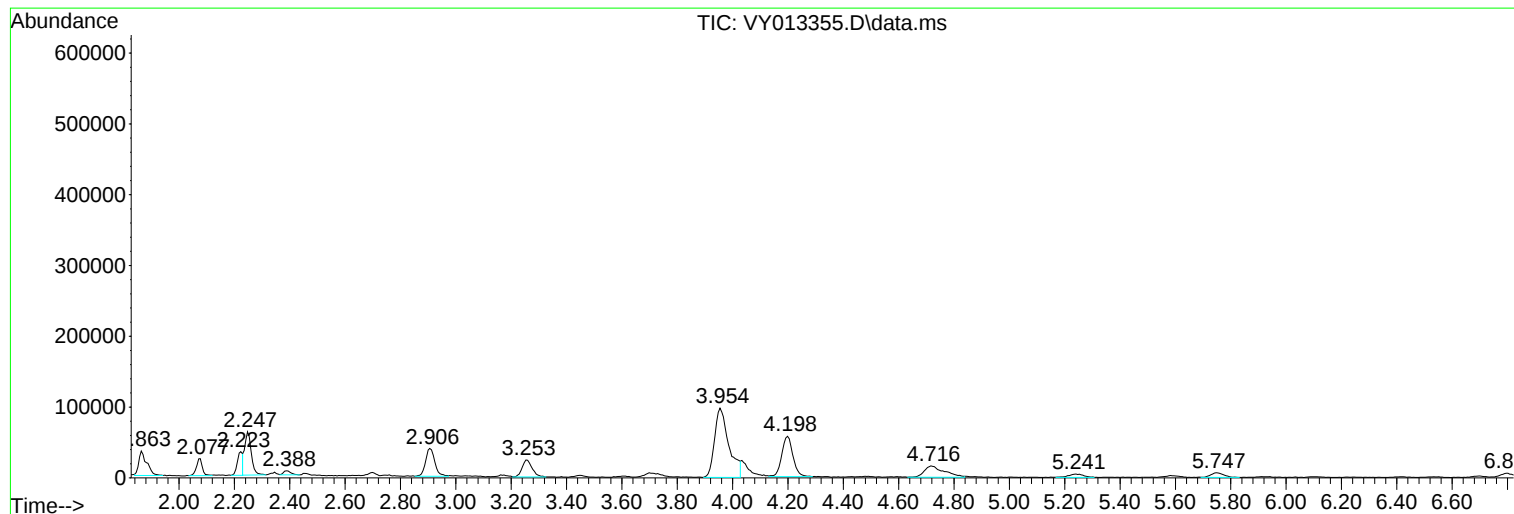
Instrument :
MSVOA_Y
ClientSampleId :
20230307-29-1

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Instrument :
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ClientSampleId :
20230307-29-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041223S.M
Quant Title : SW846 8260

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



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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20230307-29-1

