LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030123\
Data File : BG056782.D
Acq On : 2 Mar 2023 4:07
Operator : CG/JU
Sample : 01649-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DBZW5

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-BG022323.M
Title : SVOA CALIBRATION

Signal : TIC: BG056782.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.972	70	74	82	rBV	13550	22089	5.59%	0.432%
2	4.154	103	105	109	rVB2	2353	2241	0.57%	0.044%
3	4.383	142	144	150	rVB3	2657	3895	0.98%	0.076%
4	4.712	198	200	204	rBV3	1910	3076	0.78%	0.060%
5	4.971	242	244	246	rBV	1208	955	0.24%	0.019%
6	5.441	320	324	331	rVB3	7266	11664	2.95%	0.228%
7	6.487	500	502	505	rBV	969	951	0.24%	0.019%
8	6.769	549	550	554	rVB2	1372	1096	0.28%	0.021%
9	7.538	675	681	690	rVB2	64550	114356	28.91%	2.238%
10	7.720	706	712	718	rBV2	37811	61352	15.51%	1.200%
11	7.879	735	739	742	rBV4	2041	2627	0.66%	0.051%
12	7.938	744	749	757	rVV	50834	84411	21.34%	1.652%
13	8.014	760	762	765	rBV2	947	931	0.24%	0.018%
14	8.420	825	831	838	rBV	63430	106320	26.88%	2.080%
15	9.101	941	947	955	rBV	66912	114767	29.02%	2.246%
16	9.242	966	971	979	rBV4	4503	9160	2.32%	0.179%
17	9.589	1023	1030	1039	rVB2	54357	97227	24.58%	1.902%
18	9.965	1091	1094	1100	rVB	1599	2376	0.60%	0.046%
19	10.317	1148	1154	1161	rVB2	47347	83261	21.05%	1.629%
20	10.858	1237	1246	1253	rBV2	74419	128047	32.38%	2.506%
21	11.069	1277	1282	1287	rBV4	8887	12640	3.20%	0.247%
22	11.258	1306	1314	1321	rBV	92658	162561	41.10%	3.181%
23	11.375	1327	1334	1342	rBV3	46095	84736	21.43%	1.658%
24	12.809	1572	1578	1583	rVB2	1372	1713	0.43%	0.034%
25	12.867	1583	1588	1593	rBV4	13243	20702	5.23%	0.405%
26	13.191	1640	1643	1647	rBV2	487	1049	0.27%	0.021%
27	13.737	1731	1736	1742	rVB3	13286	16542	4.18%	0.324%
28	13.819	1748	1750	1751	rBV	1143	1032	0.26%	0.020%
29	13.884	1758	1761	1764	rBV2	1472	1905	0.48%	0.037%
30	14.219	1814	1818	1823	rBV	533	967	0.24%	0.019%
31	14.407	1843	1850	1856	rBV	145873	209985	53.09%	4.109%
32	14.718	1897	1903	1909	rBV	157843	245706	62.13%	4.808%
33	14.988	1944	1949	1951	rBV	44422	65271	16.50%	1.277%
34	15.024	1951	1955	1962	rVB	160200	247898	62.68%	4.851%
35	15.171	1975	1980	1990	rBV	56287	90607	22.91%	1.773%
36	15.329	2003	2007	2010	rBV2	1258	1751	0.44%	0.034%

LSC Area Percent Report

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Misc :
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Instrument : BNA_G
ClientSampleId : DBZW5

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 >
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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Title : SVOA CALIBRATION

37	15.758	2076	2080	2084	rBV3	10516	11622	2.94%	0.227%
38	16.005	2115	2122	2128	rBV	204830	309506	78.26%	6.056%
39	16.099	2133	2138	2145	rVB	65534	94086	23.79%	1.841%
40	16.357	2175	2182	2186	rVB	18878	28965	7.32%	0.567%
41	17.415	2357	2362	2367	rVB2	5237	6864	1.74%	0.134%
42	17.674	2403	2406	2409	rBV2	860	1158	0.29%	0.023%
43	17.756	2413	2420	2426	rBV	223451	332766	84.14%	6.511%
44	17.856	2430	2437	2443	rVV	209082	319245	80.72%	6.247%
45	18.390	2524	2528	2531	rVB3	2929	3398	0.86%	0.066%
46	18.484	2541	2544	2546	rBV3	958	1166	0.29%	0.023%
47	18.543	2550	2554	2555	rBV2	1814	1458	0.37%	0.029%
48	18.590	2558	2562	2573	rBV2	31961	51817	13.10%	1.014%
49	18.666	2573	2575	2576	rVV2	1891	1459	0.37%	0.029%
50	18.713	2580	2583	2587	rBV3	1203	1513	0.38%	0.030%
51	18.760	2590	2591	2593	rBV	1414	986	0.25%	0.019%
52	18.819	2596	2601	2603	rBV3	1528	2741	0.69%	0.054%
53	18.849	2603	2606	2609	rBV	3793	3702	0.94%	0.072%
54	18.960	2622	2625	2628	rBV3	1025	1383	0.35%	0.027%
55	19.019	2633	2635	2640	rVB3	1545	1729	0.44%	0.034%
56	19.066	2640	2643	2646	rBV3	818	1105	0.28%	0.022%
57	19.178	2660	2662	2668	rVV2	1724	2537	0.64%	0.050%
58	19.401	2696	2700	2703	rVB3	1898	2500	0.63%	0.049%
59	19.501	2714	2717	2720	rBV4	3042	3187	0.81%	0.062%
60	19.524	2720	2721	2726	rVB3	1727	1783	0.45%	0.035%
61	19.677	2745	2747	2754	rVB7	2505	4782	1.21%	0.094%
62	19.748	2754	2759	2763	rVV5	3567	6699	1.69%	0.131%
63	19.806	2767	2769	2771	rBV2	1099	945	0.24%	0.018%
64	19.842	2771	2775	2780	rBV5	4669	6649	1.68%	0.130%
65	19.977	2795	2798	2801	rBV3	1893	2904	0.73%	0.057%
66	20.041	2806	2809	2812	rBV2	2533	4091	1.03%	0.080%
67	20.065	2812	2813	2815	rVV2	2390	1834	0.46%	0.036%
68	20.112	2815	2821	2830	rVB	278893	395492	100.00%	7.739%
69	20.218	2835	2839	2841	rBV4	7568	7972	2.02%	0.156%
70	20.312	2853	2855	2859	rVB2	2003	2058	0.52%	0.040%
71	20.453	2877	2879	2884	rBV4	4965	6019	1.52%	0.118%
72	20.535	2890	2893	2897	rBV2	10270	12783	3.23%	0.250%
73	20.588	2900	2902	2905	rVB3	3194	3961	1.00%	0.078%
74	20.929	2956	2960	2963	rVB5	3068	4074	1.03%	0.080%
75	21.064	2978	2983	2986	rBV2	11496	16674	4.22%	0.326%
76	21.263	3015	3017	3020	rBV3	1654	1726	0.44%	0.034%

