

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110722\
 Data File : VY011341.D
 Acq On : 07 Nov 2022 17:33
 Operator : KP/MD
 Sample : N5378-02
 Misc : 4.76g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SB-16-20221028-10.5-11.5

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\82Y110122S.M

Title : SW846 8260

Signal : TIC: VY011341.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	14	rVB2	10356	17627	1.46%	0.238%
2	3.942	339	348	361	rBV	18272	51057	4.22%	0.689%
3	4.186	378	388	402	rBV	33282	92898	7.67%	1.253%
4	4.710	462	474	487	rBV3	23996	75474	6.23%	1.018%
5	5.746	632	644	654	rBV4	4378	13678	1.13%	0.185%
6	6.984	837	847	860	rVB2	6264	18256	1.51%	0.246%
7	7.710	957	966	972	rBV	194236	464836	38.39%	6.270%
8	7.783	972	978	991	rVB	286598	648249	53.53%	8.744%
9	8.136	1027	1036	1049	rBV	187239	405233	33.46%	5.466%
10	8.685	1117	1126	1138	rBV	437819	848655	70.08%	11.448%
11	10.179	1363	1371	1379	rBV	690852	1210938	100.00%	16.335%
12	11.489	1578	1586	1597	rBV	551586	904240	74.67%	12.198%
13	11.843	1634	1644	1646	rBV5	8062	21421	1.77%	0.289%
14	11.995	1663	1669	1677	rVB9	5267	14280	1.18%	0.193%
15	12.233	1704	1708	1713	rVB	10332	15419	1.27%	0.208%
16	12.325	1713	1723	1725	rBV10	7340	16205	1.34%	0.219%
17	12.477	1742	1748	1759	rVB	492335	796387	65.77%	10.743%
18	12.642	1770	1775	1781	rVB4	11150	22143	1.83%	0.299%
19	12.727	1781	1789	1796	rBV10	5420	16408	1.35%	0.221%
20	12.806	1796	1802	1806	rBV7	9146	20457	1.69%	0.276%
21	12.940	1808	1824	1835	rVB8	16412	82550	6.82%	1.114%
22	13.068	1836	1845	1849	rBV4	11249	32576	2.69%	0.439%
23	13.422	1896	1903	1912	rVB	470692	717633	59.26%	9.680%
24	13.526	1912	1920	1924	rBV4	8265	18355	1.52%	0.248%
25	13.635	1931	1938	1951	rVB7	8266	29410	2.43%	0.397%
26	13.745	1951	1956	1960	rBV7	7849	14116	1.17%	0.190%
27	13.958	1986	1991	1996	rBV2	13074	20871	1.72%	0.282%
28	14.410	2056	2065	2071	rBV9	10027	23416	1.93%	0.316%
29	14.727	2103	2117	2130	rBV2	188850	574336	47.43%	7.747%
30	15.111	2173	2180	2189	rVB8	9130	32400	2.68%	0.437%
31	15.233	2194	2200	2206	rBV	49716	87765	7.25%	1.184%
32	15.428	2220	2232	2248	rVB	18296	81536	6.73%	1.100%
33	16.165	2346	2353	2360	rBV3	4494	12204	1.01%	0.165%
34	16.488	2399	2406	2413	rVB3	5211	12268	1.01%	0.165%

Sum of corrected areas: 7413297

Instrument :

MSVOA_Y

ClientSampleId :

