LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082621\
Data File : BG050013.D
Acq On : 28 Aug 2021 1:53
Operator : CG/JU
Sample : M3518-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0B42

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-BG081921.M
Title : SVOA CALIBRATION

Signal : TIC: BG050014.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.334	45	50	54	rVB5	5725	9887	1.18%	0.105%
2	3.410	61	63	64	rBV	2964	1680	0.20%	0.018%
3	3.628	98	100	105	rBV3	2978	3885	0.46%	0.041%
4	3.774	122	125	128	rBV3	9152	13982	1.66%	0.148%
5	4.092	175	179	180	rBV3	1453	2261	0.27%	0.024%
6	4.321	214	218	225	rBV3	12352	19027	2.26%	0.201%
7	4.744	287	290	294	rVB4	6521	8844	1.05%	0.094%
8	4.791	297	298	303	rVB3	1113	1361	0.16%	0.014%
9	4.855	306	309	311	rBV2	1071	1356	0.16%	0.014%
10	5.173	360	363	366	rBV4	1224	1535	0.18%	0.016%
11	6.535	593	595	600	rVB3	1799	1901	0.23%	0.020%
12	7.023	676	678	681	rBV	1351	1750	0.21%	0.019%
13	7.135	690	697	711	rVB	134842	240650	28.60%	2.547%
14	7.287	717	723	735	rVB	85229	153689	18.27%	1.626%
15	7.499	752	759	766	rBV	130326	227392	27.03%	2.406%
16	7.569	769	771	773	rBV2	1576	1587	0.19%	0.017%
17	7.963	831	838	846	rBV	102911	174856	20.78%	1.850%
18	8.198	874	878	879	rBV	1153	1324	0.16%	0.014%
19	8.685	954	961	969	rBV	169971	297953	35.41%	3.153%
20	9.138	1031	1038	1049	rVB	133735	233300	27.73%	2.469%
21	9.314	1065	1068	1070	rVB	1424	1583	0.19%	0.017%
22	9.866	1155	1162	1170	rVB	122527	225003	26.74%	2.381%
23	9.931	1170	1173	1176	rBV2	1454	1379	0.16%	0.015%
24	10.412	1248	1255	1268	rBV	169074	309839	36.83%	3.279%
25	10.548	1272	1278	1288	rBV	99448	181828	21.61%	1.924%
26	10.724	1307	1308	1311	rBV	1417	1400	0.17%	0.015%
27	10.783	1311	1318	1327	rVB	140158	251176	29.85%	2.658%
28	10.924	1335	1342	1351	rBV2	118070	224844	26.72%	2.379%
29	11.029	1357	1360	1365	rVB3	1085	1769	0.21%	0.019%
30	11.329	1407	1411	1413	rBV2	1075	1305	0.16%	0.014%
31	11.758	1480	1484	1485	rBV	1584	1536	0.18%	0.016%
32	12.380	1583	1590	1597	rVB2	2976	6282	0.75%	0.066%
33	12.938	1682	1685	1687	rBV	1027	1537	0.18%	0.016%
34	13.220	1730	1733	1736	rVV3	2222	2518	0.30%	0.027%
35	13.262	1736	1740	1743	rVB	1134	1546	0.18%	0.016%
36	13.502	1776	1781	1789	rBV	22204	37454	4.45%	0.396%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082621\
Data File : BG050013.D
Acq On : 28 Aug 2021 1:53
Operator : CG/JU
Sample : M3518-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0B42

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-BG081921.M
Title : SVOA CALIBRATION

