LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062824\
Data File : BG061799.D
Acq On : 29 Jun 2024 9:55
Operator : MA/JU
Sample : P2897-19
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0T67

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-BG062024.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BG061799.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.455	23	28	32	rBV3	17700	28846	1.49%	0.114%
2	3.596	48	52	53	rBV4	4087	4996	0.26%	0.020%
3	3.725	69	74	83	rBV	31446	56524	2.92%	0.224%
4	3.872	96	99	113	rBV	217302	399789	20.64%	1.586%
5	4.213	153	157	161	rVV3	6291	8880	0.46%	0.035%
6	4.718	240	243	246	rBV4	3375	3935	0.20%	0.016%
7	5.135	311	314	317	rVV3	9117	12905	0.67%	0.051%
8	5.347	348	350	352	rBV2	3283	3773	0.19%	0.015%
9	5.517	376	379	382	rBV3	3278	3503	0.18%	0.014%
10	5.781	421	424	427	rBV	3940	4965	0.26%	0.020%
11	6.110	475	480	486	rBV2	13254	23971	1.24%	0.095%
12	6.157	486	488	491	rVV2	3084	3615	0.19%	0.014%
13	6.328	514	517	520	rVB3	3735	4234	0.22%	0.017%
14	6.880	606	611	614	rBV2	2635	4676	0.24%	0.019%
15	7.027	632	636	637	rBV2	2665	4227	0.22%	0.017%
16	7.156	652	658	659	rBV4	2647	3725	0.19%	0.015%
17	7.203	659	666	675	rVV	379725	633746	32.71%	2.514%
18	7.380	689	696	704	rBV	249620	409539	21.14%	1.625%
19	7.521	716	720	723	rBV6	2790	4133	0.21%	0.016%
20	7.585	723	731	737	rBV	331737	571951	29.52%	2.269%
21	7.638	737	740	743	rVV2	9287	10231	0.53%	0.041%
22	7.732	752	756	758	rBV2	3267	3637	0.19%	0.014%
23	8.055	803	811	818	rBV	298631	510332	26.34%	2.024%
24	8.102	818	819	825	rVB4	7847	9961	0.51%	0.040%
25	8.748	923	929	938	rVB2	425916	744172	38.41%	2.952%
26	9.066	978	983	985	rBV2	2400	3690	0.19%	0.015%
27	9.219	1000	1009	1018	rVB	345913	608967	31.43%	2.416%
28	9.371	1031	1035	1039	rBV5	5038	7362	0.38%	0.029%
29	9.771	1096	1103	1109	rBV2	37776	66404	3.43%	0.263%
30	9.941	1125	1132	1142	rVB2	297558	528225	27.26%	2.095%
31	10.482	1217	1224	1231	rVB	432194	767567	39.62%	3.045%
32	10.617	1244	1247	1250	rBV3	3346	4152	0.21%	0.016%
33	10.864	1281	1289	1298	rBV	442618	802594	41.43%	3.184%
34	10.946	1300	1303	1305	rBV	4073	4179	0.22%	0.017%
35	10.999	1305	1312	1319	rBV	426777	774354	39.97%	3.072%
36	11.387	1373	1378	1383	rBV4	19838	29645	1.53%	0.118%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062824\
Data File : BG061799.D
Acq On : 29 Jun 2024 9:55
Operator : MA/JU
Sample : P2897-19
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0T67

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-BG062024.MA.M
Title : SVOA CALIBRATION