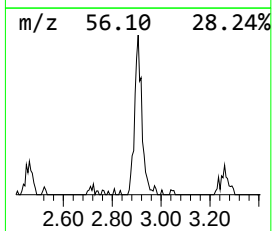
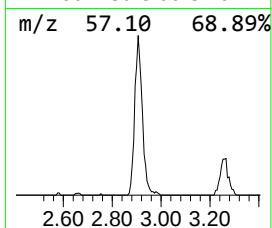
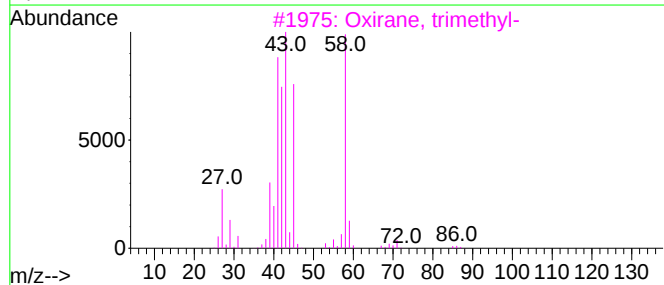
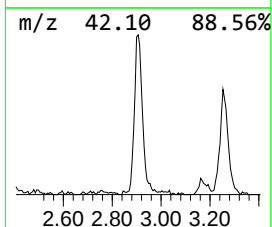
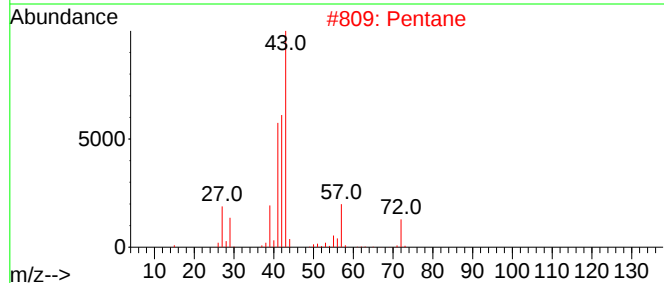
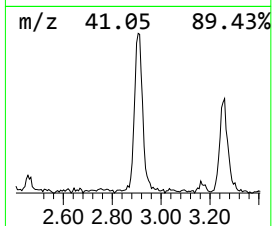
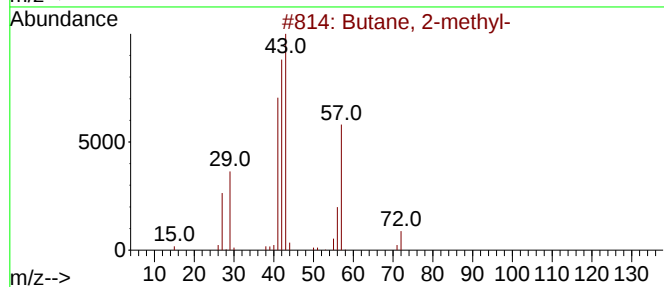
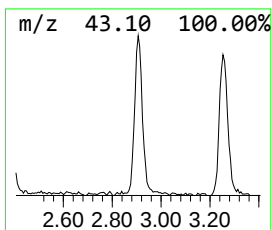
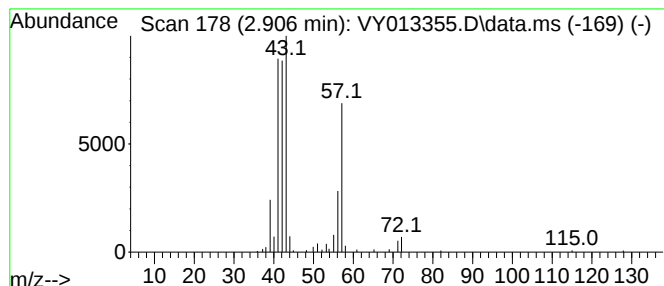
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041223S.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.906	7.32 ug/l	89986	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			Pentane	72	C5H12	000109-66-0	40
3			Oxirane, trimethyl-	86	C5H10O	005076-19-7	39
4			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	33
5			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	12