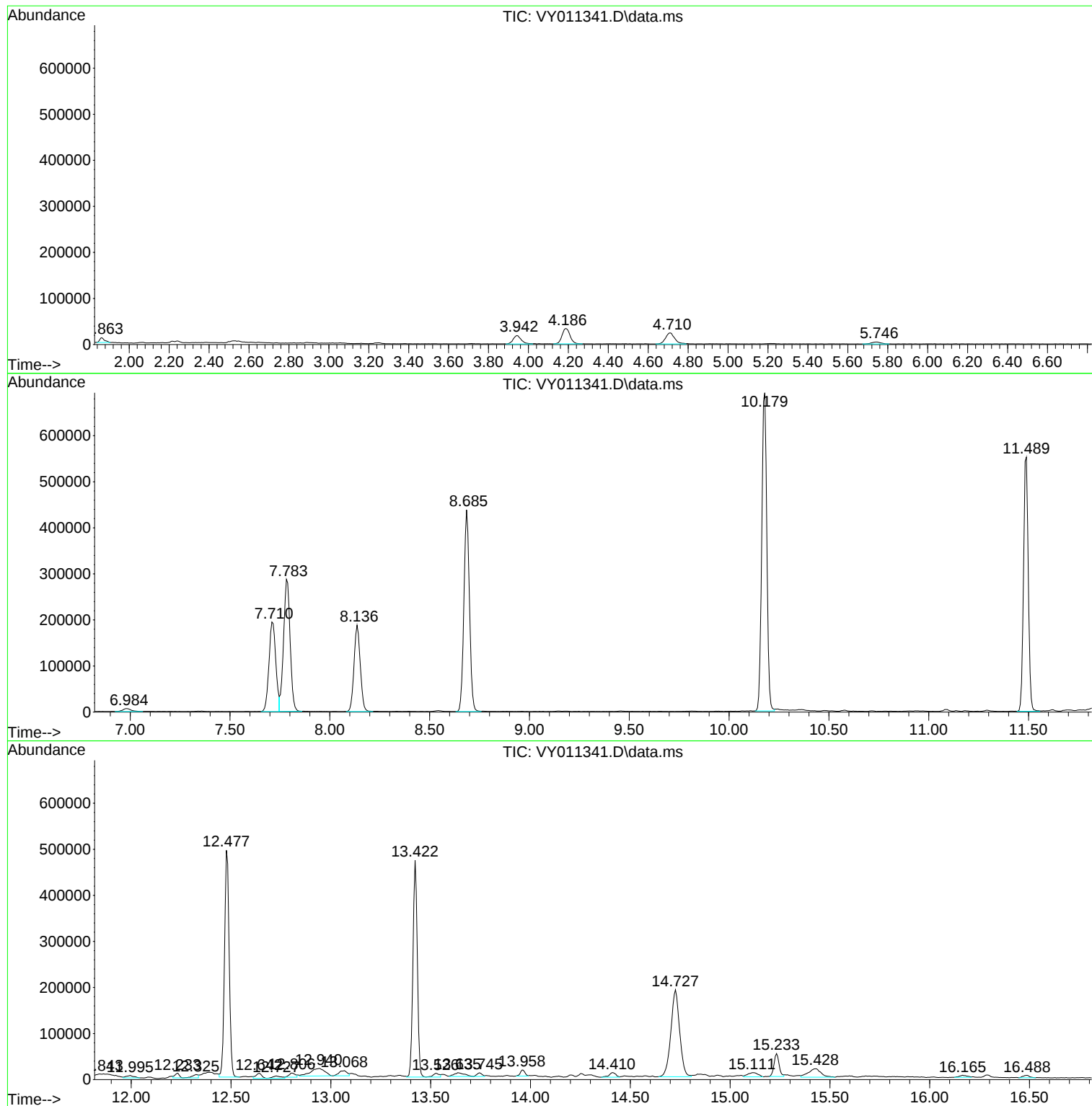
SB-16-20221028-10.5-11.5

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y110122S.M
Quant Title : SW846 8260