37	14.025	1864	1870	1878	rBV	321006	470389	55.91%	4.978%
38	14.319	1913	1920	1929	rBV	348324	535680	63.67%	5.669%
39	14.624	1966	1972	1980	rVB	237464	359797	42.76%	3.807%
40	14.777	1995	1998	1999	rBV	1871	1847	0.22%	0.020%
41	14.848	2004	2010	2023	rBV	106032	218449	25.96%	2.312%
42	15.124	2053	2057	2058	rVB3	1412	1624	0.19%	0.017%
43	15.341	2089	2094	2095	rBV	1032	1350	0.16%	0.014%
44	15.359	2095	2097	2101	rVV3	1914	2304	0.27%	0.024%
45	15.412	2103	2106	2108	rVB2	2026	1783	0.21%	0.019%
46	15.617	2135	2141	2151	rVB	430952	671938	79.87%	7.110%
47	15.752	2158	2164	2172	rBV	142254	217637	25.87%	2.303%
48	15.811	2172	2174	2177	rVV	1441	1902	0.23%	0.020%
49	15.864	2179	2183	2187	rVB3	3575	4188	0.50%	0.044%
50	16.070	2211	2218	2222	rBV3	4653	5717	0.68%	0.060%
51	16.316	2255	2260	2269	rVB2	12531	22650	2.69%	0.240%
52	16.510	2290	2293	2296	rVB	1518	1766	0.21%	0.019%
53	17.250	2413	2419	2422	rBV2	2361	3481	0.41%	0.037%
54	17.380	2434	2441	2448	rBV	295535	449697	53.45%	4.759%
55	17.479	2451	2458	2465	rVB2	427992	646252	76.81%	6.839%
56	17.567	2471	2473	2477	rVB	1139	1319	0.16%	0.014%
57	17.791	2510	2511	2517	rVB	2460	2902	0.34%	0.031%
58	17.908	2528	2531	2534	rVB	1567	1444	0.17%	0.015%
59	17.943	2534	2537	2540	rVB	1638	1347	0.16%	0.014%
60	18.032	2547	2552	2557	rVB	35691	40435	4.81%	0.428%
61	18.196	2578	2580	2581	rBV	1603	1376	0.16%	0.015%
62	18.331	2600	2603	2606	rVB	2776	3731	0.44%	0.039%
63	18.425	2615	2619	2620	rBV	2000	1559	0.19%	0.016%
64	18.531	2635	2637	2639	rBV2	1618	1627	0.19%	0.017%
65	18.619	2647	2652	2655	rBV3	4302	7687	0.91%	0.081%
66	18.719	2667	2669	2673	rVV3	1840	1661	0.20%	0.018%
67	18.772	2675	2678	2682	rVB4	5580	6739	0.80%	0.071%
68	18.860	2691	2693	2695	rBV2	1965	1909	0.23%	0.020%
69	19.101	2731	2734	2735	rBV2	2484	2254	0.27%	0.024%
70	19.165	2743	2745	2747	rBV2	4478	4591	0.55%	0.049%
71	19.201	2747	2751	2759	rVB2	57805	72969	8.67%	0.772%
72	19.330	2767	2773	2777	rBV2	21984	29042	3.45%	0.307%
73	19.412	2783	2787	2790	rBV	5765	10258	1.22%	0.109%
74	19.465	2794	2796	2801	rVB5	2916	3308	0.39%	0.035%
75	19.524	2804	2806	2807	rBV2	1929	1840	0.22%	0.019%
76	19.588	2813	2817	2822	rVB7	1880	2679	0.32%	0.028%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082621\
Data File : BG050013.D
Acq On : 28 Aug 2021 1:53
Operator : CG/JU
Sample : M3518-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0B42

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-BG081921.M
Title : SVOA CALIBRATION

77	19.700	2835	2836	2840	rBV3	2186	1590	0.19%	0.017%
78	19.770	2842	2848	2855	rVB	598951	841336	100.00%	8.903%
79	19.894	2867	2869	2872	rBV3	1761	1881	0.22%	0.020%
80	19.917	2872	2873	2877	rVB3	2456	2212	0.26%	0.023%
81	20.193	2919	2920	2923	rBV2	2377	1990	0.24%	0.021%
82	20.281	2933	2935	2942	rVB7	6993	9957	1.18%	0.105%
83	20.381	2949	2952	2958	rVB6	4833	8879	1.06%	0.094%
84	20.499	2970	2972	2975	rBV4	3051	2820	0.34%	0.030%
85	20.593	2986	2988	2989	rBV2	3046	1356	0.16%	0.014%
86	20.616	2989	2992	2996	rVB3	20224	21344	2.54%	0.226%
87	20.757	3014	3016	3017	rBV2	3074	1923	0.23%	0.020%
88	20.775	3017	3019	3022	rBV4	4764	5512	0.66%	0.058%
89	21.028	3060	3062	3063	rBV	3934	2309	0.27%	0.024%
90	21.292	3102	3107	3108	rBV4	32569	46306	5.50%	0.490%
91	21.650	3162	3168	3175	rVB	305077	471551	56.05%	4.990%
92	22.420	3296	3299	3300	rBV3	7001	7589	0.90%	0.080%
93	23.918	3548	3554	3563	rVB3	44639	102694	12.21%	1.087%
94	24.311	3619	3621	3622	rBV2	5021	3666	0.44%	0.039%
95	24.652	3669	3679	3691	rVB2	282216	792342	94.18%	8.385%
96	24.875	3708	3717	3729	rVB2	173668	496386	59.00%	5.253%
97	25.375	3798	3802	3810	rVB9	10988	27652	3.29%	0.293%
98	25.486	3819	3821	3822	rBV2	5673	3834	0.46%	0.041%
99	25.986	3899	3906	3917	rVB6	41440	123668	14.70%	1.309%
100	32.400	4997	4998	5000	rVB2	5704	2848	0.34%	0.030%