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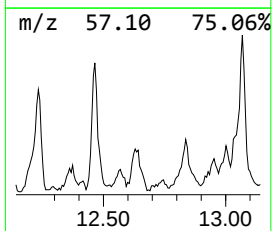
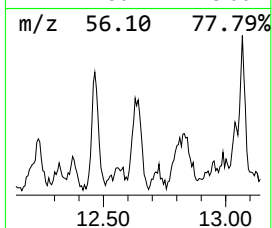
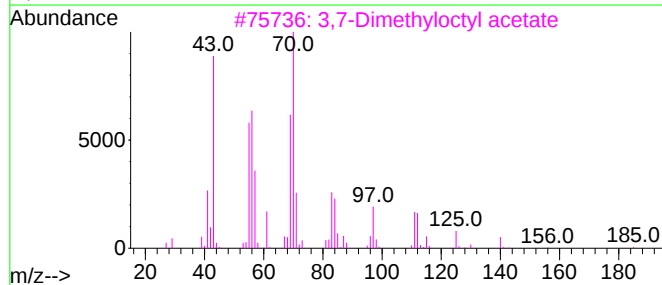
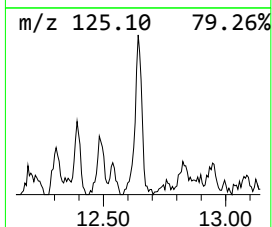
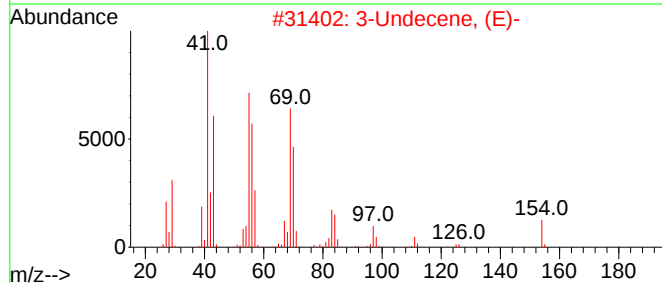
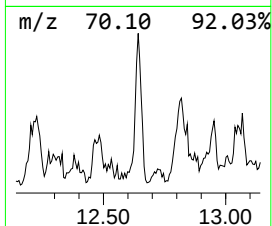
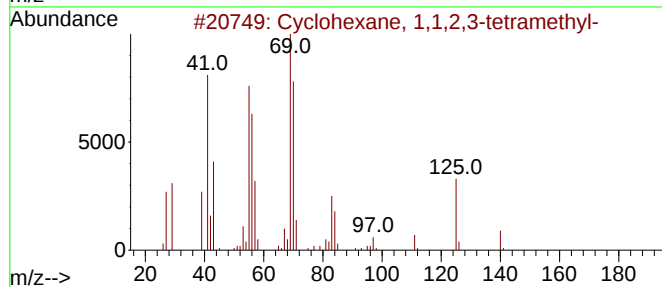
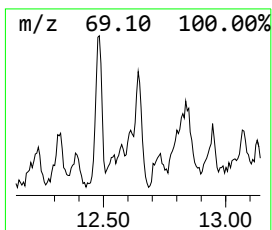
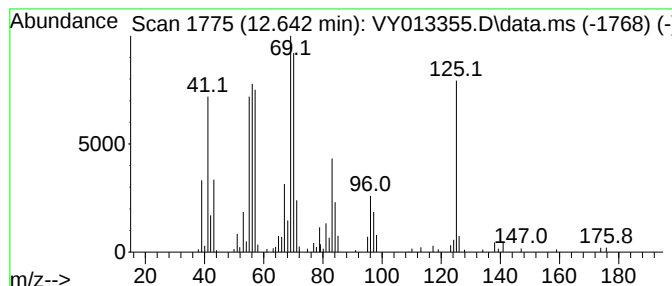
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041223S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclohexane, 1,1,2,3-tetram... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.642	8.76 ug/l	141942	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	64
2			3-Undecene, (E)-	154	C11H22	001002-68-2	50
3			3,7-Dimethyloctyl acetate	200	C12H24O2	020780-49-8	43
4			Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	38
5			3-Dodecene, (E)-	168	C12H24	007206-14-6	38