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



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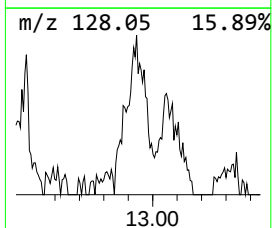
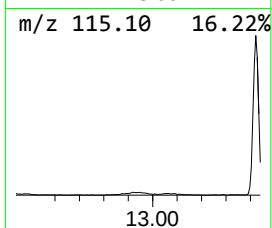
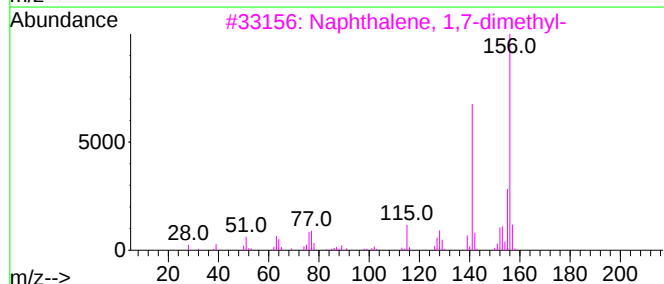
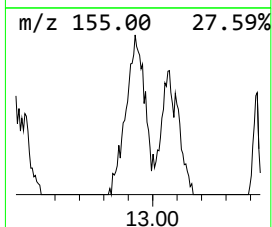
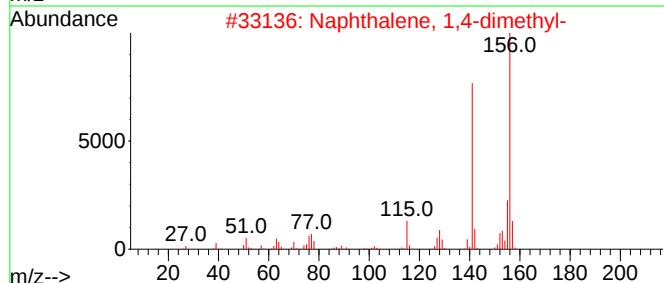
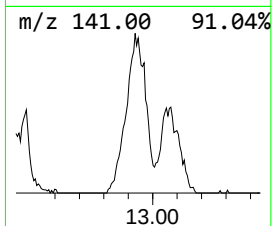
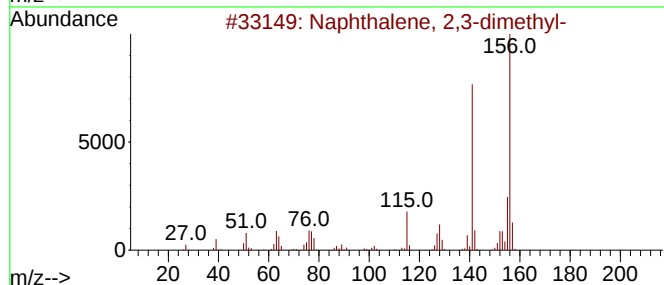
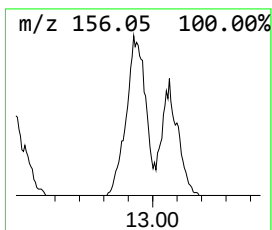
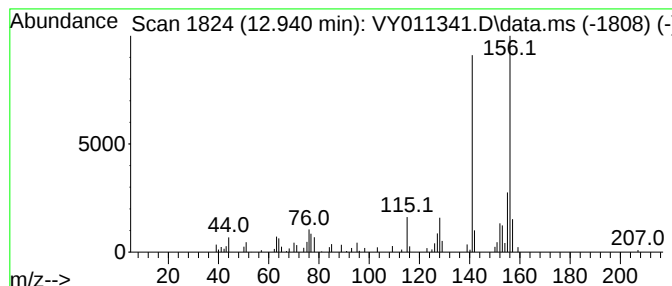
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y110122S.M
Quant Title : SW846 8260

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

Peak Number 2 Naphthalene, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.940	5.75 ug/l	82550	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	95
2			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	95
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	95
4			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	94
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	94



