LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031622\
Data File : VX027473.D
Acq On : 16 Mar 2022 16:03
Operator : JC/MD
Sample : N1950-10RE
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3222RE

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_X\Method\82X030822W.M
Title : SW846 8260

Signal : TIC: VX027473.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.313	31	37	39	rBV5	26471	58745	2.75%	0.236%
2	1.563	70	78	83	rVB6	20480	51075	2.39%	0.206%
3	2.057	154	159	168	rBV	147878	233813	10.94%	0.941%
4	2.538	230	238	244	rBV	31972	61155	2.86%	0.246%
5	5.391	694	706	721	rBV2	217502	634873	29.71%	2.555%
6	5.556	721	733	750	rVB	370739	1046898	48.99%	4.214%
7	5.958	788	799	821	rBV	217005	589164	27.57%	2.371%
8	6.763	920	931	946	rBV	545523	1319967	61.77%	5.313%
9	8.653	1234	1241	1249	rBV	1122716	1758550	82.29%	7.078%
10	10.055	1464	1471	1485	rBV	1195108	1571233	73.52%	6.324%
11	10.403	1523	1528	1536	rBV	31388	45701	2.14%	0.184%
12	10.647	1562	1568	1575	rBV	31885	45331	2.12%	0.182%
13	11.085	1634	1640	1646	rBV	961456	1235374	57.81%	4.973%
14	11.573	1714	1720	1724	rBV2	28327	37063	1.73%	0.149%
15	12.024	1788	1794	1801	rBV	1234631	1493322	69.88%	6.011%
16	12.091	1801	1805	1813	rVB	16476	25151	1.18%	0.101%
17	12.219	1821	1826	1828	rBV	41204	53032	2.48%	0.213%
18	12.244	1828	1830	1838	rVV2	28616	41353	1.94%	0.166%
19	12.701	1901	1905	1913	rVB2	19895	31822	1.49%	0.128%
20	12.927	1933	1942	1945	rBV2	19807	37660	1.76%	0.152%
21	13.170	1978	1982	1993	rVB	32657	53829	2.52%	0.217%
22	13.292	1998	2002	2008	rVB2	78074	106364	4.98%	0.428%
23	13.420	2020	2023	2028	rVB	23852	30629	1.43%	0.123%
24	13.548	2040	2044	2046	rBV	20857	25971	1.22%	0.105%
25	13.585	2046	2050	2054	rBV3	36816	46606	2.18%	0.188%
26	13.658	2056	2062	2070	rVB3	96114	168780	7.90%	0.679%
27	13.780	2079	2082	2090	rVB2	11934	23628	1.11%	0.095%
28	13.896	2090	2101	2105	rBV2	194138	525853	24.61%	2.117%
29	14.079	2127	2131	2132	rBV	52055	62721	2.93%	0.252%
30	14.103	2132	2135	2142	rVB	56816	75768	3.55%	0.305%
31	14.219	2148	2154	2158	rBV4	239900	407526	19.07%	1.640%
32	14.250	2158	2159	2167	rVB	83029	87843	4.11%	0.354%
33	14.329	2167	2172	2185	rBV	673586	1330210	62.24%	5.354%
34	14.481	2192	2197	2200	rBV3	50713	67991	3.18%	0.274%
35	14.530	2200	2205	2207	rBV	748735	946421	44.29%	3.809%
36	14.560	2207	2210	2221	rVB	1338435	2137074	100.00%	8.602%

LSC Area Percent Report

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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3222RE

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_X\Method\82X030822W.M
Title : SW846 8260

37	14.719	2231	2236	2241	rBV2	335677	471231	22.05%	1.897%
38	14.786	2241	2247	2250	rVV2	458890	801080	37.48%	3.224%
39	14.823	2250	2253	2262	rVV2	753281	1238079	57.93%	4.983%
40	14.908	2262	2267	2270	rVV	364692	595015	27.84%	2.395%
41	14.957	2271	2275	2279	rVV	773137	1253628	58.66%	5.046%
42	14.993	2279	2281	2291	rVB	312004	404542	18.93%	1.628%
43	15.085	2291	2296	2299	rBV2	66110	105947	4.96%	0.426%
44	15.146	2299	2306	2316	rVV3	576908	1240286	58.04%	4.992%
45	15.225	2317	2319	2322	rVB	34034	34999	1.64%	0.141%
46	15.268	2322	2326	2328	rBV	78999	116475	5.45%	0.469%
47	15.292	2328	2330	2334	rVV	103419	129761	6.07%	0.522%
48	15.329	2334	2336	2342	rVB3	37783	71302	3.34%	0.287%
49	15.475	2355	2360	2364	rBV2	219967	382598	17.90%	1.540%
50	15.579	2373	2377	2378	rBV3	28565	38511	1.80%	0.155%
51	15.615	2378	2383	2386	rVV	309467	459122	21.48%	1.848%
52	15.652	2386	2389	2396	rVB	172704	254335	11.90%	1.024%
53	15.737	2398	2403	2408	rBV3	30207	51392	2.40%	0.207%
54	15.835	2409	2419	2425	rBV6	91614	278155	13.02%	1.120%
55	15.987	2439	2444	2453	rVB2	52829	104701	4.90%	0.421%
56	16.328	2494	2500	2512	rVB3	83601	198741	9.30%	0.800%
57	16.481	2520	2525	2530	rBV5	11098	23095	1.08%	0.093%
58	16.542	2530	2535	2539	rBV6	9591	22464	1.05%	0.090%
59	16.597	2540	2544	2550	rVB	27693	47025	2.20%	0.189%
60	16.658	2550	2554	2559	rBV2	21657	53107	2.49%	0.214%