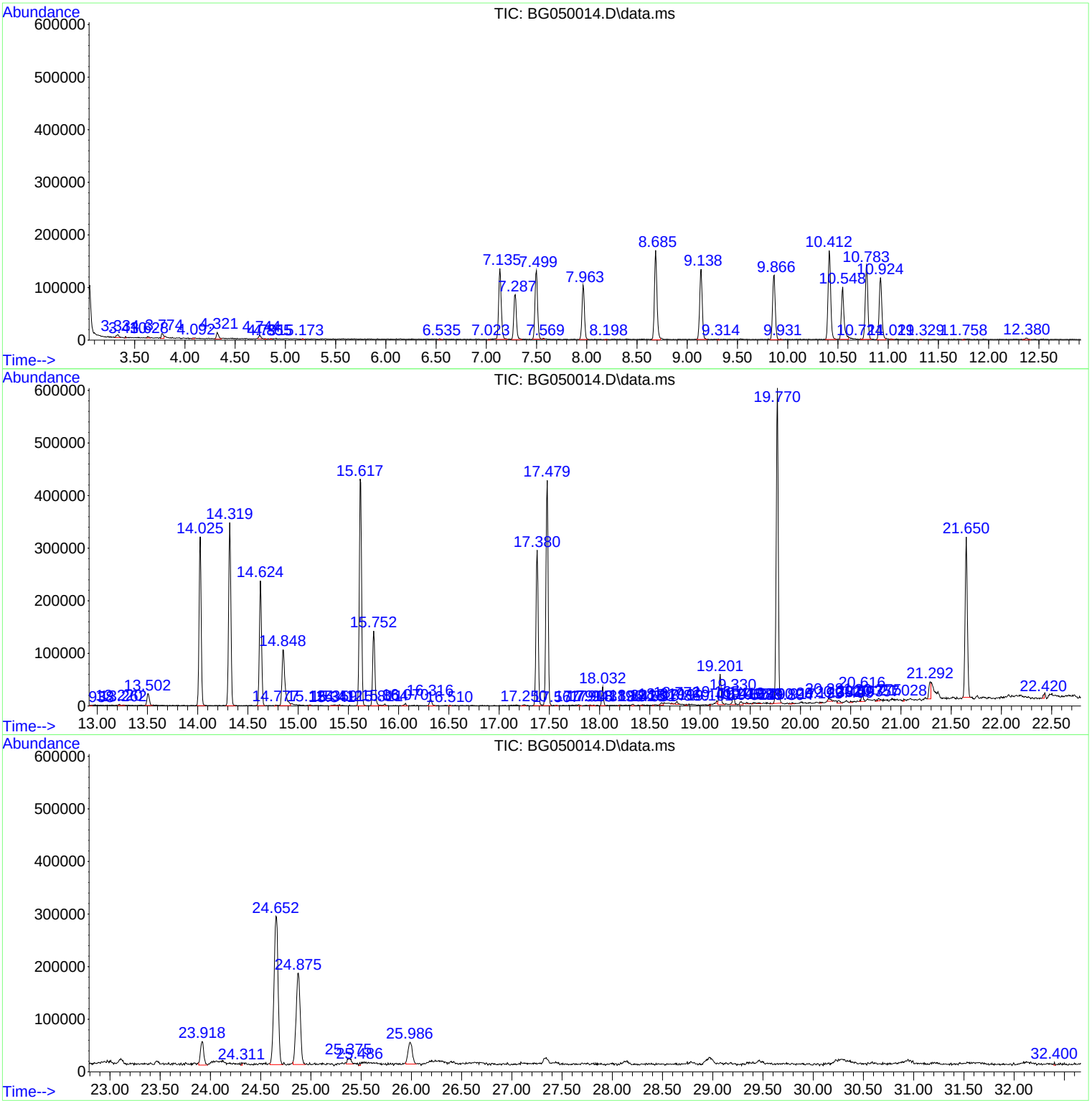
Sum of corrected areas: 9449992

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082621\
Data File : BG050013.D
Acq On : 28 Aug 2021 1:53
Operator : CG/JU
Sample : M3518-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0B42

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SFAM-EPA-BG081921.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082621\
Data File : BG050013.D
Acq On : 28 Aug 2021 1:53
Operator : CG/JU
Sample : M3518-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0B42

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SFAM-EPA-BG081921.M
Quant Title : SVOA CALIBRATION

