LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062022\
Data File : BG053955.D
Acq On : 20 Jun 2022 19:18
Operator : CG/JU
Sample : N3358-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EW4R7

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062022.M
Title : SVOA CALIBRATION

Signal : TIC: BG053955.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.502	14	19	24	rBV5	3976	6750	0.19%	0.062%
2	3.919	87	90	104	rVB2	12917	27535	0.78%	0.251%
3	4.072	111	116	122	rVB3	4230	6789	0.19%	0.062%
4	4.160	127	131	137	rVB4	2307	3952	0.11%	0.036%
5	7.233	647	654	655	rBV	22651	34268	0.97%	0.313%
6	7.397	675	682	691	rBV	62585	109000	3.09%	0.994%
7	7.609	711	718	726	rVB	66517	118330	3.36%	1.080%
8	8.079	791	798	805	rBV	64262	112310	3.19%	1.025%
9	8.772	908	916	925	rBB2	60739	109160	3.10%	0.996%
10	9.236	988	995	1005	rBV	86461	157579	4.47%	1.438%
11	9.959	1112	1118	1126	rBV	69651	129198	3.66%	1.179%
12	10.500	1204	1210	1223	rBV	106251	201780	5.72%	1.841%
13	10.793	1252	1260	1267	rBV	77588	133338	3.78%	1.216%
14	10.887	1268	1276	1284	rVB	86566	162483	4.61%	1.482%
15	11.011	1290	1297	1306	rBV	74096	145109	4.12%	1.324%
16	11.222	1329	1333	1340	rVB3	10274	19480	0.55%	0.178%
17	11.451	1366	1372	1378	rBV4	2377	6260	0.18%	0.057%
18	11.710	1410	1416	1417	rBV3	2957	4982	0.14%	0.045%
19	11.745	1417	1422	1429	rVB7	4124	10001	0.28%	0.091%
20	11.892	1442	1447	1457	rBV2	14655	35065	0.99%	0.320%
21	11.980	1457	1462	1469	rVV9	7377	24366	0.69%	0.222%
22	12.033	1469	1471	1480	rVV6	4894	10706	0.30%	0.098%
23	12.227	1493	1504	1515	rBV	1875513	3526204	100.00%	32.170%
24	12.333	1520	1522	1532	rVB3	4804	8757	0.25%	0.080%
25	13.537	1719	1727	1732	rBV2	13126	19810	0.56%	0.181%
26	13.590	1732	1736	1744	rVB4	3417	6705	0.19%	0.061%
27	13.948	1792	1797	1802	rVB3	2189	3716	0.11%	0.034%
28	14.101	1815	1823	1830	rBV	258613	385536	10.93%	3.517%
29	14.395	1866	1873	1879	rBV	246908	412126	11.69%	3.760%
30	14.442	1879	1881	1887	rVB2	8436	11614	0.33%	0.106%
31	14.701	1918	1925	1932	rBV	161232	260762	7.39%	2.379%
32	14.877	1950	1955	1961	rBV2	21002	36695	1.04%	0.335%
33	14.924	1961	1963	1970	rVB	7972	10645	0.30%	0.097%
34	15.547	2065	2069	2073	rVB4	3746	4981	0.14%	0.045%
35	15.693	2087	2094	2101	rBV	378855	595573	16.89%	5.433%
36	15.799	2105	2112	2123	rBV	112022	174286	4.94%	1.590%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062022\
Data File : BG053955.D
Acq On : 20 Jun 2022 19:18
Operator : CG/JU
Sample : N3358-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EW4R7

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062022.M
Title : SVOA CALIBRATION

37	15.934	2129	2135	2138	rBV2	4494	6839	0.19%	0.062%
38	17.444	2385	2392	2398	rBV	227568	361776	10.26%	3.301%
39	17.544	2402	2409	2417	rVB	444766	694637	19.70%	6.337%
40	18.337	2539	2544	2549	rBV3	7903	13000	0.37%	0.119%
41	19.395	2719	2724	2728	rBV2	6679	9720	0.28%	0.089%
42	19.460	2731	2735	2741	rBV	6091	9802	0.28%	0.089%
43	19.830	2791	2798	2812	rVB	598209	907932	25.75%	8.283%
44	21.357	3052	3058	3067	rBV	34185	61321	1.74%	0.559%
45	21.716	3113	3119	3127	rBV	263451	446456	12.66%	4.073%
46	23.238	3375	3378	3384	rVB7	3814	6673	0.19%	0.061%
47	24.060	3515	3518	3527	rVB6	4509	10710	0.30%	0.098%
48	24.759	3625	3637	3653	rVB2	315031	923064	26.18%	8.421%
49	24.977	3663	3674	3691	rVB2	154234	464244	13.17%	4.235%
50	26.193	3872	3881	3886	rBV9	6528	19221	0.55%	0.175%