Sum of corrected areas: 24844087

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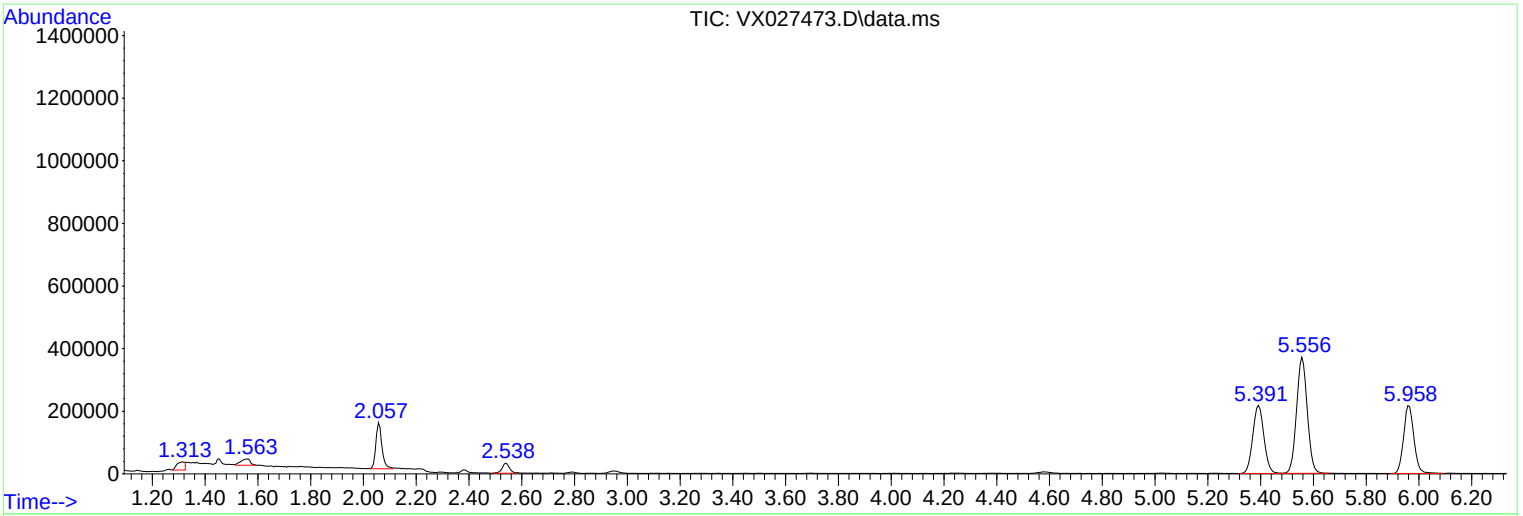
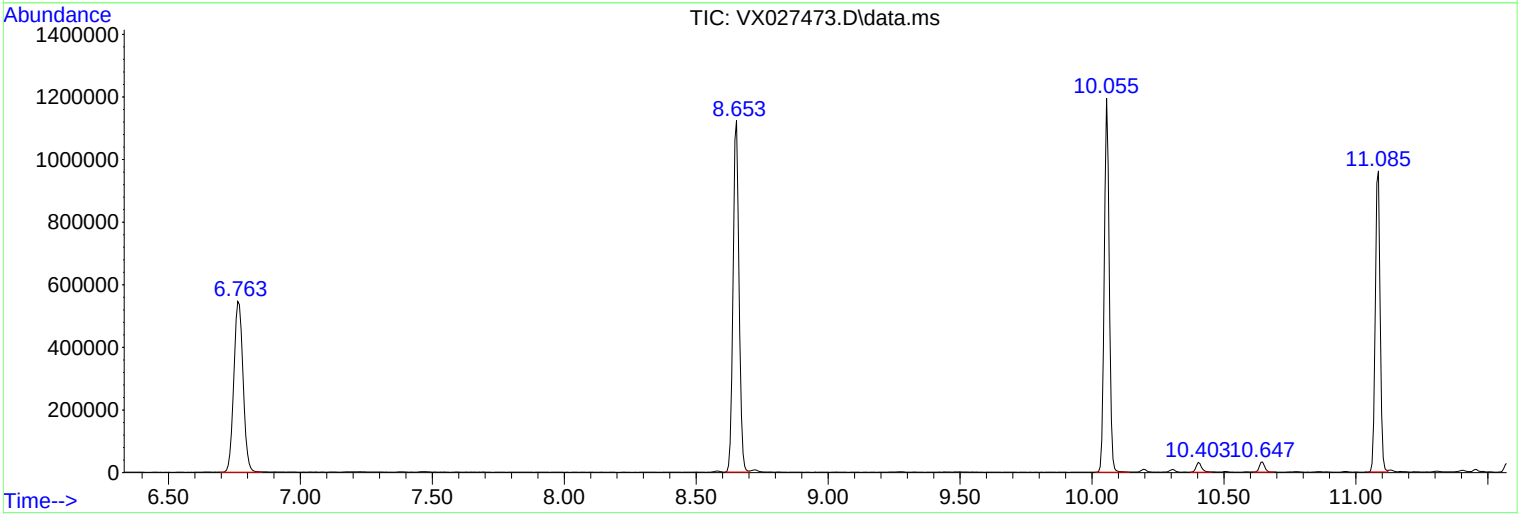
ALS Vial : 13 Sample Multiplier: 1

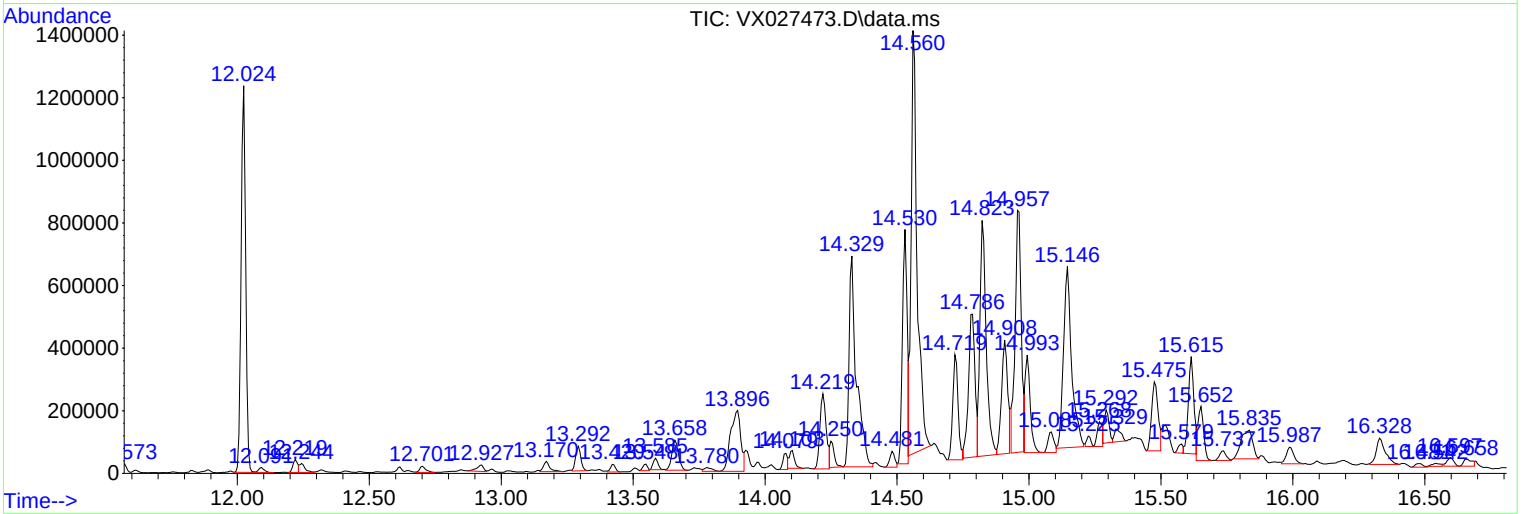
Instrument :
MSVOA_X
ClientSampleId :
3222RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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







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Data File : VX027473.D
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Instrument :
MSVOA_X
ClientSampleId :
3222RE