37	11.598	1407	1414	1425	rBV3	47092	97324	5.02%	0.386%
38	12.121	1500	1503	1508	rBV4	2244	3841	0.20%	0.015%
39	12.233	1520	1522	1526	rVB2	2969	4169	0.22%	0.017%
40	12.333	1537	1539	1542	rVB4	4947	4406	0.23%	0.017%
41	12.362	1542	1544	1547	rBV	2866	3903	0.20%	0.015%
42	12.438	1553	1557	1558	rBV2	5871	7837	0.40%	0.031%
43	12.450	1558	1559	1564	rVV2	8609	6838	0.35%	0.027%
44	12.579	1577	1581	1582	rBV2	3902	4538	0.23%	0.018%
45	12.650	1589	1593	1595	rBV2	2964	3686	0.19%	0.015%
46	12.797	1613	1618	1620	rVB2	3497	3465	0.18%	0.014%
47	12.908	1633	1637	1638	rVB2	3171	3512	0.18%	0.014%
48	13.173	1681	1682	1687	rVB4	3156	3719	0.19%	0.015%
49	13.649	1759	1763	1766	rBV3	3103	4299	0.22%	0.017%
50	13.801	1787	1789	1791	rVB2	3722	3437	0.18%	0.014%
51	13.825	1791	1793	1795	rBV2	3993	4012	0.21%	0.016%
52	13.860	1795	1799	1803	rVV3	6390	7826	0.40%	0.031%
53	13.925	1805	1810	1817	rVB2	54753	85687	4.42%	0.340%
54	14.089	1832	1838	1844	rBV	774010	1099033	56.73%	4.360%
55	14.383	1880	1888	1895	rVB	813177	1330865	68.69%	5.279%
56	14.571	1918	1920	1923	rVB3	5781	4038	0.21%	0.016%
57	14.683	1932	1939	1948	rBV	700948	1081979	55.85%	4.292%
58	14.741	1948	1949	1954	rVB4	5460	6777	0.35%	0.027%
59	14.818	1957	1962	1964	rBV2	19782	28791	1.49%	0.114%
60	14.865	1964	1970	1975	rBV	392330	628381	32.43%	2.493%
61	14.929	1975	1981	1996	rVB	940627	1533344	79.14%	6.082%
62	15.458	2067	2071	2072	rBV3	4790	6902	0.36%	0.027%
63	15.523	2077	2082	2085	rBV4	19276	28100	1.45%	0.111%
64	15.676	2097	2108	2115	rBV	1095681	1694655	87.47%	6.722%
65	15.781	2120	2126	2132	rBV2	235974	352640	18.20%	1.399%
66	15.917	2146	2149	2150	rBV3	4128	4236	0.22%	0.017%
67	15.975	2156	2159	2160	rBV	3270	3905	0.20%	0.015%
68	16.028	2166	2168	2173	rVB5	4544	6150	0.32%	0.024%
69	16.210	2196	2199	2200	rBV3	3814	4011	0.21%	0.016%
70	16.310	2210	2216	2223	rBV4	38012	60246	3.11%	0.239%
71	16.528	2250	2253	2254	rBV	5205	5926	0.31%	0.024%
72	16.557	2257	2258	2261	rBV2	4009	4453	0.23%	0.018%
73	16.722	2284	2286	2290	rVB5	4689	4834	0.25%	0.019%
74	17.015	2335	2336	2338	rBV2	4983	3922	0.20%	0.016%
75	17.074	2344	2346	2349	rBV3	4518	4728	0.24%	0.019%
76	17.168	2360	2362	2365	rVB4	8658	8727	0.45%	0.035%

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Operator : MA/JU
Sample : P2897-19
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0T67

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

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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Title : SVOA CALIBRATION

77	17.197	2365	2367	2368	rBV2	4946	3513	0.18%	0.014%
78	17.338	2387	2391	2396	rVB4	6846	9953	0.51%	0.039%
79	17.427	2400	2406	2412	rBV	880210	1329515	68.62%	5.274%
80	17.526	2417	2423	2433	rVB	1194487	1749686	90.31%	6.941%
81	17.603	2433	2436	2440	rVB5	13440	19948	1.03%	0.079%
82	17.662	2442	2446	2450	rBV7	12749	22081	1.14%	0.088%
83	17.779	2464	2466	2468	rBV3	6154	6299	0.33%	0.025%
84	17.955	2494	2496	2498	rVB3	5598	3575	0.18%	0.014%
85	18.090	2515	2519	2525	rVB7	12280	21592	1.11%	0.086%
86	18.308	2552	2556	2561	rBV3	48475	75528	3.90%	0.300%
87	18.490	2583	2587	2590	rBV5	9585	15699	0.81%	0.062%
88	18.649	2611	2614	2618	rVB5	9658	13318	0.69%	0.053%
89	18.796	2636	2639	2642	rBV5	6342	8187	0.42%	0.032%
90	19.330	2728	2730	2732	rVB2	6741	4922	0.25%	0.020%
91	19.354	2732	2734	2735	rBV2	6783	4950	0.26%	0.020%
92	19.377	2735	2738	2743	rVB6	17172	27387	1.41%	0.109%
93	19.442	2747	2749	2752	rVV2	17706	18653	0.96%	0.074%
94	19.471	2752	2754	2756	rVB2	12243	11578	0.60%	0.046%
95	19.806	2805	2811	2821	rBV	1321133	1937395	100.00%	7.685%
96	21.334	3067	3071	3079	rBV2	176145	278090	14.35%	1.103%
97	21.686	3125	3131	3138	rVB2	764726	1232406	63.61%	4.889%
98	21.892	3162	3166	3173	rBV4	31980	51707	2.67%	0.205%
99	24.683	3632	3641	3653	rVB2	672602	1833511	94.64%	7.273%
100	24.900	3670	3678	3687	rBV2	473899	1303445	67.28%	5.170%

