LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122221\
Data File : BG051769.D
Acq On : 23 Dec 2021 4:03
Operator : CG/JU
Sample : M5090-12
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BG3E2

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-BG121421.M
Title : SVOA CALIBRATION

Signal : TIC: BG051769.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.602	13	19	23	rBV2	7760	12666	1.06%	0.114%
2	4.031	88	92	99	rBV	26760	46179	3.88%	0.414%
3	4.383	145	152	153	rBV3	2395	3525	0.30%	0.032%
4	4.747	210	214	220	rVB3	3397	5436	0.46%	0.049%
5	5.317	308	311	315	rVB2	1302	1902	0.16%	0.017%
6	6.310	477	480	482	rVB	1958	1891	0.16%	0.017%
7	6.886	572	578	585	rBV3	11577	17319	1.45%	0.155%
8	7.344	650	656	659	rBV4	2031	3091	0.26%	0.028%
9	7.403	659	666	674	rVV2	40043	70531	5.92%	0.632%
10	7.573	689	695	706	rVB	122123	210035	17.64%	1.882%
11	7.796	724	733	740	rBV	128072	221706	18.62%	1.987%
12	8.272	806	814	819	rBV	134642	238820	20.05%	2.140%
13	8.501	850	853	854	rBV2	1683	1662	0.14%	0.015%
14	8.877	910	917	923	rBV2	1753	3964	0.33%	0.036%
15	8.965	923	932	940	rBV	106977	186758	15.68%	1.674%
16	9.095	948	954	959	rBV2	9437	16319	1.37%	0.146%
17	9.371	996	1001	1006	rBV3	15539	24354	2.04%	0.218%
18	9.441	1006	1013	1023	rVB	163766	307166	25.79%	2.753%
19	9.594	1035	1039	1043	rVB	1707	1919	0.16%	0.017%
20	10.170	1130	1137	1145	rVB	130254	233664	19.62%	2.094%
21	10.716	1223	1230	1237	rBV2	187518	345795	29.04%	3.099%
22	10.998	1272	1278	1284	rBV5	7874	15598	1.31%	0.140%
23	11.109	1287	1297	1303	rBV	190649	332135	27.89%	2.976%
24	11.227	1309	1317	1328	rBV	174332	322655	27.09%	2.891%
25	11.750	1402	1406	1412	rBV3	2049	3175	0.27%	0.028%
26	12.255	1488	1492	1495	rBV2	2299	2864	0.24%	0.026%
27	12.355	1501	1509	1517	rBV2	35878	58906	4.95%	0.528%
28	12.678	1560	1564	1570	rBV2	2924	4375	0.37%	0.039%
29	13.518	1702	1707	1709	rBV3	1983	2978	0.25%	0.027%
30	13.806	1748	1756	1764	rBV2	35765	58325	4.90%	0.523%
31	14.293	1833	1839	1846	rBV	411880	608031	51.06%	5.449%
32	14.605	1884	1892	1901	rVB	445531	702033	58.95%	6.291%
33	14.904	1935	1943	1950	rBV	304159	479725	40.28%	4.299%
34	14.969	1950	1954	1958	rBV3	4479	6718	0.56%	0.060%
35	15.069	1964	1971	1981	rBV	26542	48005	4.03%	0.430%
36	15.298	2005	2010	2016	rBV4	1701	2780	0.23%	0.025%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122221\
Data File : BG051769.D
Acq On : 23 Dec 2021 4:03
Operator : CG/JU
Sample : M5090-12
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BG3E2

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-BG121421.M
Title : SVOA CALIBRATION

