

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121421\
 Data File : BG051506.D
 Acq On : 14 Dec 2021 16:39
 Operator : CG/JU
 Sample : M4960-03RX
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

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: BG051506.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.610	16	21	27	rBV3	7066	11592	1.13%	0.140%
2	3.881	63	67	68	rBV2	1045	1579	0.15%	0.019%
3	4.057	94	97	101	rBV2	8979	13522	1.31%	0.164%
4	4.227	124	126	127	rBV2	2142	1532	0.15%	0.019%
5	4.356	146	148	151	rBV3	1283	1411	0.14%	0.017%
6	4.392	151	154	160	rVB5	3153	5692	0.55%	0.069%
7	4.756	212	216	226	rVB6	3806	7786	0.76%	0.094%
8	4.920	241	244	245	rBV2	1706	1424	0.14%	0.017%
9	4.997	255	257	259	rBV	1305	1488	0.14%	0.018%
10	5.337	308	315	319	rBV6	4026	7474	0.73%	0.091%
11	5.778	389	390	395	rVB4	1891	2360	0.23%	0.029%
12	5.972	419	423	426	rBV2	1303	1807	0.18%	0.022%
13	6.360	483	489	490	rBV	1788	2626	0.26%	0.032%
14	7.076	608	611	613	rVB	1439	1572	0.15%	0.019%
15	7.217	631	635	636	rBV2	1504	1859	0.18%	0.023%
16	7.364	654	660	661	rBV2	1484	2076	0.20%	0.025%
17	7.417	663	669	675	rBV2	35906	62678	6.09%	0.759%
18	7.593	693	699	706	rBV	88710	148389	14.42%	1.798%
19	7.811	729	736	743	rVB2	94344	166102	16.14%	2.012%
20	8.122	787	789	791	rBV	1387	1636	0.16%	0.020%
21	8.292	811	818	824	rBV2	99357	176849	17.19%	2.143%
22	8.345	824	827	834	rVB2	13232	19261	1.87%	0.233%
23	8.521	854	857	859	rBV2	1831	2258	0.22%	0.027%
24	8.886	918	919	924	rBV3	1551	1810	0.18%	0.022%
25	8.980	929	935	942	rBV	86089	147470	14.33%	1.787%
26	9.115	954	958	966	rVB3	5539	8861	0.86%	0.107%
27	9.250	978	981	984	rBV2	1048	1660	0.16%	0.020%
28	9.391	998	1005	1010	rBV3	10275	18650	1.81%	0.226%
29	9.455	1010	1016	1024	rVB	122827	210531	20.46%	2.551%
30	9.661	1048	1051	1055	rVB2	1529	2524	0.25%	0.031%
31	10.190	1133	1141	1152	rBV	93326	171240	16.64%	2.075%
32	10.730	1225	1233	1242	rBV	138152	252316	24.52%	3.057%
33	11.024	1281	1283	1288	rVB3	2826	3019	0.29%	0.037%
34	11.124	1293	1300	1308	rVV	138158	252610	24.55%	3.061%
35	11.177	1308	1309	1313	rVV2	2871	2586	0.25%	0.031%
36	11.247	1313	1321	1330	rVB	101294	176409	17.15%	2.137%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121421\
 Data File : BG051506.D
 Acq On : 14 Dec 2021 16:39
 Operator : CG/JU
 Sample : M4960-03RX
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