Sum of corrected areas: 25209485

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062824\
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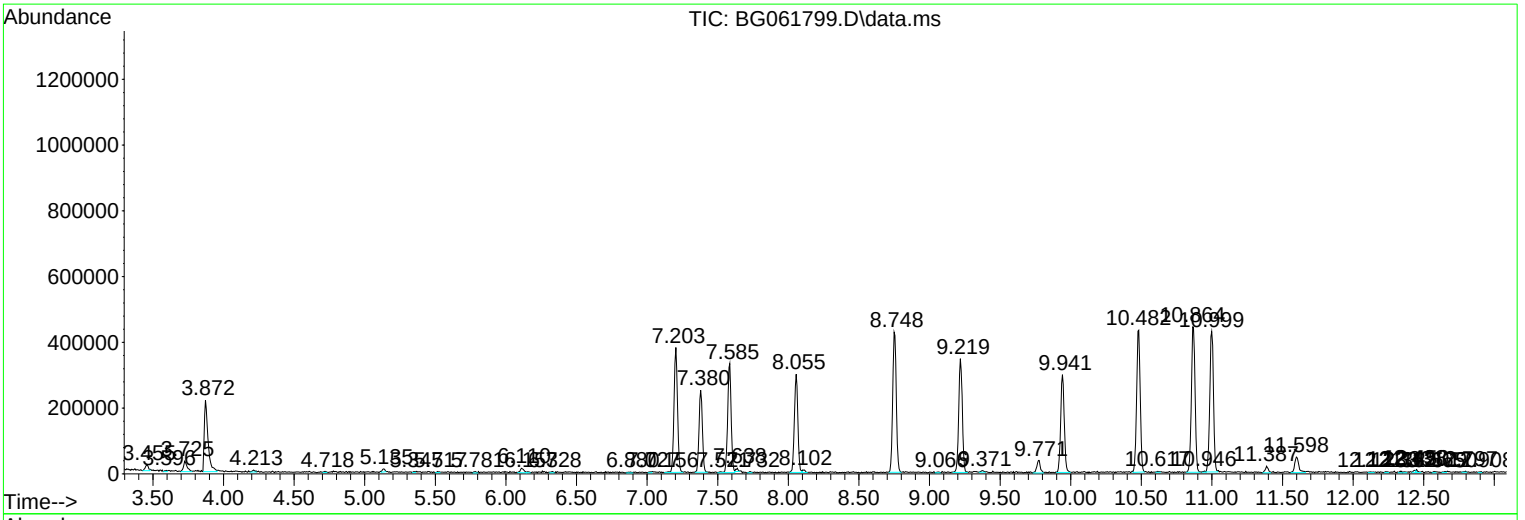
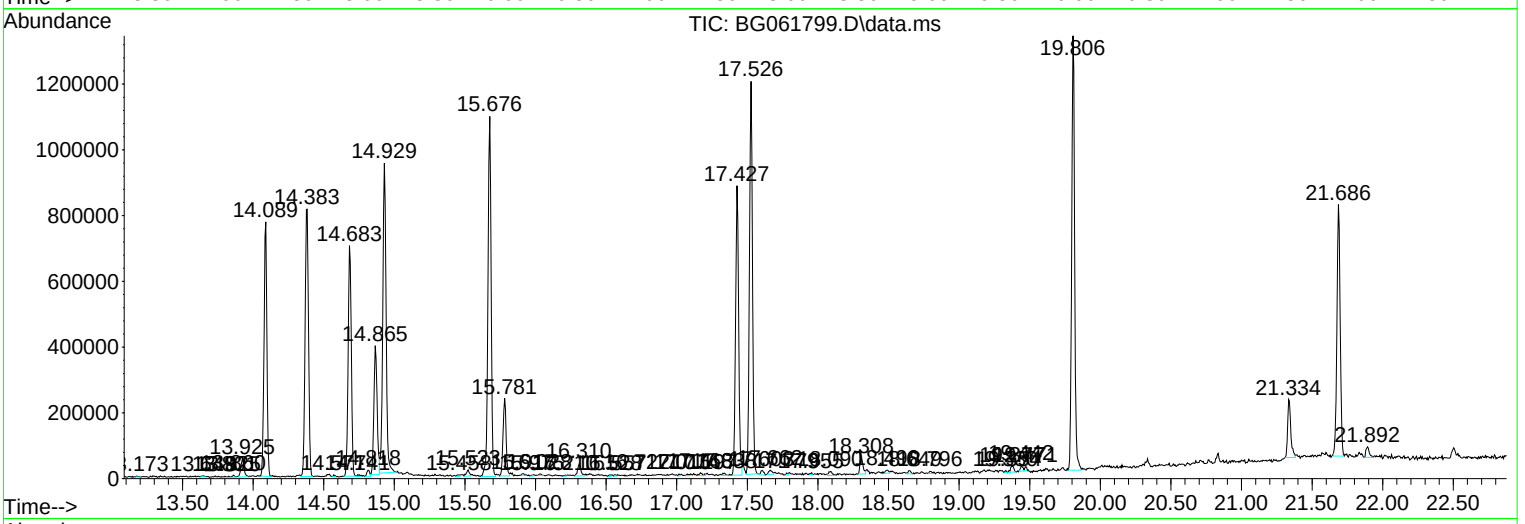
Sample : P2897-19
Misc :
ALS Vial : 28 Sample Multiplier: 1

