LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111524\
Data File : BG063469.D
Acq On : 16 Nov 2024 20:59
Operator : RC/JU
Sample : P4829-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : E29W6

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-BG110624.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BG063469.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.300	34	36	43	rVB	25886	41215	1.01%	0.111%
2	3.441	58	60	62	rBV3	6792	6001	0.15%	0.016%
3	3.711	102	106	118	rBV	73943	128422	3.16%	0.345%
4	4.017	156	158	160	rBV3	6068	5736	0.14%	0.015%
5	4.134	176	178	186	rVB6	5829	9868	0.24%	0.027%
6	4.316	207	209	213	rVB5	5446	6123	0.15%	0.016%
7	5.691	440	443	447	rBV4	5321	7621	0.19%	0.020%
8	6.402	560	564	569	rBV4	6633	8745	0.22%	0.024%
9	6.972	657	661	662	rBV2	7058	8867	0.22%	0.024%
10	7.007	662	667	677	rVB	112721	217930	5.36%	0.586%
11	7.166	688	694	703	rBV	294199	485030	11.93%	1.305%
12	7.366	723	728	739	rBV	357380	609048	14.98%	1.638%
13	7.830	801	807	813	rBV	305843	530767	13.06%	1.428%
14	7.894	814	818	827	rVB	75082	125377	3.08%	0.337%
15	8.541	921	928	939	rBV	362049	637808	15.69%	1.716%
16	8.652	942	947	953	rVB2	37378	66589	1.64%	0.179%
17	8.928	988	994	998	rBV2	40243	69606	1.71%	0.187%
18	8.987	998	1004	1013	rVB	399529	693100	17.05%	1.864%
19	9.169	1030	1035	1045	rBV6	38194	121997	3.00%	0.328%
20	9.410	1074	1076	1081	rVB4	10504	13567	0.33%	0.036%
21	9.710	1119	1127	1134	rBV	359263	663909	16.33%	1.786%
22	10.250	1212	1219	1230	rBV	546848	1005161	24.73%	2.704%
23	10.397	1241	1244	1249	rBV6	7117	12880	0.32%	0.035%
24	10.438	1249	1251	1254	rVB2	7169	7100	0.17%	0.019%
25	10.532	1263	1267	1274	rVB4	44179	74305	1.83%	0.200%
26	10.621	1274	1282	1289	rBV	482071	810792	19.95%	2.181%
27	10.668	1289	1290	1295	rVV5	10941	13686	0.34%	0.037%
28	10.756	1299	1305	1316	rVB	192785	377094	9.28%	1.014%
29	10.914	1329	1332	1334	rBV3	5152	6790	0.17%	0.018%
30	11.061	1353	1357	1358	rVB2	6789	7217	0.18%	0.019%
31	11.085	1358	1361	1365	rBV3	5039	7808	0.19%	0.021%
32	11.214	1380	1383	1386	rBV3	4355	6084	0.15%	0.016%
33	11.273	1389	1393	1398	rVB3	19653	36293	0.89%	0.098%
34	11.525	1434	1436	1440	rVB4	4352	5908	0.15%	0.016%
35	12.213	1547	1553	1557	rBV7	8466	17842	0.44%	0.048%
36	12.454	1592	1594	1599	rVB3	6207	9579	0.24%	0.026%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111524\
Data File : BG063469.D
Acq On : 16 Nov 2024 20:59
Operator : RC/JU
Sample : P4829-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E29W6

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-BG110624.MA.M
Title : SVOA CALIBRATION