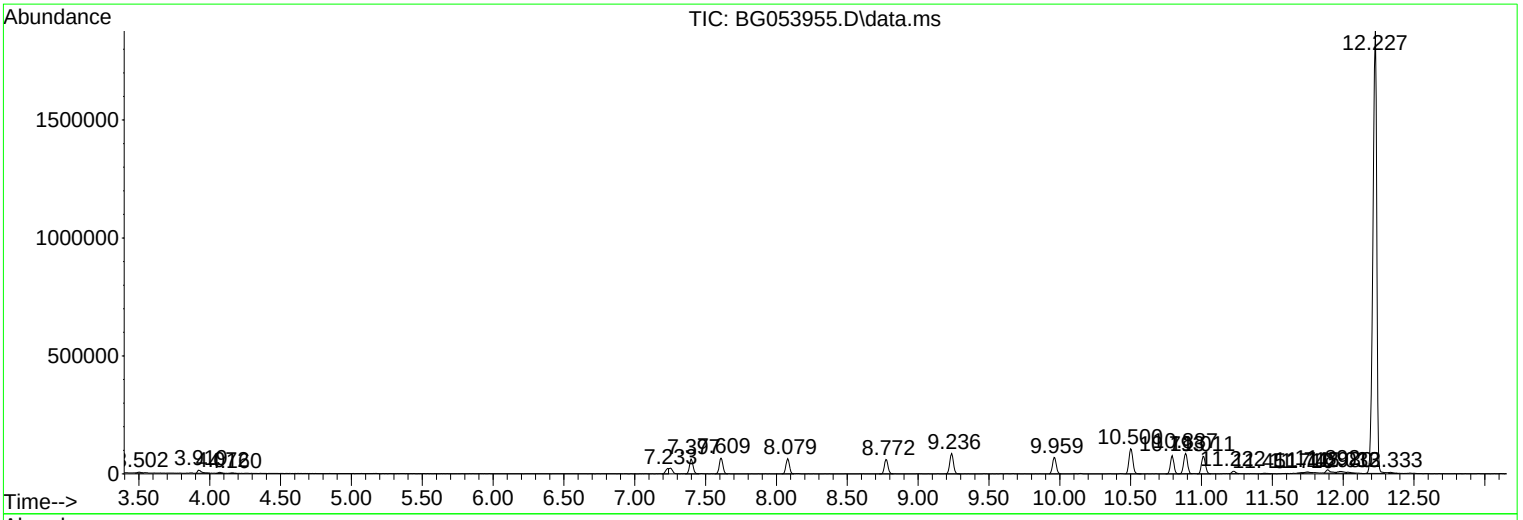
Sum of corrected areas: 10961246

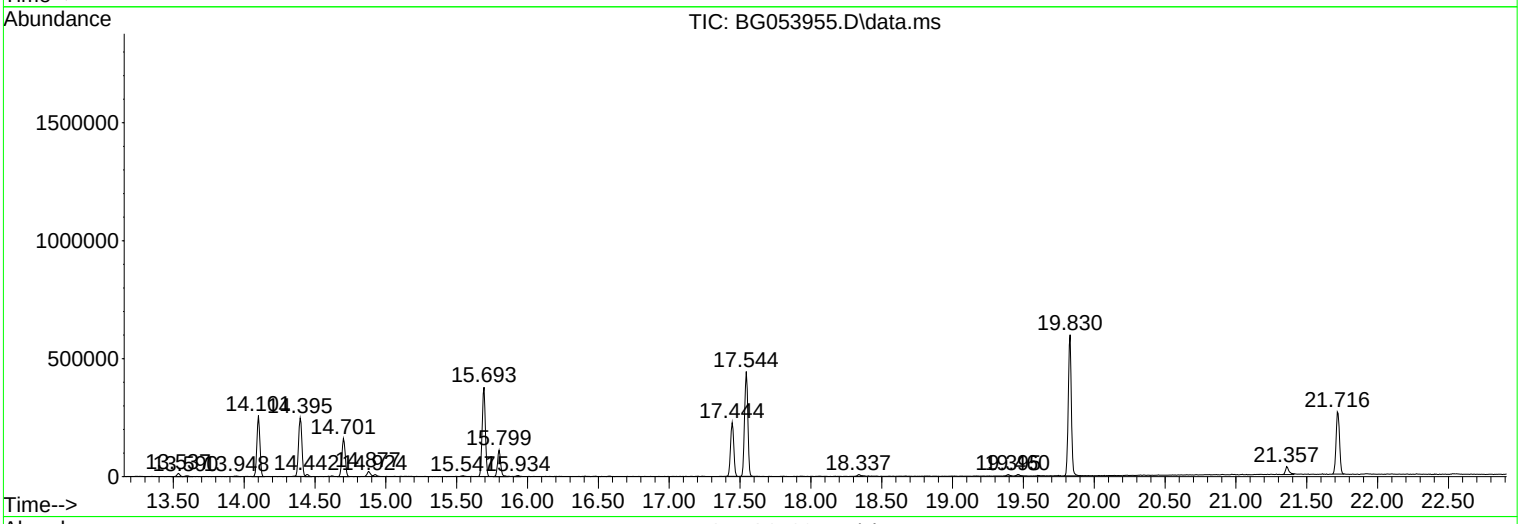
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062022\
Data File : BG053955.D
Acq On : 20 Jun 2022 19:18
Operator : CG/JU
Sample : N3358-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