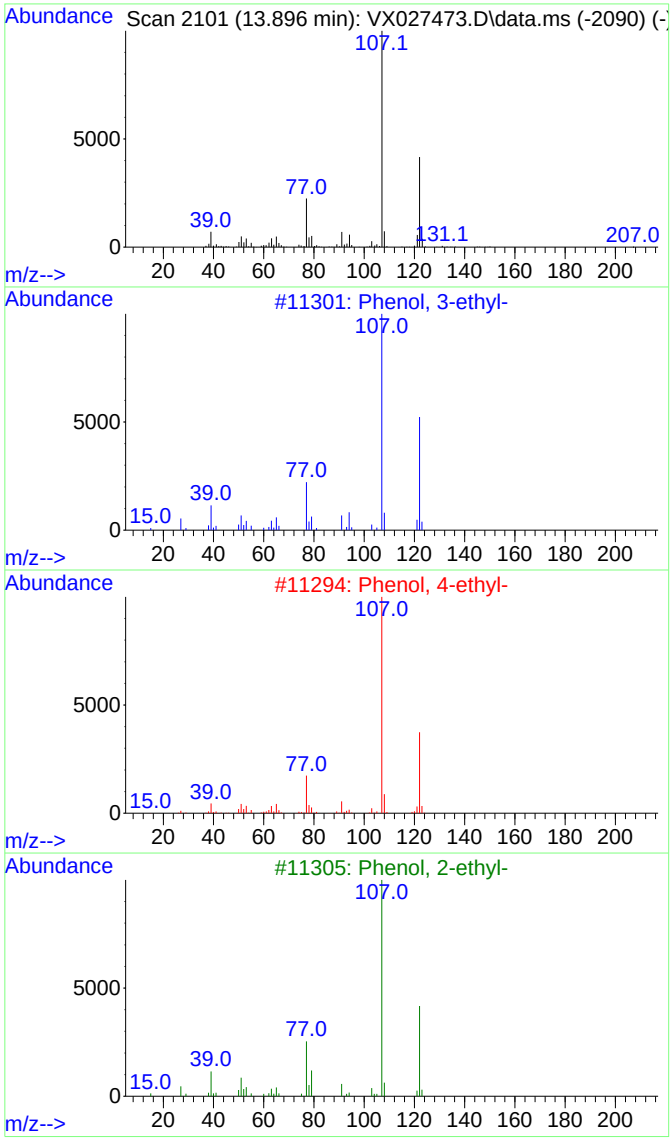
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

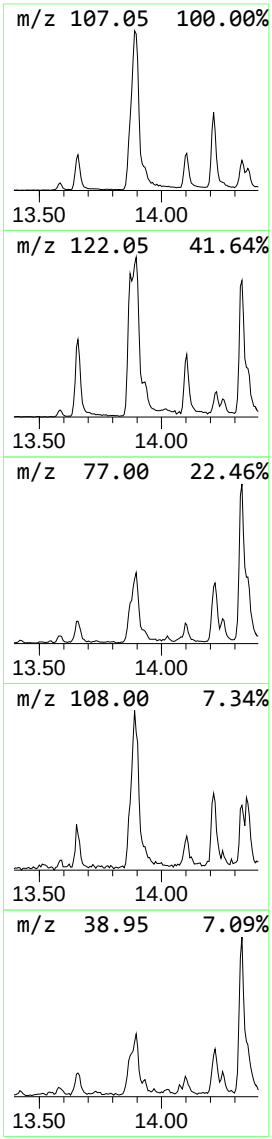
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Phenol, 3-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.896	17.61 ug/l	525853	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-ethyl-	122	C8H10O	000620-17-7	97
2	Phenol, 4-ethyl-	122	C8H10O	000123-07-9	91
3	Phenol, 2-ethyl-	122	C8H10O	000090-00-6	91
4	Phenol, 3,4-dimethyl-	122	C8H10O	000095-65-8	78
5	Silane, 1,3-butadiynyltrimethyl-	122	C7H10Si	004526-06-1	59





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Operator : JC/MD
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3222RE

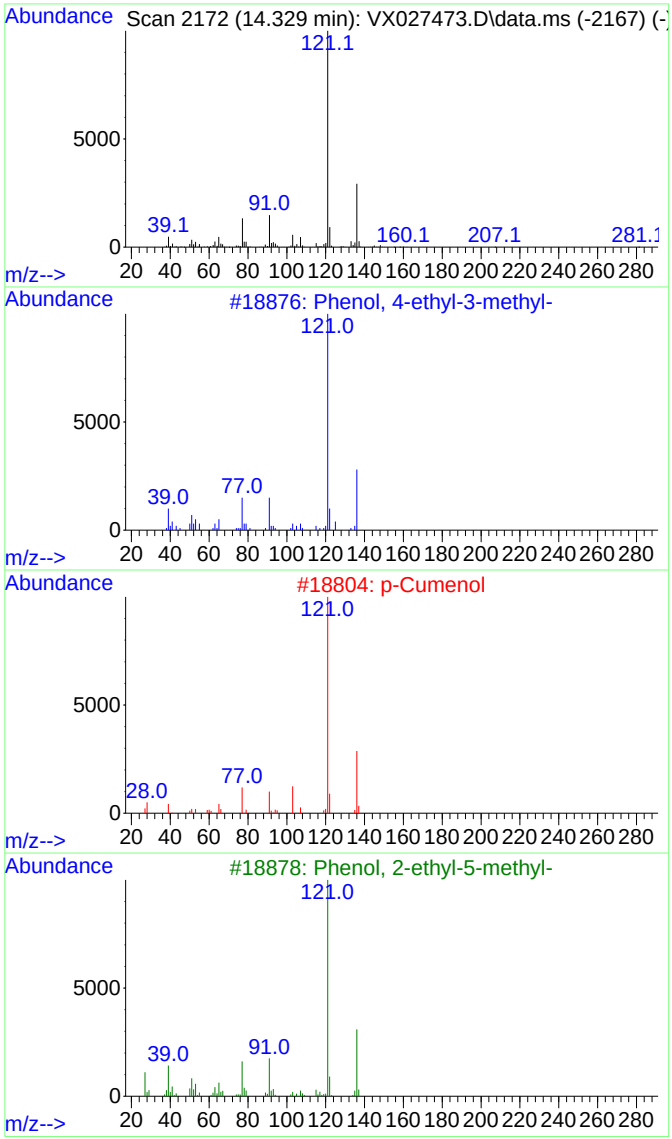
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