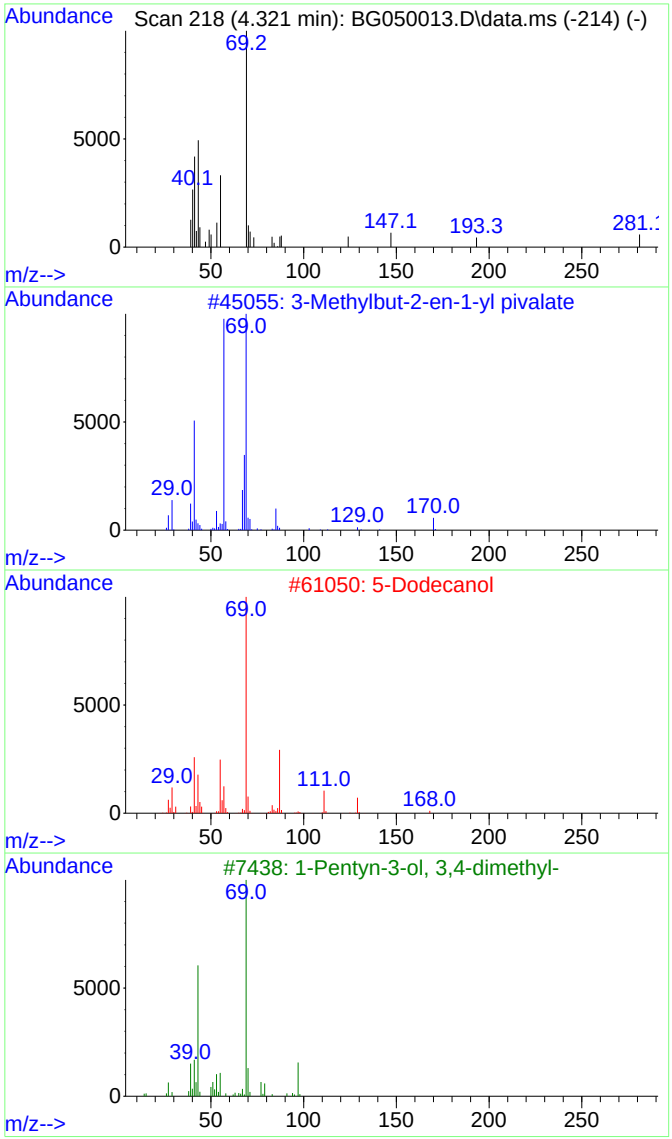
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

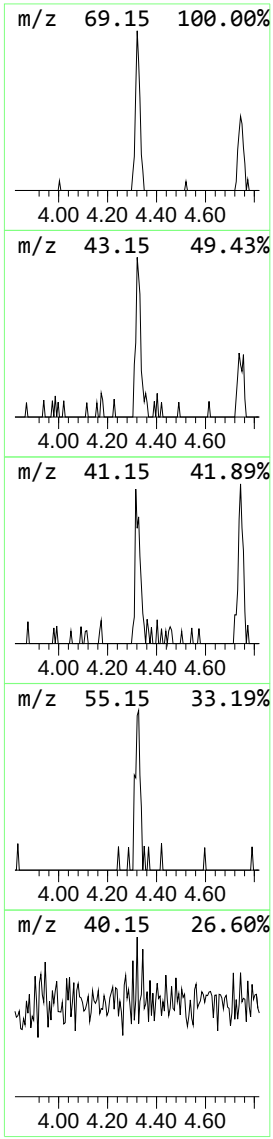
****

Peak Number 1 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.321	2.18 ng/ul	19027	1,4-Dichlorobenzene-d4	7.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methylbut-2-en-1-yl pivalate	170	C10H18O2	211429-71-9	36
2	5-Dodecanol	186	C12H26O	010203-33-5	36
3	1-Pentyn-3-ol, 3,4-dimethyl-	112	C7H12O	001482-15-1	36
4	4-Trifluoroacetoxyoctane	226	C10H17F3O2	116465-17-9	36
5	1-Undecyn-4-ol	168	C11H20O	022127-86-2	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082621\
Data File : BG050013.D
Acq On : 28 Aug 2021 1:53
Operator : CG/JU
Sample : M3518-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0B42

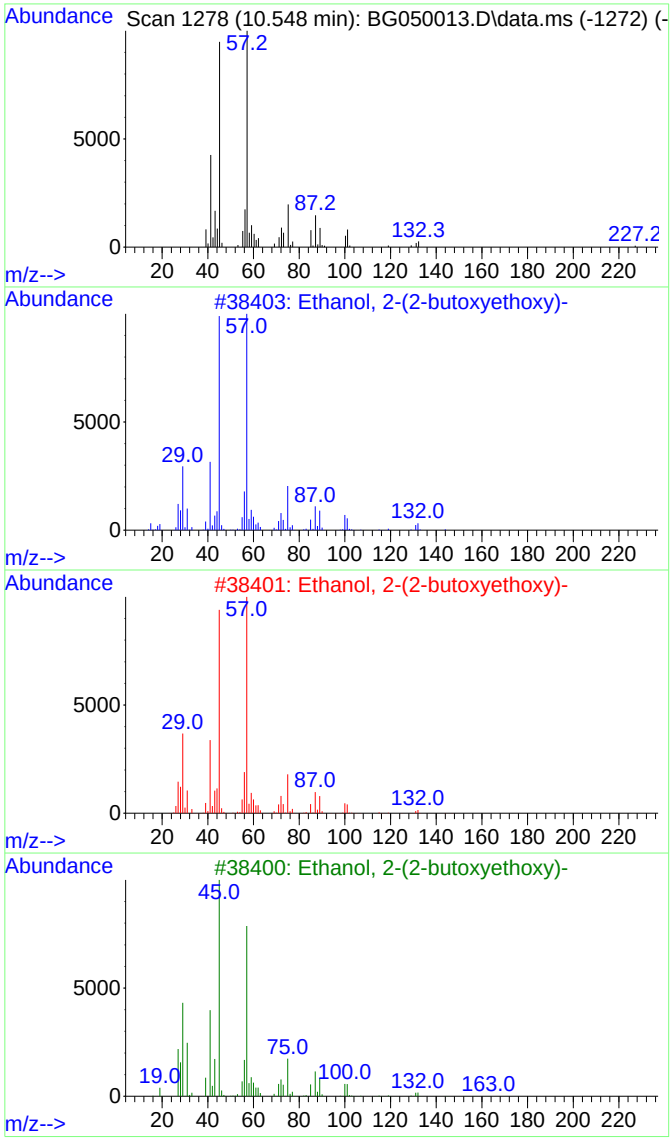
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SFAM-EPA-BG081921.M
Quant Title : SVOA CALIBRATION