37	12.524	1603	1606	1611	rVB3	3909	6154	0.15%	0.017%
38	12.665	1628	1630	1633	rBV4	4949	5690	0.14%	0.015%
39	12.824	1652	1657	1660	rBV6	9212	16998	0.42%	0.046%
40	12.918	1670	1673	1679	rVB7	8152	10563	0.26%	0.028%
41	12.983	1682	1684	1687	rBV4	4617	6428	0.16%	0.017%
42	13.071	1695	1699	1705	rBV6	11667	20353	0.50%	0.055%
43	13.229	1725	1726	1730	rVB2	6886	5881	0.14%	0.016%
44	13.265	1730	1732	1735	rBV4	5519	6114	0.15%	0.016%
45	13.312	1735	1740	1745	rVV2	69026	107847	2.65%	0.290%
46	13.359	1745	1748	1754	rVB5	13172	23902	0.59%	0.064%
47	13.876	1829	1836	1847	rVB	1203292	1676060	41.23%	4.508%
48	13.993	1853	1856	1857	rBV3	5948	6826	0.17%	0.018%
49	14.046	1863	1865	1867	rBV	7653	7036	0.17%	0.019%
50	14.163	1874	1885	1894	rBV	1137282	1825958	44.92%	4.911%
51	14.469	1927	1937	1946	rBV2	822618	1268048	31.20%	3.411%
52	14.551	1946	1951	1954	rVB5	5014	6796	0.17%	0.018%
53	14.698	1969	1976	1983	rBV4	78248	169346	4.17%	0.455%
54	15.145	2046	2052	2057	rBV4	15099	28346	0.70%	0.076%
55	15.280	2069	2075	2081	rVB5	31597	72457	1.78%	0.195%
56	15.462	2099	2106	2117	rVB	1654643	2589359	63.70%	6.965%
57	15.591	2122	2128	2138	rBV	529706	852193	20.97%	2.292%
58	15.691	2143	2145	2153	rVV7	11538	27634	0.68%	0.074%
59	15.779	2153	2160	2164	rVV	2344703	2992914	73.63%	8.050%
60	15.826	2164	2168	2177	rVV	221632	385523	9.48%	1.037%
61	15.891	2177	2179	2182	rVB3	6051	5987	0.15%	0.016%
62	16.085	2209	2212	2213	rVB3	7025	6639	0.16%	0.018%
63	16.819	2332	2337	2340	rBV2	12460	17024	0.42%	0.046%
64	16.901	2345	2351	2357	rBV7	10792	24938	0.61%	0.067%
65	17.136	2388	2391	2394	rVB4	4374	5709	0.14%	0.015%
66	17.219	2394	2405	2415	rBV	1104021	1676343	41.24%	4.509%
67	17.319	2415	2422	2429	rBV2	2069785	3216245	79.13%	8.651%
68	17.507	2450	2454	2458	rVB	23793	29675	0.73%	0.080%
69	17.889	2513	2519	2528	rVB	252497	346932	8.54%	0.933%
70	18.018	2538	2541	2545	rVB6	7511	9593	0.24%	0.026%
71	18.065	2547	2549	2552	rVB3	6050	6441	0.16%	0.017%
72	18.124	2557	2559	2564	rBV6	7599	12202	0.30%	0.033%
73	18.188	2564	2570	2574	rBV3	124846	183451	4.51%	0.493%
74	18.276	2583	2585	2588	rBV4	5287	7260	0.18%	0.020%
75	18.370	2599	2601	2604	rVB3	14680	14929	0.37%	0.040%
76	18.406	2604	2607	2609	rBV3	8769	11934	0.29%	0.032%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111524\
Data File : BG063469.D
Acq On : 16 Nov 2024 20:59
Operator : RC/JU
Sample : P4829-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E29W6

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-BG110624.MA.M
Title : SVOA CALIBRATION

77	18.423	2609	2610	2615	rVB5	13401	9907	0.24%	0.027%
78	18.646	2644	2648	2654	rVB8	14780	21927	0.54%	0.059%
79	18.699	2654	2657	2660	rBV4	9437	13283	0.33%	0.036%
80	18.876	2684	2687	2689	rBV4	7025	9813	0.24%	0.026%
81	18.970	2701	2703	2707	rVB4	12167	16458	0.40%	0.044%
82	19.022	2710	2712	2714	rBV3	6783	7088	0.17%	0.019%
83	19.181	2735	2739	2746	rBV4	40866	62734	1.54%	0.169%
84	19.252	2746	2751	2755	rBV	36120	54419	1.34%	0.146%
85	19.622	2807	2814	2829	rBV	2942923	4064664	100.00%	10.933%
86	19.851	2851	2853	2859	rBV6	15908	21384	0.53%	0.058%
87	20.092	2892	2894	2895	rBV2	10434	7036	0.17%	0.019%
88	21.478	3123	3130	3139	rBV2	1225491	1956390	48.13%	5.262%
89	22.589	3314	3319	3327	rBV2	227430	381106	9.38%	1.025%
90	24.305	3601	3611	3624	rVB	1533880	3922836	96.51%	10.551%
91	24.510	3637	3646	3659	rVB	778365	2080251	51.18%	5.595%