LSC Area Percent Report

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Misc :
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Instrument : BNA_G
ClientSampleId : DBZW5

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Integrator: RTE
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Title : SVOA CALIBRATION

77	21.598	3072	3074	3075	rBV2	3115	2369	0.60%	0.046%
78	21.639	3076	3081	3098	rVB4	48002	103061	26.06%	2.017%
79	22.062	3146	3153	3160	rVB2	201381	353988	89.51%	6.927%
80	22.145	3165	3167	3168	rBV2	2054	1267	0.32%	0.025%
81	22.491	3223	3226	3233	rVB6	8573	11406	2.88%	0.223%
82	22.909	3289	3297	3299	rBV6	11705	24956	6.31%	0.488%
83	23.625	3413	3419	3428	rVB7	14372	32632	8.25%	0.639%
84	23.996	3480	3482	3483	rBV	2006	1309	0.33%	0.026%
85	24.524	3567	3572	3579	rVB4	20242	42877	10.84%	0.839%
86	25.253	3695	3696	3700	rBV3	1892	1956	0.49%	0.038%
87	25.341	3700	3711	3721	rVV2	126957	361248	91.34%	7.069%
88	25.588	3743	3753	3766	rVB	118824	345583	87.38%	6.762%
89	26.463	3899	3902	3904	rBV4	2422	3139	0.79%	0.061%
90	26.563	3917	3919	3921	rBV3	1985	1250	0.32%	0.024%
91	26.663	3934	3936	3938	rBV2	2049	1423	0.36%	0.028%
92	26.833	3956	3965	3976	rVB4	22657	69509	17.58%	1.360%
93	26.980	3979	3990	3991	rBV7	8988	22687	5.74%	0.444%
94	27.403	4060	4062	4067	rVB5	2378	2263	0.57%	0.044%
95	27.832	4133	4135	4137	rBV2	1761	1915	0.48%	0.037%
96	27.973	4158	4159	4160	rBV	2344	1110	0.28%	0.022%
97	29.025	4337	4338	4339	rBV	2637	1308	0.33%	0.026%
98	30.946	4663	4665	4667	rBV3	1837	1745	0.44%	0.034%
99	31.404	4741	4743	4744	rBV	3356	2262	0.57%	0.044%
100	31.469	4744	4754	4755	rBV6	17380	38087	9.63%	0.745%

Sum of corrected areas: 5110556

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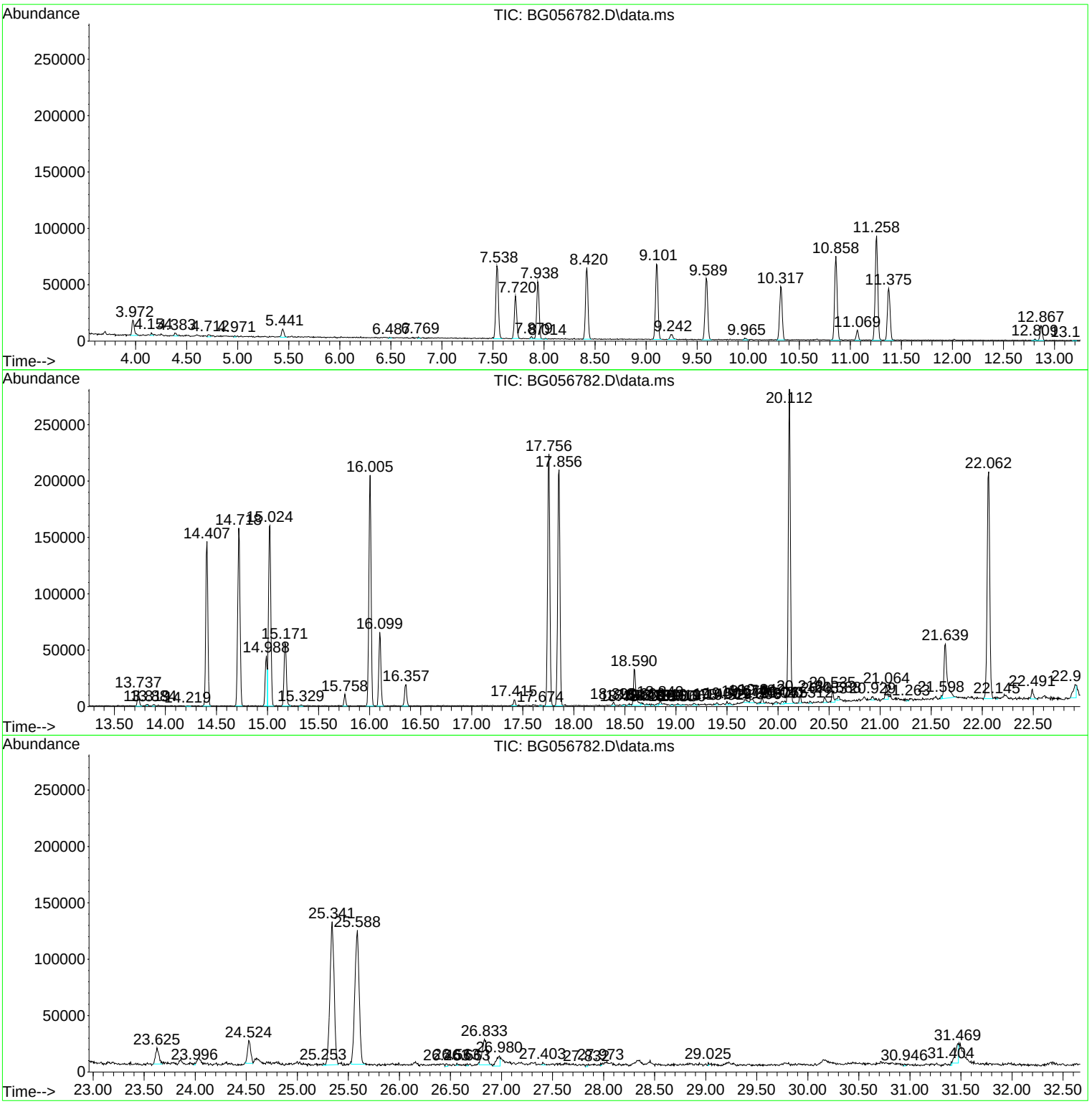
BNA_G
ClientSampleId :
DBZW5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

