LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111521\
Data File : BG051038.D
Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

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-BG110321.M
Title : SVOA CALIBRATION

Signal : TIC: BG051038.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.854	558	573	581	rBV3	64421	171181	0.14%	0.058%
2	7.618	653	703	708	rBV3	12447530	122897213	100.00%	41.420%
3	7.741	718	724	729	rVV	1993016	2717201	2.21%	0.916%
4	7.800	729	734	744	rVB6	52940	147749	0.12%	0.050%
5	8.240	803	809	817	rVB	140106	249258	0.20%	0.084%
6	8.769	890	899	908	rVB	665284	1229193	1.00%	0.414%
7	8.946	922	929	934	rBV	81852	147436	0.12%	0.050%
8	9.004	934	939	945	rVV	186673	328971	0.27%	0.111%
9	9.075	945	951	969	rVB	144296	306442	0.25%	0.103%
10	9.416	1002	1009	1017	rVB	73127	136335	0.11%	0.046%
11	10.685	1218	1225	1233	rBV	73548	140831	0.11%	0.047%
12	10.814	1235	1247	1261	rBV5	47198	170335	0.14%	0.057%
13	10.973	1267	1274	1280	rBV	176278	347009	0.28%	0.117%
14	11.055	1282	1288	1296	rVB	220900	420119	0.34%	0.142%
15	11.184	1303	1310	1330	rBV2	50144	241512	0.20%	0.081%
16	11.619	1374	1384	1402	rBV	1652852	3714910	3.02%	1.252%
17	11.842	1402	1422	1427	rBV2	3593388	17810043	14.49%	6.003%
18	12.048	1441	1457	1493	rVB3	804305	5148995	4.19%	1.735%
19	12.389	1506	1515	1530	rVB	853952	1439268	1.17%	0.485%
20	13.094	1623	1635	1642	rBV2	103287	246840	0.20%	0.083%
21	13.240	1645	1660	1678	rVV	1395924	3630400	2.95%	1.224%
22	13.546	1699	1712	1733	rBV	1178533	2920507	2.38%	0.984%
23	14.104	1801	1807	1816	rBV	133433	262678	0.21%	0.089%
24	14.245	1824	1831	1838	rVB	154776	246590	0.20%	0.083%
25	14.551	1877	1883	1892	rVV	165999	277214	0.23%	0.093%
26	14.850	1927	1934	1943	rVB	350384	562434	0.46%	0.190%
27	15.832	2093	2101	2111	rBV	1215856	1909673	1.55%	0.644%
28	17.594	2391	2401	2409	rBV	393552	635145	0.52%	0.214%
29	17.694	2412	2418	2426	rBV	220416	358666	0.29%	0.121%
30	17.823	2436	2440	2449	rVB3	106852	204618	0.17%	0.069%
31	18.023	2467	2474	2478	rVV3	115376	257684	0.21%	0.087%
32	18.082	2480	2484	2491	rVV3	156735	283945	0.23%	0.096%
33	18.205	2501	2505	2511	rVV	216719	365142	0.30%	0.123%
34	18.458	2542	2548	2559	rBV	264178	467716	0.38%	0.158%
35	18.769	2589	2601	2610	rBV	3565425	6178412	5.03%	2.082%
36	19.045	2629	2648	2652	rBV	14404724	53060505	43.17%	17.883%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111521\
Data File : BG051038.D
Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

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-BG110321.M
Title : SVOA CALIBRATION

37	19.316	2688	2694	2702	rVV	857893	1675197	1.36%	0.565%
38	19.463	2702	2719	2728	rVV	14376372	49115023	39.96%	16.553%
39	19.533	2728	2731	2738	rVV3	182583	380530	0.31%	0.128%
40	19.633	2740	2748	2755	rVV	425938	1025139	0.83%	0.346%
41	19.721	2759	2763	2769	rVV2	179443	299431	0.24%	0.101%
42	19.786	2769	2774	2786	rVB3	305455	671443	0.55%	0.226%
43	19.980	2802	2807	2810	rBV	302711	441883	0.36%	0.149%
44	20.009	2810	2812	2816	rVB	117797	125664	0.10%	0.042%
45	20.144	2831	2835	2841	rVB	169607	227148	0.18%	0.077%
46	20.326	2860	2866	2870	rBV2	79740	164173	0.13%	0.055%
47	20.473	2885	2891	2893	rBV	357841	594055	0.48%	0.200%
48	20.585	2901	2910	2916	rBV5	175387	683994	0.56%	0.231%
49	20.655	2919	2922	2929	rVV3	223467	452610	0.37%	0.153%
50	20.714	2929	2932	2938	rVB2	117995	175422	0.14%	0.059%
51	20.802	2940	2947	2951	rBV2	135244	240657	0.20%	0.081%
52	20.926	2965	2968	2981	rVB5	106823	294592	0.24%	0.099%
53	21.296	3028	3031	3039	rVB3	105761	166197	0.14%	0.056%
54	21.431	3049	3054	3060	rBV	203763	439230	0.36%	0.148%
55	21.501	3060	3066	3069	rBV	218917	410606	0.33%	0.138%
56	21.590	3076	3081	3086	rVB	878784	1299497	1.06%	0.438%
57	21.648	3086	3091	3094	rVV	493644	792445	0.64%	0.267%
58	21.678	3094	3096	3110	rVB	427095	785216	0.64%	0.265%
59	21.901	3128	3134	3143	rVB2	347760	660375	0.54%	0.223%
60	22.107	3163	3169	3181	rVB	500539	1120167	0.91%	0.378%
61	23.411	3386	3391	3402	rVB4	78198	198324	0.16%	0.067%
62	25.062	3666	3672	3683	rVB2	113260	348924	0.28%	0.118%
63	25.303	3702	3713	3725	rVB2	193480	672107	0.55%	0.227%
64	25.438	3728	3736	3749	rVB2	107887	320314	0.26%	0.108%
65	26.454	3897	3909	3928	rBV4	283051	1364916	1.11%	0.460%
66	26.866	3968	3979	4002	rBV3	132619	677747	0.55%	0.228%
67	27.518	4078	4090	4117	rBV6	179660	1253307	1.02%	0.422%