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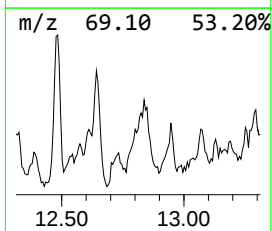
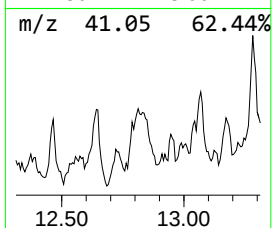
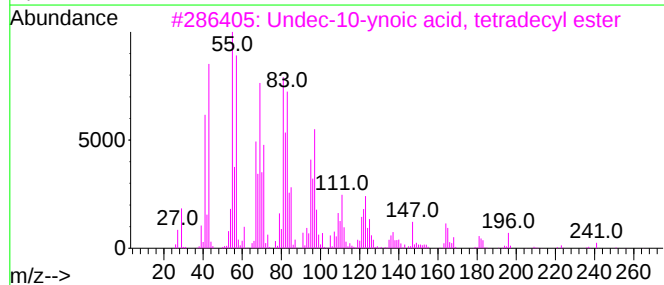
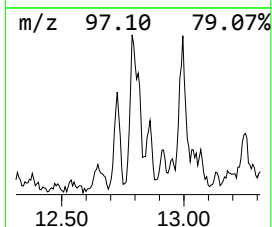
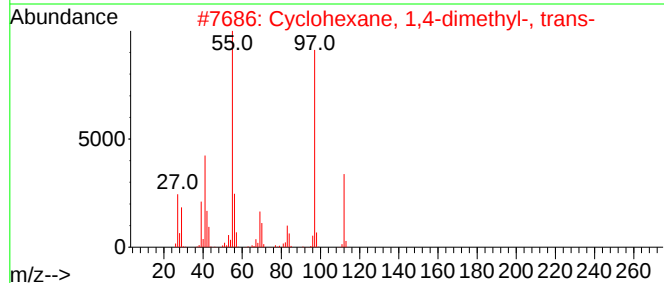
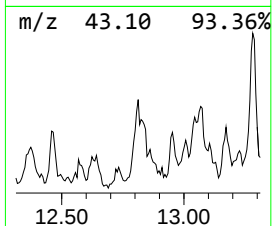
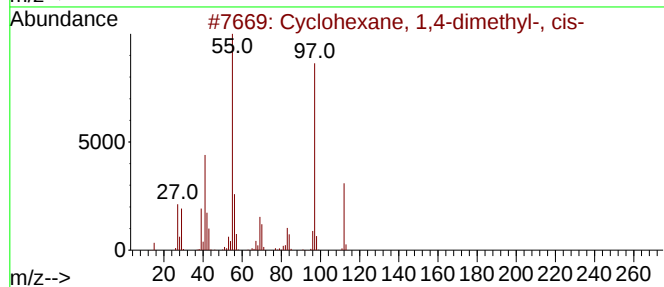
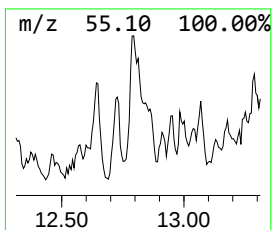
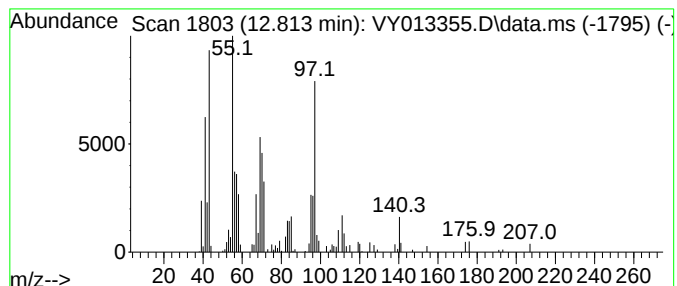
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041223S.M
Quant Title : SW846 8260

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

Peak Number 5 unknown12.813 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.813	13.54 ug/l	219309	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	38
2			Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	38
3			Undec-10-ynoic acid, tetradecyl ...	378	C25H46O2	1000406-16-7	38
4			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	38
5			7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	35