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



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Instrument :
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ClientSampleId :
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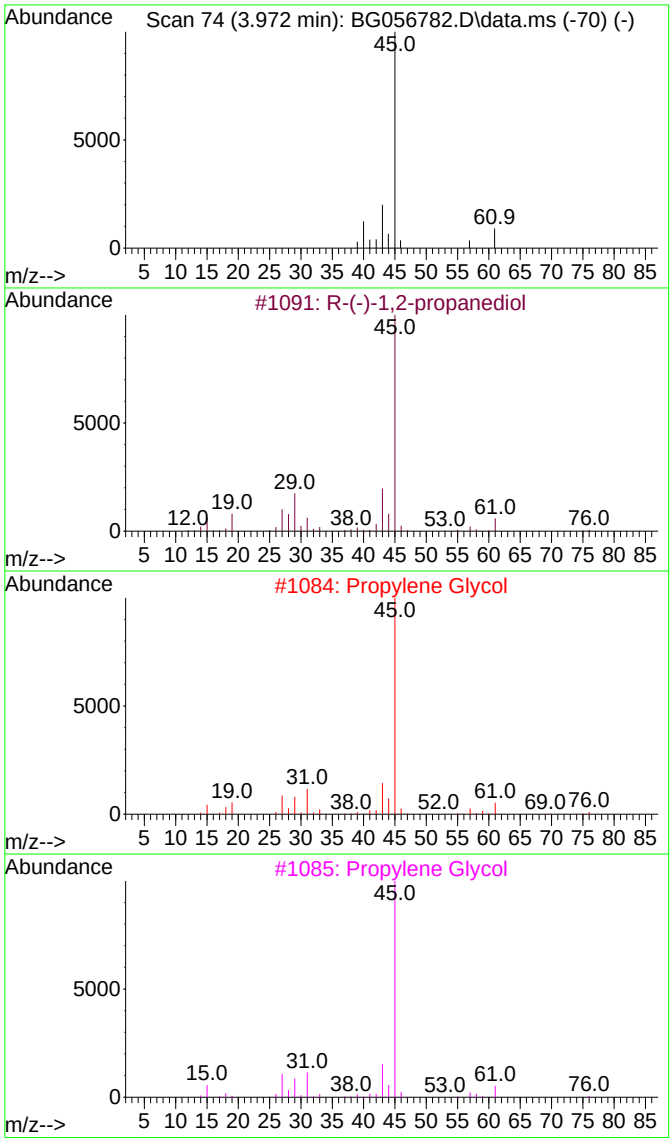
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

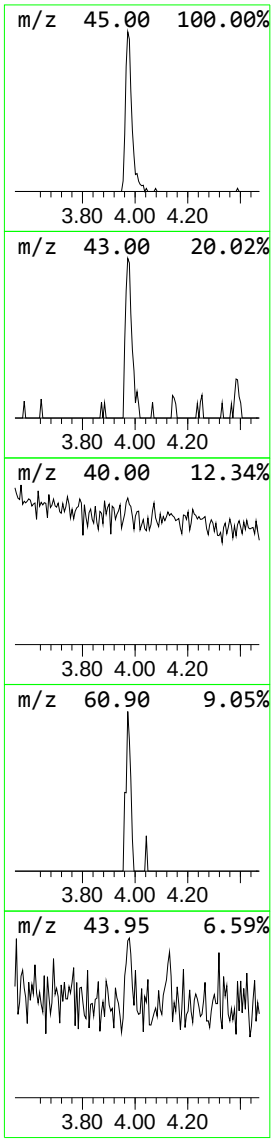
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 R-(-)-1,2-propanediol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.972	4.16 ng/ul	22089	1,4-Dichlorobenzene-d4	8.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2	Propylene Glycol	76	C3H8O2	000057-55-6	9
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Propylene Glycol	76	C3H8O2	000057-55-6	9
5	Formamide	45	CH3NO	000075-12-7	5





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Data File : BG056782.D
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

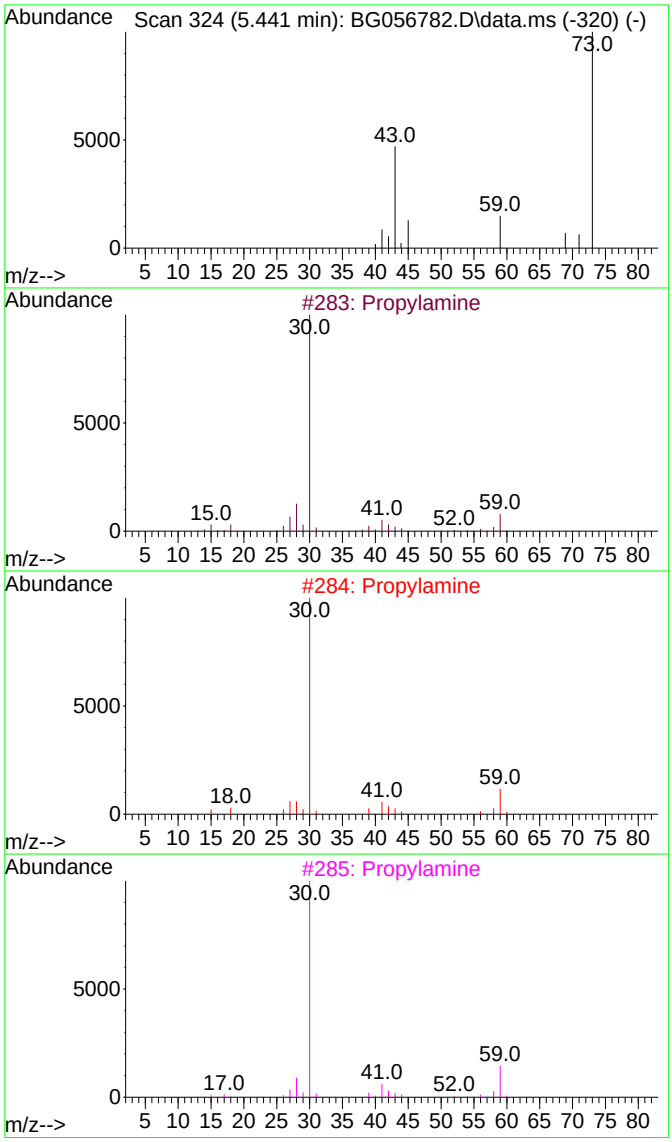
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

