LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050423\
Data File : BG057309.D
Acq On : 4 May 2023 20:12
Operator : CG/JU
Sample : PB152587BL
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SBLK587

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-BG042823.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BG057309.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.093	91	94	108	rVB	31894	58432	11.25%	1.215%
2	5.350	306	308	310	rBV3	1225	895	0.17%	0.019%
3	5.503	332	334	336	rBV3	940	868	0.17%	0.018%
4	5.585	346	348	349	rBV	986	665	0.13%	0.014%
5	5.609	351	352	354	rBV	1500	1244	0.24%	0.026%
6	5.744	372	375	376	rBV3	1214	1009	0.19%	0.021%
7	6.325	473	474	476	rVB2	1074	695	0.13%	0.014%
8	6.490	500	502	504	rBV2	842	748	0.14%	0.016%
9	6.602	520	521	524	rBV3	557	666	0.13%	0.014%
10	6.919	572	575	578	rBV2	965	1449	0.28%	0.030%
11	6.978	583	585	588	rVV3	619	703	0.14%	0.015%
12	7.160	615	616	618	rBV2	654	564	0.11%	0.012%
13	7.307	639	641	644	rVB2	774	709	0.14%	0.015%
14	7.330	644	645	646	rBV	1174	639	0.12%	0.013%
15	7.512	669	676	684	rBV	49615	88580	17.06%	1.841%
16	7.677	697	704	713	rBV	37351	62492	12.03%	1.299%
17	7.900	735	742	749	rBV2	50824	86059	16.57%	1.789%
18	8.058	767	769	772	rVB4	527	630	0.12%	0.013%
19	8.376	816	823	829	rBV	43006	69963	13.47%	1.454%
20	8.822	896	899	902	rVB2	782	704	0.14%	0.015%
21	9.075	935	942	949	rBV	64753	112543	21.67%	2.340%
22	9.175	957	959	961	rBV	659	629	0.12%	0.013%
23	9.263	971	974	977	rVB3	588	747	0.14%	0.016%
24	9.292	977	979	981	rBV	494	574	0.11%	0.012%
25	9.445	1002	1005	1007	rVB	657	546	0.11%	0.011%
26	9.551	1016	1023	1033	rVB	52300	93514	18.01%	1.944%
27	9.633	1035	1037	1041	rVB	691	773	0.15%	0.016%
28	9.921	1084	1086	1088	rVB2	836	657	0.13%	0.014%
29	10.050	1105	1108	1110	rBV2	507	606	0.12%	0.013%
30	10.132	1119	1122	1125	rVB2	584	590	0.11%	0.012%
31	10.226	1135	1138	1139	rVB	622	576	0.11%	0.012%
32	10.279	1141	1147	1155	rVB2	44560	81210	15.64%	1.688%
33	10.755	1225	1228	1231	rBV2	608	888	0.17%	0.018%
34	10.825	1234	1240	1250	rBV2	63013	117342	22.59%	2.439%
35	11.043	1274	1277	1279	rBV2	578	751	0.14%	0.016%
36	11.213	1299	1306	1312	rVB	59795	108076	20.81%	2.247%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050423\
Data File : BG057309.D
Acq On : 4 May 2023 20:12
Operator : CG/JU
Sample : PB152587BL
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SBLK587

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-BG042823.MA.M
Title : SVOA CALIBRATION