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	11.641	1386	1388	1396	rVB2	1297	2314	0.22%	0.028%
38	11.782	1406	1412	1413	rBV4	1322	2102	0.20%	0.025%
39	11.870	1423	1427	1428	rBV2	1346	1427	0.14%	0.017%
40	12.222	1484	1487	1489	rBV2	1072	1447	0.14%	0.018%
41	12.399	1514	1517	1519	rVB2	1299	1513	0.15%	0.018%
42	12.422	1519	1521	1525	rBV	1463	1920	0.19%	0.023%
43	12.698	1562	1568	1573	rVB2	4152	5526	0.54%	0.067%
44	12.980	1614	1616	1619	rVB2	1740	1571	0.15%	0.019%
45	13.286	1667	1668	1671	rBV3	2165	2251	0.22%	0.027%
46	13.385	1681	1685	1686	rVB3	1645	1700	0.17%	0.021%
47	13.479	1698	1701	1702	rBV2	1577	1489	0.14%	0.018%
48	13.532	1705	1710	1716	rVB6	3654	7654	0.74%	0.093%
49	13.756	1743	1748	1751	rBV3	5955	9071	0.88%	0.110%
50	13.814	1753	1758	1763	rVB4	11251	22547	2.19%	0.273%
51	14.314	1836	1843	1850	rBV	324672	458386	44.55%	5.554%
52	14.443	1862	1865	1868	rVB2	1487	1482	0.14%	0.018%
53	14.549	1881	1883	1885	rBV2	1370	1656	0.16%	0.020%
54	14.619	1887	1895	1901	rVV	321997	513912	49.95%	6.227%
55	14.919	1939	1946	1954	rVB	243373	390675	37.97%	4.733%
56	14.989	1954	1958	1963	rBV3	5056	8754	0.85%	0.106%
57	15.071	1966	1972	1978	rVB2	40663	63739	6.19%	0.772%
58	15.365	2020	2022	2025	rBV3	1204	1765	0.17%	0.021%
59	15.447	2033	2036	2037	rBV2	1456	1412	0.14%	0.017%
60	15.582	2056	2059	2063	rVB4	2857	4767	0.46%	0.058%
61	15.653	2068	2071	2073	rVB	1327	1412	0.14%	0.017%
62	15.700	2077	2079	2080	rBV	1810	1641	0.16%	0.020%
63	15.906	2107	2114	2123	rBV	434460	675144	65.62%	8.180%
64	16.005	2125	2131	2138	rVV	142948	208351	20.25%	2.524%
65	16.264	2170	2175	2179	rBV3	8097	14832	1.44%	0.180%
66	16.581	2228	2229	2230	rBV	3352	1471	0.14%	0.018%
67	16.622	2234	2236	2237	rBV2	1921	1635	0.16%	0.020%
68	16.728	2252	2254	2257	rBV2	1476	1826	0.18%	0.022%
69	17.069	2310	2312	2313	rBV	2829	1766	0.17%	0.021%
70	17.556	2393	2395	2397	rBV2	2196	1491	0.14%	0.018%
71	17.668	2408	2414	2420	rBV	326807	512260	49.79%	6.207%
72	17.768	2424	2431	2437	rBV	549725	843927	82.02%	10.225%
73	17.938	2455	2460	2463	rBV6	6566	10659	1.04%	0.129%
74	18.326	2521	2526	2531	rBV2	73169	92567	9.00%	1.122%
75	18.614	2572	2575	2580	rVB	18025	20454	1.99%	0.248%
76	20.041	2812	2818	2824	rBV	697326	1028906	100.00%	12.466%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121421\
Data File : BG051506.D
Acq On : 14 Dec 2021 16:39
Operator : CG/JU
Sample : M4960-03RX
Misc :
ALS Vial : 5 Sample Multiplier: 1

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	21.986	3144	3149	3157	rVB	328380	574628	55.85%	6.962%
78	25.252	3698	3705	3716	rVB2	307366	858852	83.47%	10.406%

Sum of corrected areas: 8253561

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121421\
Data File : BG051506.D
Acq On : 14 Dec 2021 16:39
Operator : CG/JU
Sample : M4960-03RX
Misc :
ALS Vial : 5 Sample Multiplier: 1