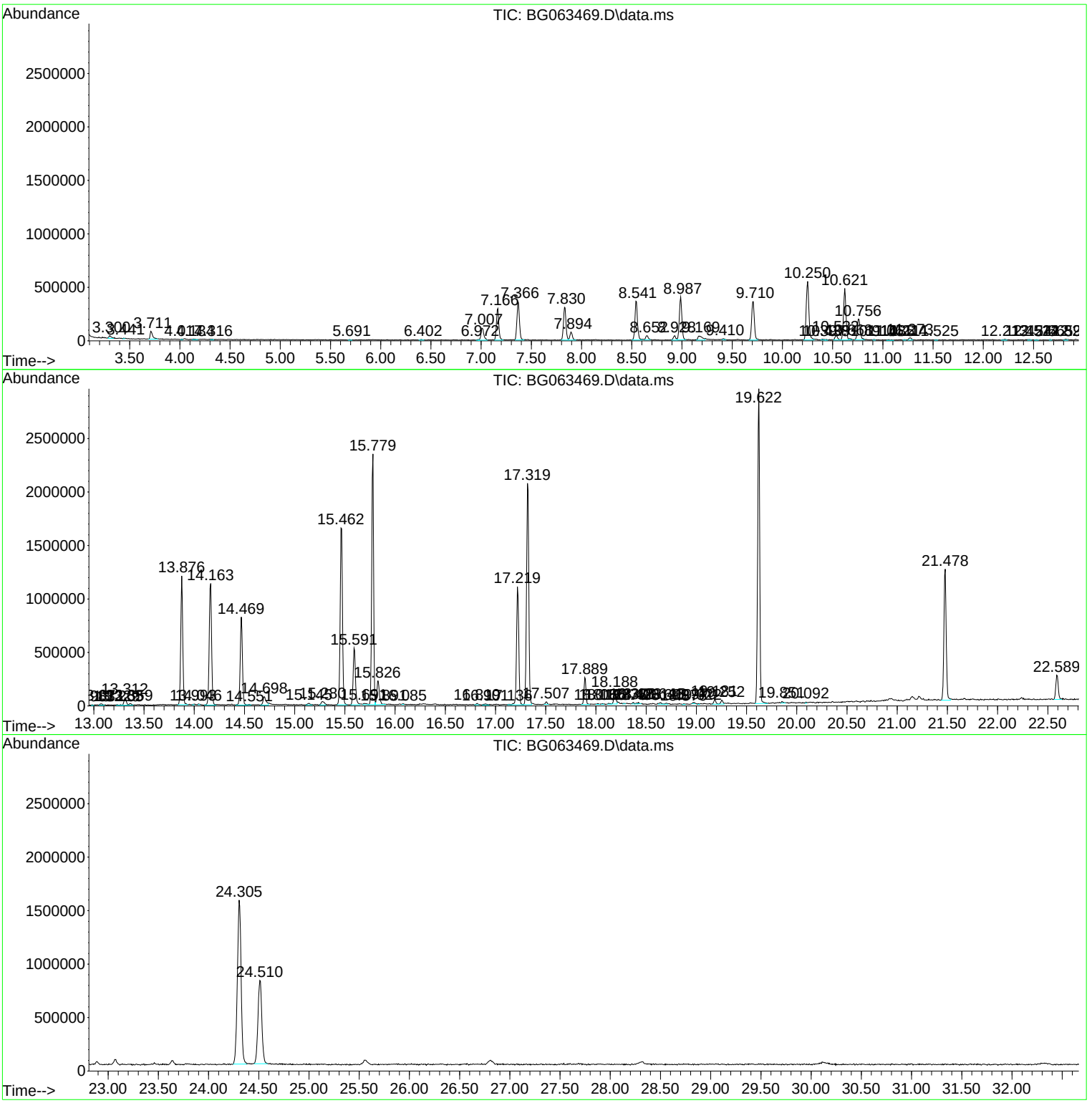
Sum of corrected areas: 37178889

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111524\
Data File : BG063469.D
Acq On : 16 Nov 2024 20:59
Operator : RC/JU
Sample : P4829-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E29W6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110624.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111524\
Data File : BG063469.D
Acq On : 16 Nov 2024 20:59
Operator : RC/JU
Sample : P4829-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E29W6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110624.MA.M
Quant Title : SVOA CALIBRATION