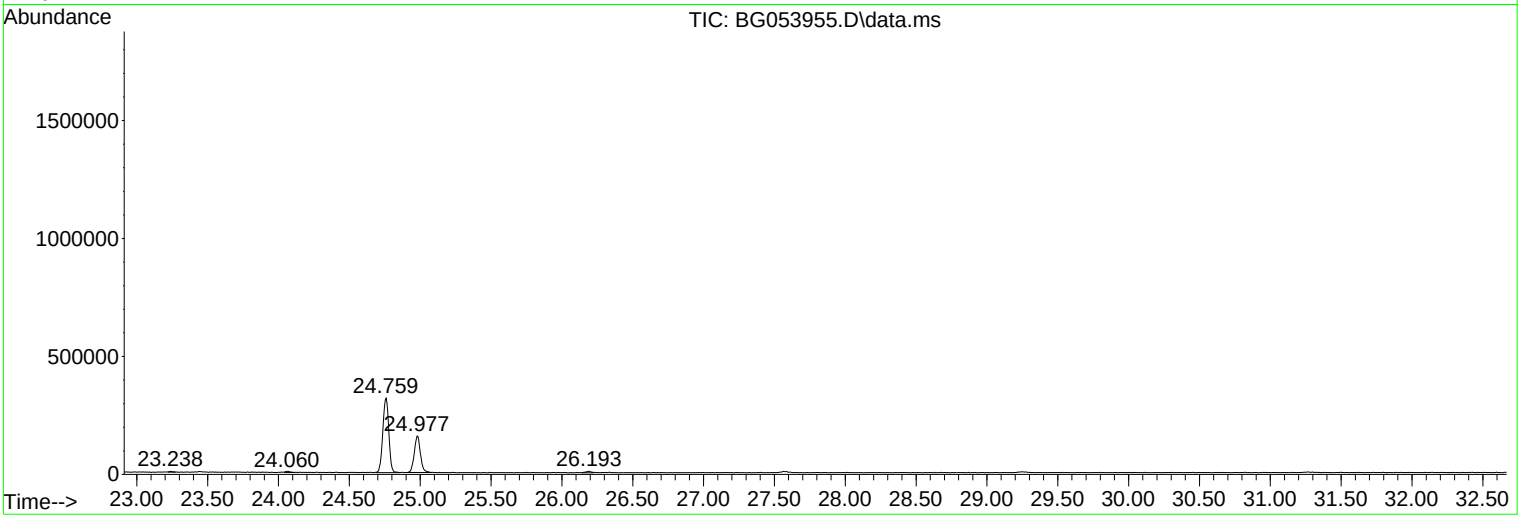
Instrument :
BNA_G
ClientSampleId :
EW4R7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062022.M
Quant Title : SVOA CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062022\
Data File : BG053955.D
Acq On : 20 Jun 2022 19:18
Operator : CG/JU
Sample : N3358-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EW4R7