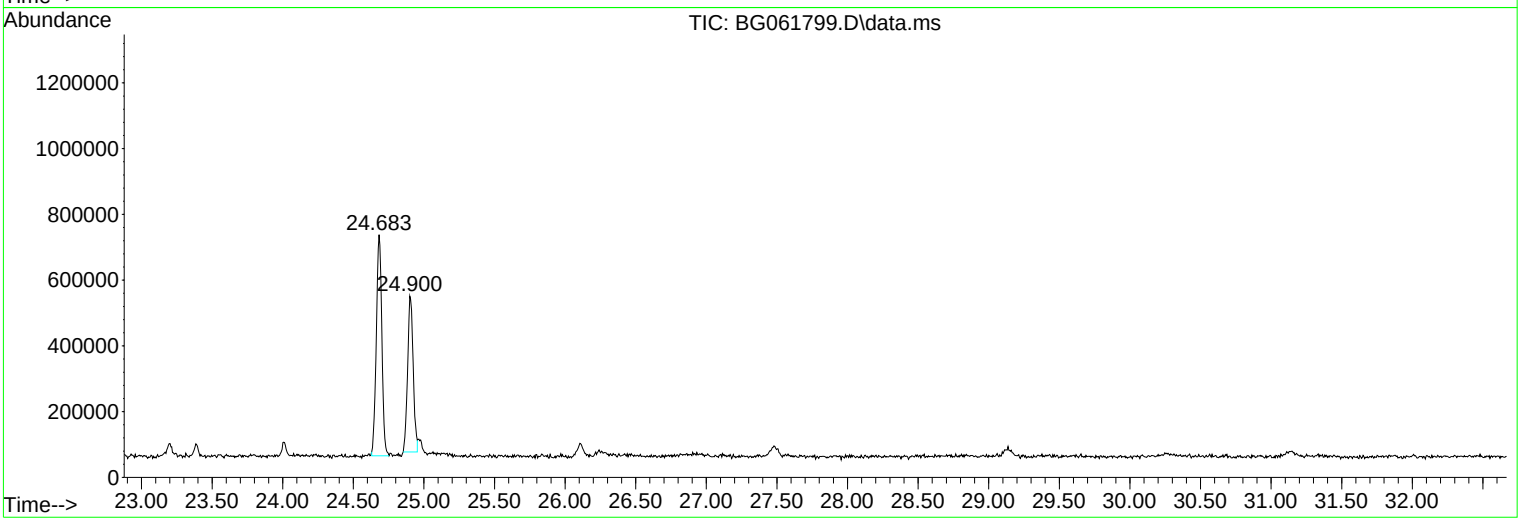
Instrument :
BNA_G
ClientSampleId :
C0T67