Sum of corrected areas: 296708503

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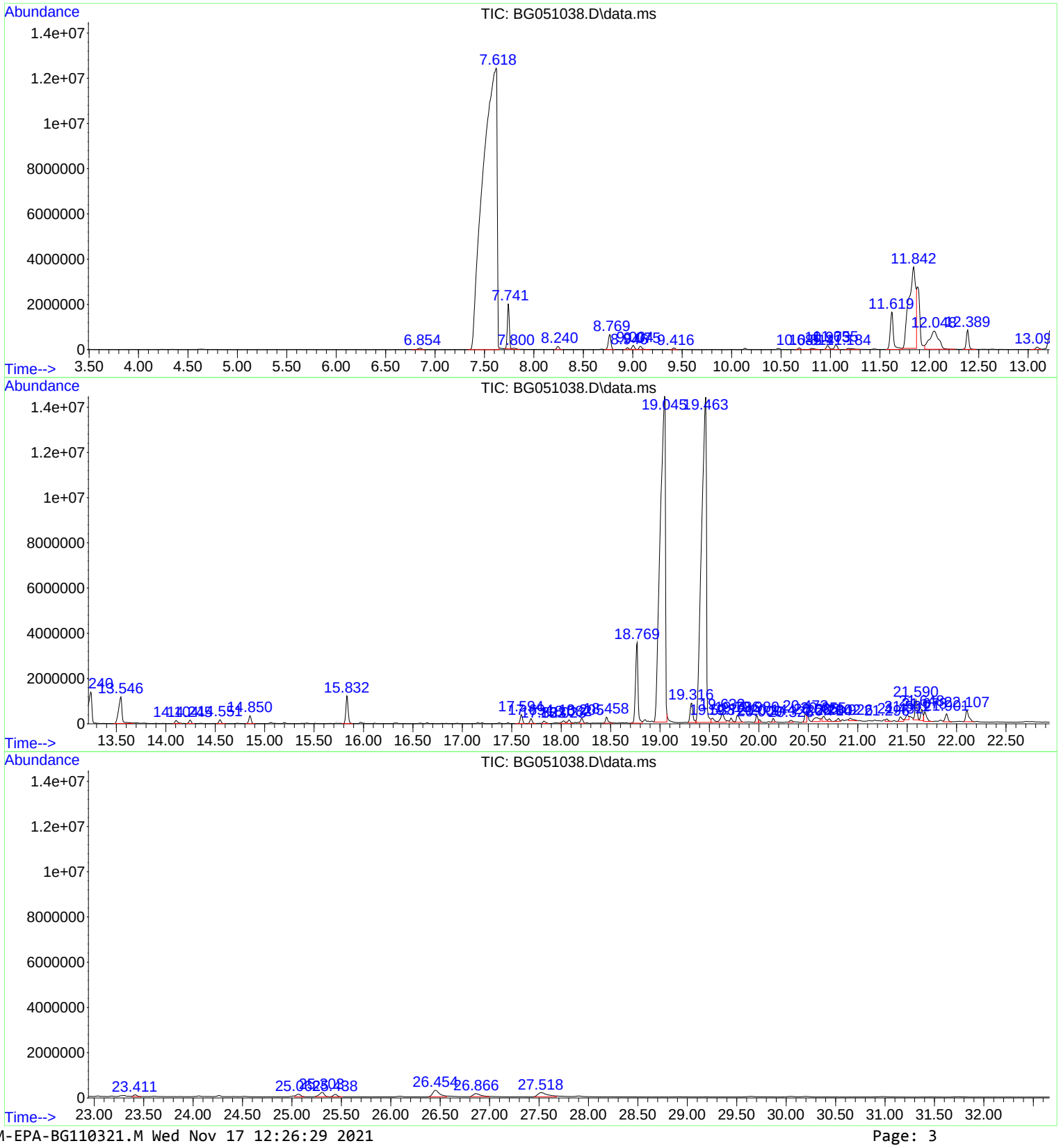
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

Quant Title :

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111521\
Data File : BG051038.D
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Operator : CG/JU
Sample : M4615-05
Misc :
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Instrument :
BNA_G
ClientSampleId :
C0V04

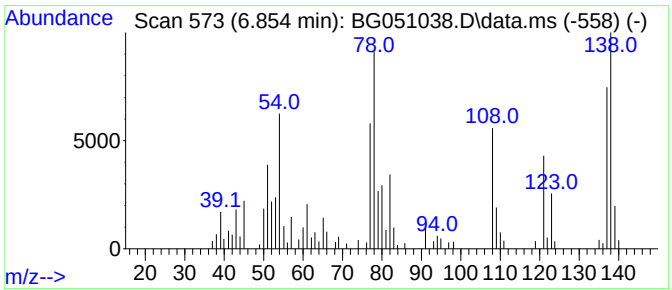
Quant Title :

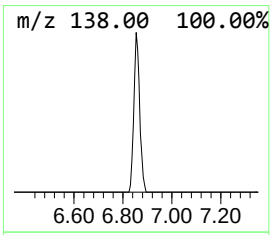
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

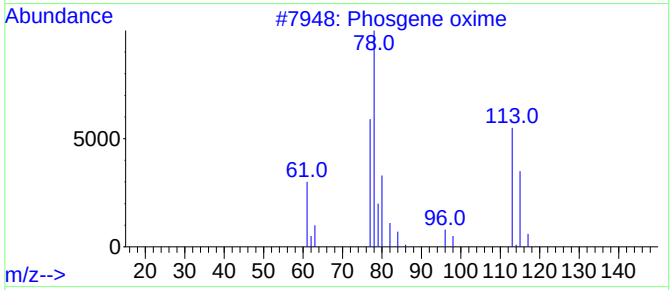
****
Peak Number 1 unknown-01 Concentration Rank 26

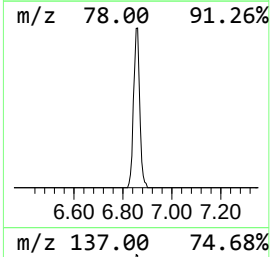
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.854	13.74 ng/ul	171181	1,4-Dichlorobenzene-d4	8.240