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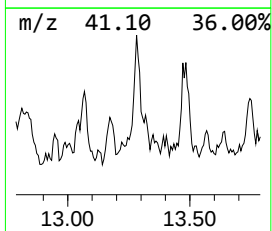
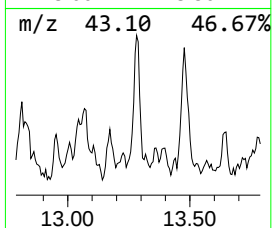
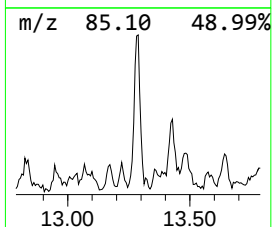
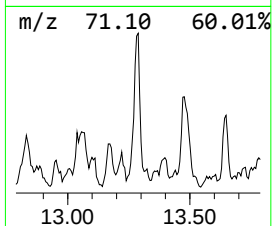
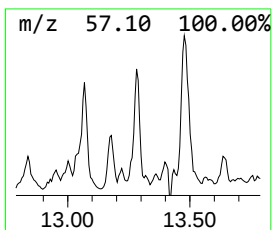
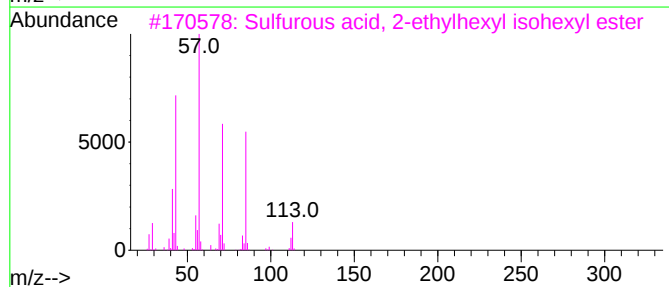
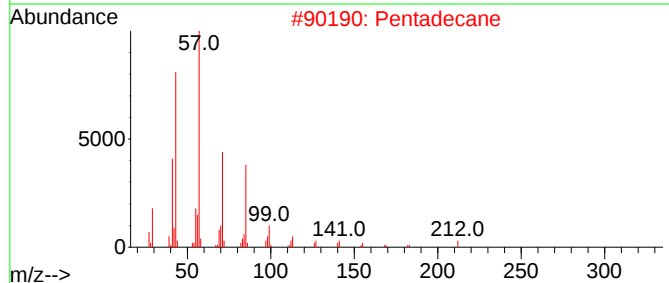
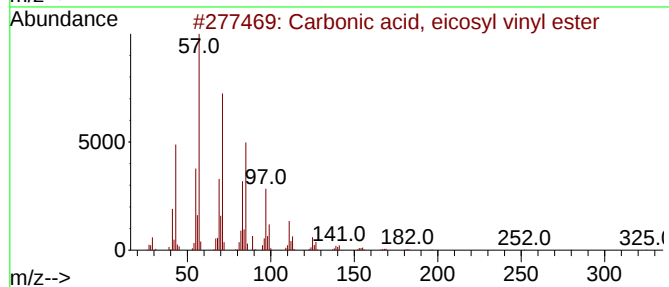
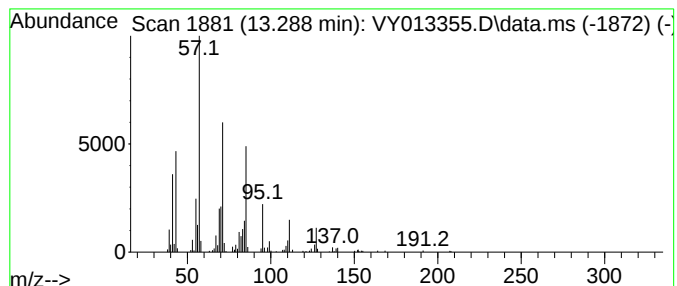
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Quant Title : SW846 8260

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

Peak Number 6 Carbonic acid, eicosyl vinyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.288	10.81 ug/l	175098	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	59
2			Pentadecane	212	C15H32	000629-62-9	53
3			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	47
4			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	47
5			Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041923\
Data File : VY013355.D
Acq On : 19 Apr 2023 19:02
Operator : KP/MD
Sample : 02366-05
Misc : 4.35g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20230307-29-1