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

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







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Data File : BG061799.D
Acq On : 29 Jun 2024 9:55
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Instrument :
BNA_G
ClientSampleId :
C0T67

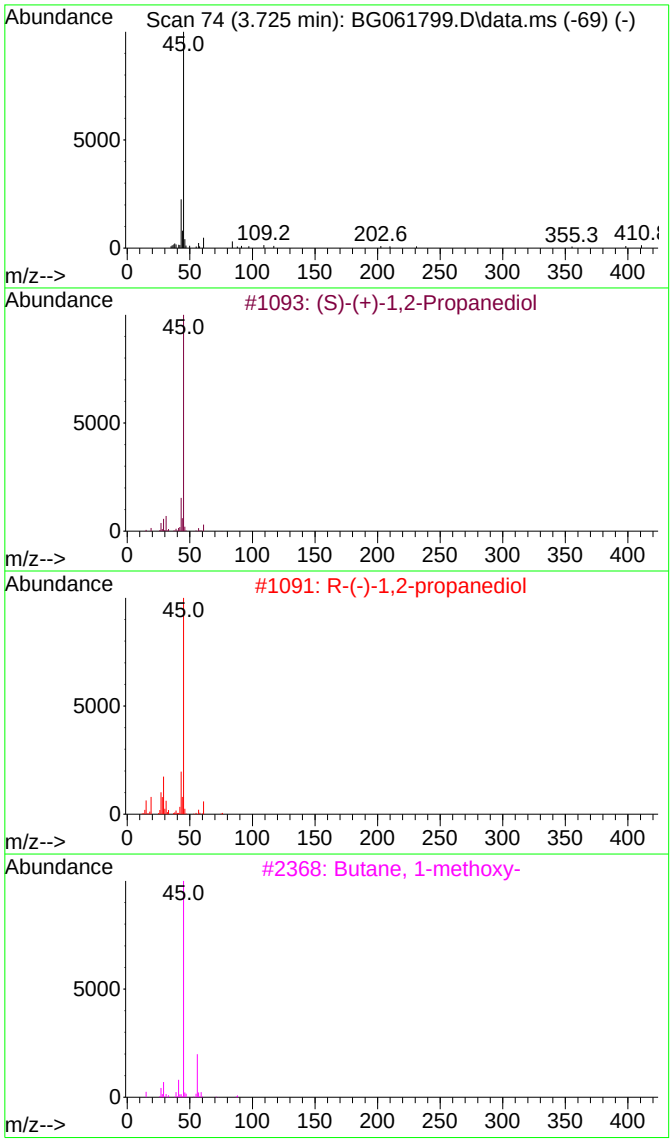
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

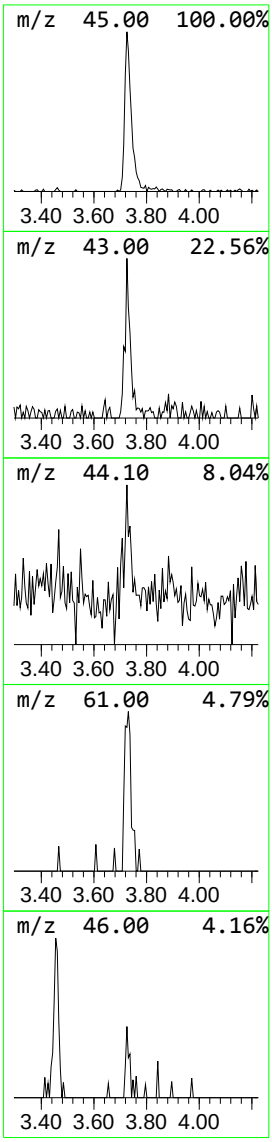
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.725	2.22 ng/ul	56524	1,4-Dichlorobenzene-d4	8.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	39
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	39
3	Butane, 1-methoxy-	88	C5H12O	000628-28-4	9
4	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	9
5	2,2-Dichloroethyl methyl ether	128	C3H6Cl2O	034862-07-2	9