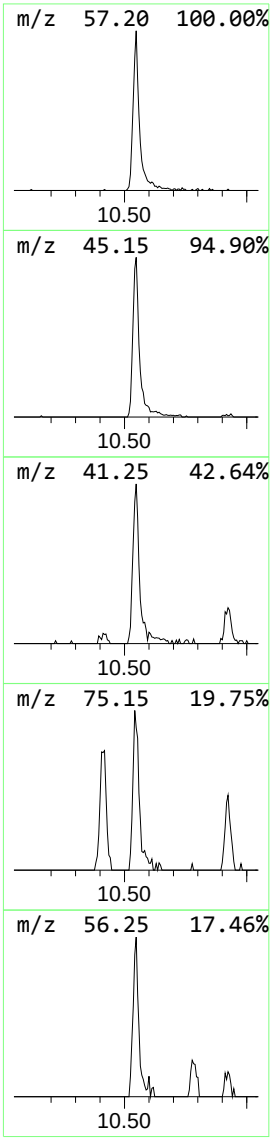
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.548	14.48 ng/ul	181828	Naphthalene-d8	10.783

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
4	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
5	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082621\
Data File : BG050013.D
Acq On : 28 Aug 2021 1:53
Operator : CG/JU
Sample : M3518-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0B42

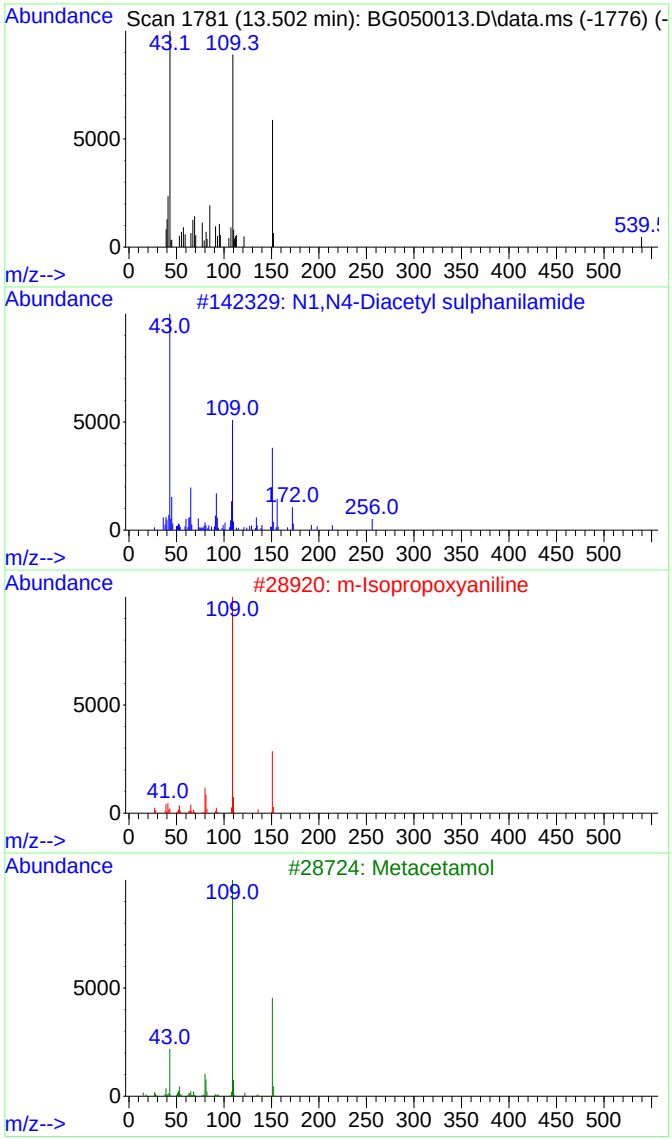
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SFAM-EPA-BG081921.M
Quant Title : SVOA CALIBRATION