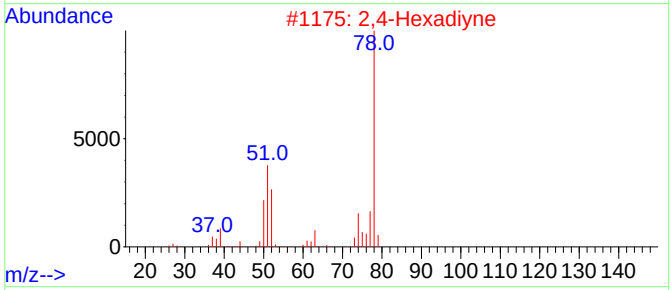
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosgene oxime	113	CHCl2NO	001794-86-1	47
2	2,4-Hexadiyne	78	C6H6	002809-69-0	46
3	Benzene	78	C6H6	000071-43-2	43
4	Benzenamine, N-hydroxy-N-nitroso-	138	C6H6N2O2	000148-97-0	43
5	Pyridine, 2-nitro-	124	C5H4N2O2	015009-91-3	38

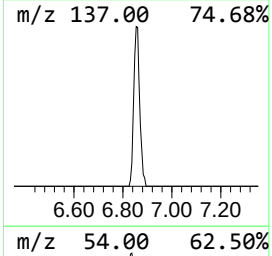


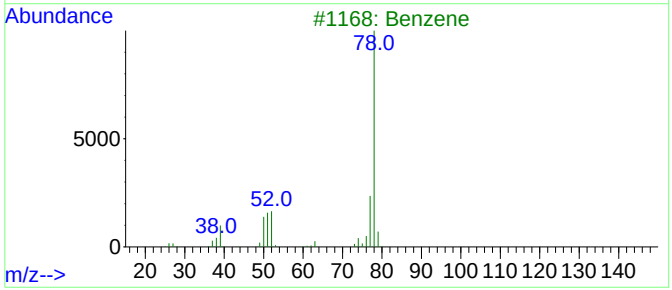


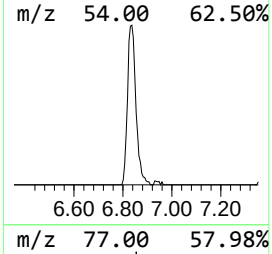


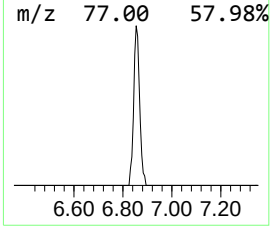












Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111521\
Data File : BG051038.D
Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

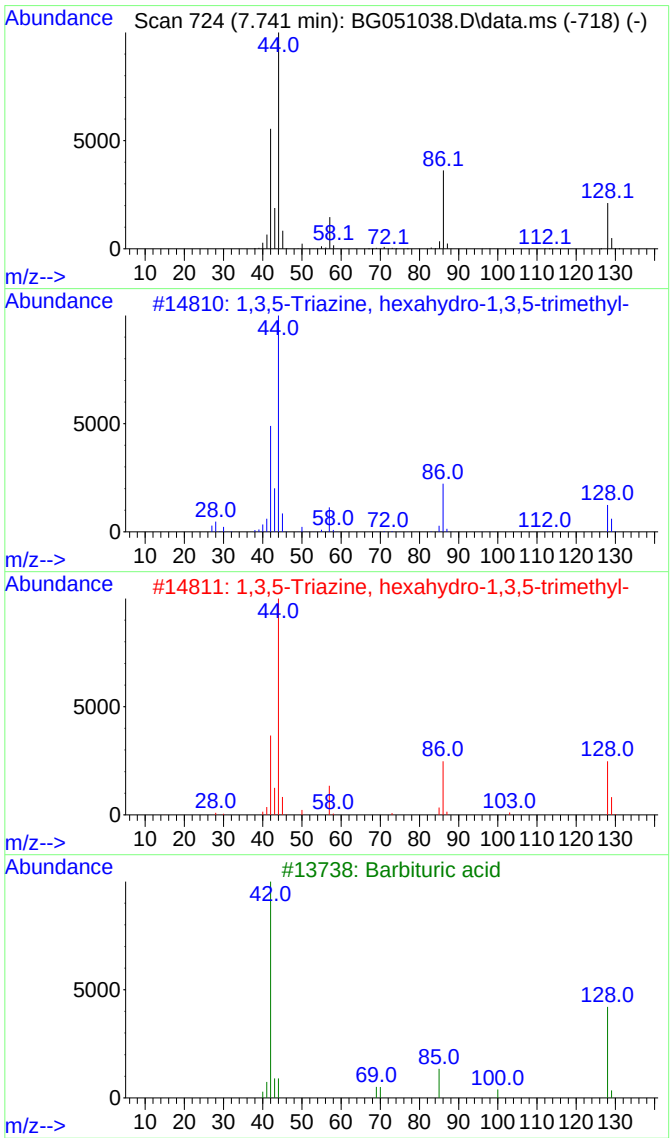
Quant Title :

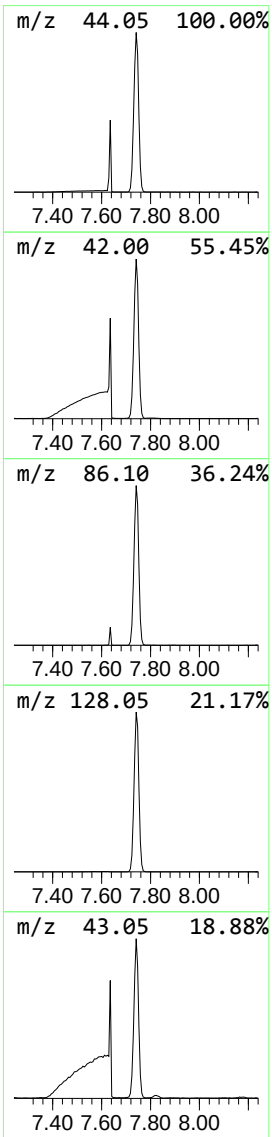
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1,3,5-Triazine, hexahydro-1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.741	218.02 ng/ul	2717200	1,4-Dichlorobenzene-d4	8.240

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine, hexahydro-1,3,5-...	129	C6H15N3	000108-74-7	80
2	1,3,5-Triazine, hexahydro-1,3,5-...	129	C6H15N3	000108-74-7	80
3	Barbituric acid	128	C4H4N2O3	000067-52-7	9
4	Piperazine	86	C4H10N2	000110-85-0	9
5	n-Butylethylenediamine	116	C6H16N2	019522-69-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111521\
Data File : BG051038.D
Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