37	11.342	1321	1328	1335	rBV	62807	118586	22.83%	2.465%
38	12.006	1438	1441	1442	rBV	684	700	0.13%	0.015%
39	12.599	1540	1542	1545	rBV	618	532	0.10%	0.011%
40	12.770	1568	1571	1577	rVB	1366	2083	0.40%	0.043%
41	13.210	1643	1646	1653	rVB	345	587	0.11%	0.012%
42	13.345	1664	1669	1674	rBV	298	602	0.12%	0.013%
43	13.839	1750	1753	1757	rBV3	1056	1383	0.27%	0.029%
44	14.368	1838	1843	1850	rBV	161410	234484	45.15%	4.875%
45	14.685	1891	1897	1904	rBV	170074	263467	50.73%	5.477%
46	14.984	1941	1948	1956	rVB	125958	197937	38.11%	4.115%
47	15.172	1975	1980	1993	rBV2	45688	92885	17.89%	1.931%
48	15.255	1993	1994	1997	rVV3	1566	1526	0.29%	0.032%
49	15.284	1997	1999	2002	rVV2	702	798	0.15%	0.017%
50	15.325	2005	2006	2011	rVB	464	553	0.11%	0.011%
51	15.971	2109	2116	2125	rVB	242407	354702	68.30%	7.374%
52	16.089	2131	2136	2145	rBV	56627	91508	17.62%	1.902%
53	17.504	2376	2377	2380	rBV	470	543	0.10%	0.011%
54	17.728	2408	2415	2422	rVB	199470	291194	56.07%	6.054%
55	17.828	2425	2432	2443	rBV	290510	438662	84.47%	9.119%
56	17.916	2444	2447	2451	rVB2	512	630	0.12%	0.013%
57	19.167	2655	2660	2662	rBV3	656	1149	0.22%	0.024%
58	19.326	2683	2687	2690	rVV3	814	754	0.15%	0.016%
59	19.537	2719	2723	2724	rBV3	684	765	0.15%	0.016%
60	19.578	2726	2730	2731	rBV2	802	881	0.17%	0.018%
61	19.625	2736	2738	2740	rBV2	1181	935	0.18%	0.019%
62	19.655	2740	2743	2747	rVV3	3657	5026	0.97%	0.104%
63	19.725	2751	2755	2761	rVB2	3955	5489	1.06%	0.114%
64	19.772	2761	2763	2764	rVB2	1240	716	0.14%	0.015%
65	19.795	2764	2767	2768	rBV2	951	1060	0.20%	0.022%
66	19.878	2778	2781	2782	rBV3	719	794	0.15%	0.017%
67	19.925	2787	2789	2791	rBV2	895	771	0.15%	0.016%
68	19.954	2791	2794	2796	rBV3	1507	1369	0.26%	0.028%
69	19.989	2798	2800	2802	rBV2	1301	922	0.18%	0.019%
70	20.007	2802	2803	2805	rBV2	917	721	0.14%	0.015%
71	20.089	2811	2817	2824	rVB	355822	519332	100.00%	10.796%
72	20.154	2827	2828	2831	rVB3	1488	993	0.19%	0.021%
73	20.195	2833	2835	2838	rBV3	1472	1612	0.31%	0.034%
74	20.254	2842	2845	2846	rBV3	1392	1377	0.27%	0.029%
75	20.312	2853	2855	2856	rBV2	1190	589	0.11%	0.012%
76	20.354	2860	2862	2864	rBV2	1162	983	0.19%	0.020%

LSC Area Percent Report

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Acq On : 4 May 2023 20:12
Operator : CG/JU
Sample : PB152587BL
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SBLK587

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-BG042823.MA.M
Title : SVOA CALIBRATION

77	20.383	2865	2867	2869	rBV4	1305	847	0.16%	0.018%
78	20.406	2869	2871	2873	rBV2	1374	1229	0.24%	0.026%
79	20.606	2903	2905	2906	rBV2	1954	1603	0.31%	0.033%
80	21.711	3089	3093	3098	rVB	13035	20216	3.89%	0.420%
81	22.040	3142	3149	3155	rVB2	174391	298058	57.39%	6.196%
82	23.661	3419	3425	3435	rVB6	11451	23494	4.52%	0.488%
83	24.777	3608	3615	3627	rVB6	16215	45071	8.68%	0.937%
84	25.041	3659	3660	3662	rBV2	3778	2440	0.47%	0.051%
85	25.312	3696	3706	3719	rVB2	154516	450193	86.69%	9.359%
86	25.552	3738	3747	3759	rVB2	93544	279445	53.81%	5.809%
87	25.699	3770	3772	3774	rBV3	3045	2537	0.49%	0.053%
88	26.157	3842	3850	3859	rVB5	18047	53019	10.21%	1.102%
89	26.904	3975	3977	3978	rBV2	2559	1431	0.28%	0.030%
90	27.068	4003	4005	4006	rBV2	2359	1584	0.31%	0.033%
91	27.879	4130	4143	4155	rBV6	18461	83621	16.10%	1.738%
92	28.401	4230	4232	4233	rBV2	2609	1993	0.38%	0.041%
93	28.877	4311	4313	4315	rBV3	2381	1569	0.30%	0.033%
94	29.465	4411	4413	4414	rBV2	2800	2257	0.43%	0.047%
95	30.845	4646	4648	4650	rBV3	2228	2312	0.45%	0.048%