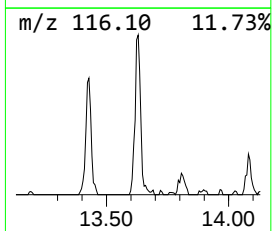
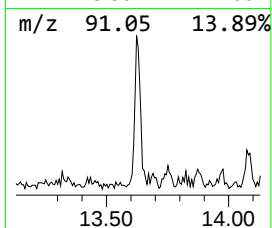
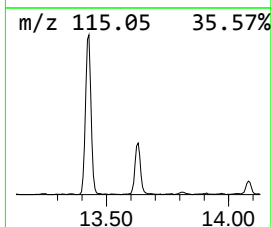
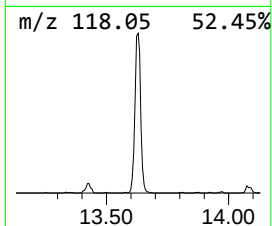
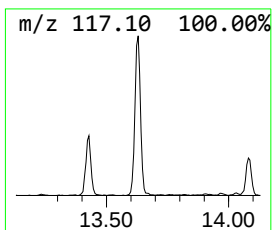
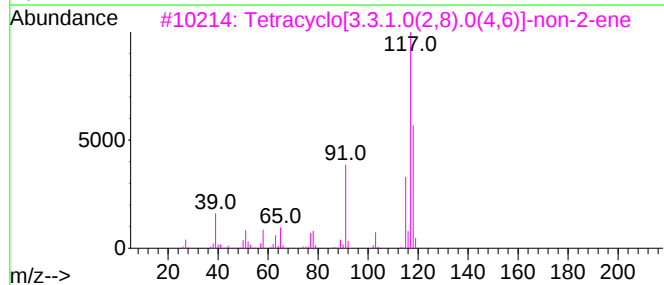
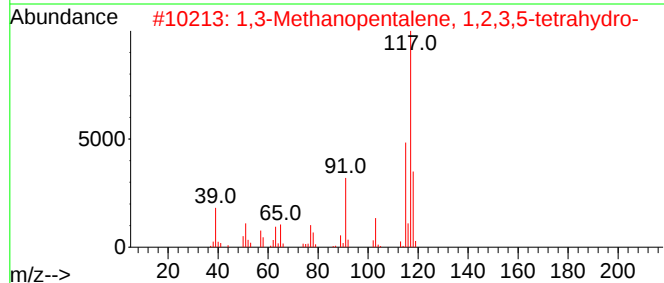
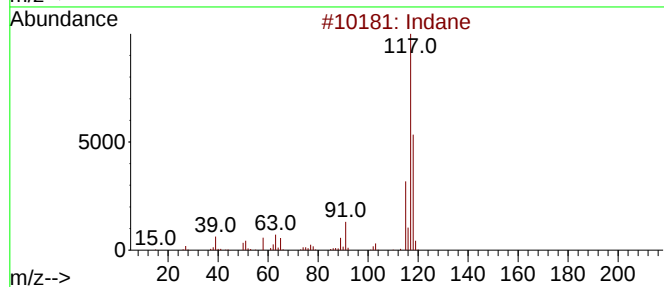
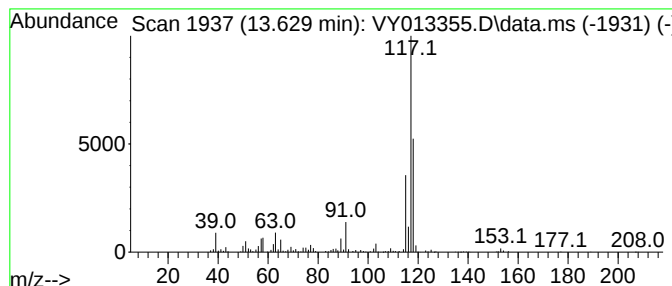
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Quant Title : SW846 8260

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

Peak Number 7 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.630	14.60 ug/l	236510	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			1,3-Methanopentalene, 1,2,3,5-te...	118	C9H10	128600-88-4	64
3			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
4			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	59
5			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041923\
Data File : VY013355.D
Acq On : 19 Apr 2023 19:02
Operator : KP/MD
Sample : 02366-05
Misc : 4.35g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20230307-29-1