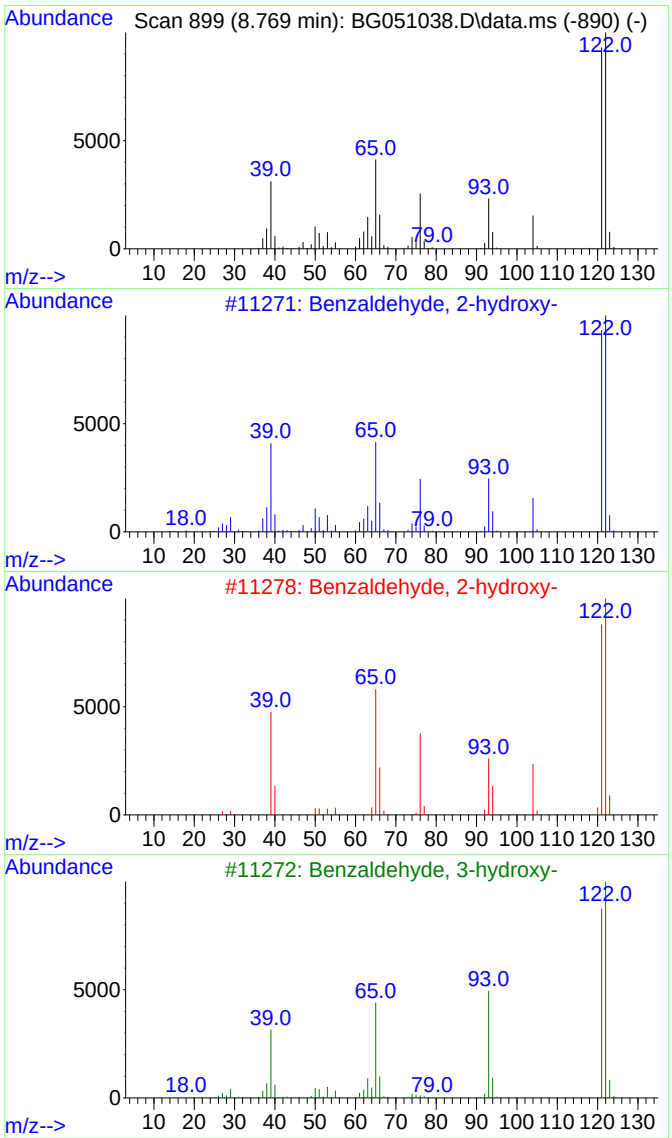
Quant Title :

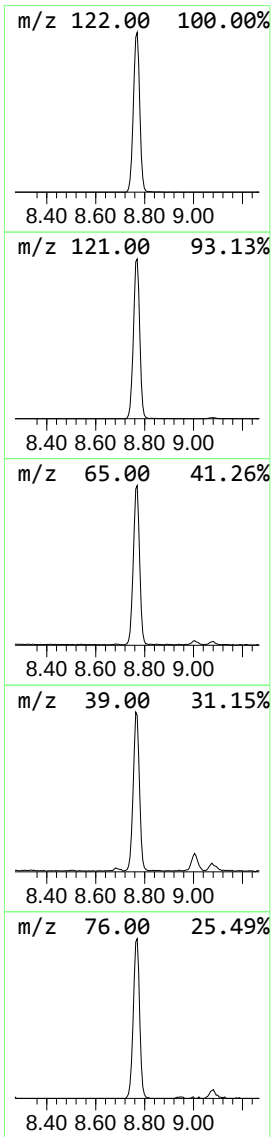
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzaldehyde, 2-hydroxy- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.769	98.63 ng/ul	1229190	1,4-Dichlorobenzene-d4	8.240

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 2-hydroxy-	122	C7H6O2	000090-02-8	96
2	Benzaldehyde, 2-hydroxy-	122	C7H6O2	000090-02-8	94
3	Benzaldehyde, 3-hydroxy-	122	C7H6O2	000100-83-4	93
4	Benzaldehyde, 3-hydroxy-	122	C7H6O2	000100-83-4	91
5	Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111521\
Data File : BG051038.D
Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

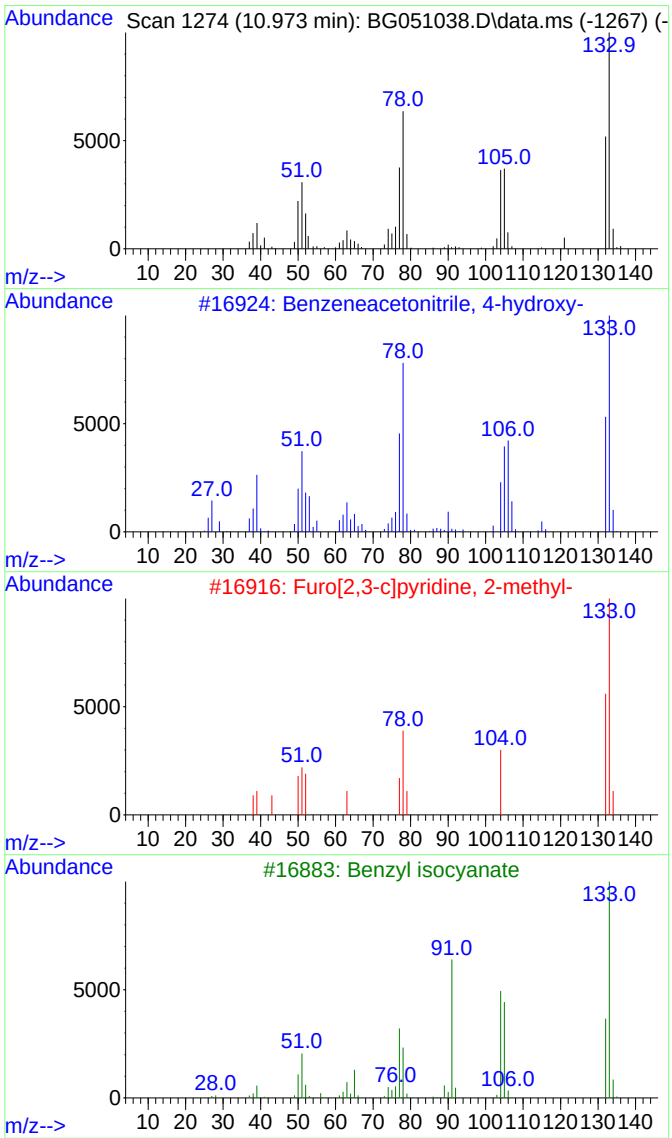
Quant Title :