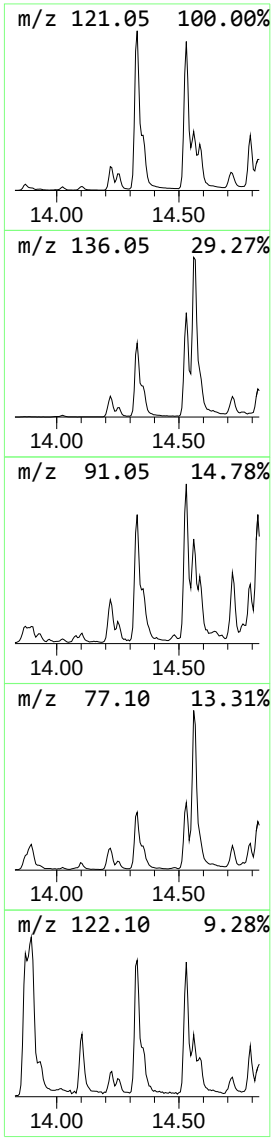
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Phenol, 4-ethyl-3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	44.54 ug/l	1330210	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-ethyl-3-methyl-	136	C9H12O	001123-94-0	91
2	p-Cumenol	136	C9H12O	000099-89-8	91
3	Phenol, 2-ethyl-5-methyl-	136	C9H12O	001687-61-2	91
4	Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	90
5	Benzene, 1-ethyl-4-methoxy-	136	C9H12O	001515-95-3	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031622\
Data File : VX027473.D
Acq On : 16 Mar 2022 16:03
Operator : JC/MD
Sample : N1950-10RE
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3222RE

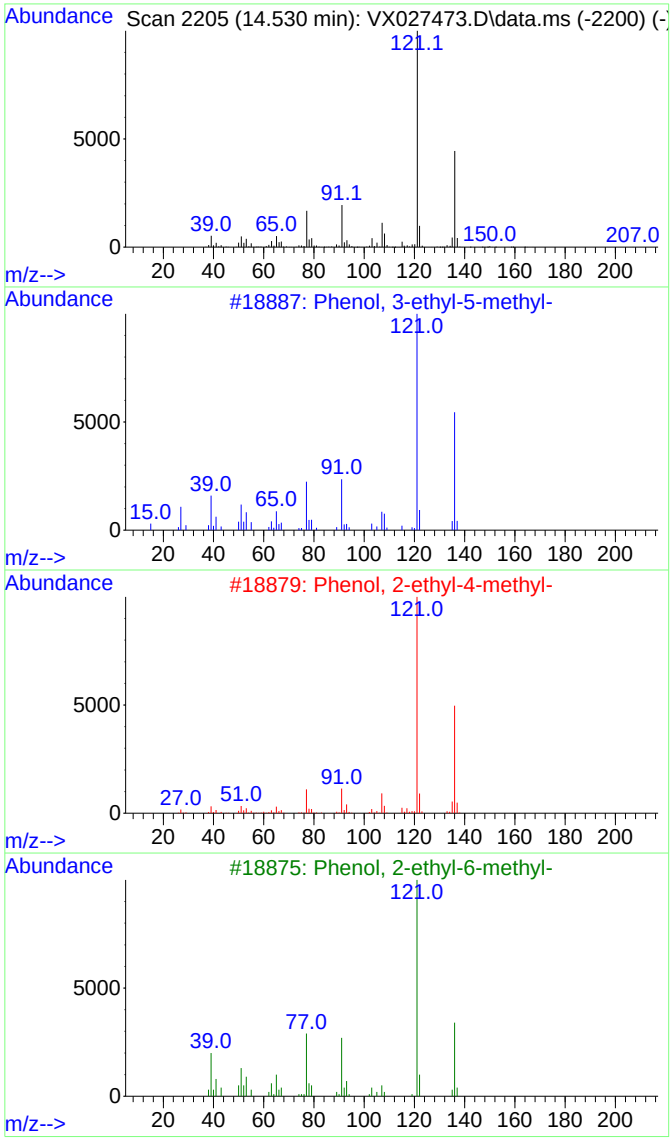
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

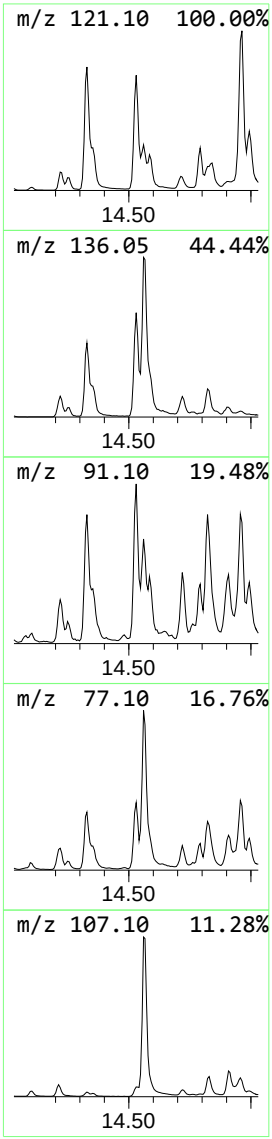
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Phenol, 3-ethyl-5-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.530	31.69 ug/l	946421	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-ethyl-5-methyl-	136	C9H12O	000698-71-5	94
2	Phenol, 2-ethyl-4-methyl-	136	C9H12O	003855-26-3	91
3	Phenol, 2-ethyl-6-methyl-	136	C9H12O	001687-64-5	90
4	1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	86
5	Phenol, 2-ethyl-5-methyl-	136	C9H12O	001687-61-2	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031622\
Data File : VX027473.D
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3222RE

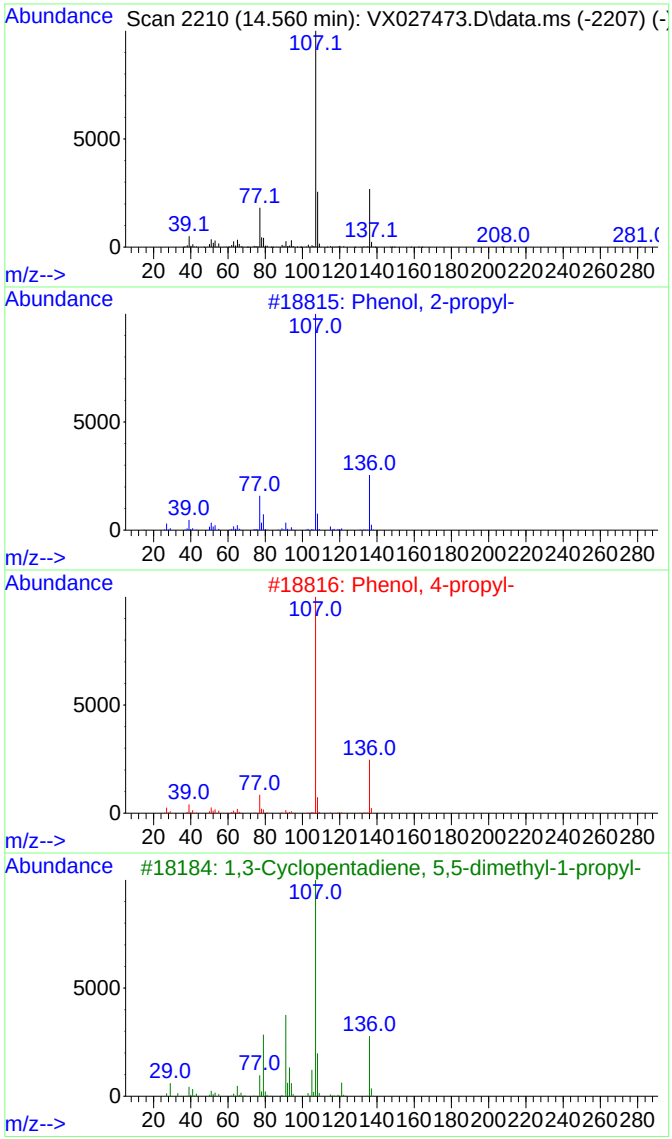
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