Sum of corrected areas: 4810255

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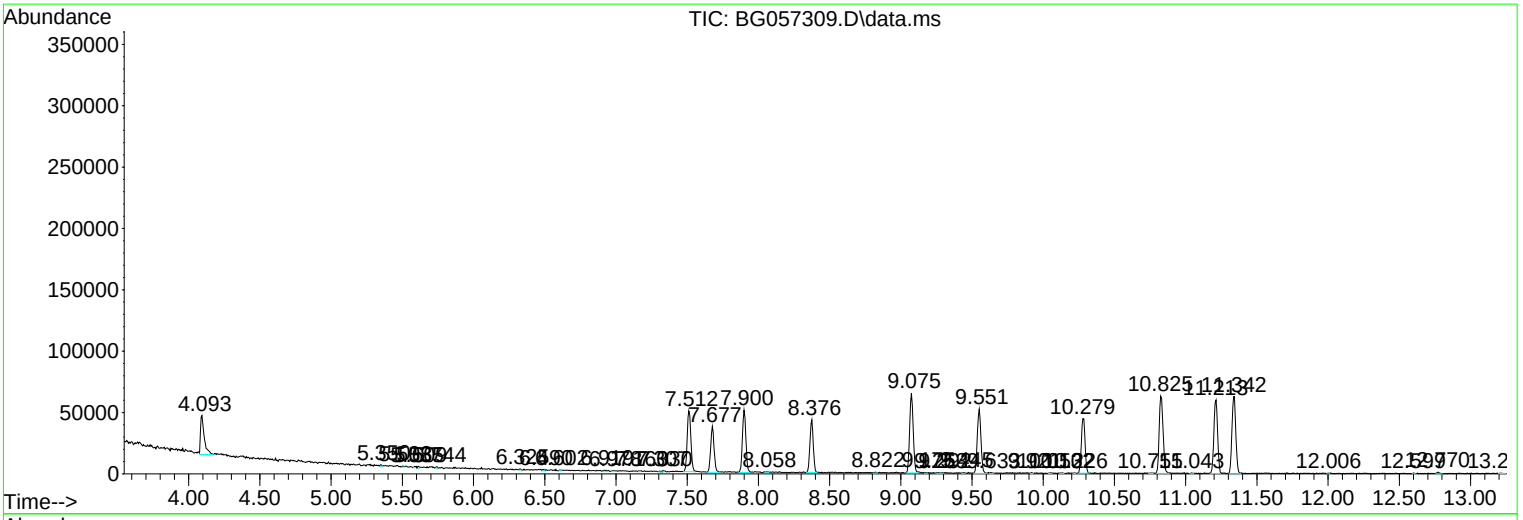
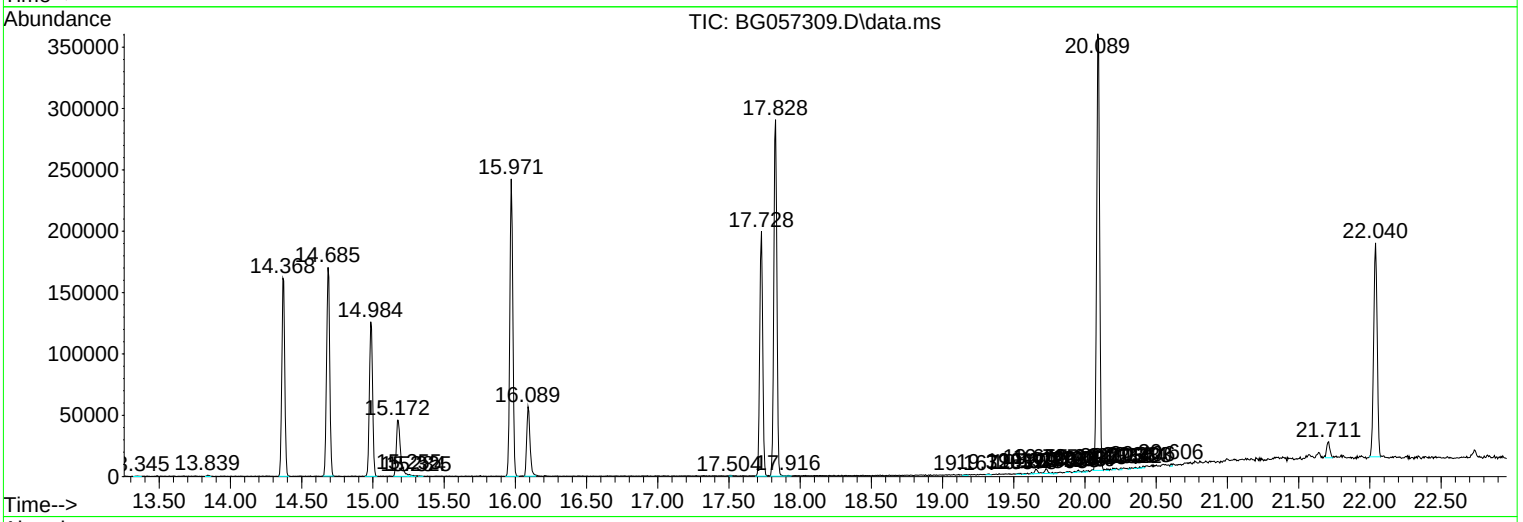
Acq On : 4 May 2023 20:12
Operator : CG/JU
Sample : PB152587BL
Misc :
ALS Vial : 14 Sample Multiplier: 1