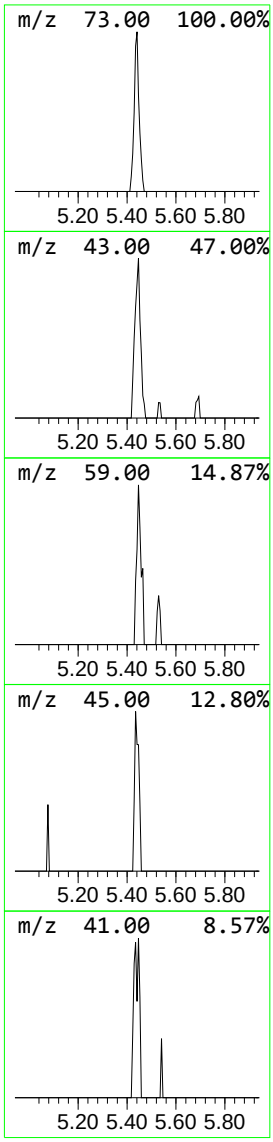
****

Peak Number 2 unknown-01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.441	2.19 ng/ul	11664	1,4-Dichlorobenzene-d4	8.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylamine	59	C3H9N	000107-10-8	4
2	Propylamine	59	C3H9N	000107-10-8	4
3	Propylamine	59	C3H9N	000107-10-8	4
4	Propylamine	59	C3H9N	000107-10-8	4
5	Isobutylamine	73	C4H11N	000078-81-9	4





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

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

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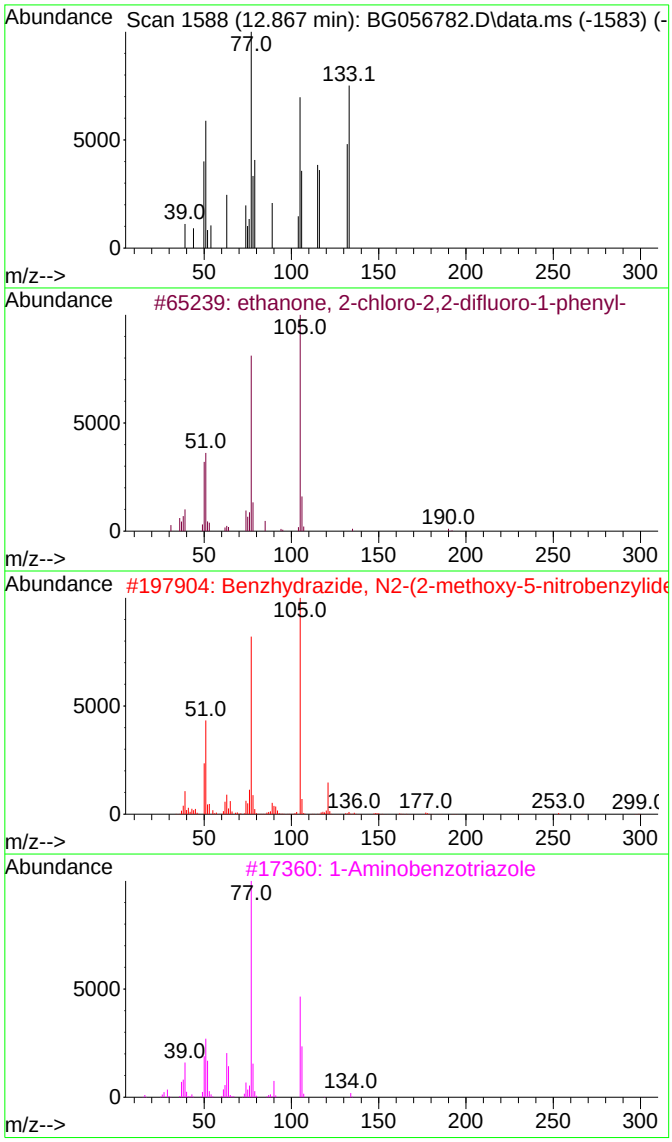
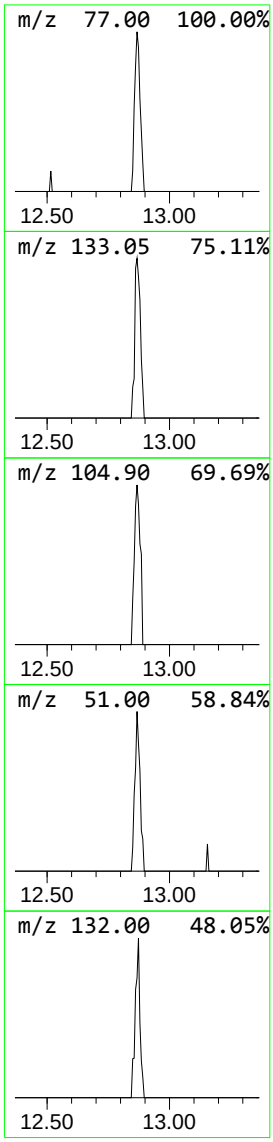
Peak Number 3 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.867	2.55 ng/ul	20702	Naphthalene-d8	11.258