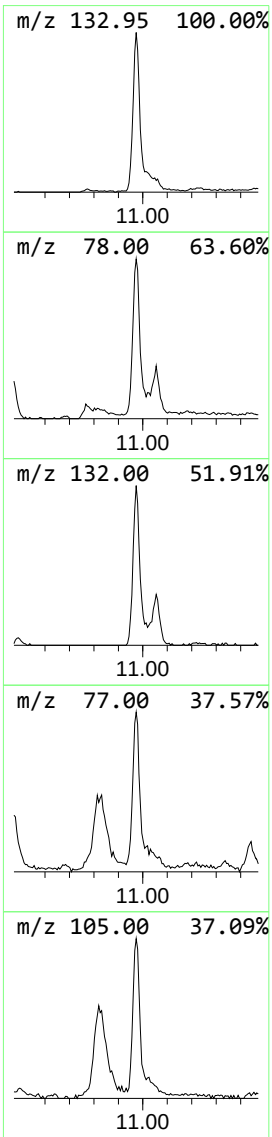
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzeneacetonitrile, 4-hydr... Concentration Rank 24

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.973	16.52 ng/ul	347009	Naphthalene-d8	11.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetonitrile, 4-hydroxy-	133	C8H7NO	014191-95-8	93
2	Furo[2,3-c]pyridine, 2-methyl-	133	C8H7NO	069022-76-0	74
3	Benzyl isocyanate	133	C8H7NO	003173-56-6	72
4	Benzene, 1-isocyanato-4-methyl-	133	C8H7NO	000622-58-2	72
5	Benzyl isocyanate	133	C8H7NO	003173-56-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111521\
Data File : BG051038.D
Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

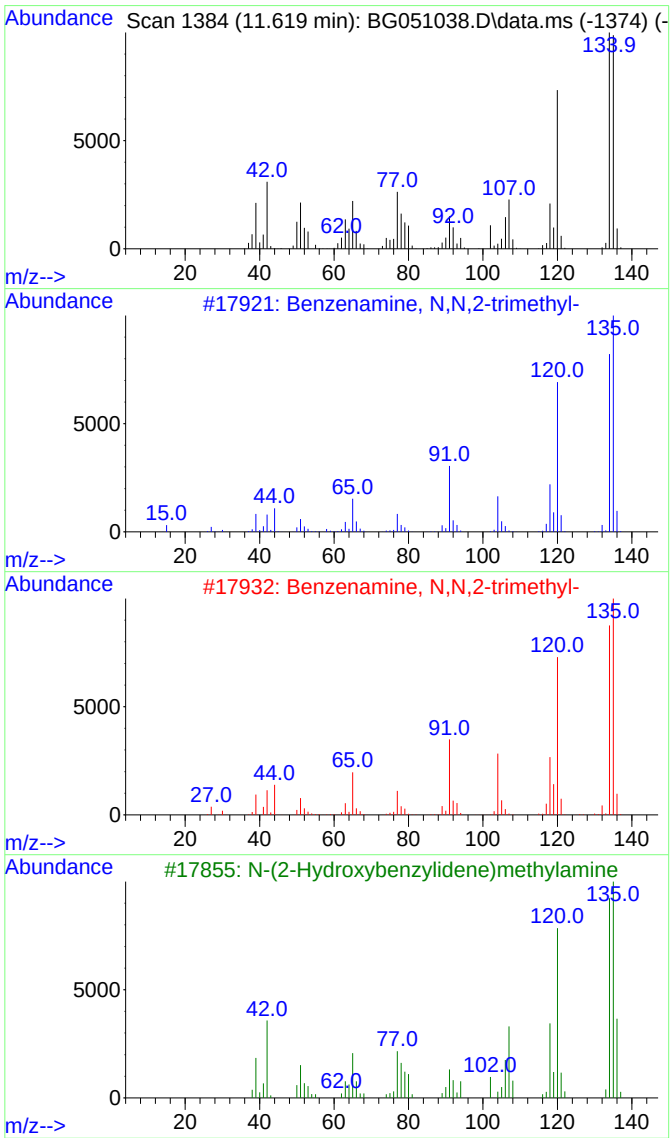
Quant Title :

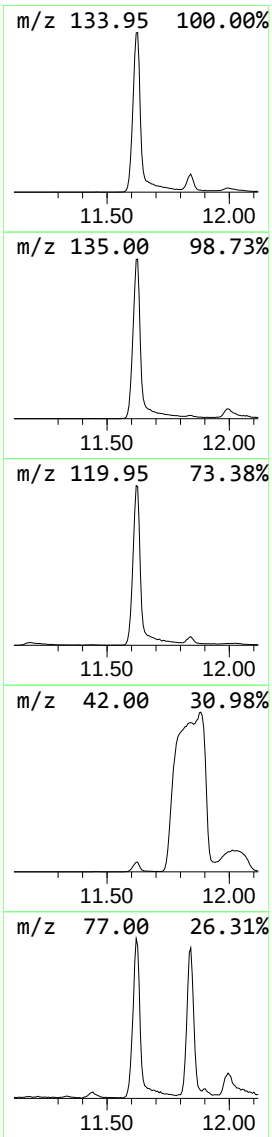
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzenamine, N,N,2-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.619	176.85 ng/ul	3714910	Naphthalene-d8	11.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, N,N,2-trimethyl-	135	C9H13N	000609-72-3	83
2	Benzenamine, N,N,2-trimethyl-	135	C9H13N	000609-72-3	80
3	N-(2-Hydroxybenzylidene)methylamine	135	C8H9NO	1000433-53-5	74
4	Furo[3,2-b]pyridine, 2,3-dihydro...	135	C8H9NO	069022-81-7	68
5	Benzenamine, N,N,2-trimethyl-	135	C9H13N	000609-72-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111521\
Data File : BG051038.D
Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

Quant Title :