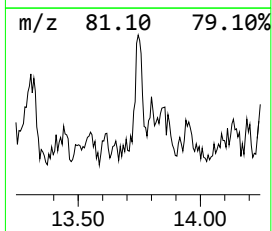
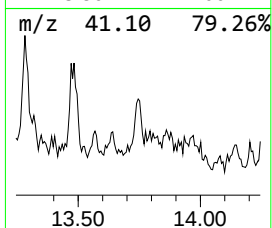
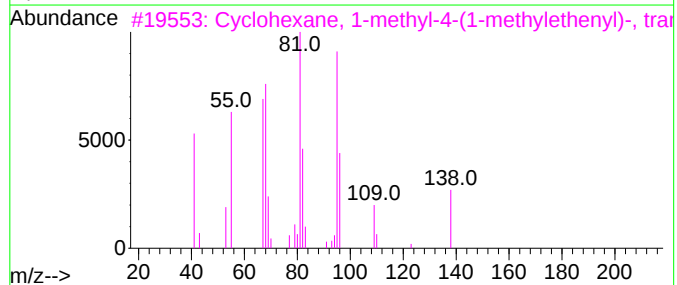
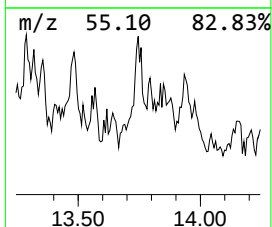
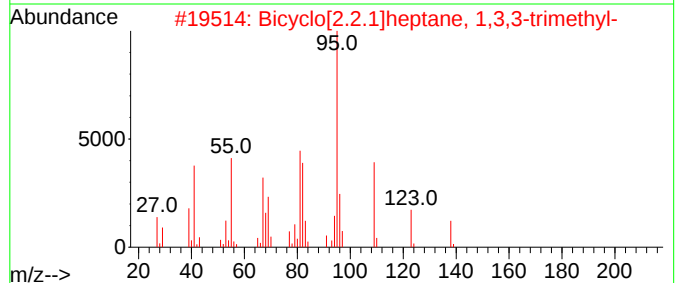
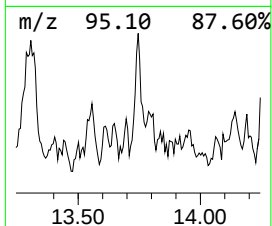
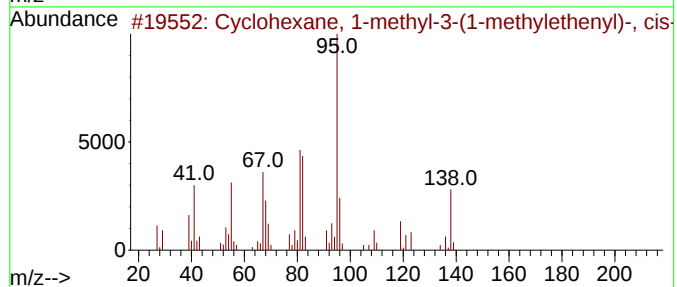
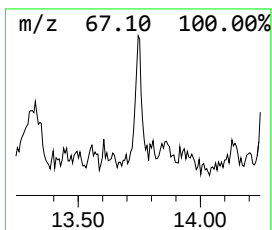
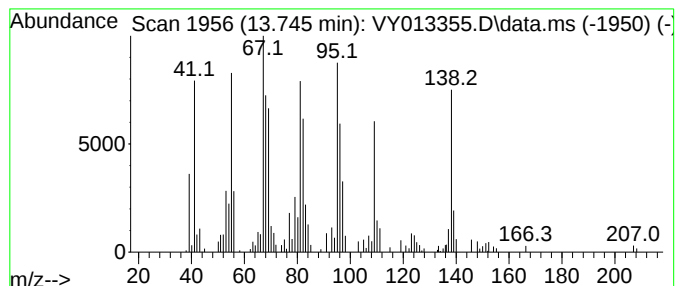
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041223S.M
Quant Title : SW846 8260

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

Peak Number 8 Cyclohexane, 1-methyl-3-(1-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.745	6.62 ug/l	107196	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-methyl-3-(1-methy...	138	C10H18	024399-15-3	91
2			Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	90
3			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-25-0	76
4			Naphthalene, decahydro-	138	C10H18	000091-17-8	76
5			Spiro[4.5]decane	138	C10H18	000176-63-6	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041923\
Data File : VY013355.D
Acq On : 19 Apr 2023 19:02
Operator : KP/MD
Sample : 02366-05
Misc : 4.35g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20230307-29-1