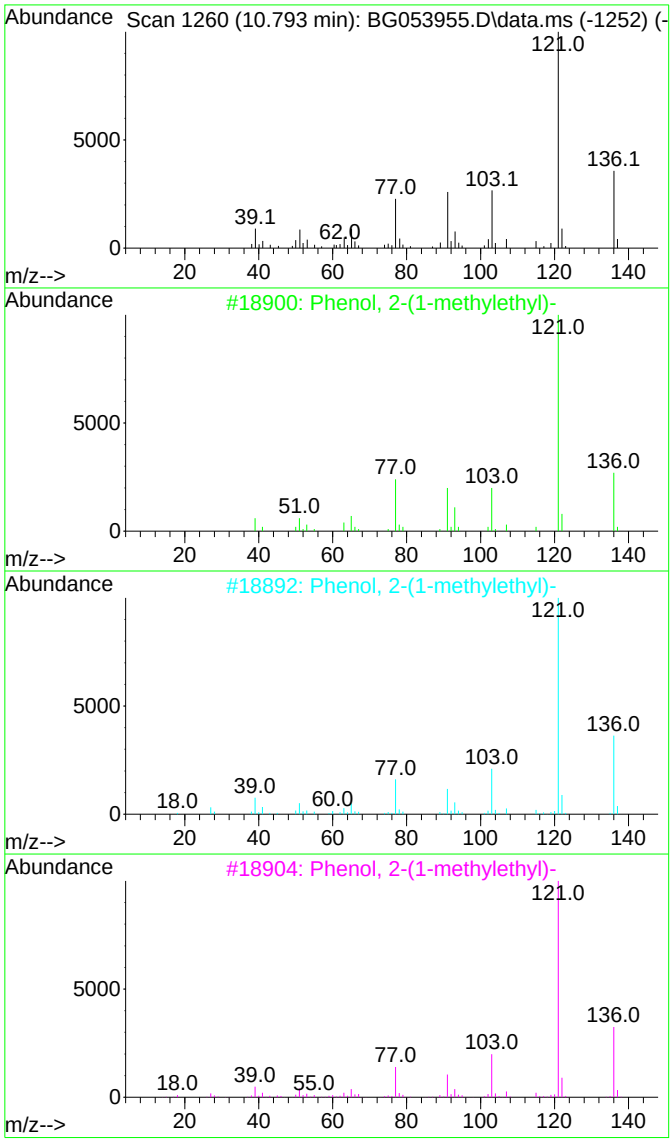
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062022.M
Quant Title : SVOA CALIBRATION

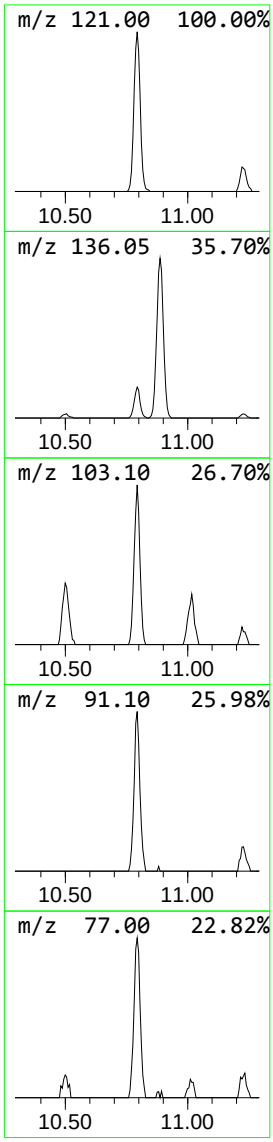
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.793	16.41 ng/ul	133338	Naphthalene-d8	10.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	94
2	Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	91
3	Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	91
4	p-Cumenol	136	C9H12O	000099-89-8	87
5	Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062022\
Data File : BG053955.D
Acq On : 20 Jun 2022 19:18
Operator : CG/JU
Sample : N3358-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EW4R7

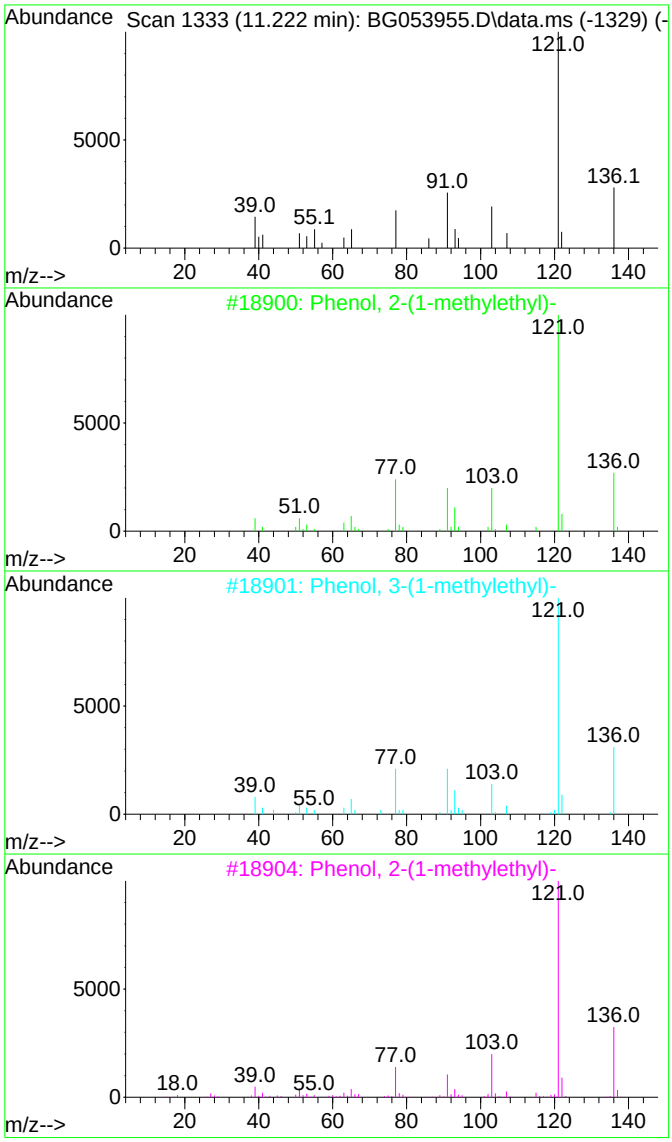
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062022.M
Quant Title : SVOA CALIBRATION