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Instrument :
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ClientSampleId :
C0T67

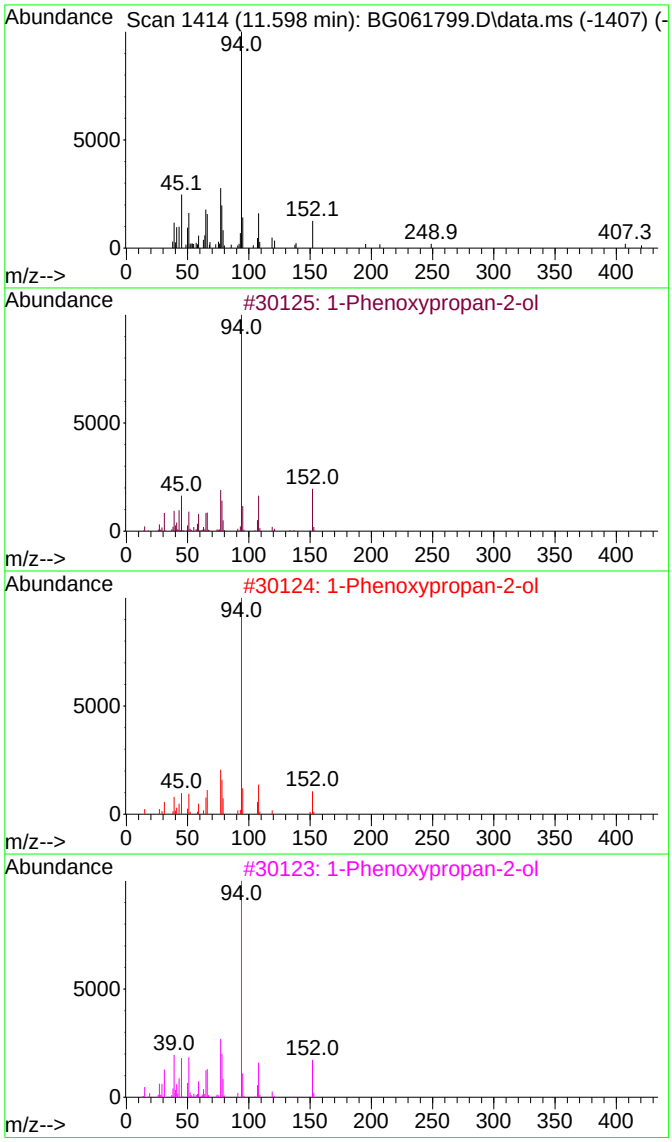
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

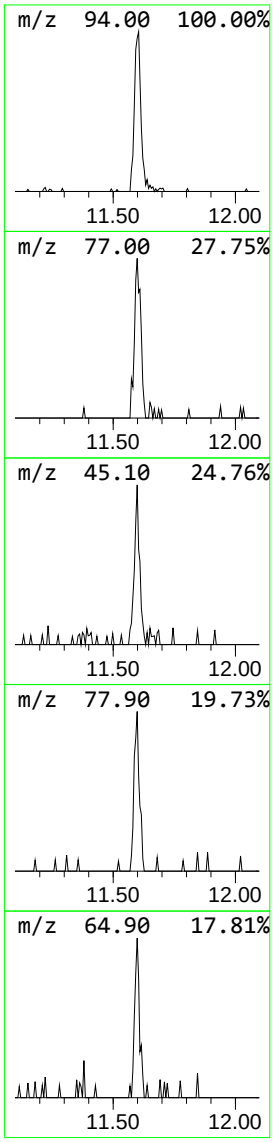
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.598	2.43 ng/ul	97324	Naphthalene-d8	10.870

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	91
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	91
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	90
4	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	72
5	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	58