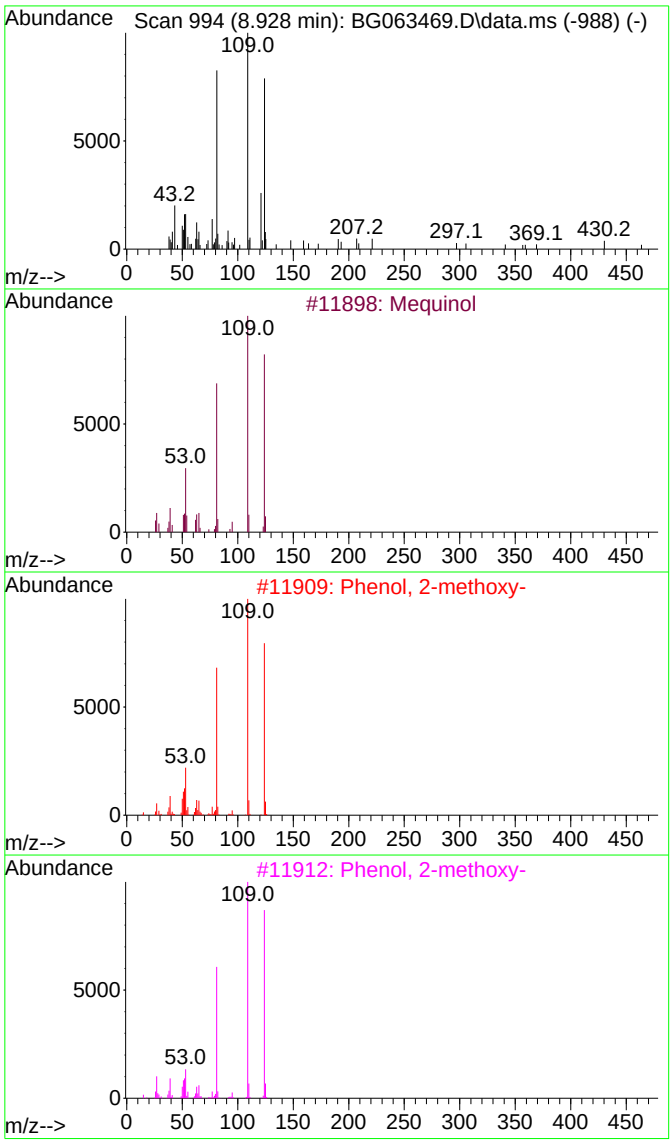
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

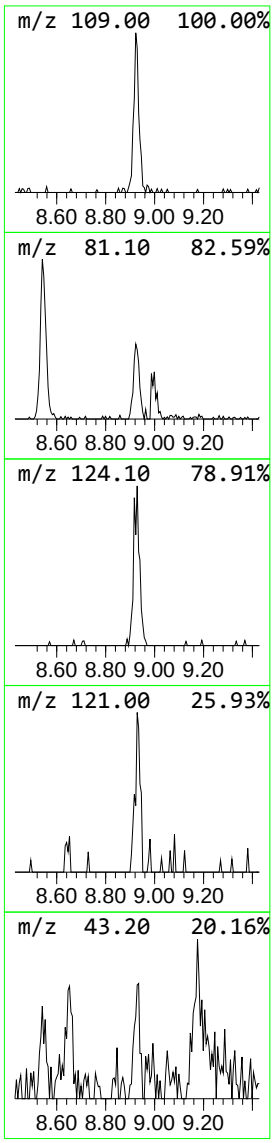
****

Peak Number 2 Mequinol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.928	2.62 ng/ul	69606	1,4-Dichlorobenzene-d4	7.830