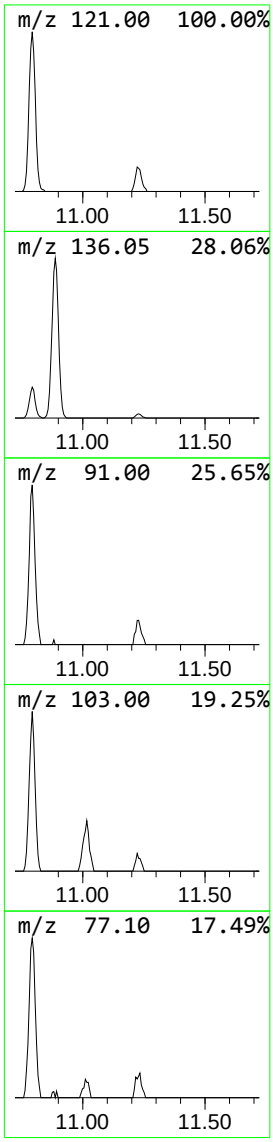
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Phenol, 3-(1-methylethyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.222	2.40 ng/ul	19480	Naphthalene-d8	10.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	90
2	Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	86
3	Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	83
4	p-Cumenol	136	C9H12O	000099-89-8	80
5	p-Cumenol	136	C9H12O	000099-89-8	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062022\
Data File : BG053955.D
Acq On : 20 Jun 2022 19:18
Operator : CG/JU
Sample : N3358-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EW4R7

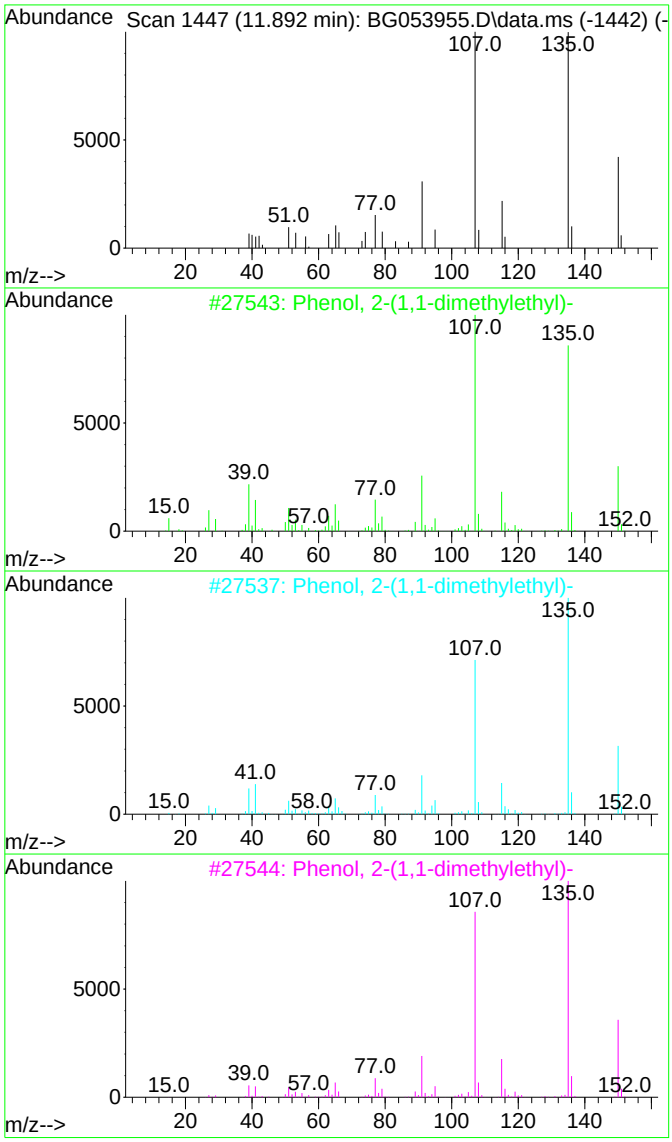
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062022.M
Quant Title : SVOA CALIBRATION