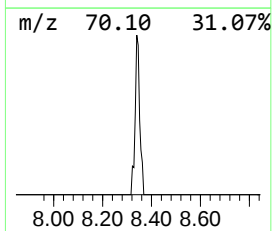
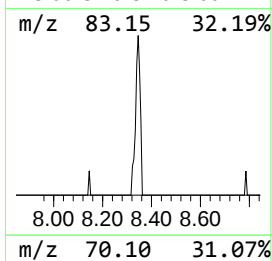
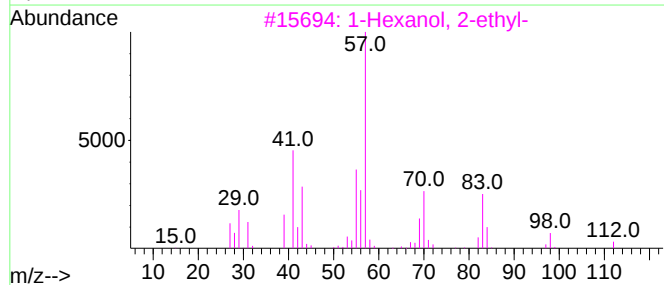
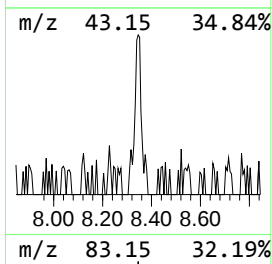
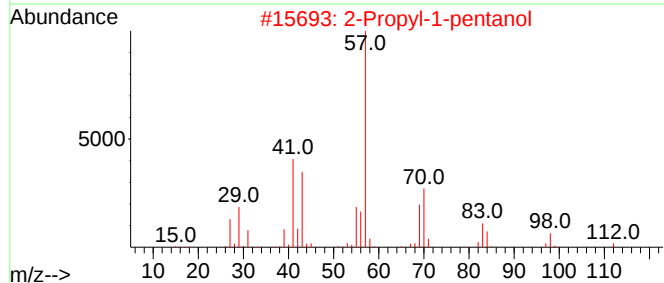
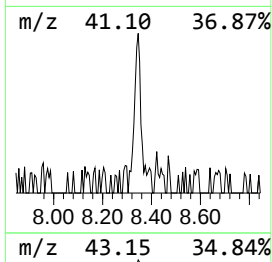
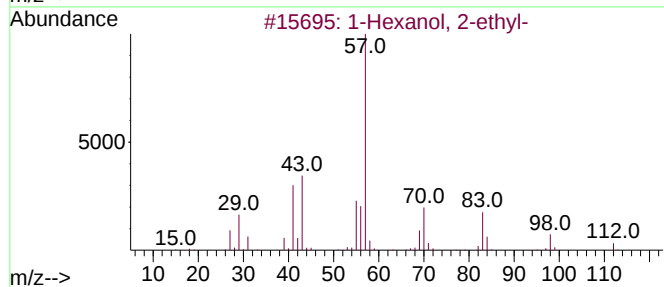
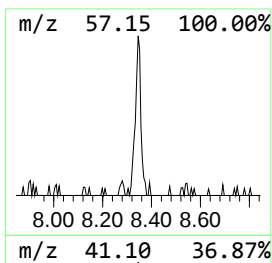
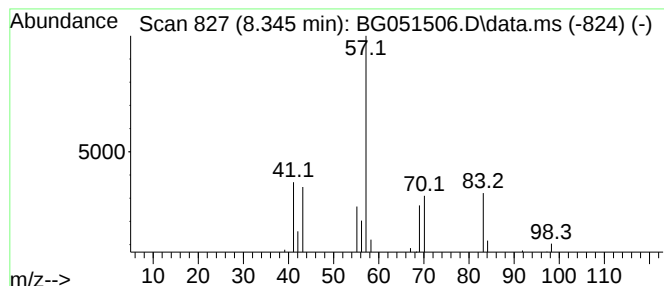
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.345	2.18 ng/ul	19261	1,4-Dichlorobenzene-d4	8.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
2	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	64
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
4	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	50
5	1-Pentanol, 2-ethyl-4-methyl-			130	C8H18O	000106-67-2	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121421\
Data File : BG051506.D
Acq On : 14 Dec 2021 16:39
Operator : CG/JU
Sample : M4960-03RX
Misc :
ALS Vial : 5 Sample Multiplier: 1