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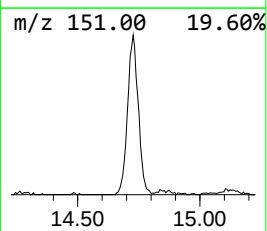
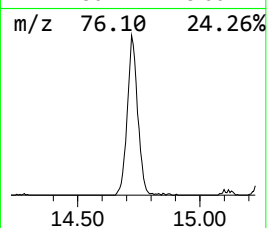
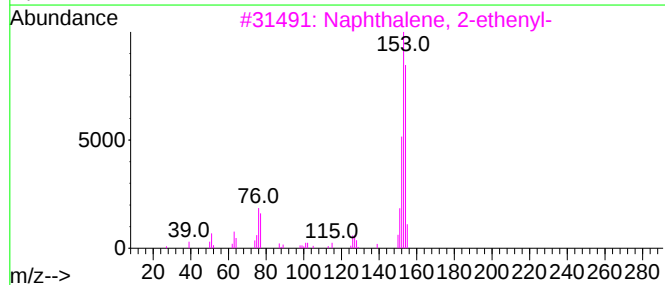
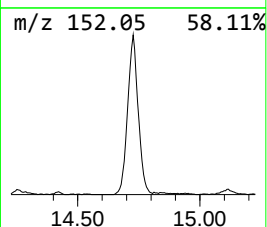
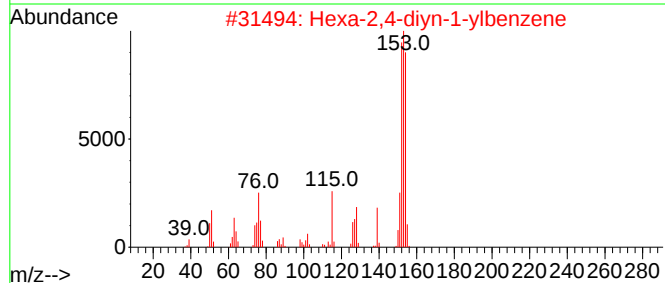
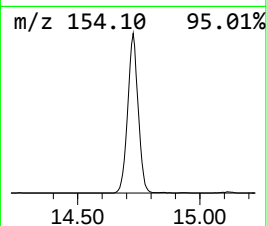
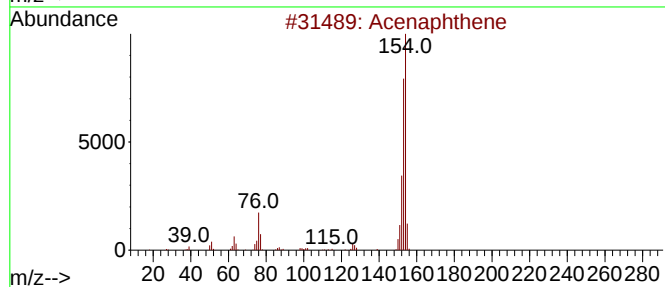
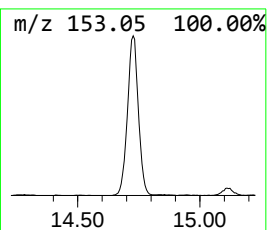
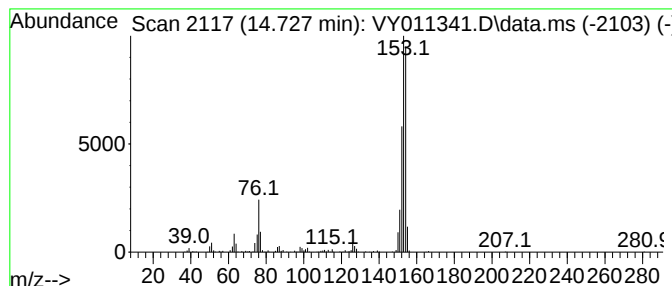
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y110122S.M
Quant Title : SW846 8260

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

Peak Number 3 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.727	40.02 ug/l	574336	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	93
2			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	53
3			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	53
4			3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50
5			1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	40