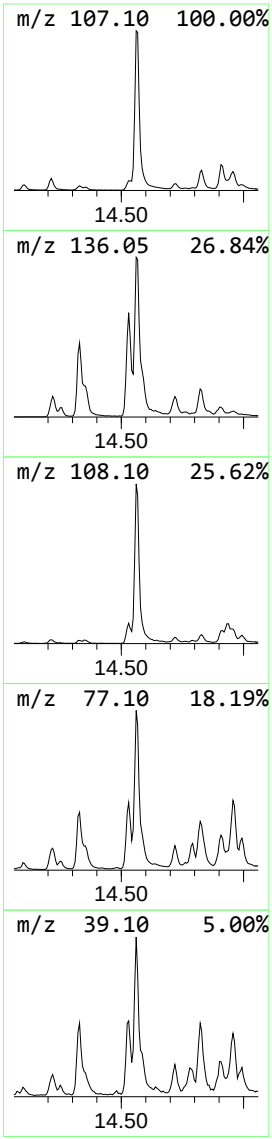
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Phenol, 2-propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.560	71.55 ug/l	2137070	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-propyl-	136	C9H12O	000644-35-9	74
2	Phenol, 4-propyl-	136	C9H12O	000645-56-7	74
3	1,3-Cyclopentadiene, 5,5-dimethy...	136	C10H16	1000163-57-1	43
4	Phenol, 4-ethyl-	122	C8H10O	000123-07-9	42
5	o-Toluidine	107	C7H9N	000095-53-4	33





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

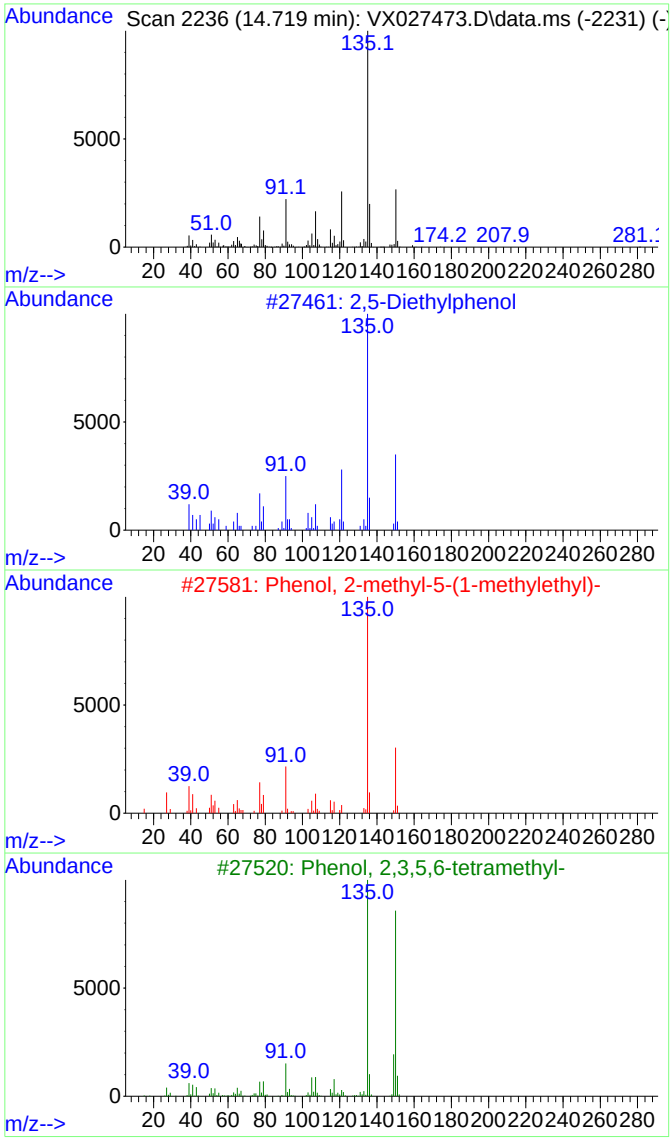
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

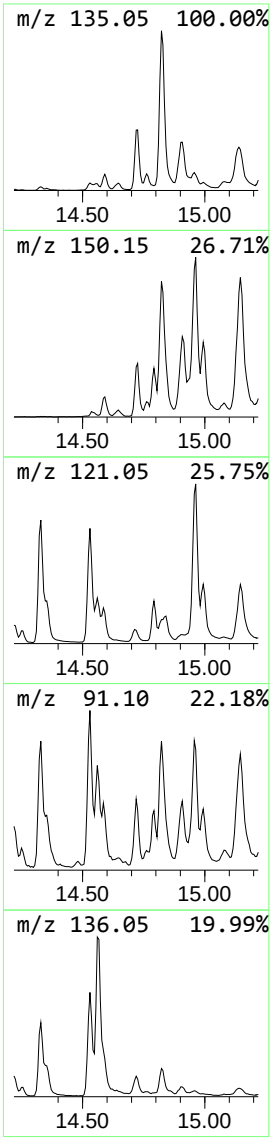
****

Peak Number 5 2,5-Diethylphenol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.719	15.78 ug/l	471231	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Diethylphenol	150	C10H14O	000876-20-0	86
2	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	000499-75-2	81
3	Phenol, 2,3,5,6-tetramethyl-	150	C10H14O	000527-35-5	72
4	4-Hydroxy-2-methylacetophenone	150	C9H10O2	000875-59-2	68
5	Thymol	150	C10H14O	000089-83-8	64





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ALS Vial : 13 Sample Multiplier: 1

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MSVOA_X
ClientSampleId :
3222RE