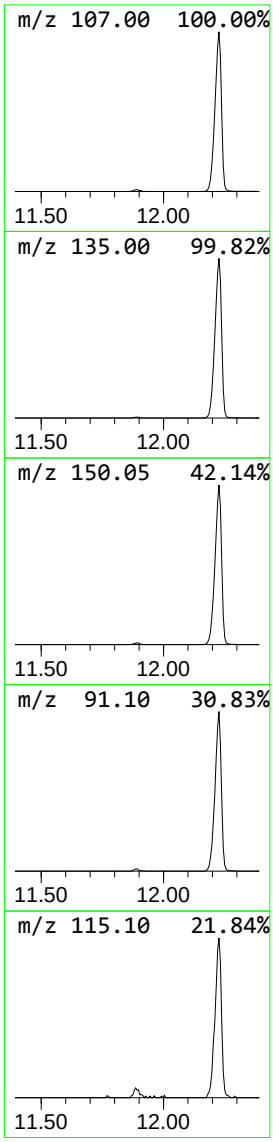
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	4.32 ng/ul	35065	Naphthalene-d8	10.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	90
2	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	83
3	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	83
4	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	58
5	3-Methoxyacetophenone	150	C9H10O2	000586-37-8	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062022\
Data File : BG053955.D
Acq On : 20 Jun 2022 19:18
Operator : CG/JU
Sample : N3358-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EW4R7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062022.M
Quant Title : SVOA CALIBRATION

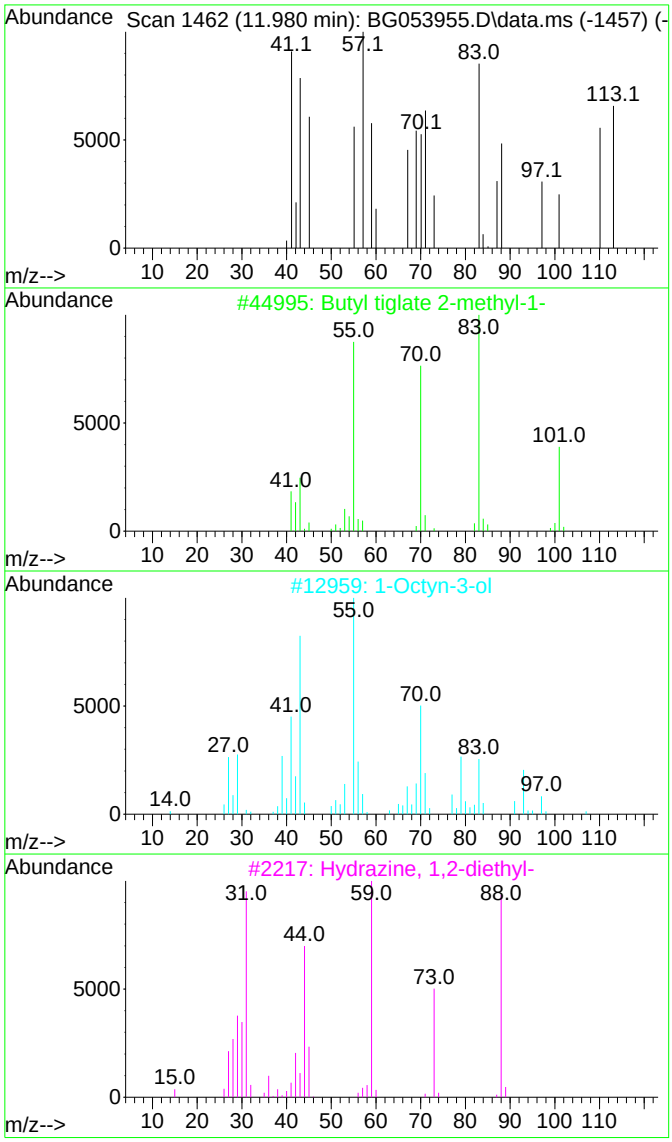
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