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mequinol	124	C7H8O2	000150-76-5	86
2	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	86
3	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	78
4	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	78
5	Mequinol	124	C7H8O2	000150-76-5	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111524\
Data File : BG063469.D
Acq On : 16 Nov 2024 20:59
Operator : RC/JU
Sample : P4829-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E29W6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110624.MA.M
Quant Title : SVOA CALIBRATION

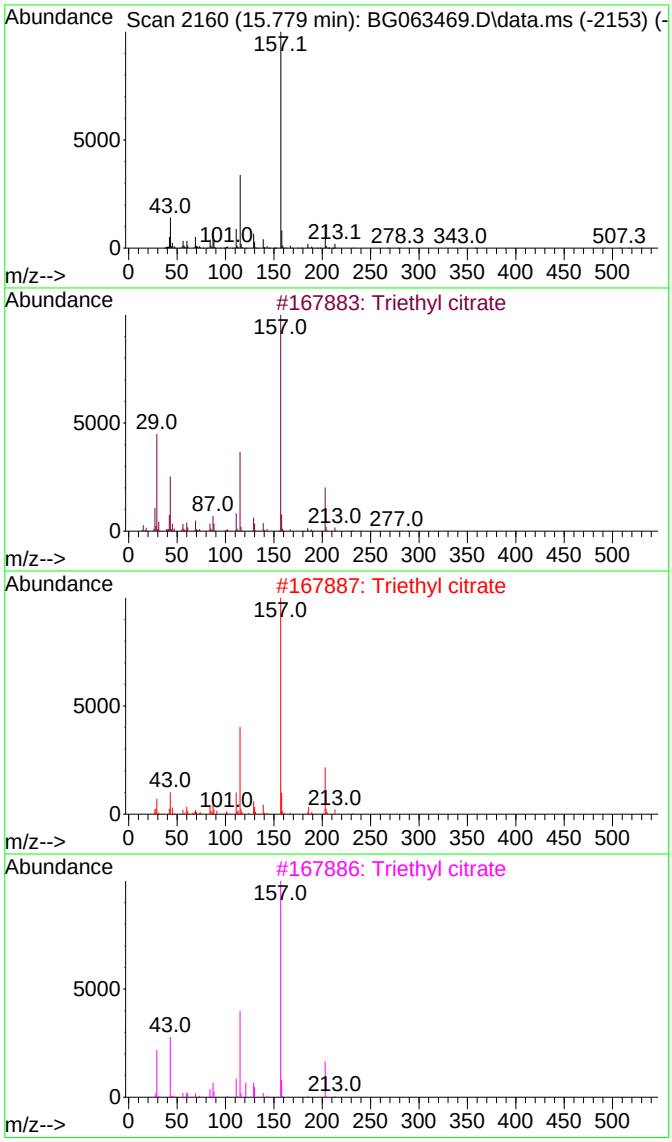
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

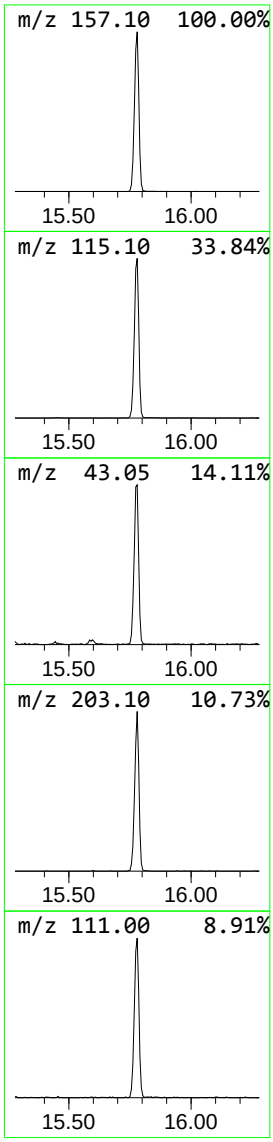
****

Peak Number 4 Triethyl citrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.779	47.21 ng/ul	2992910	Acenaphthene-d10	14.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	87
2	Triethyl citrate	276	C12H20O7	000077-93-0	64
3	Triethyl citrate	276	C12H20O7	000077-93-0	59
4	Triethyl citrate	276	C12H20O7	000077-93-0	58
5	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111524\
Data File : BG063469.D
Acq On : 16 Nov 2024 20:59
Operator : RC/JU
Sample : P4829-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E29W6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110624.MA.M
Quant Title : SVOA CALIBRATION