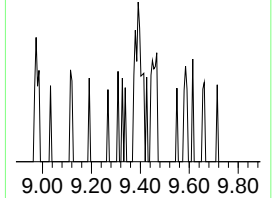
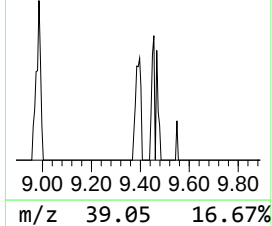
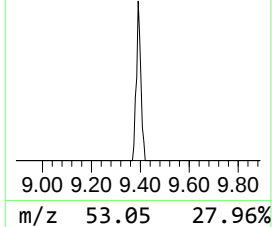
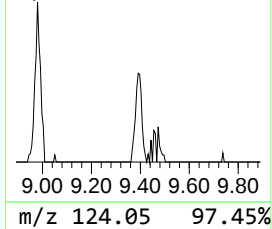
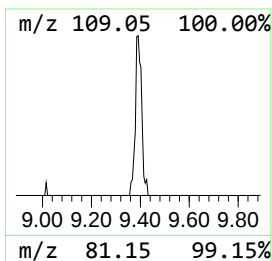
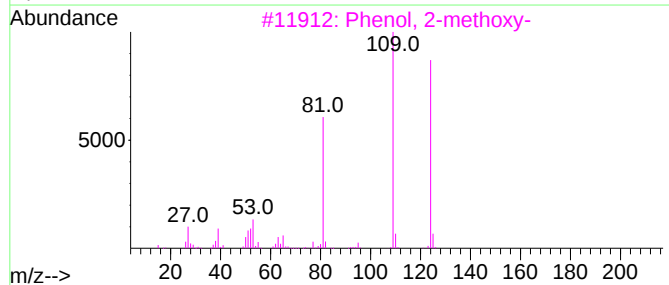
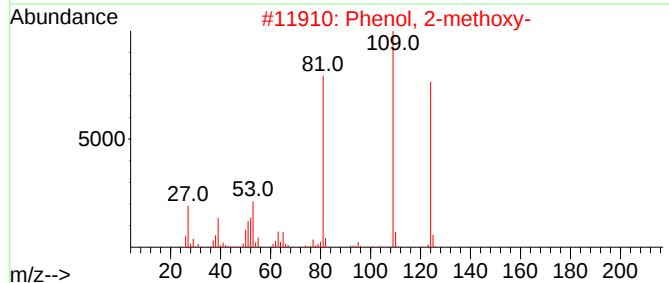
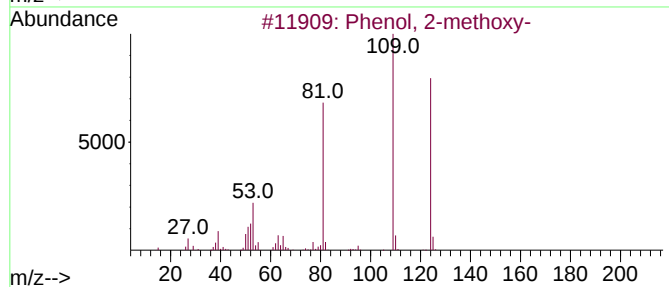
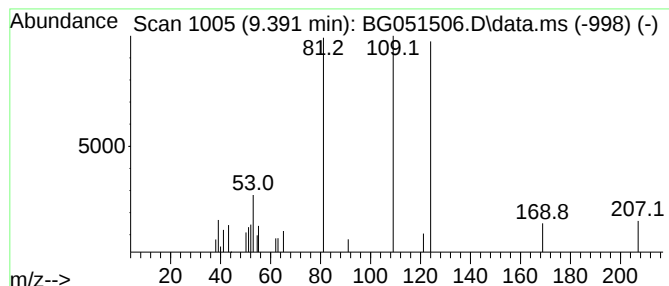
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Phenol, 2-methoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.391	2.11 ng/ul	18650	1,4-Dichlorobenzene-d4	8.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	80
2			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	80
3			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	72
4			Formic acid, 2-methoxyphenyl ester	152	C8H8O3	1000368-70-7	64
5			Mequinol	124	C7H8O2	000150-76-5	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121421\
Data File : BG051506.D
Acq On : 14 Dec 2021 16:39
Operator : CG/JU
Sample : M4960-03RX
Misc :
ALS Vial : 5 Sample Multiplier: 1