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	ethanone, 2-chloro-2,2-difluoro-...	190	C8H5ClF2O	1000400-22-4	38
2	Benzhydrazide, N2-(2-methoxy-5-n...	299	C15H13N3O4	349572-84-5	38
3	1-Aminobenzotriazole	134	C6H6N4	001614-12-6	37
4	2-(2-Hydroxyphenoxy)-1-phenyleth...	230	C14H14O3	328104-89-8	32
5	1,2,3-Benzotriazole-1-benzoate	239	C13H9N3O2	054769-36-7	25





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

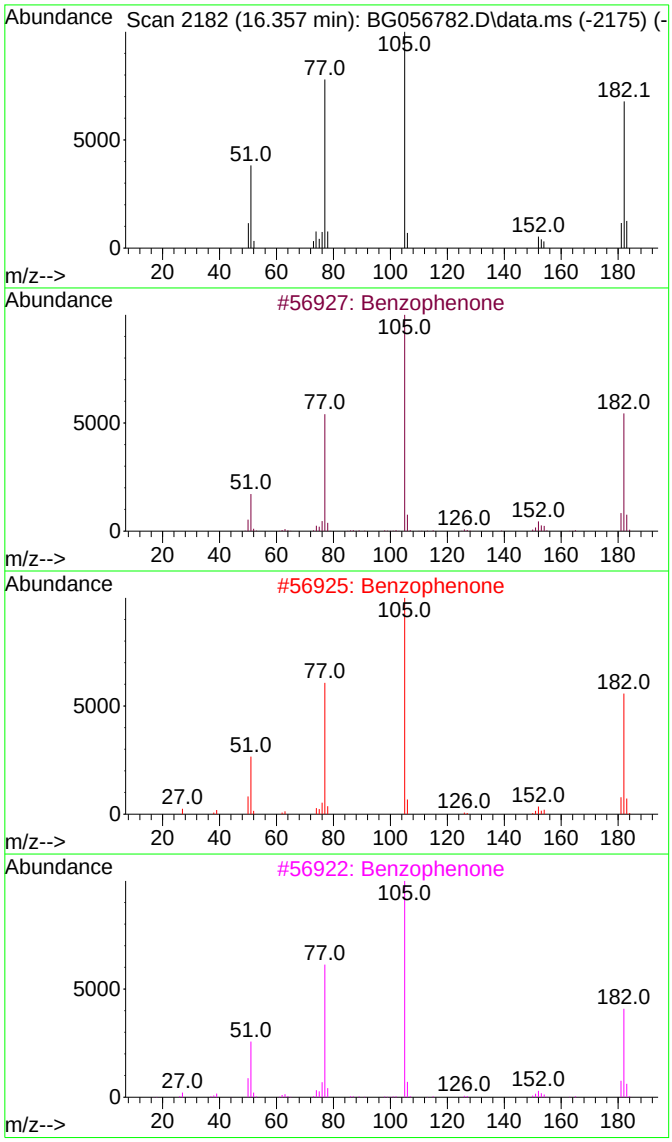
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

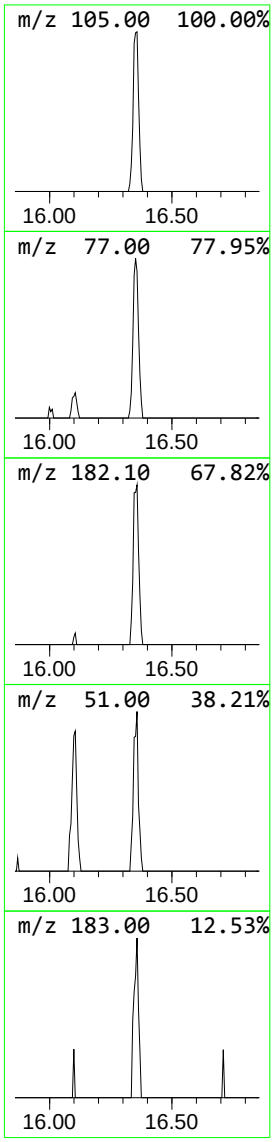
****

Peak Number 4 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.357	2.34 ng/ul	28965	Acenaphthene-d10	15.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	Benzophenone	182	C13H10O	000119-61-9	94
3	Benzophenone	182	C13H10O	000119-61-9	91
4	Benzophenone	182	C13H10O	000119-61-9	91
5	Benzophenone	182	C13H10O	000119-61-9	81





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Operator : CG/JU
Sample : 01649-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZW5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

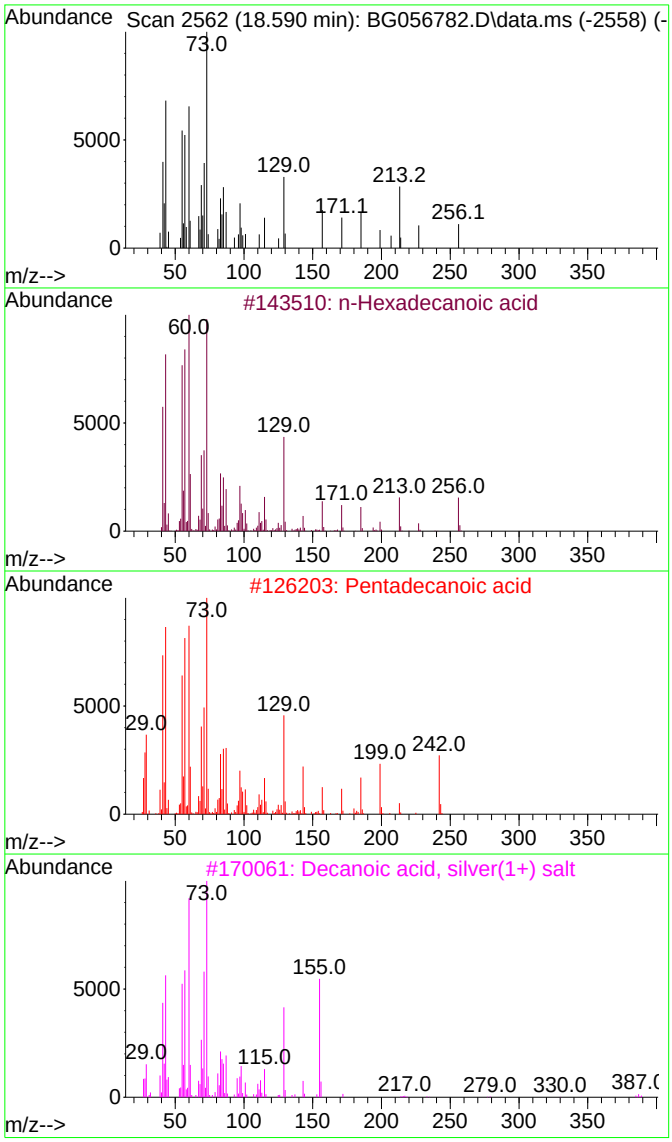
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