37	15.562	2049	2055	2062	rBV3	3644	7282	0.61%	0.065%
38	15.627	2062	2066	2069	rVB2	2105	3413	0.29%	0.031%
39	15.686	2073	2076	2084	rVB4	1811	3436	0.29%	0.031%
40	15.897	2104	2112	2121	rBV	592520	903620	75.88%	8.097%
41	15.997	2123	2129	2140	rVB	84382	131687	11.06%	1.180%
42	16.138	2148	2153	2156	rBV3	2578	3489	0.29%	0.031%
43	16.244	2167	2171	2176	rBV2	5396	7697	0.65%	0.069%
44	17.231	2336	2339	2345	rVB	1756	2460	0.21%	0.022%
45	17.436	2372	2374	2380	rVB3	1589	2443	0.21%	0.022%
46	17.654	2405	2411	2419	rBV	388452	578761	48.60%	5.186%
47	17.753	2419	2428	2438	rBV	685538	1021488	85.77%	9.154%
48	17.912	2452	2455	2461	rVB2	1570	1950	0.16%	0.017%
49	18.311	2517	2523	2529	rVB	117523	160659	13.49%	1.440%
50	18.635	2575	2578	2583	rVB3	1934	2783	0.23%	0.025%
51	19.557	2730	2735	2737	rBV4	901	1575	0.13%	0.014%
52	19.592	2737	2741	2749	rVB5	8042	12385	1.04%	0.111%
53	19.663	2749	2753	2757	rBV3	8589	12053	1.01%	0.108%
54	19.927	2795	2798	2801	rVB3	6373	6676	0.56%	0.060%
55	19.962	2801	2804	2806	rVB3	1452	1628	0.14%	0.015%
56	20.027	2809	2815	2826	rBV	815768	1190910	100.00%	10.672%
57	20.262	2852	2855	2856	rBV2	1838	1571	0.13%	0.014%
58	20.532	2899	2901	2904	rBV4	2039	1789	0.15%	0.016%
59	20.579	2907	2909	2912	rBV3	1854	2041	0.17%	0.018%
60	20.602	2912	2913	2915	rBV2	2758	1766	0.15%	0.016%
61	20.661	2919	2923	2925	rBV3	2565	3095	0.26%	0.028%
62	20.973	2973	2976	2980	rVB4	11064	10997	0.92%	0.099%
63	21.014	2980	2983	2986	rBV3	6622	10444	0.88%	0.094%
64	21.260	3023	3025	3028	rVB4	3244	2420	0.20%	0.022%
65	21.578	3075	3079	3082	rBV5	5063	7717	0.65%	0.069%
66	21.971	3139	3146	3156	rVB	362503	625029	52.48%	5.601%
67	22.159	3176	3178	3185	rVB5	5979	9976	0.84%	0.089%
68	22.341	3207	3209	3211	rBV2	2899	2239	0.19%	0.020%
69	22.682	3265	3267	3275	rBV4	2333	4071	0.34%	0.036%
70	22.823	3289	3291	3297	rVB6	7014	9062	0.76%	0.081%
71	24.474	3567	3572	3579	rVB6	13683	31374	2.63%	0.281%
72	25.231	3689	3701	3714	rBV2	363435	1070307	89.87%	9.591%
73	25.472	3731	3742	3760	rVB2	180900	617058	51.81%	5.529%
74	25.948	3821	3823	3825	rBV3	2862	2470	0.21%	0.022%
75	26.030	3835	3837	3839	rBV3	2746	2436	0.20%	0.022%
76	26.436	3904	3906	3908	rBV3	2404	1567	0.13%	0.014%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122221\
Data File : BG051769.D
Acq On : 23 Dec 2021 4:03
Operator : CG/JU
Sample : M5090-12
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BG3E2

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-BG121421.M
Title : SVOA CALIBRATION

77	26.788	3959	3966	3977	rVB7	17259	56176	4.72%	0.503%
78	28.280	4213	4220	4221	rBV5	13278	21078	1.77%	0.189%
79	30.877	4660	4662	4665	rBV4	2666	3228	0.27%	0.029%
80	32.574	4949	4951	4952	rBV	2950	2098	0.18%	0.019%