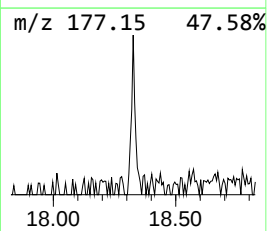
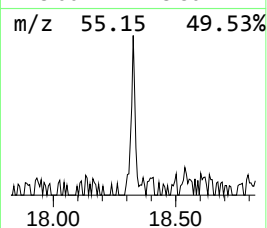
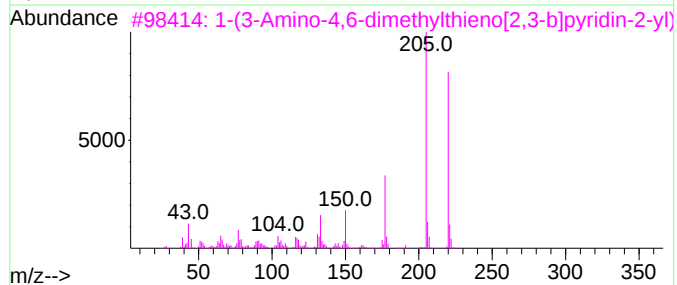
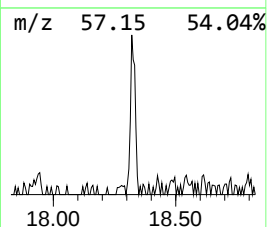
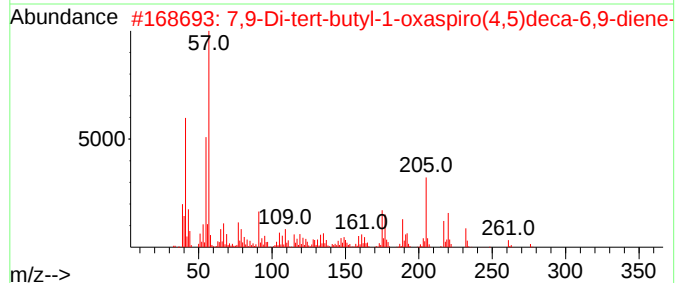
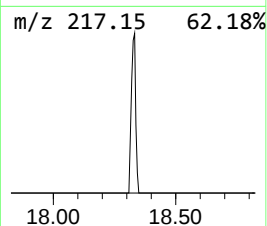
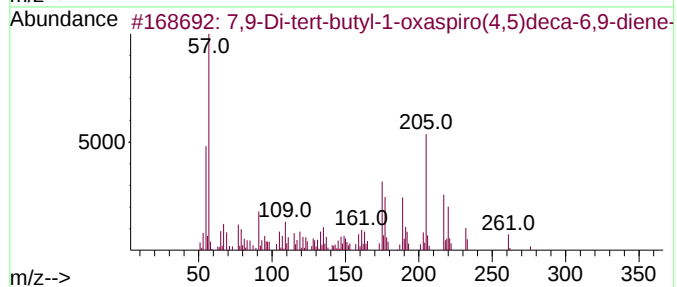
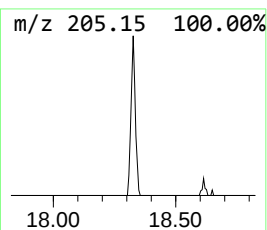
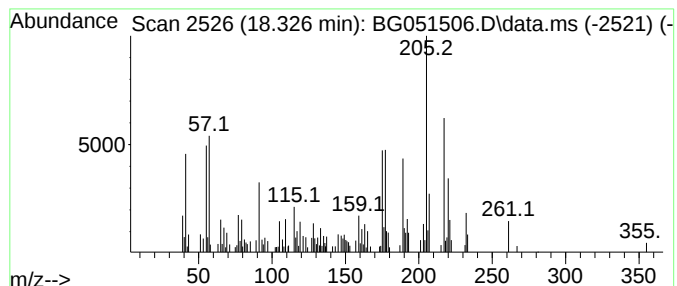
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.326	3.61 ng/ul	92567	Phenanthrene-d10	17.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	83		
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	49		
3	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	45		
4	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	43		
5	2,4-Diamino-6-nitroquinazoline	205	C8H7N5O2	007154-34-9	42		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121421\
Data File : BG051506.D
Acq On : 14 Dec 2021 16:39
Operator : CG/JU
Sample : M4960-03RX
Misc :
ALS Vial : 5 Sample Multiplier: 1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	8.345	2.2	ng/ul	19261	1	8.292	176849	20.0
Phenol, 2-methoxy-	9.391	2.1	ng/ul	18650	1	8.292	176849	20.0
7,9-Di-tert-but...	18.326	3.6	ng/ul	92567	4	17.668	512260	20.0