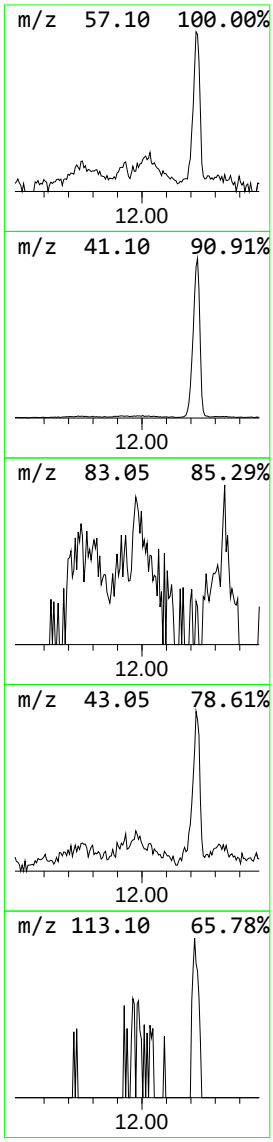
****

Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.980	3.00 ng/ul	24366	Naphthalene-d8	10.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl tiglate 2-methyl-1-	170	C10H18O2	1000383-67-9	10
2	1-Octyn-3-ol	126	C8H14O	000818-72-4	10
3	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	9
4	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	9
5	4-Cyanothiazole	110	C4H2N2S	001452-15-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062022\
Data File : BG053955.D
Acq On : 20 Jun 2022 19:18
Operator : CG/JU
Sample : N3358-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EW4R7

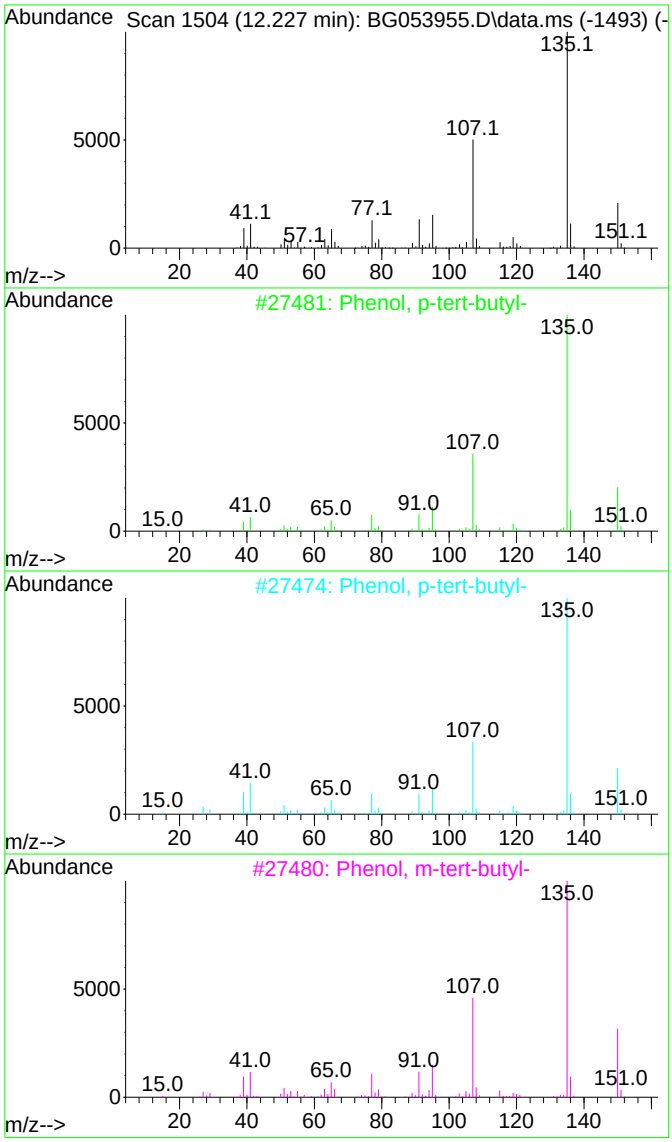
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062022.M
Quant Title : SVOA CALIBRATION

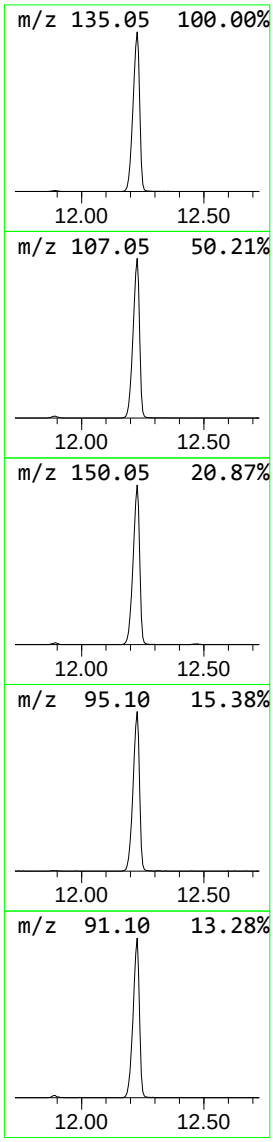
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phenol, p-tert-butyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.227	434.04 ng/ul	3526200	Naphthalene-d8	10.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	97
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	94
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	91
4	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	91
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062022\
Data File : BG053955.D
Acq On : 20 Jun 2022 19:18
Operator : CG/JU
Sample : N3358-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EW4R7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062022.M
Quant Title : SVOA CALIBRATION