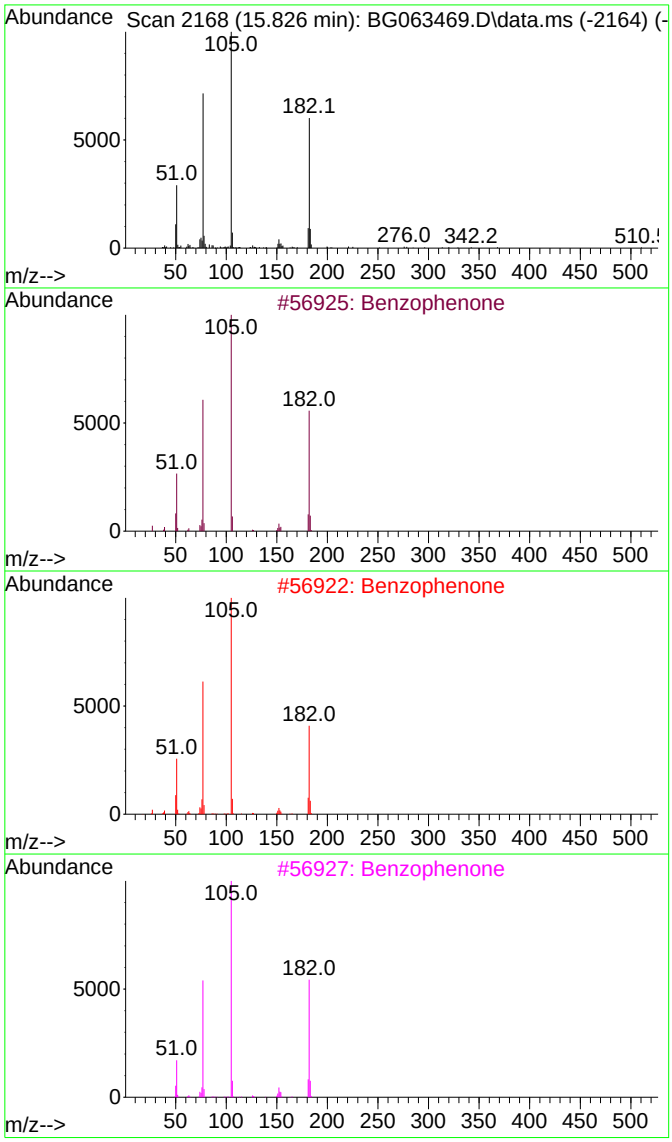
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

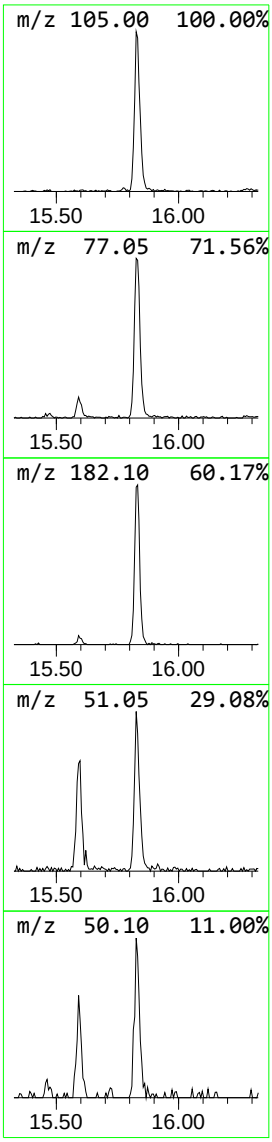
****

Peak Number 5 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.826	6.08 ng/ul	385523	Acenaphthene-d10	14.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	94
2	Benzophenone	182	C13H10O	000119-61-9	94
3	Benzophenone	182	C13H10O	000119-61-9	91
4	Benzophenone	182	C13H10O	000119-61-9	90
5	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111524\
Data File : BG063469.D
Acq On : 16 Nov 2024 20:59
Operator : RC/JU
Sample : P4829-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E29W6