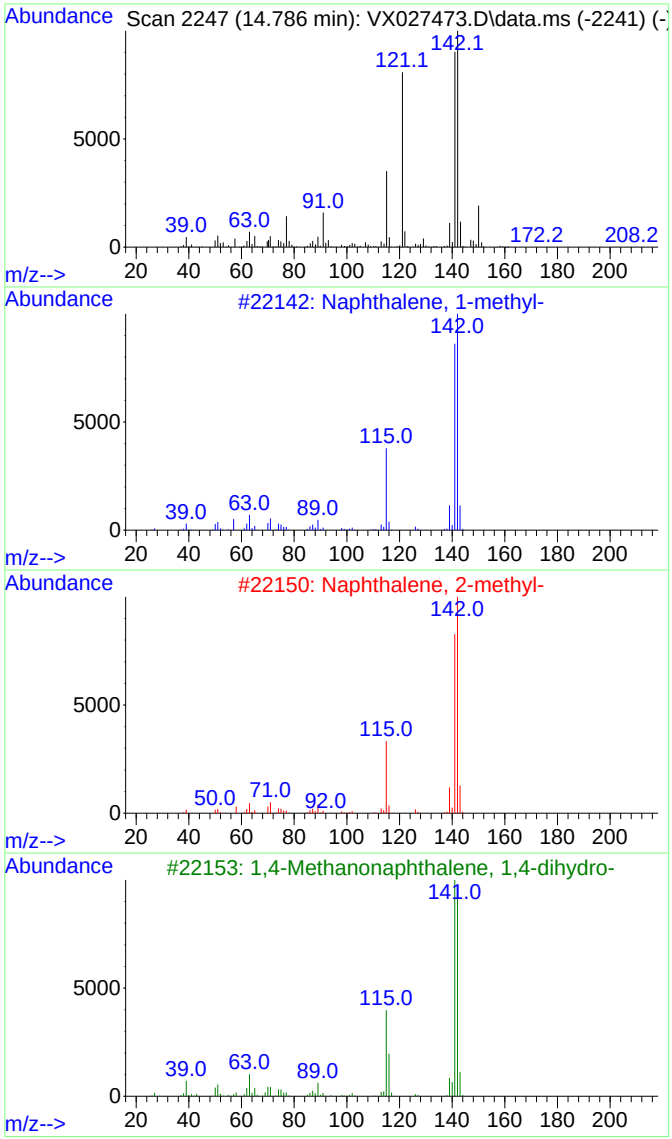
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

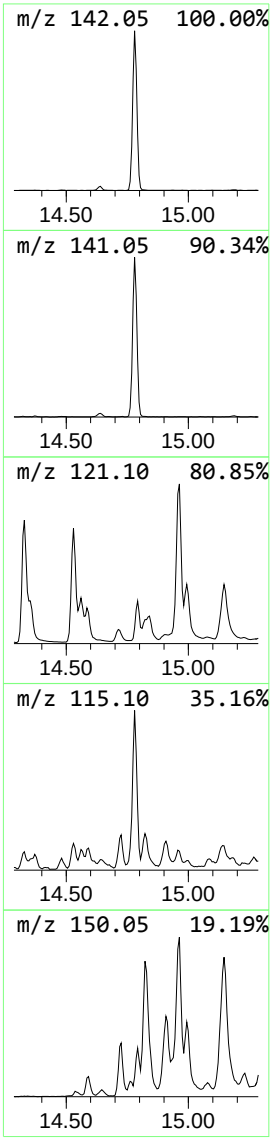
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,4-Methanonaphthalene, 1,4... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	26.82 ug/l	801080	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	78
4	Benzocycloheptatriene	142	C11H10	000264-09-5	64
5	2-Methyl-6-propylphenol	150	C10H14O	003520-52-3	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031622\
Data File : VX027473.D
Acq On : 16 Mar 2022 16:03
Operator : JC/MD
Sample : N1950-10RE
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3222RE

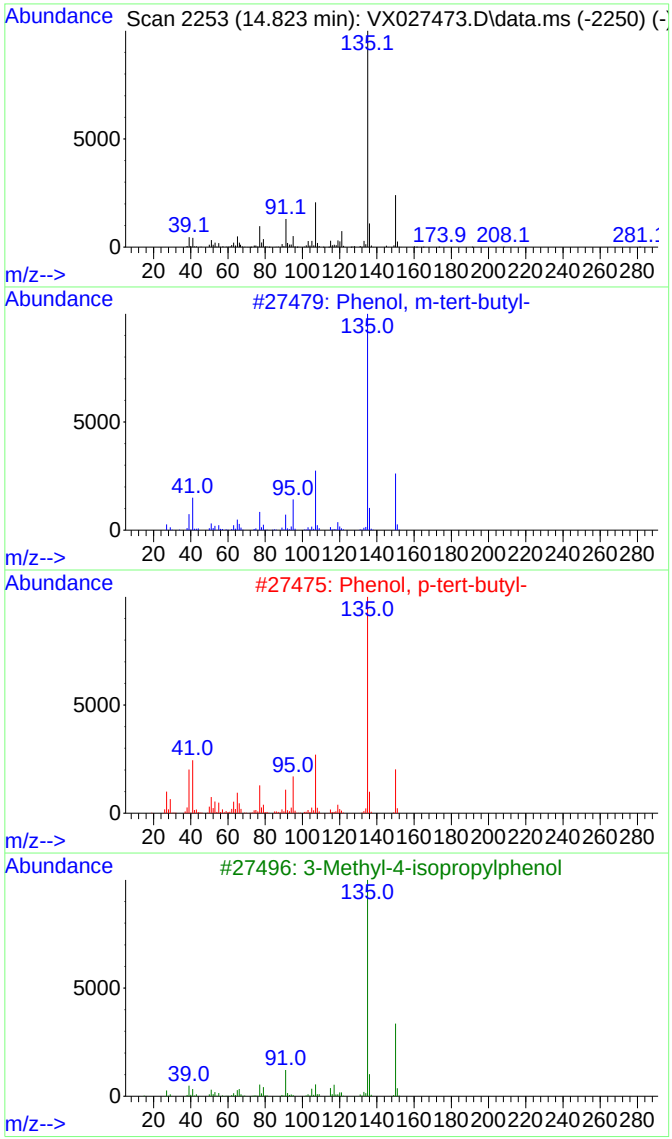
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

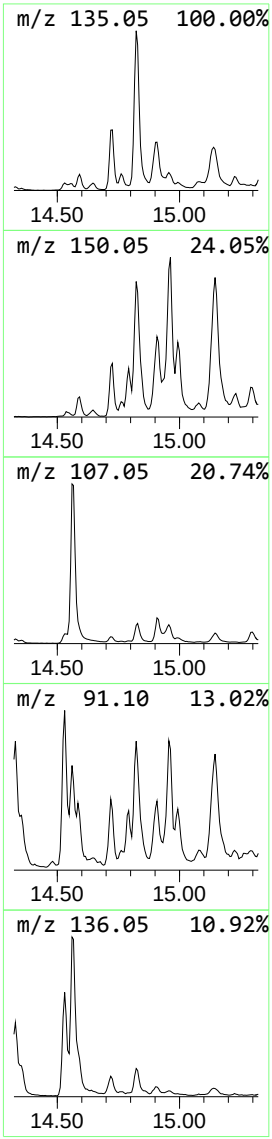
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phenol, m-tert-butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.823	41.45 ug/l	1238080	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	87
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	87
3	3-Methyl-4-isopropylphenol	150	C10H14O	003228-02-2	81
4	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	72
5	o-Isopropylanisole	150	C10H14O	002944-47-0	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031622\
Data File : VX027473.D
Acq On : 16 Mar 2022 16:03
Operator : JC/MD
Sample : N1950-10RE
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3222RE