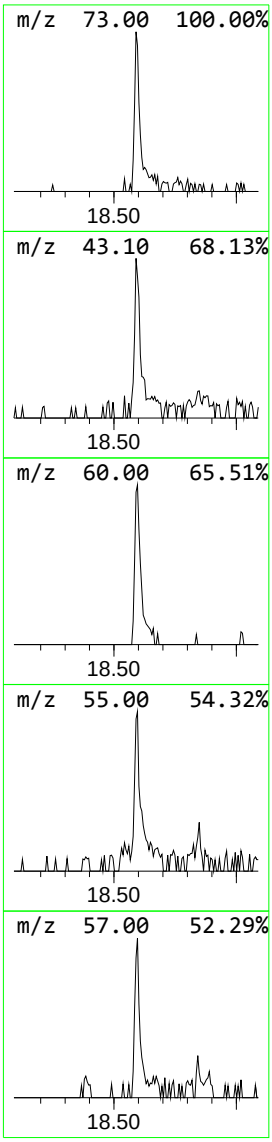
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.590	3.11 ng/ul	51817	Phenanthrene-d10	17.756

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
3	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	43
4	Tridecanoic acid	214	C13H26O2	000638-53-9	38
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	38





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Data File : BG056782.D
Acq On : 2 Mar 2023 4:07
Operator : CG/JU
Sample : 01649-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZW5

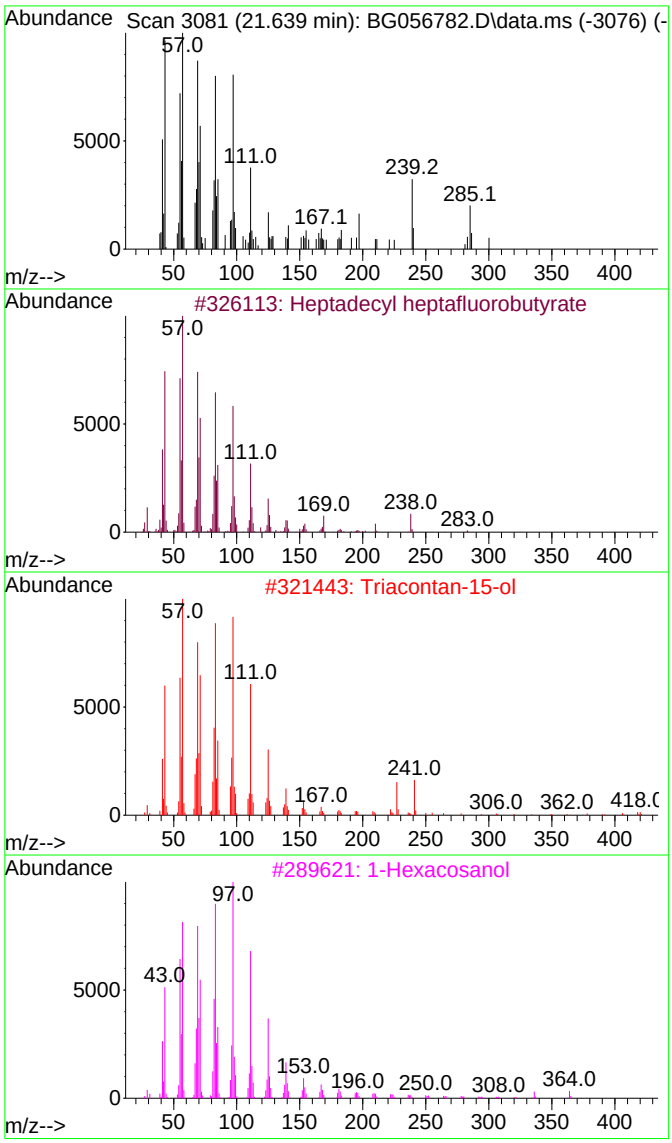
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

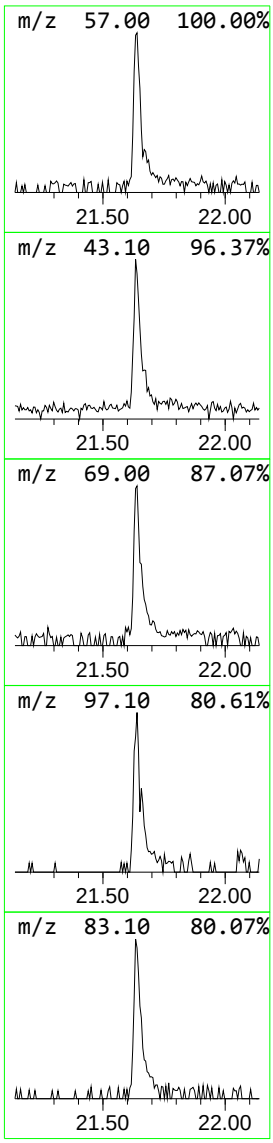
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.640	5.82 ng/ul	103061	Chrysene-d12	22.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	89
2	Triacontan-15-ol	438	C30H62O	031849-26-0	87
3	1-Hexacosanol	382	C26H54O	000506-52-5	87
4	1-Tetracosene	336	C24H48	010192-32-2	87
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030123\
Data File : BG056782.D
Acq On : 2 Mar 2023 4:07
Operator : CG/JU
Sample : 01649-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZW5