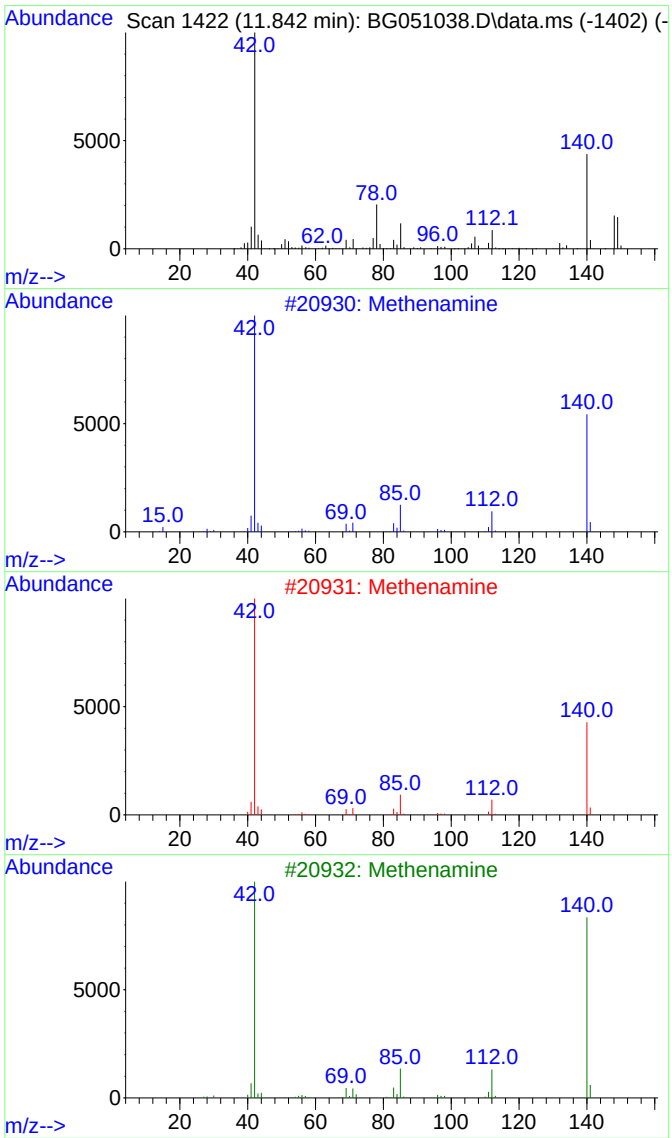
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

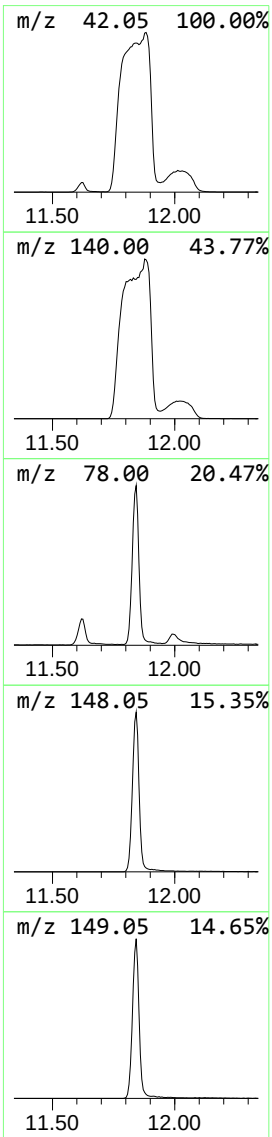
****

Peak Number 8 Methenamine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.842	847.86 ng/ul	17810000	Naphthalene-d8	11.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methenamine	140	C6H12N4	000100-97-0	94
2	Methenamine	140	C6H12N4	000100-97-0	93
3	Methenamine	140	C6H12N4	000100-97-0	76
4	Methenamine	140	C6H12N4	000100-97-0	76
5	Methenamine	140	C6H12N4	000100-97-0	68





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Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

Quant Title :

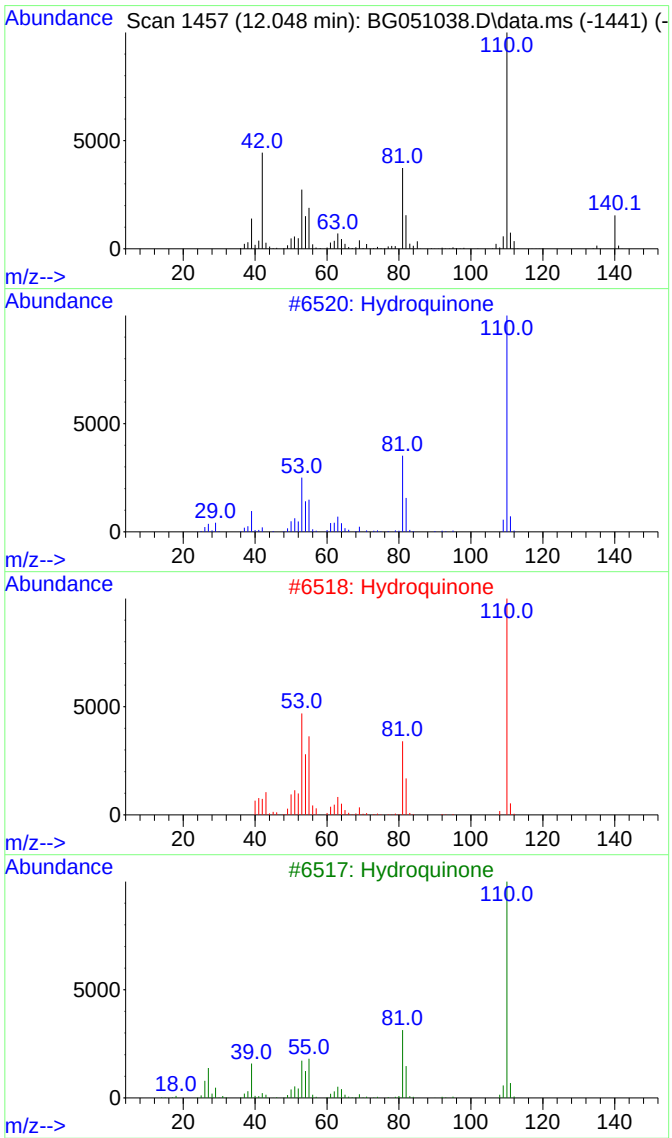
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