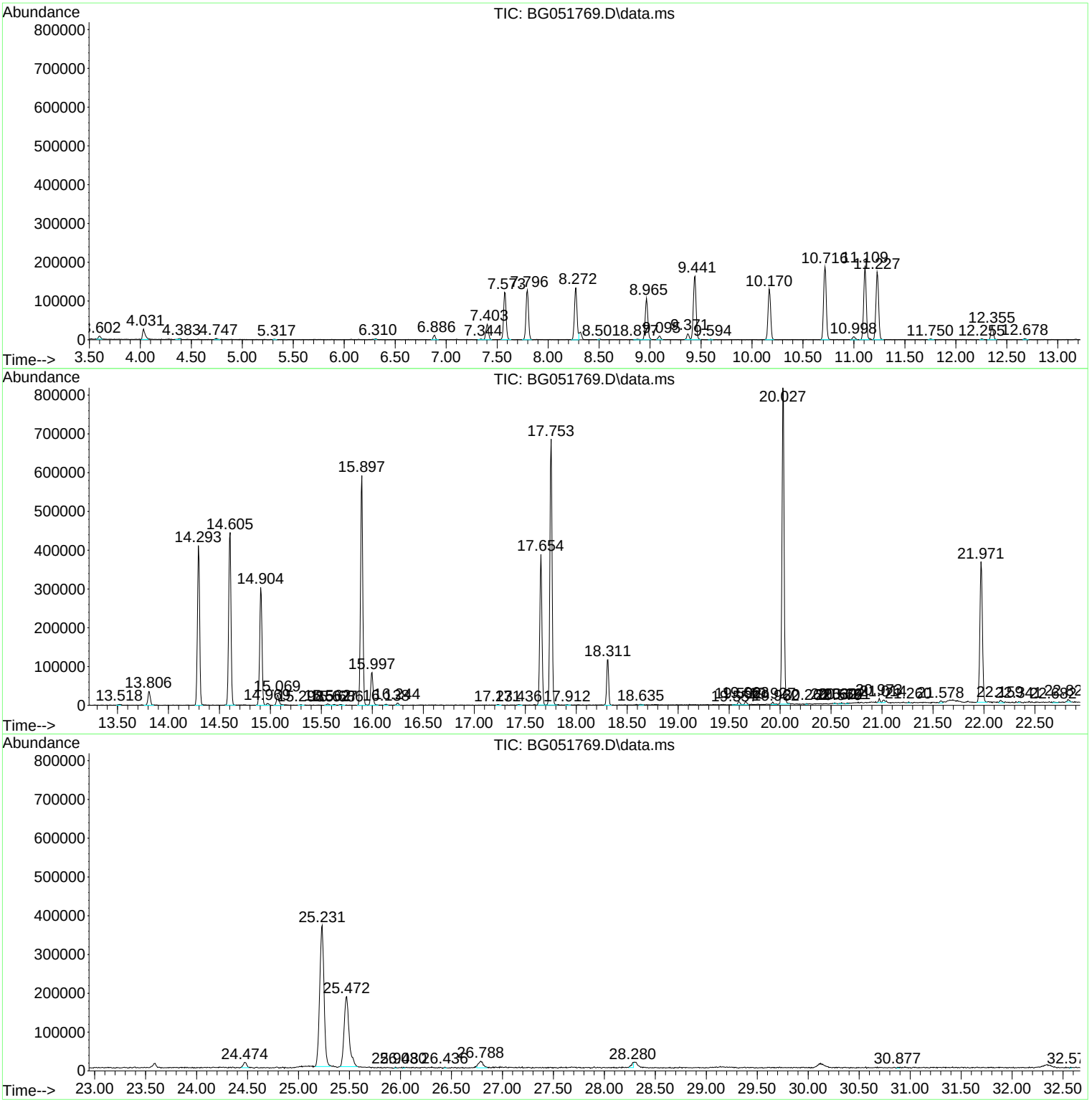
Sum of corrected areas: 11159409

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122221\
Data File : BG051769.D
Acq On : 23 Dec 2021 4:03
Operator : CG/JU
Sample : M5090-12
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BG3E2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122221\
Data File : BG051769.D
Acq On : 23 Dec 2021 4:03
Operator : CG/JU
Sample : M5090-12
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BG3E2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
Quant Title : SVOA CALIBRATION