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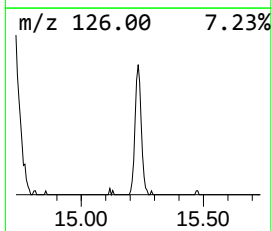
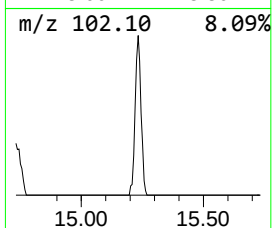
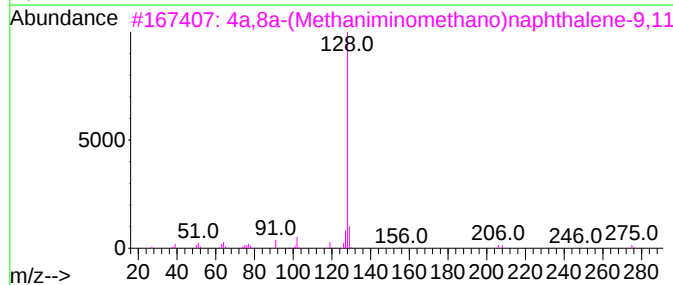
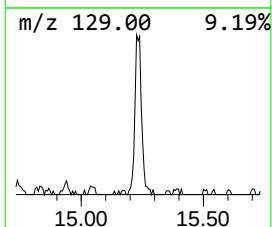
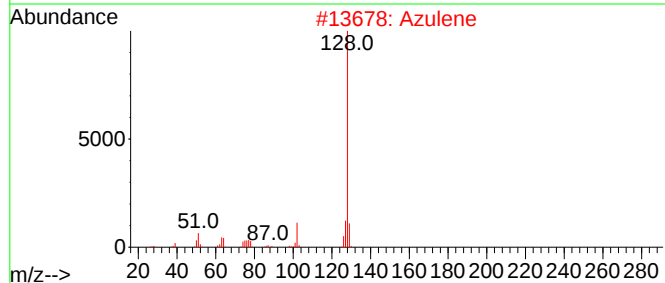
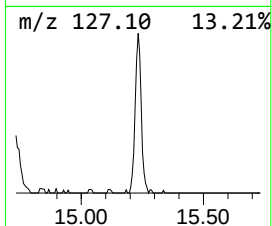
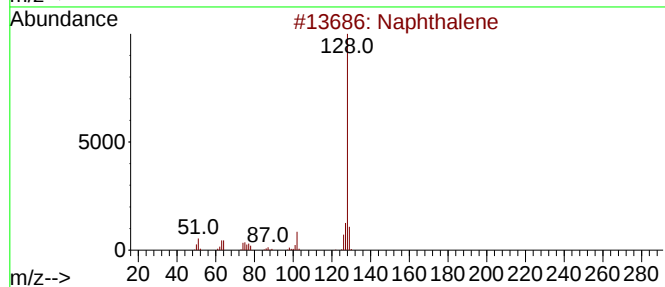
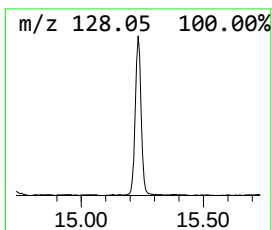
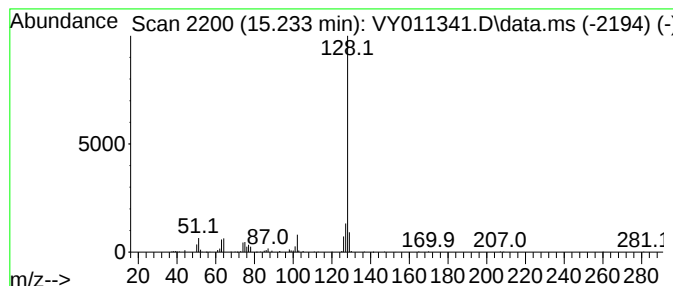
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Quant Title : SW846 8260

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

Peak Number 4 4a,8a-(Methaniminomethano)n... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.233	6.11 ug/l	87765	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	93
3			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	64
4			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	64
5			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	47