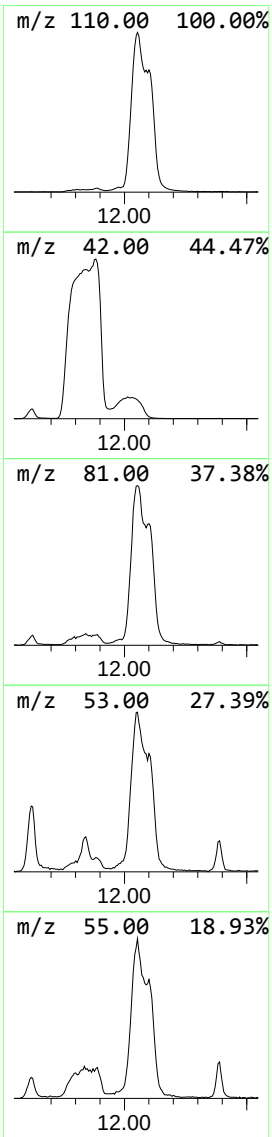
****

Peak Number 9 Hydroquinone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.048	245.12 ng/ul	5149000	Naphthalene-d8	11.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydroquinone	110	C6H6O2	000123-31-9	83
2	Hydroquinone	110	C6H6O2	000123-31-9	64
3	Hydroquinone	110	C6H6O2	000123-31-9	60
4	1-(Dimethylamino)pyrrole	110	C6H10N2	078307-76-3	59
5	4(1H)-Pyrimidinone, 6-methyl-	110	C5H6N2O	003524-87-6	53





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Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

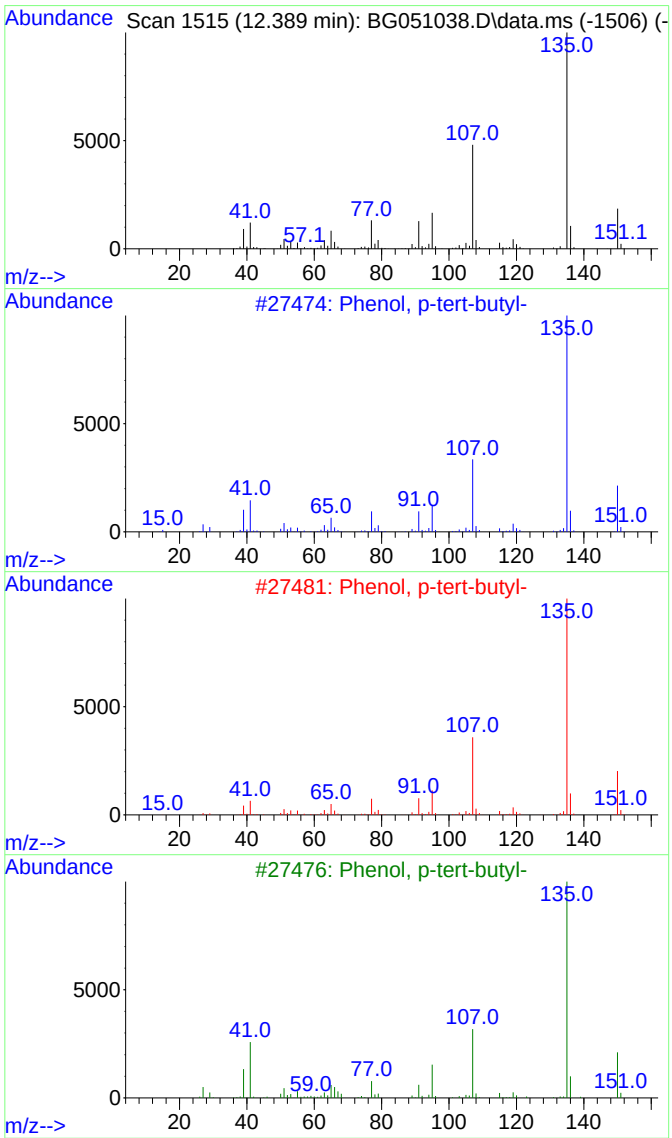
Quant Title :

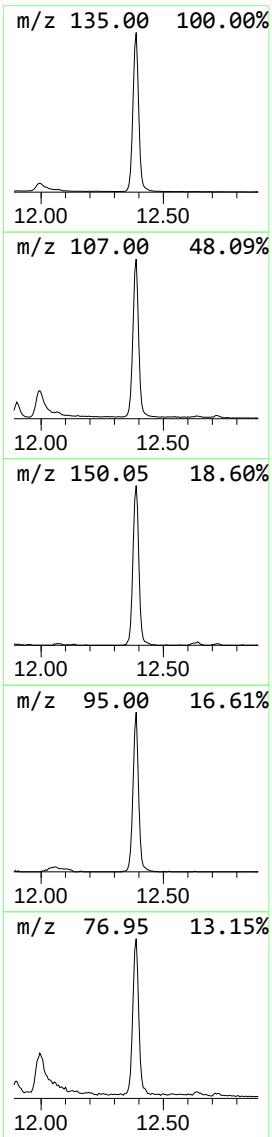
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phenol, p-tert-butyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.389	68.52 ng/ul	1439270	Naphthalene-d8	11.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	95
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	95
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	91
4	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	91
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	86





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Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

Quant Title :

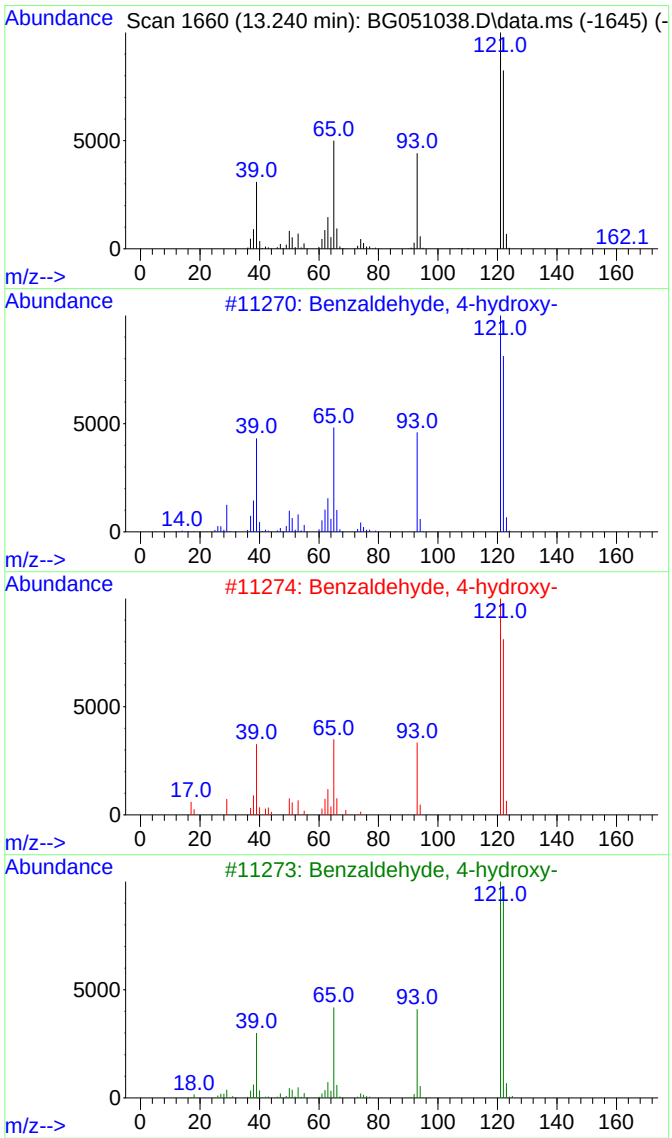
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