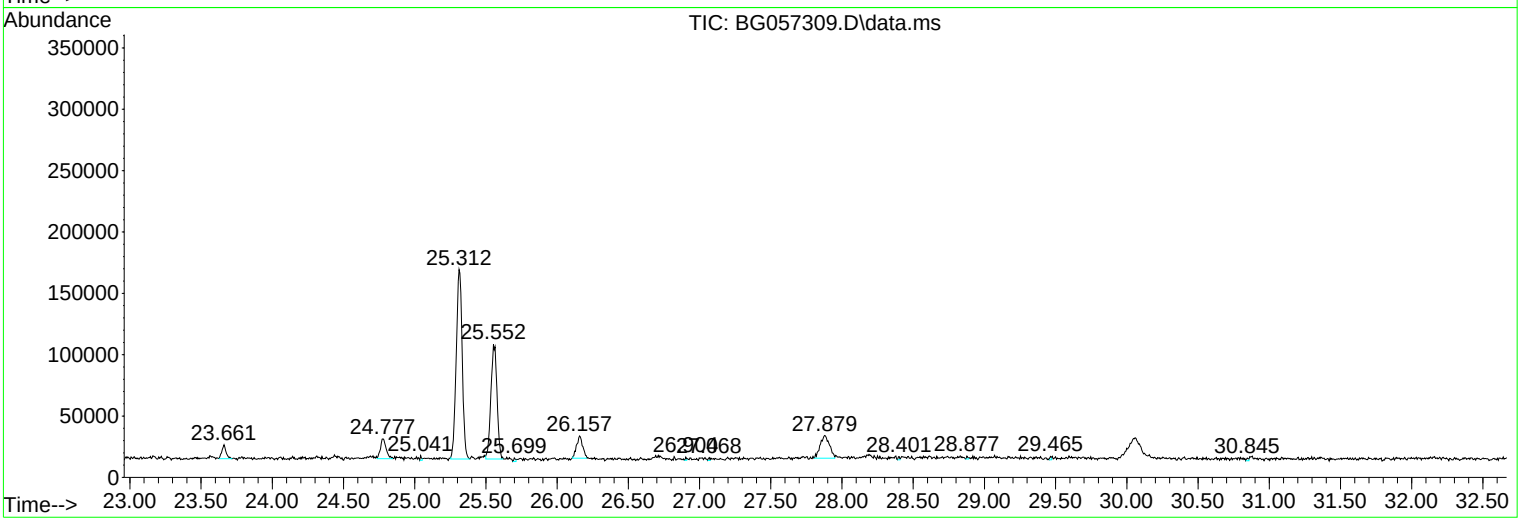
Instrument :
BNA_G
ClientSampleId :
SBLK587