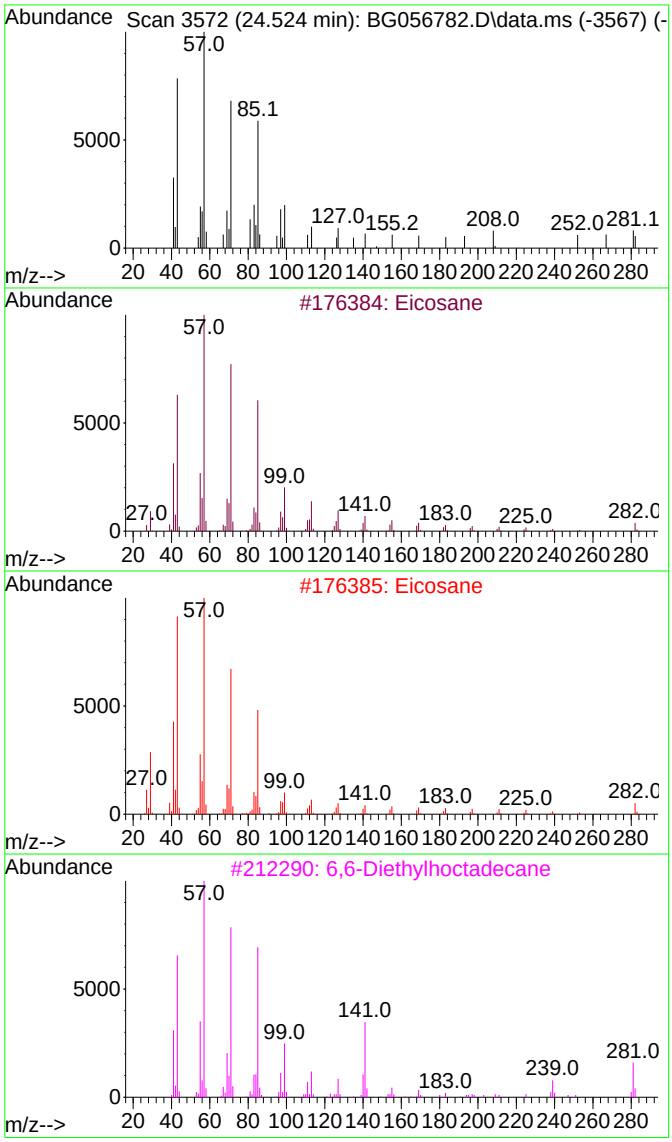
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

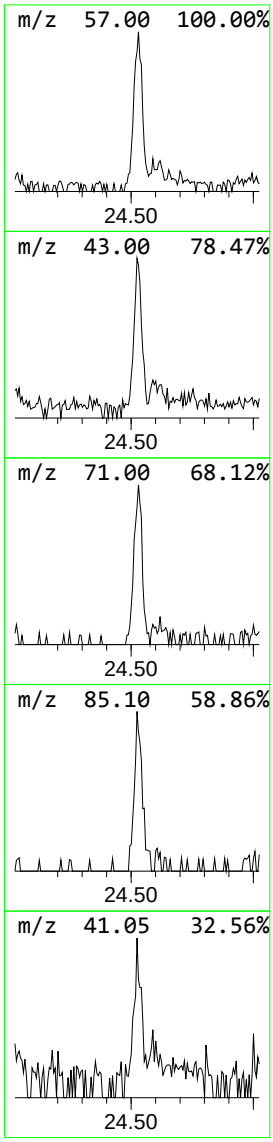
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.524	2.48 ng/ul	42877	Perylene-d12	25.588

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Eicosane	282	C20H42	000112-95-8	89
3	6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	86
4	2-Methyltetracosane	352	C25H52	001560-78-7	83
5	Heptacosane	380	C27H56	000593-49-7	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030123\
Data File : BG056782.D
Acq On : 2 Mar 2023 4:07
Operator : CG/JU
Sample : 01649-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZW5

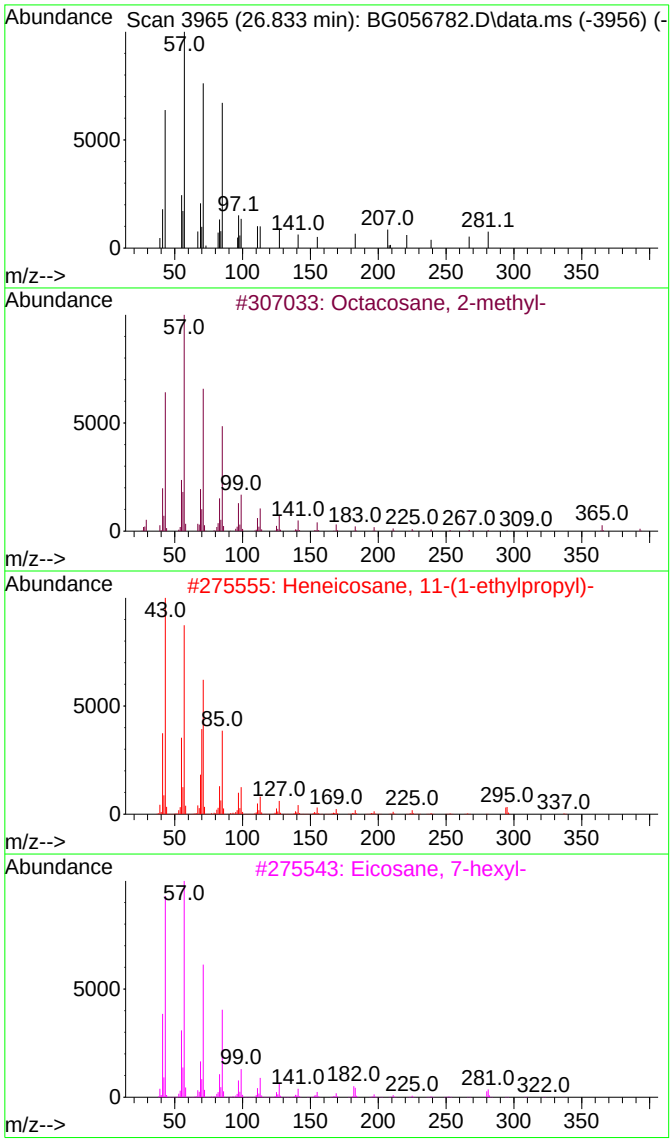
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