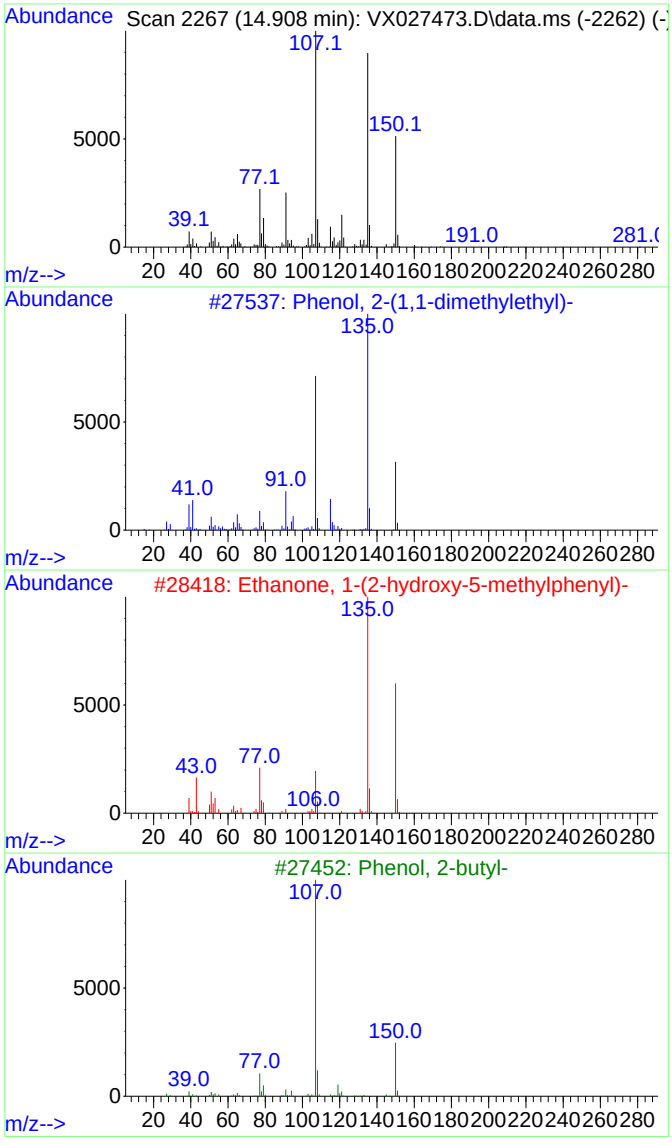
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

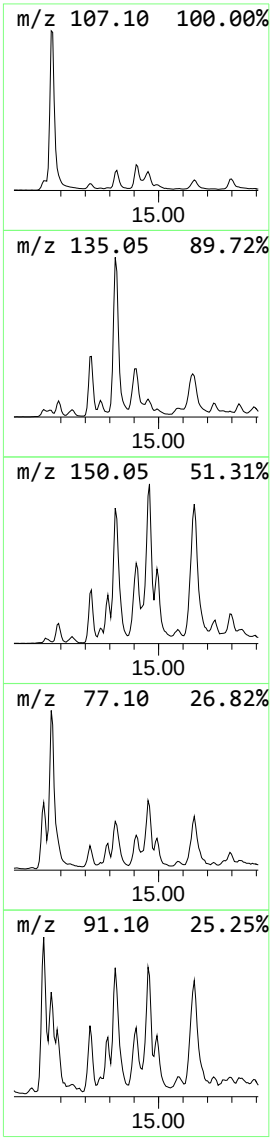
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Phenol, 2-(1,1-dimethylethyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.908	19.92 ug/l	595015	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	83
2	Ethanone, 1-(2-hydroxy-5-methylp...	150	C9H10O2	001450-72-2	53
3	Phenol, 2-butyl-	150	C10H14O	003180-09-4	53
4	3-Methoxyacetophenone	150	C9H10O2	000586-37-8	52
5	Benzene, 1-methoxy-4-(1-methylet...	150	C10H14O	004132-48-3	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031622\
Data File : VX027473.D
Acq On : 16 Mar 2022 16:03
Operator : JC/MD
Sample : N1950-10RE
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3222RE

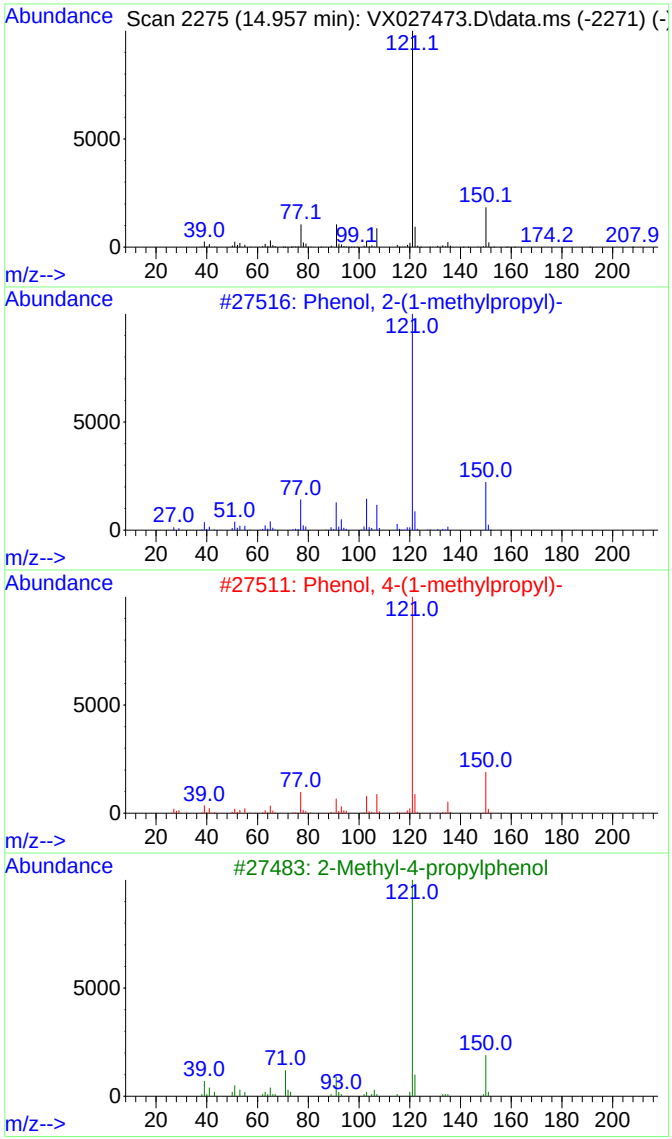
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