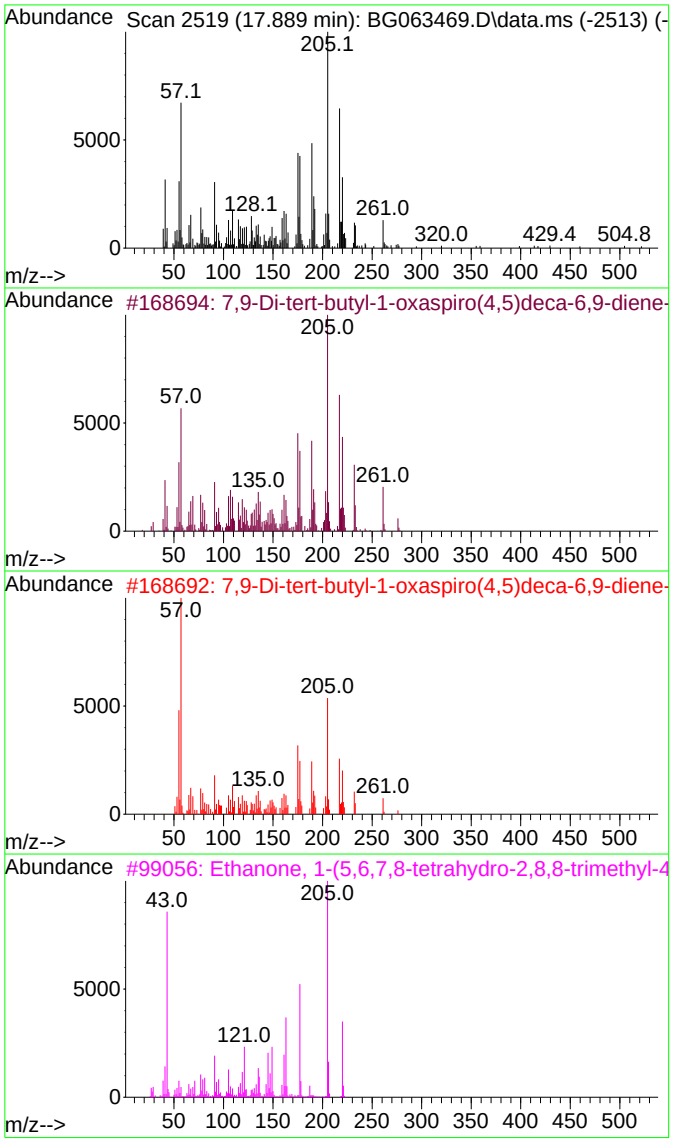
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110624.MA.M
Quant Title : SVOA CALIBRATION

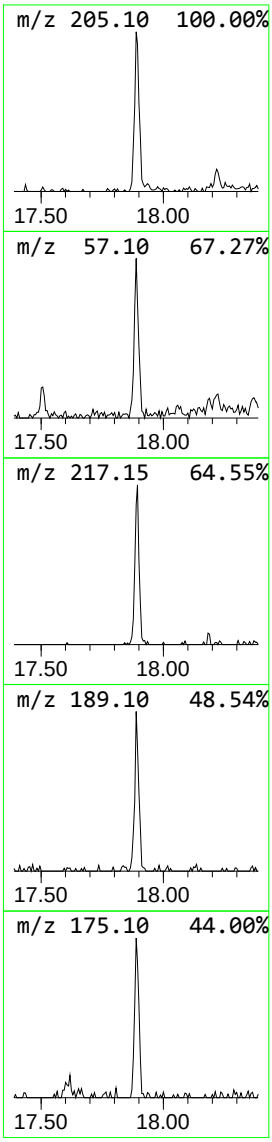
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.889	4.14 ng/ul	346932	Phenanthrene-d10	17.219

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	90
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	64
3	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	46
4	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	43
5	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111524\
Data File : BG063469.D
Acq On : 16 Nov 2024 20:59
Operator : RC/JU
Sample : P4829-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E29W6