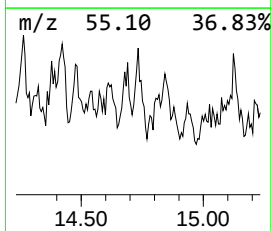
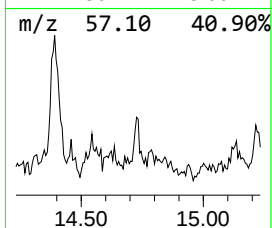
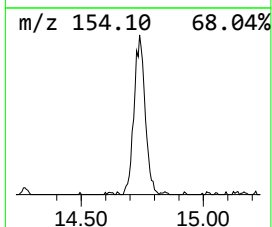
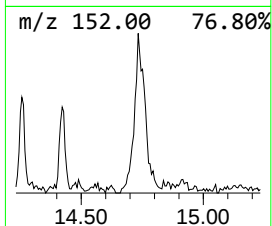
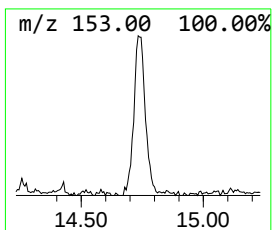
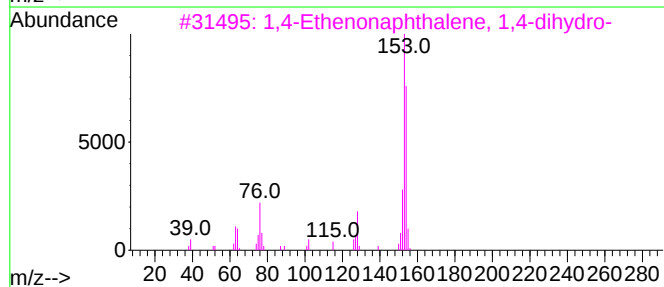
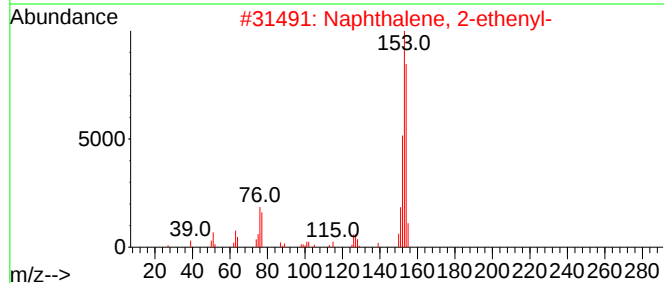
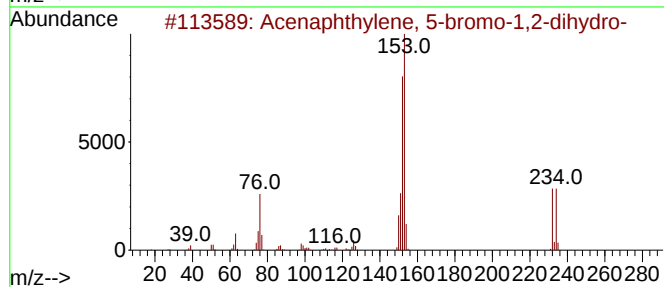
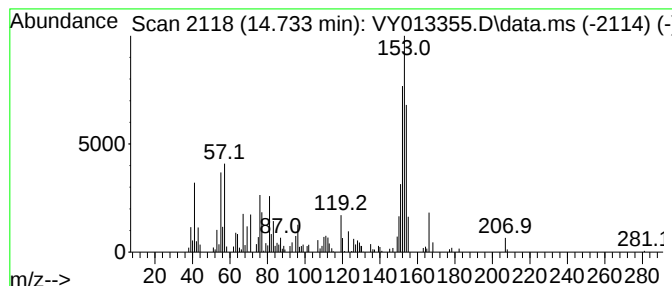
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041223S.M
Quant Title : SW846 8260

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

Peak Number 10 Acenaphthylene, 5-bromo-1,2... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.733	6.67 ug/l	108127	1,4-Dichlorobenzene-d4	13.428

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acenaphthylene, 5-bromo-1,2-dihy...	232	C12H9Br	002051-98-1	59
2		Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	50
3		1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	49
4		Acenaphthene	154	C12H10	000083-32-9	45
5		Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041923\
Data File : VY013355.D
Acq On : 19 Apr 2023 19:02
Operator : KP/MD
Sample : 02366-05
Misc : 4.35g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20230307-29-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041223S.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	2.906	7.3	ug/l	89986	1	7.789	614443	50.0
Cyclohexane, 1,...	12.642	8.8	ug/l	141942	4	13.428	809964	50.0
unknown12.813	12.813	13.5	ug/l	219309	4	13.428	809964	50.0
Carbonic acid, ...	13.288	10.8	ug/l	175098	4	13.428	809964	50.0
Indane	13.630	14.6	ug/l	236510	4	13.428	809964	50.0
Cyclohexane, 1-...	13.745	6.6	ug/l	107196	4	13.428	809964	50.0
Acenaphthylene,...	14.733	6.7	ug/l	108127	4	13.428	809964	50.0