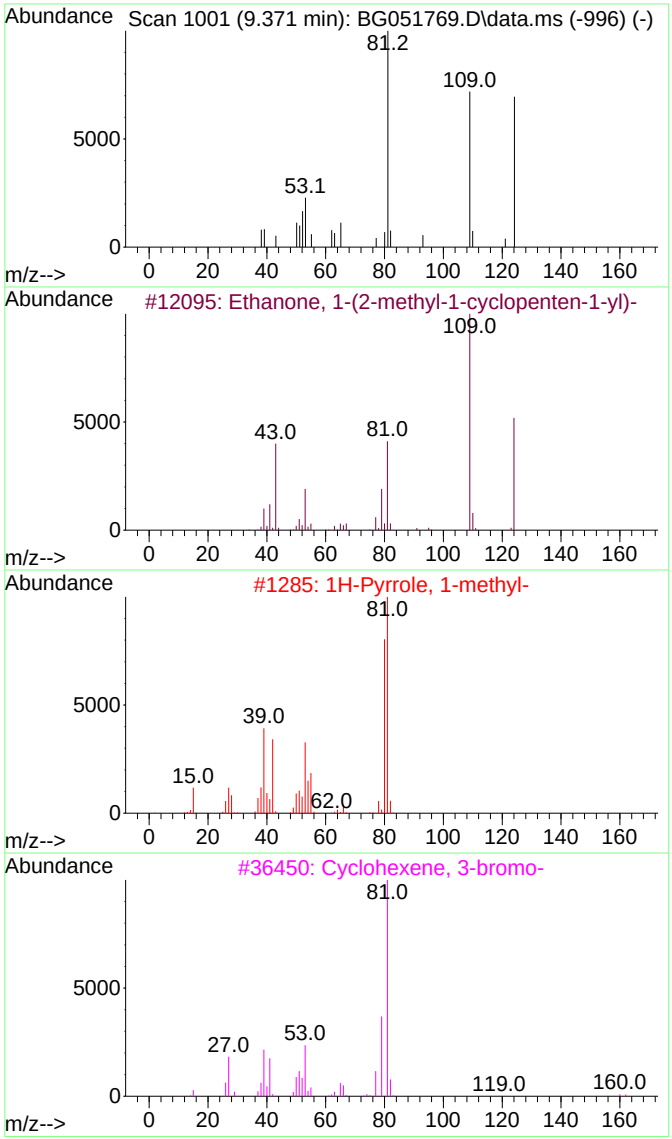
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

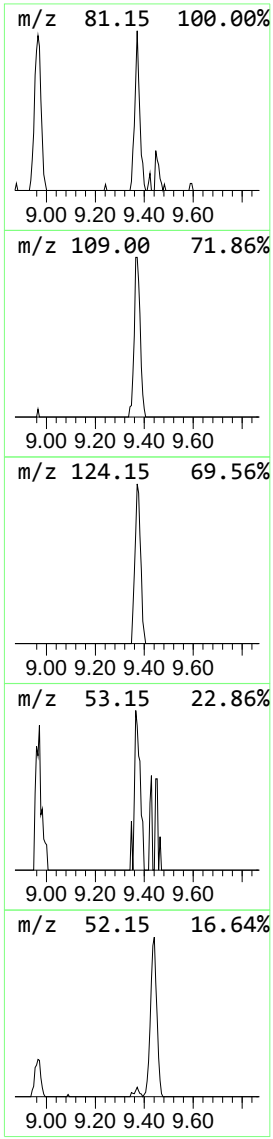
****

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.371	2.04 ng/ul	24354	1,4-Dichlorobenzene-d4	8.272

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(2-methyl-1-cyclopen...	124	C8H12O	003168-90-9	37
2	1H-Pyrrole, 1-methyl-	81	C5H7N	000096-54-8	35
3	Cyclohexene, 3-bromo-	160	C6H9Br	001521-51-3	32
4	Nicotinyl alcohol	109	C6H7NO	000100-55-0	27
5	1H-Pyrrole, 1-methyl-	81	C5H7N	000096-54-8	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122221\
Data File : BG051769.D
Acq On : 23 Dec 2021 4:03
Operator : CG/JU
Sample : M5090-12
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BG3E2