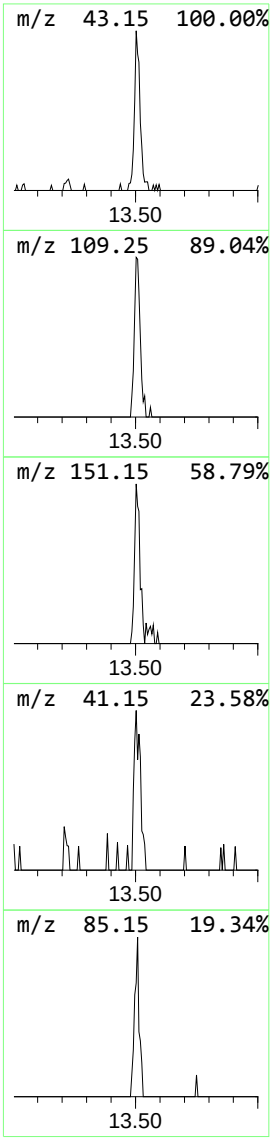
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 N1,N4-Diacetyl sulphanilamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.502	2.08 ng/ul	37454	Acenaphthene-d10	14.624

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N1,N4-Diacetyl sulphanilamide	256	C10H12N2O4S	005626-90-4	53
2	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	52
3	Metacetamol	151	C8H9NO2	000621-42-1	52
4	Tiocarlide	400	C23H32N2O2S	000910-86-1	50
5	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082621\
Data File : BG050013.D
Acq On : 28 Aug 2021 1:53
Operator : CG/JU
Sample : M3518-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0B42

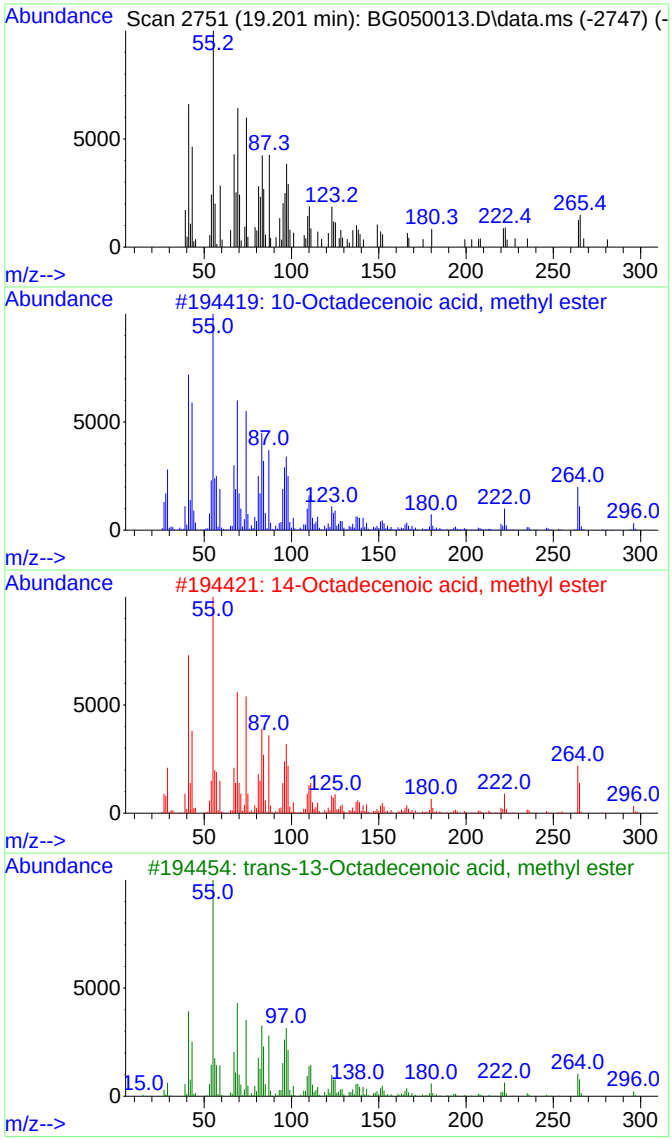
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SFAM-EPA-BG081921.M
Quant Title : SVOA CALIBRATION