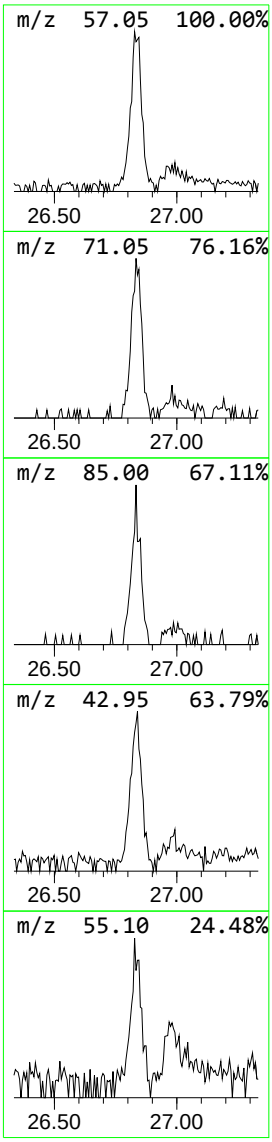
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.833	4.02 ng/ul	69509	Perylene-d12	25.588

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
4	Hentriacontane	437	C31H64	000630-04-6	87
5	Pentacosane	352	C25H52	000629-99-2	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030123\
Data File : BG056782.D
Acq On : 2 Mar 2023 4:07
Operator : CG/JU
Sample : 01649-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZW5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

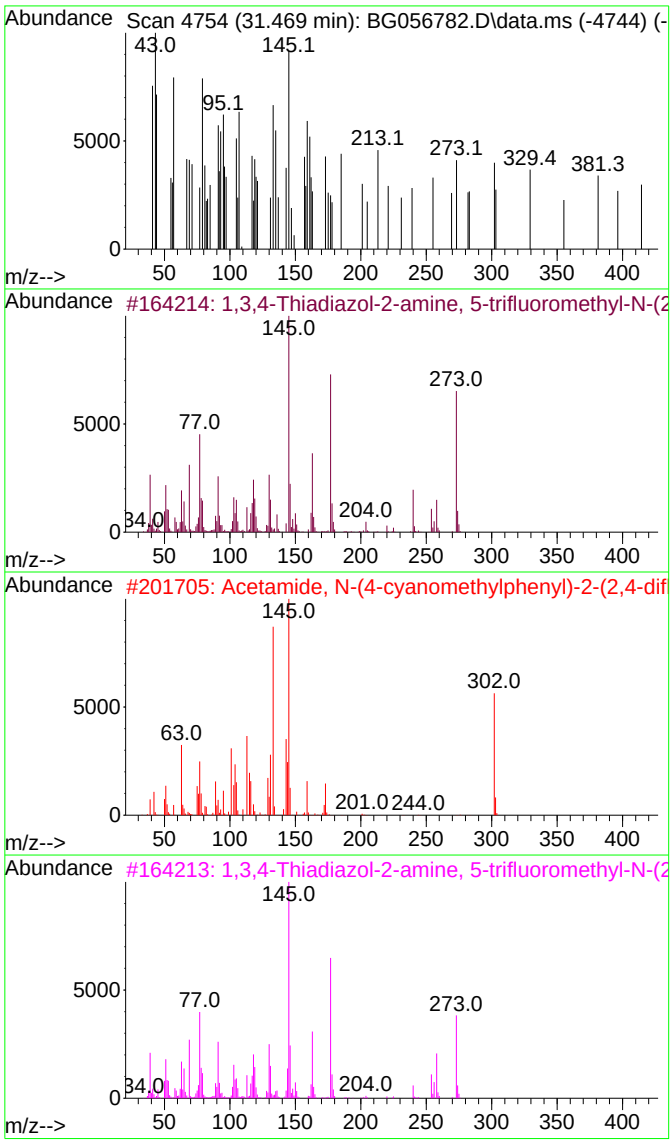
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

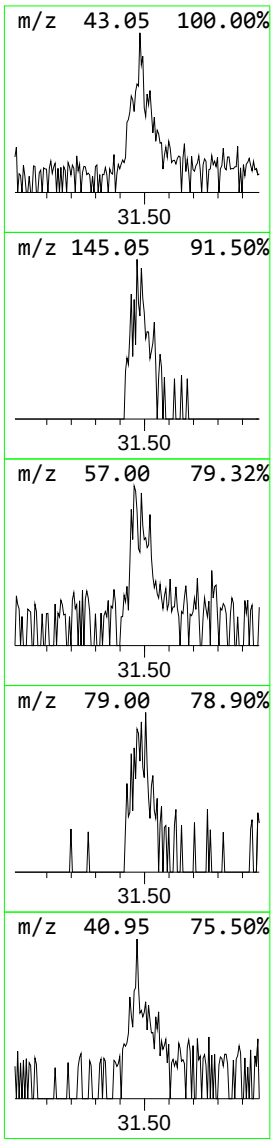
****

Peak Number 9 unknown-03 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.469	2.20 ng/ul	38087	Perylene-d12	25.588

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4-Thiadiazol-2-amine, 5-trif...	273	C11H10F3N3S	1000267-89-8	27
2	Acetamide, N-(4-cyanomethylpheny...	302	C16H12F2N2O2	1000303-56-0	27
3	1,3,4-Thiadiazol-2-amine, 5-trif...	273	C11H10F3N3S	284488-18-2	16
4	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	11
5	Sebacic acid, hexyl 2,3,6-triflu...	430	C23H33F3O4	1000380-79-5	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030123\
Data File : BG056782.D
Acq On : 2 Mar 2023 4:07
Operator : CG/JU
Sample : 01649-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZW5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.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
R-(-)-1,2-propa...	3.972	4.2	ng/ul	22089	1	8.420	106320	20.0
unknown-01	5.441	2.2	ng/ul	11664	1	8.420	106320	20.0
unknown-02	12.867	2.5	ng/ul	20702	2	11.258	162561	20.0
Benzophenone	16.357	2.3	ng/ul	28965	3	15.018	247898	20.0
n-Hexadecanoic ...	18.590	3.1	ng/ul	51817	4	17.756	332766	20.0
Heptadecyl hept...	21.640	5.8	ng/ul	103061	5	22.063	353988	20.0
(DEL) Alkane: S...	24.524	2.5	ng/ul	42877	6	25.588	345583	20.0
(DEL) Alkane: S...	26.833	4.0	ng/ul	69509	6	25.588	345583	20.0
unknown-03	31.469	2.2	ng/ul	38087	6	25.588	345583	20.0