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.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\BG050423\
Data File : BG057309.D
Acq On : 4 May 2023 20:12
Operator : CG/JU
Sample : PB152587BL
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Instrument :
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ClientSampleId :
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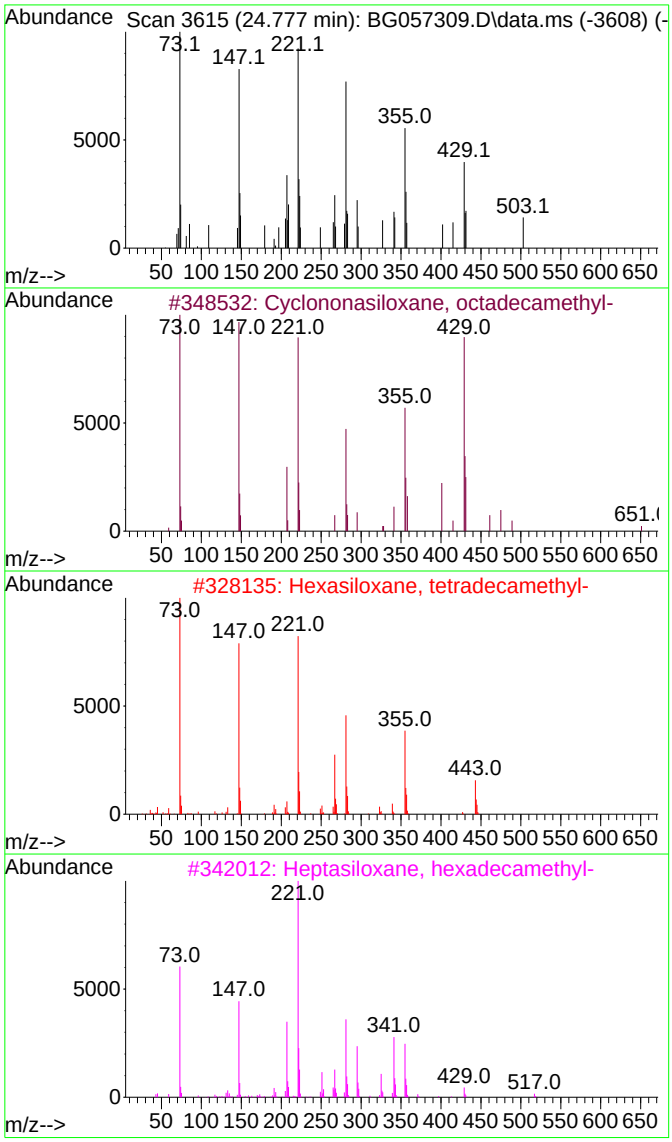
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

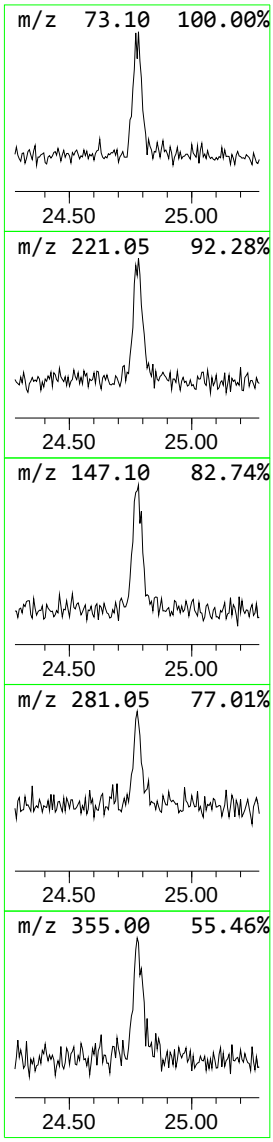
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cyclononasiloxane, octadeca... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.777	3.23 ng/ul	45071	Perylene-d12	25.558

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	64
2	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	38
3	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	37
4	1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	37
5	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050423\
Data File : BG057309.D
Acq On : 4 May 2023 20:12
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SBLK587

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

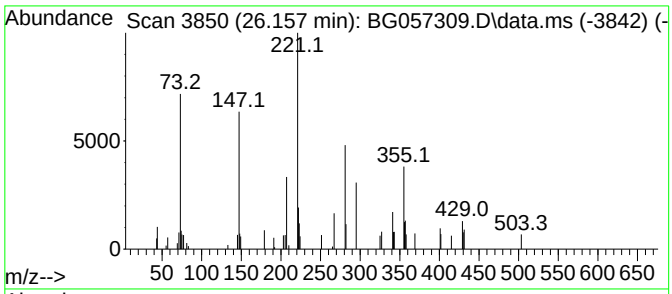
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