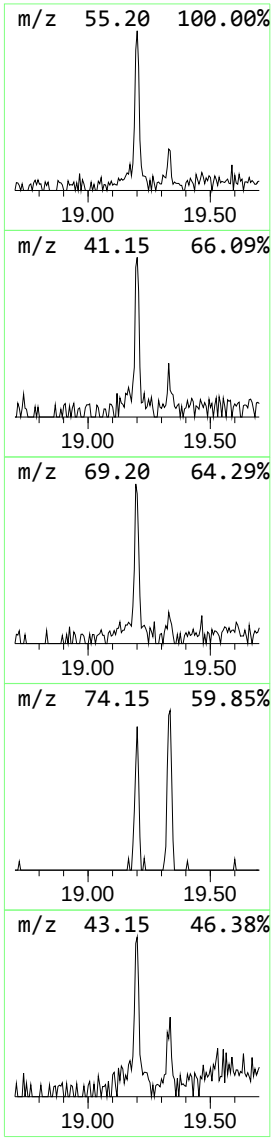
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 10-Octadecenoic acid, methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.201	3.25 ng/ul	72969	Phenanthrene-d10	17.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	90
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	90
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	87
4	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	86
5	(Z)-Methyl hexadec-11-enoate	268	C17H32O2	000822-05-9	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082621\
Data File : BG050013.D
Acq On : 28 Aug 2021 1:53
Operator : CG/JU
Sample : M3518-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0B42

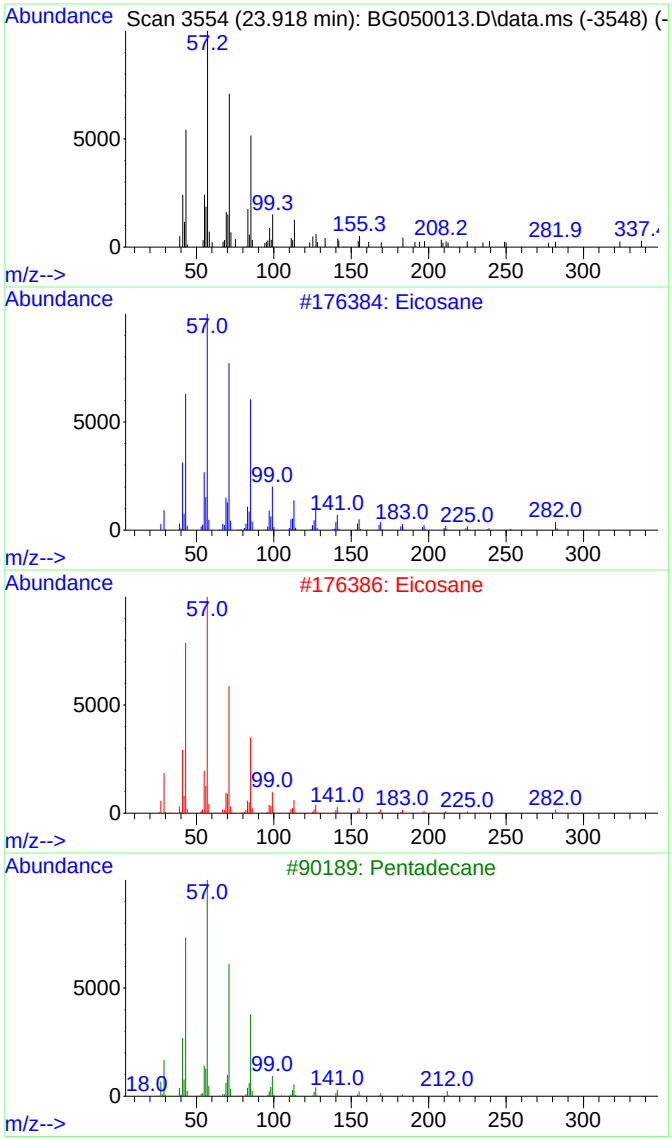
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SFAM-EPA-BG081921.M
Quant Title : SVOA CALIBRATION

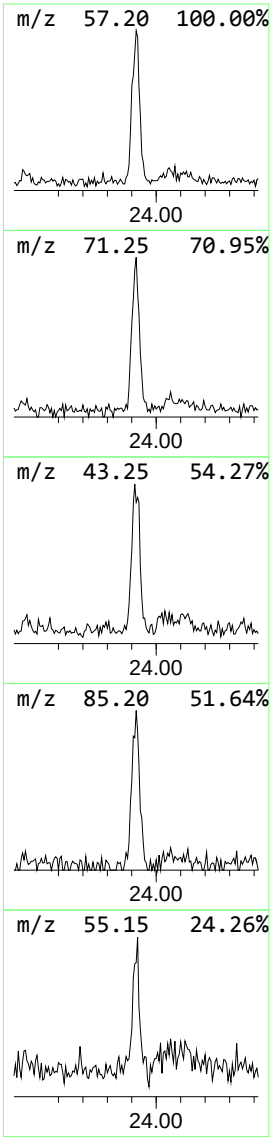
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.918	4.14 ng/ul	102694	Perylene-d12	24.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Eicosane	282	C20H42	000112-95-8	89
3	Pentadecane	212	C15H32	000629-62-9	87
4	Pentadecane	212	C15H32	000629-62-9	87
5	Docosane	310	C22H46	000629-97-0	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082621\
Data File : BG050013.D
Acq On : 28 Aug 2021 1:53
Operator : CG/JU
Sample : M3518-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0B42