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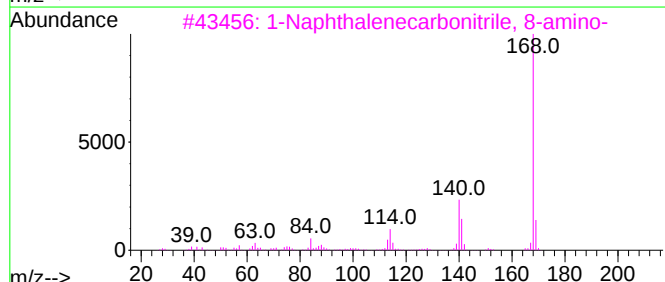
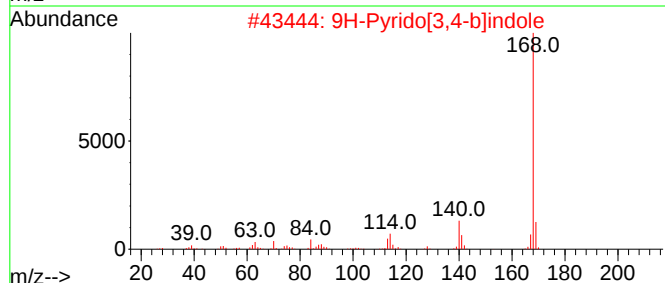
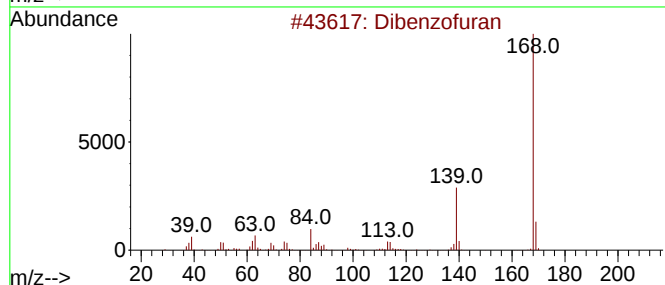
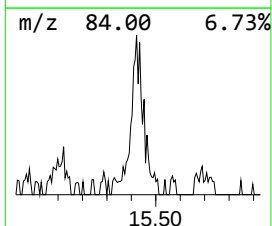
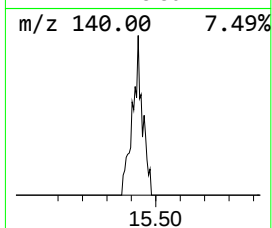
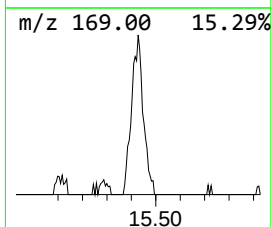
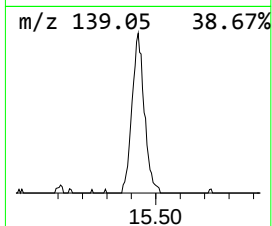
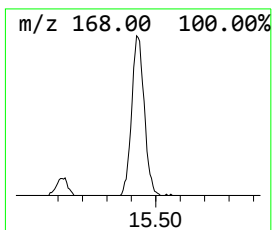
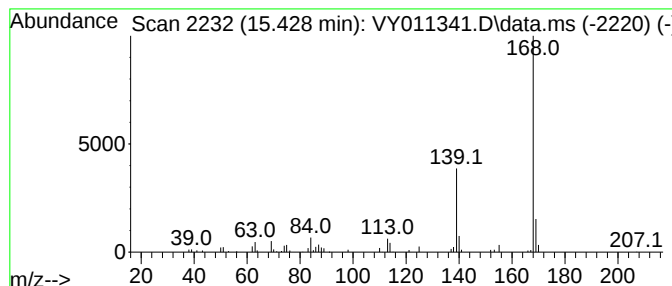
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y110122S.M
Quant Title : SW846 8260

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

Peak Number 5 9H-Pyrido[3,4-b]indole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.428	5.68 ug/l	81536	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzofuran	168	C12H8O	000132-64-9	86
2			9H-Pyrido[3,4-b]indole	168	C11H8N2	000244-63-3	53
3			1-Naphthalenecarbonitrile, 8-amino-	168	C11H8N2	038515-13-8	52
4			4-Fluoro-1,3-benzothiazol-2-ylamine	168	C7H5FN2S	020358-06-9	50
5			1(2H)-Acenaphthylenone	168	C12H8O	002235-15-6	45



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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
Naphthalene, 2,...	12.940	5.8	ug/l	82550	4	13.422	717633	50.0
Hexa-2,4-diyne-1...	14.727	40.0	ug/l	574336	4	13.422	717633	50.0
4a,8a-(Methanim...	15.233	6.1	ug/l	87765	4	13.422	717633	50.0
9H-Pyrido[3,4-b...	15.428	5.7	ug/l	81536	4	13.422	717633	50.0