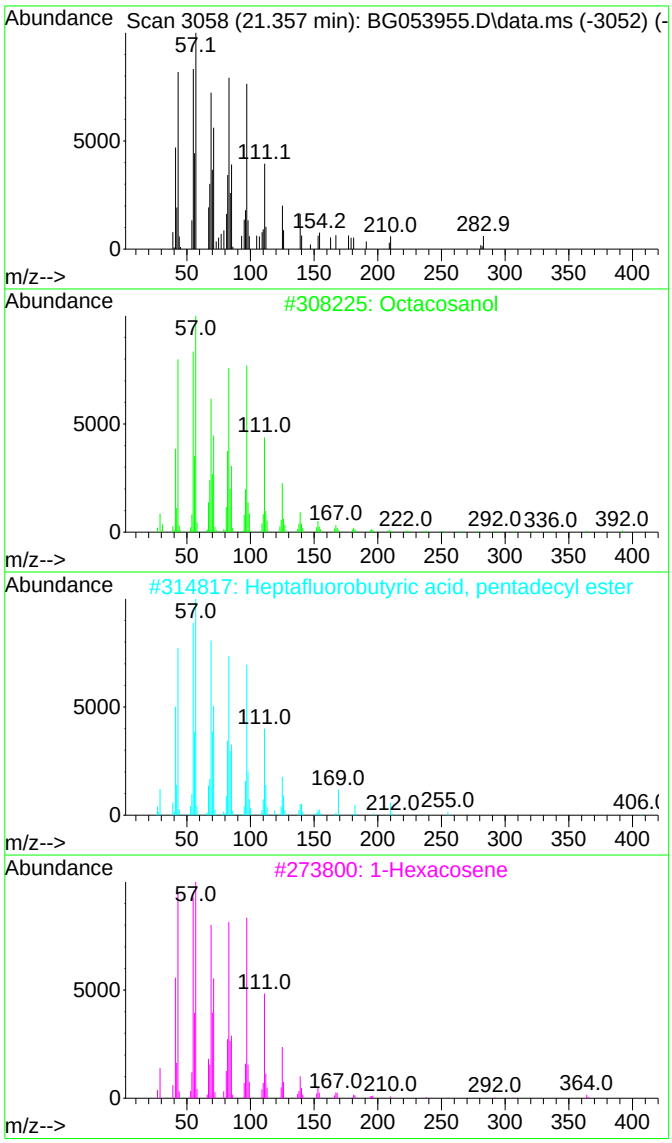
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

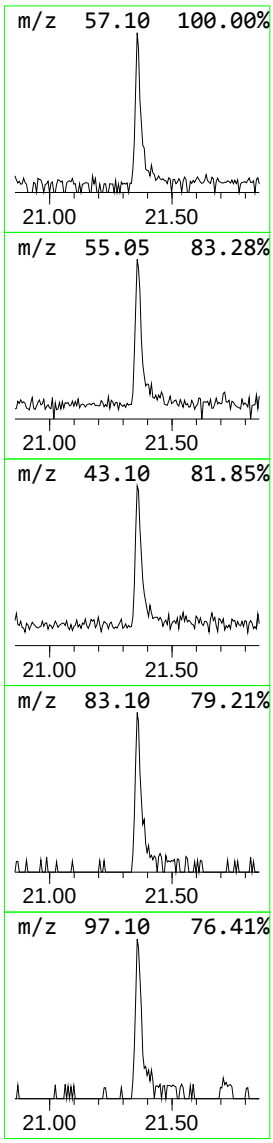
****

Peak Number 6 Octacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.357	2.75 ng/ul	61321	Chrysene-d12	21.716

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	95
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	1-Hexacosene	364	C26H52	018835-33-1	93
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062022\
Data File : BG053955.D
Acq On : 20 Jun 2022 19:18
Operator : CG/JU
Sample : N3358-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EW4R7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062022.M
Quant Title : SVOA CALIBRATION

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, 2-(1-me...	10.793	16.4	ng/ul	133338	2	10.887	162483	20.0
Phenol, 3-(1-me...	11.222	2.4	ng/ul	19480	2	10.887	162483	20.0
Phenol, 2-(1,1-...	11.892	4.3	ng/ul	35065	2	10.887	162483	20.0
unknown-01	11.980	3.0	ng/ul	24366	2	10.887	162483	20.0
Phenol, p-tert-...	12.227	434.0	ng/ul	3526200	2	10.887	162483	20.0
Octacosanol	21.357	2.8	ng/ul	61321	5	21.716	446456	20.0