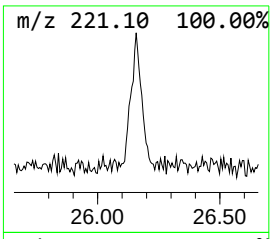
****

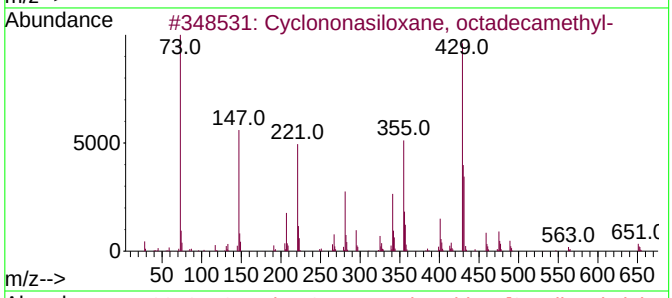
Peak Number 2 unknown-01 Concentration Rank 2

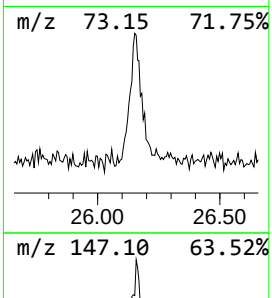
R.T.	EstConc	Area	Relative to ISTD	R.T.
26.157	3.79 ng/ul	53019	Perylene-d12	25.558

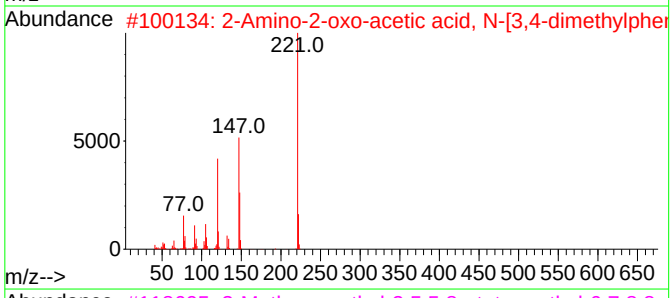
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	47
2	2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	32
3	3-Methoxymethyl-2,5,5,8a-tetrame...	236	C15H24O2	064201-73-6	27
4	.alpha.-Tetraloxime, 5,6-dimethoxy-	221	C12H15NO3	023923-10-6	25
5	4-Hydroxybenzyl alcohol, 2TBDMS ...	352	C19H36O2Si2	1000364-43-9	25

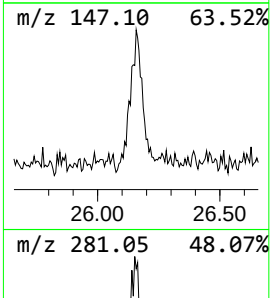


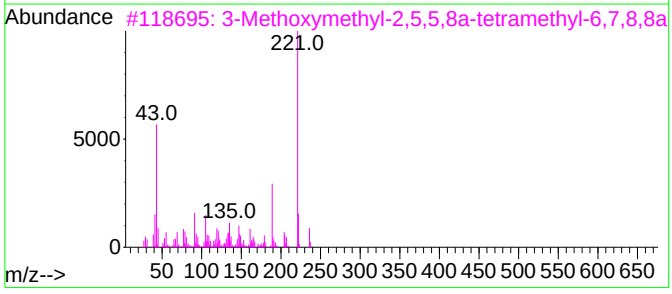


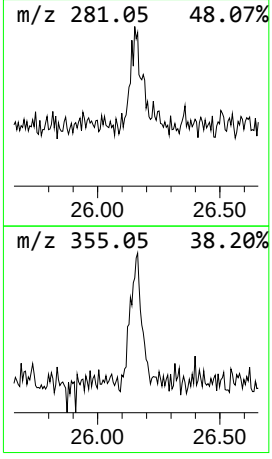












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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SBLK587