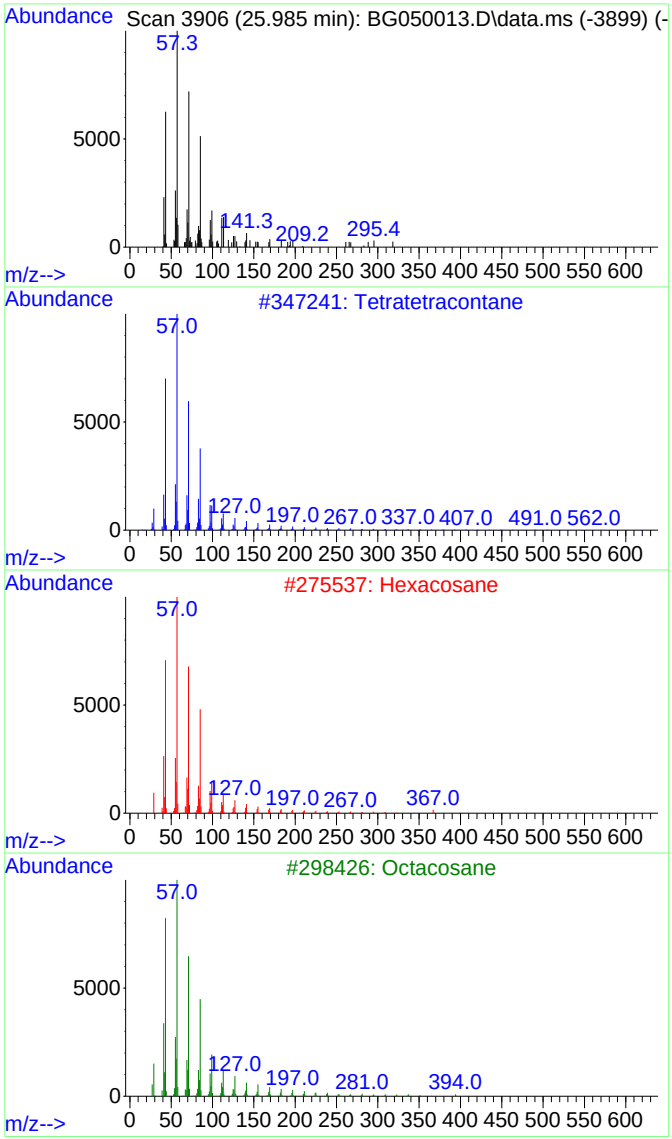
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SFAM-EPA-BG081921.M
Quant Title : SVOA CALIBRATION

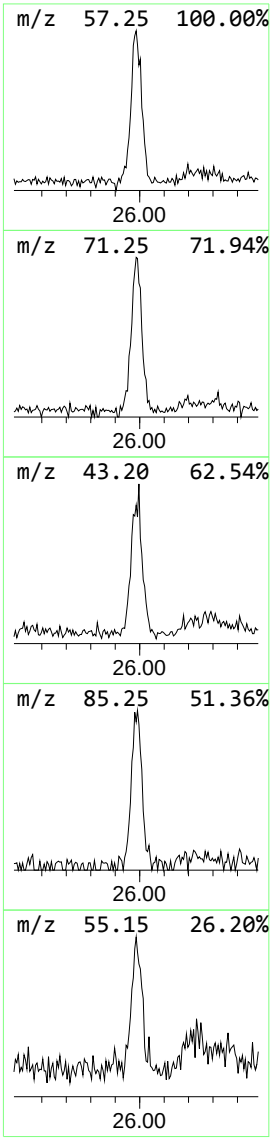
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.985	4.98 ng/ul	123668	Perylene-d12	24.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	87
2	Hexacosane	366	C26H54	000630-01-3	87
3	Octacosane	394	C28H58	000630-02-4	86
4	Eicosane	282	C20H42	000112-95-8	86
5	Octacosane	394	C28H58	000630-02-4	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082621\
Data File : BG050013.D
Acq On : 28 Aug 2021 1:53
Operator : CG/JU
Sample : M3518-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0B42

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SFAM-EPA-BG081921.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	4.321	2.2	ng/ul	19027	1	7.963	174856	20.0
Ethanol, 2-(2-b...	10.548	14.5	ng/ul	181828	2	10.783	251176	20.0
N1,N4-Diacetyl ...	13.502	2.1	ng/ul	37454	3	14.624	359797	20.0
10-Octadecenoic...	19.201	3.3	ng/ul	72969	4	17.380	449697	20.0
(DEL) Alkane: S...	23.918	4.1	ng/ul	102694	6	24.875	496386	20.0
(DEL) Alkane: S...	25.985	5.0	ng/ul	123668	6	24.875	496386	20.0