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Sample : P2897-19
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ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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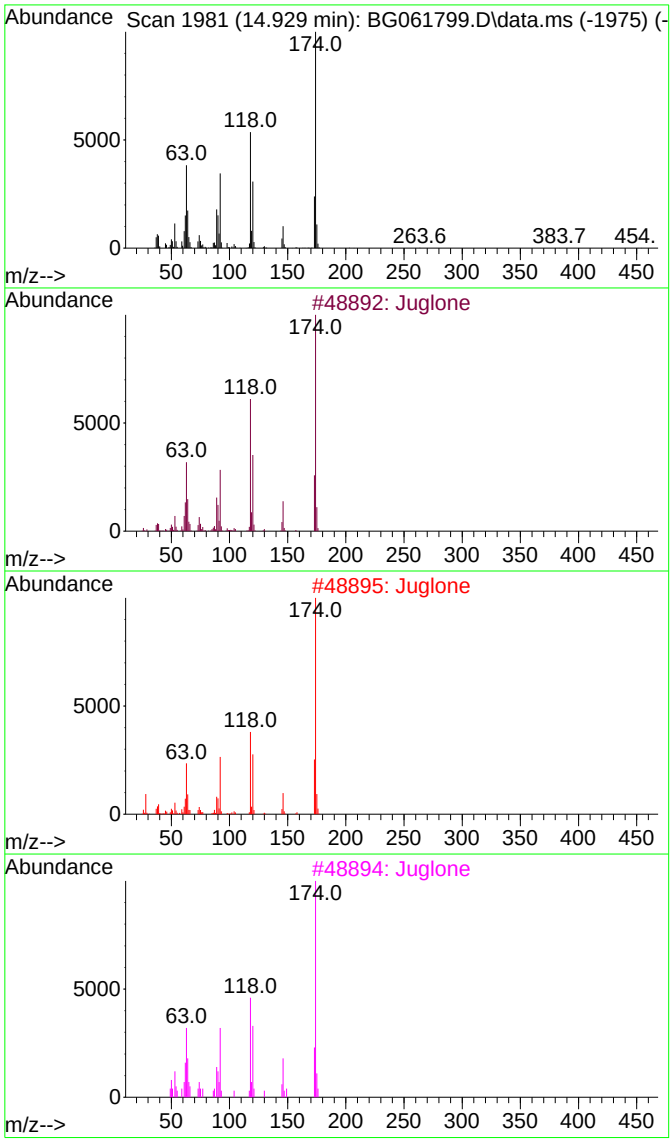
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

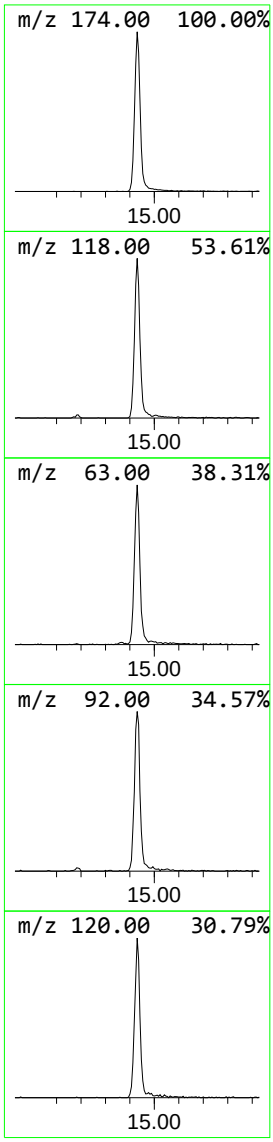
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Juglone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	28.34 ng/ul	1533340	Acenaphthene-d10	14.683

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Juglone	174	C10H6O3	000481-39-0	97
2	Juglone	174	C10H6O3	000481-39-0	97
3	Juglone	174	C10H6O3	000481-39-0	94
4	Juglone	174	C10H6O3	000481-39-0	94
5	2,3-Dihydro-4-methyl-1H-1,5-benz...	174	C10H10N2O	006276-48-8	49





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Data File : BG061799.D
Acq On : 29 Jun 2024 9:55
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Sample : P2897-19
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0T67