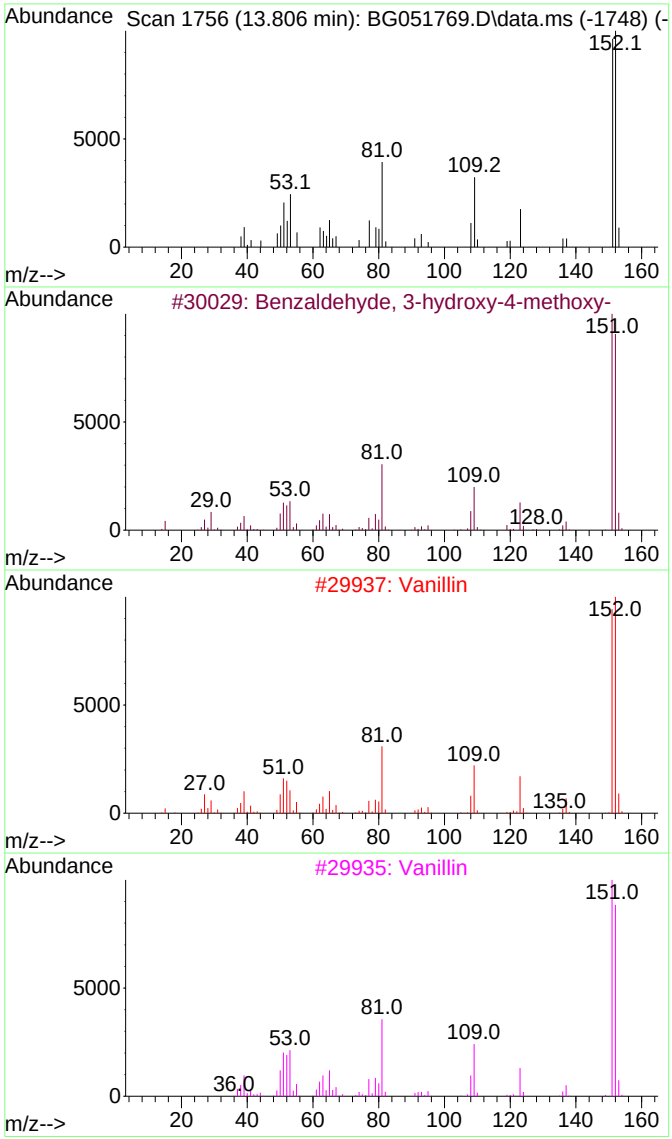
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
Quant Title : SVOA CALIBRATION

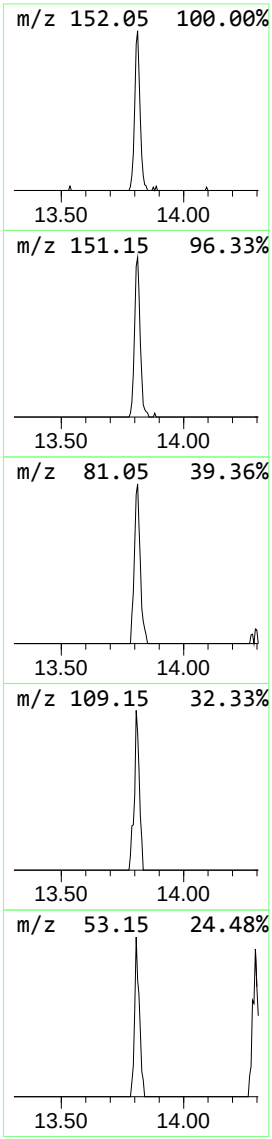
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzaldehyde, 3-hydroxy-4-m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.806	2.43 ng/ul	58325	Acenaphthene-d10	14.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	94
2	Vanillin	152	C8H8O3	000121-33-5	94
3	Vanillin	152	C8H8O3	000121-33-5	91
4	Vanillin	152	C8H8O3	000121-33-5	90
5	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122221\
Data File : BG051769.D
Acq On : 23 Dec 2021 4:03
Operator : CG/JU
Sample : M5090-12
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BG3E2