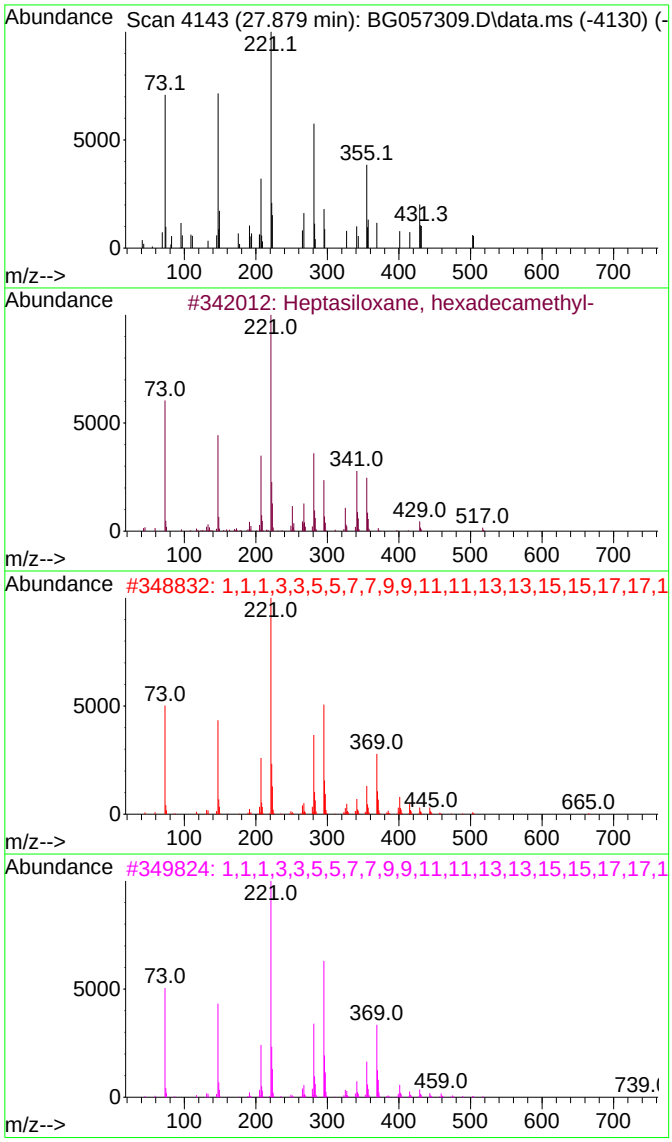
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

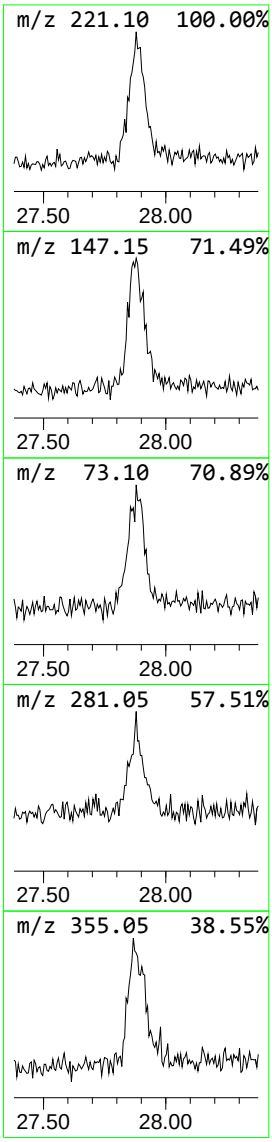
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Heptasiloxane, hexadecamethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.879	5.98 ng/ul	83621	Perylene-d12	25.558

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	53
2	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	680	C20H60O8Si9	002652-13-3	50
3	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	40
4	3,4-Bis-(methylthio)-quinoline	221	C11H11NS2	074579-34-3	25
5	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050423\
Data File : BG057309.D
Acq On : 4 May 2023 20:12
Operator : CG/JU
Sample : PB152587BL
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SBLK587

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.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
Cyclononasiloxa...	24.777	3.2	ng/ul	45071	6	25.558	279445	20.0
unknown-01	26.157	3.8	ng/ul	53019	6	25.558	279445	20.0
Heptasiloxane, ...	27.879	6.0	ng/ul	83621	6	25.558	279445	20.0