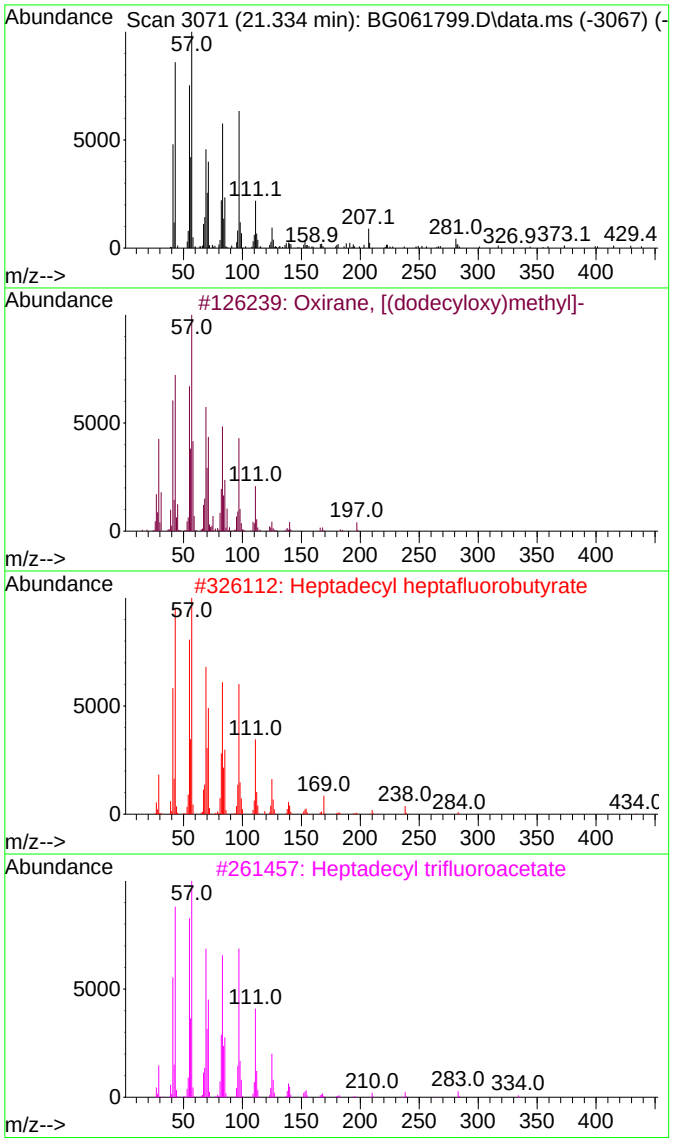
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

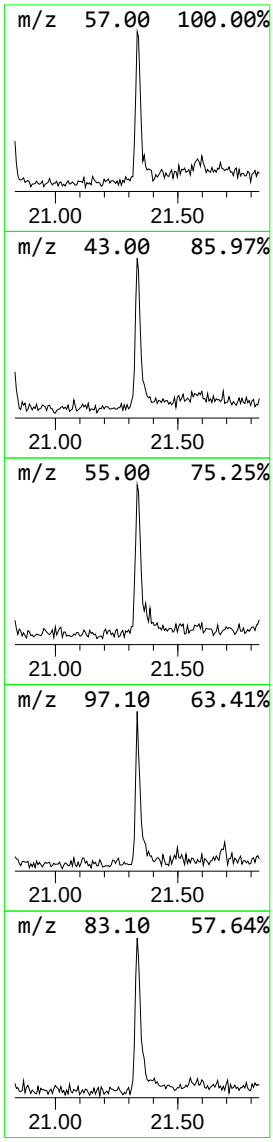
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Oxirane, [(dodecyloxy)methyl]- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.334	4.51 ng/ul	278090	Chrysene-d12	21.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	74
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	70
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	60
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	58
5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062824\
Data File : BG061799.D
Acq On : 29 Jun 2024 9:55
Operator : MA/JU
Sample : P2897-19
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.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
unknown-01	3.725	2.2	ng/ul	56524	1	8.055	510332	20.0
1-Phenoxypropan...	11.598	2.4	ng/ul	97324	2	10.870	802594	20.0
Juglone	14.930	28.3	ng/ul	1533340	3	14.683	1081980	20.0
Oxirane, [(dode...	21.334	4.5	ng/ul	278090	5	21.686	1232410	20.0