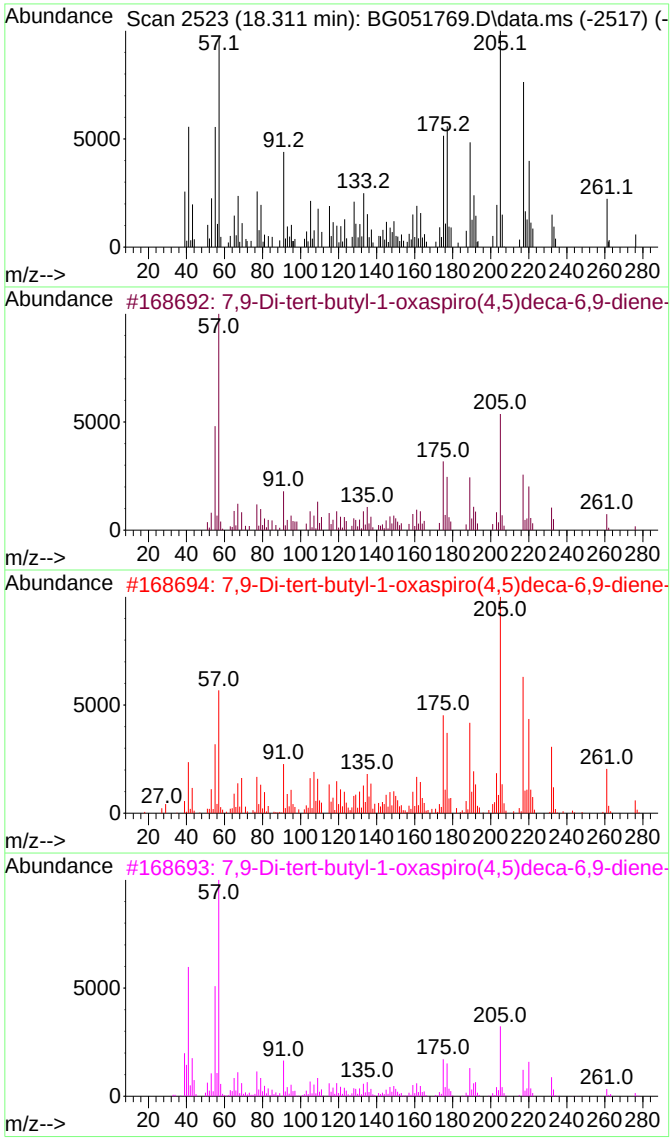
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
Quant Title : SVOA CALIBRATION

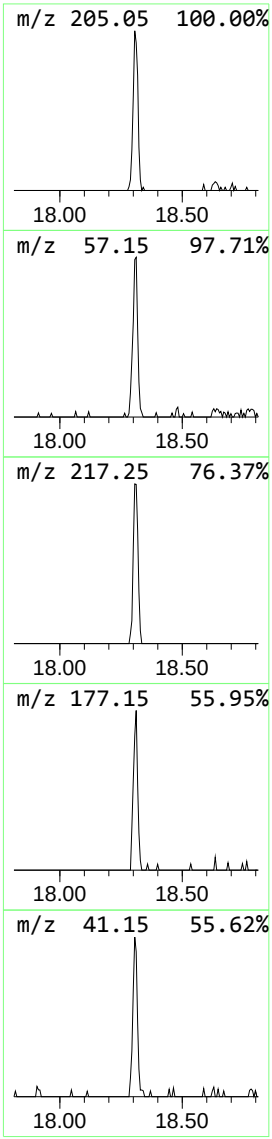
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.311	5.55 ng/ul	160659	Phenanthrene-d10	17.654

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	94
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	90
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	89
4	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	44
5	2-Hydroxy-4-methoxy-5-(2-methylb...	220	C13H16O3	2108511-28-8	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122221\
Data File : BG051769.D
Acq On : 23 Dec 2021 4:03
Operator : CG/JU
Sample : M5090-12
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BG3E2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.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
unknown-01	9.371	2.0	ng/ul	24354	1	8.272	238820	20.0
Benzaldehyde, 3...	13.806	2.4	ng/ul	58325	3	14.904	479725	20.0
7,9-Di-tert-but...	18.311	5.5	ng/ul	160659	4	17.654	578761	20.0