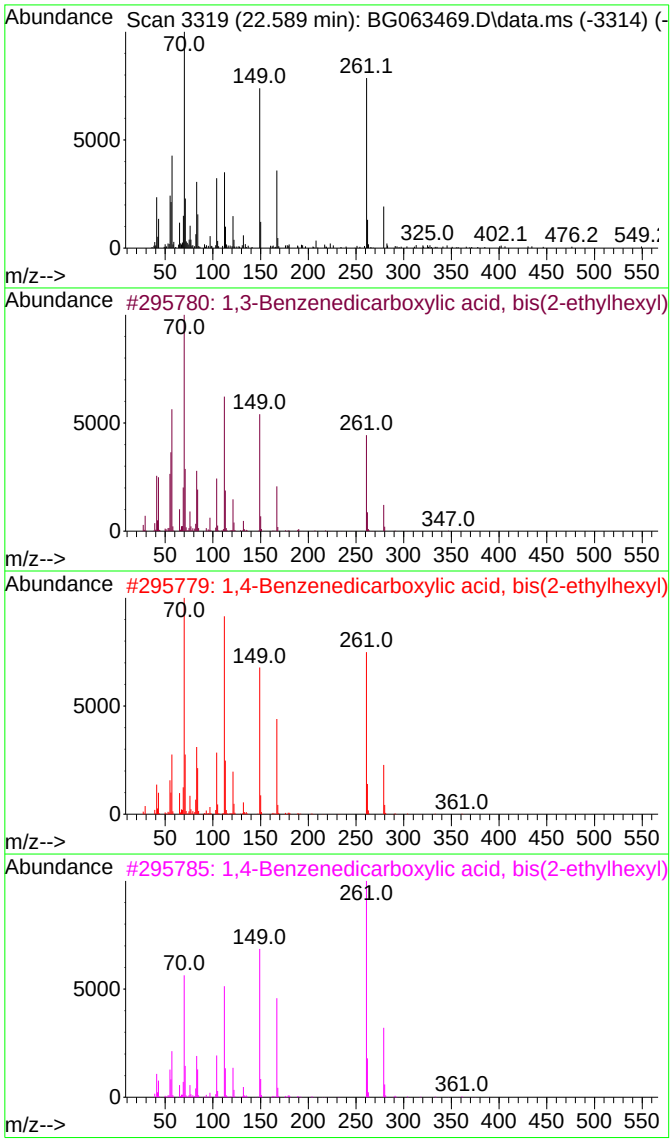
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110624.MA.M
Quant Title : SVOA CALIBRATION

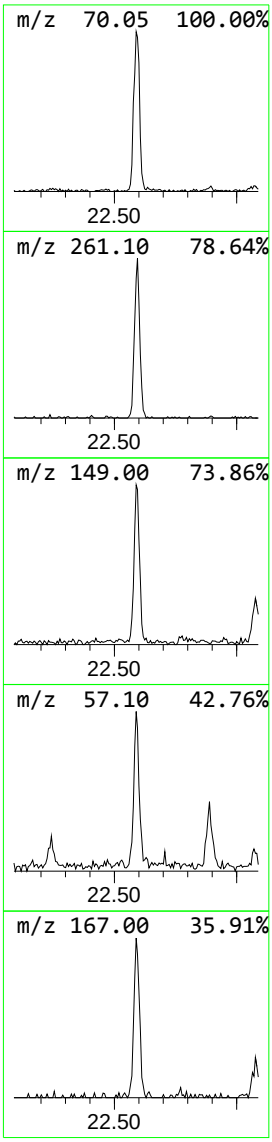
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1,3-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.589	3.90 ng/ul	381106	Chrysene-d12	21.478

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	86
2	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	86
3	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	58
4	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	52
5	Terephthalic acid, 2-methylthiop...	400	C23H28O4S	1000382-96-9	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111524\
Data File : BG063469.D
Acq On : 16 Nov 2024 20:59
Operator : RC/JU
Sample : P4829-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E29W6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110624.MA.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
Mequinol	8.928	2.6	ng/ul	69606	1	7.830	530767	20.0
Triethyl citrate	15.779	47.2	ng/ul	2992910	3	14.469	1268050	20.0
Benzophenone	15.826	6.1	ng/ul	385523	3	14.469	1268050	20.0
7,9-Di-tert-but...	17.889	4.1	ng/ul	346932	4	17.219	1676340	20.0
1,3-Benzenedica...	22.589	3.9	ng/ul	381106	5	21.478	1956390	20.0