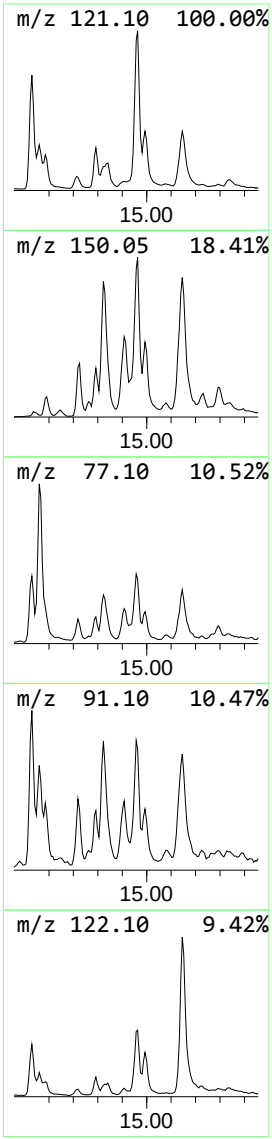
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Phenol, 2-(1-methylpropyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.957	41.97 ug/l	1253630	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	91
2	Phenol, 4-(1-methylpropyl)-	150	C10H14O	000099-71-8	91
3	2-Methyl-4-propylphenol	150	C10H14O	018441-56-0	80
4	2-Methyl-6-propylphenol	150	C10H14O	003520-52-3	78
5	Benzene, 1-methoxy-4-propyl-	150	C10H14O	000104-45-0	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031622\
Data File : VX027473.D
Acq On : 16 Mar 2022 16:03
Operator : JC/MD
Sample : N1950-10RE
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3222RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

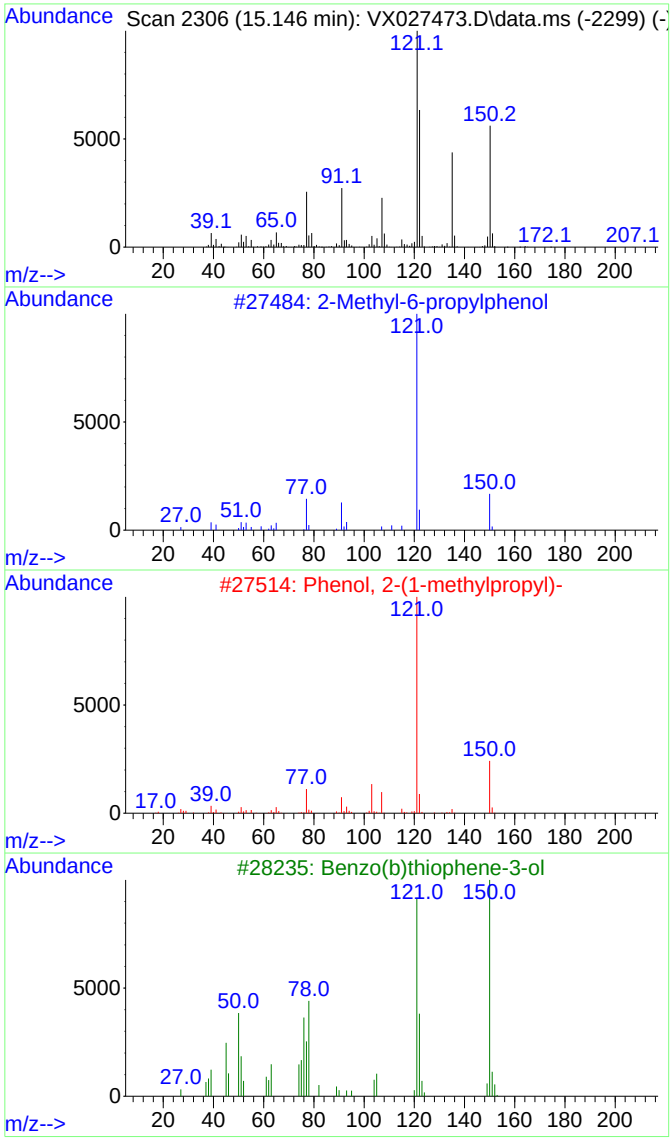
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

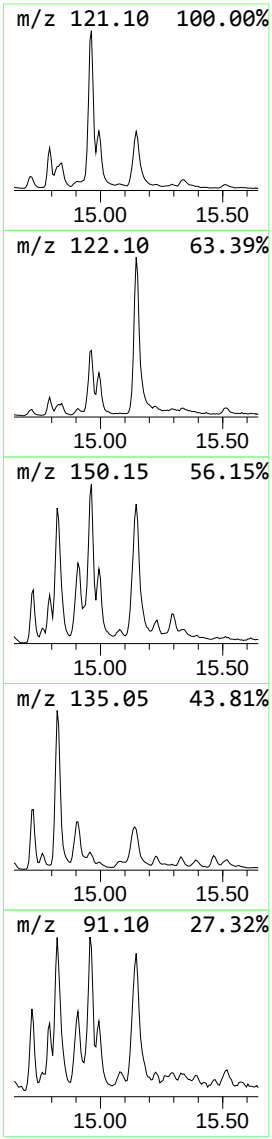
****

Peak Number 10 unknown15.146 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.146	41.53 ug/l	1240290	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-6-propylphenol	150	C10H14O	003520-52-3	49
2	Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	47
3	Benzo(b)thiophene-3-ol	150	C8H6OS	000520-72-9	47
4	4-Pyridinamine, N,N-dimethyl-	122	C7H10N2	001122-58-3	43
5	25B-NBOMe	379	C18H22BrNO3	1026511-90-9	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031622\
Data File : VX027473.D
Acq On : 16 Mar 2022 16:03
Operator : JC/MD
Sample : N1950-10RE
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3222RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Phenol, 3-ethyl-	13.896	17.6	ug/l	525853	4	12.024	1493320	50.0
Phenol, 4-ethyl...	14.329	44.5	ug/l	1330210	4	12.024	1493320	50.0
Phenol, 3-ethyl...	14.530	31.7	ug/l	946421	4	12.024	1493320	50.0
Phenol, 2-propyl-	14.560	71.5	ug/l	2137070	4	12.024	1493320	50.0
2,5-Diethylphenol	14.719	15.8	ug/l	471231	4	12.024	1493320	50.0
1,4-Methanonaph...	14.786	26.8	ug/l	801080	4	12.024	1493320	50.0
Phenol, m-tert-...	14.823	41.5	ug/l	1238080	4	12.024	1493320	50.0
Phenol, 2-(1,1-...	14.908	19.9	ug/l	595015	4	12.024	1493320	50.0
Phenol, 2-(1-me...	14.957	42.0	ug/l	1253630	4	12.024	1493320	50.0
unknown15.146	15.146	41.5	ug/l	1240290	4	12.024	1493320	50.0