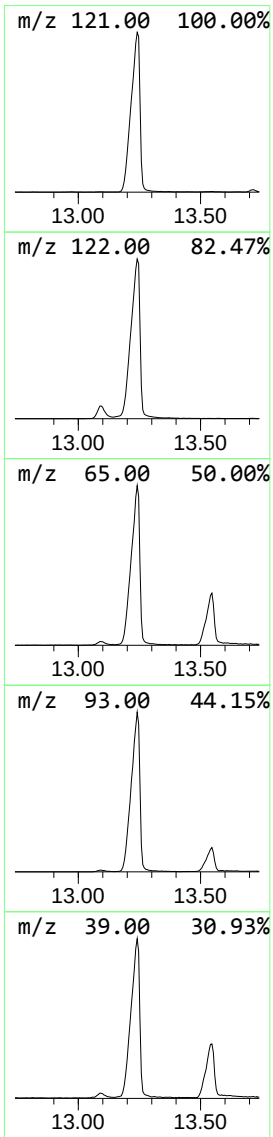
****

Peak Number 12 Benzaldehyde, 4-hydroxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.241	129.10 ng/ul	3630400	Acenaphthene-d10	14.850

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	98
2	Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	97
3	Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	95
4	Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	94
5	Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	94





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Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

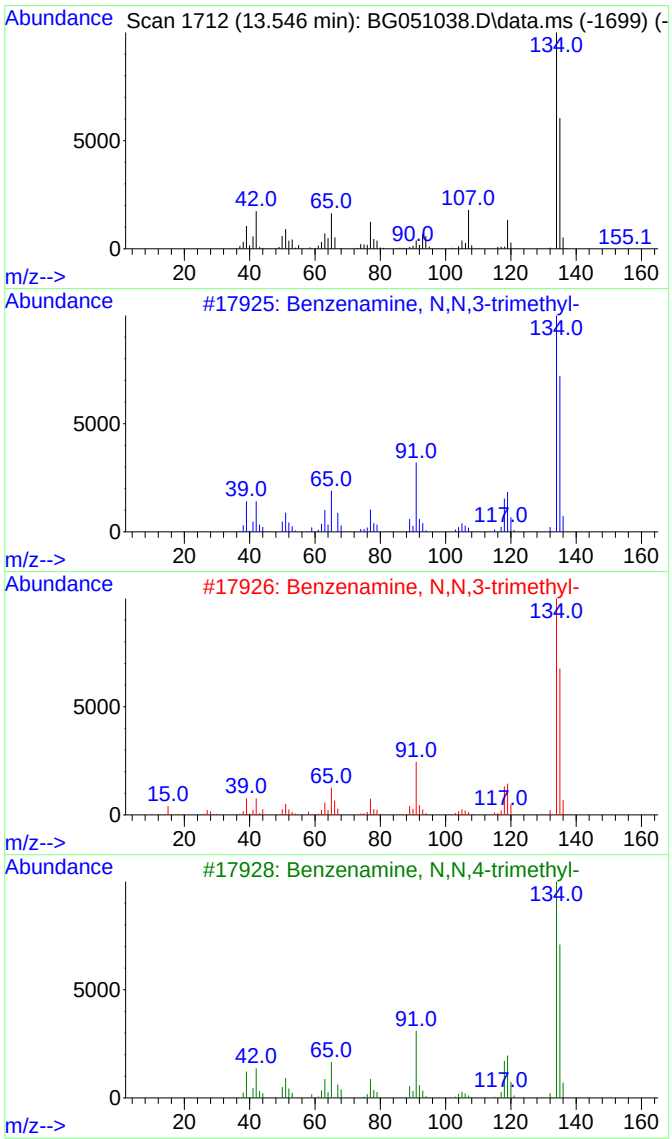
Quant Title :

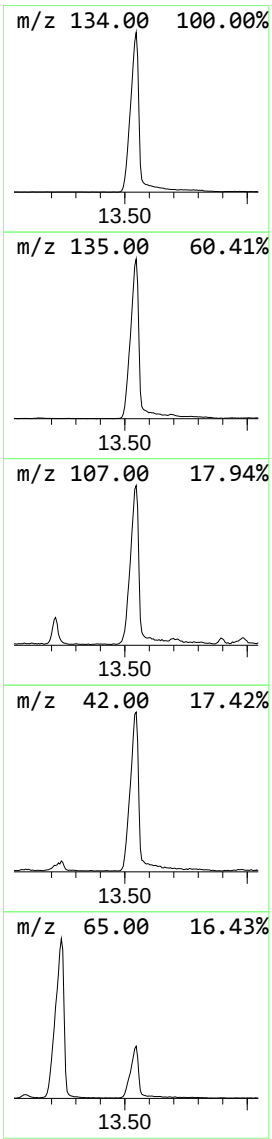
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Benzenamine, N,N,3-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.546	103.85 ng/ul	2920510	Acenaphthene-d10	14.850

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, N,N,3-trimethyl-	135	C9H13N	000121-72-2	83
2	Benzenamine, N,N,3-trimethyl-	135	C9H13N	000121-72-2	72
3	Benzenamine, N,N,4-trimethyl-	135	C9H13N	000099-97-8	72
4	Pyridine, 2-ethyl-4,6-dimethyl-	135	C9H13N	001124-35-2	72
5	Pyridine, 2,6-diethyl-	135	C9H13N	000935-28-4	64





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Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

Quant Title :

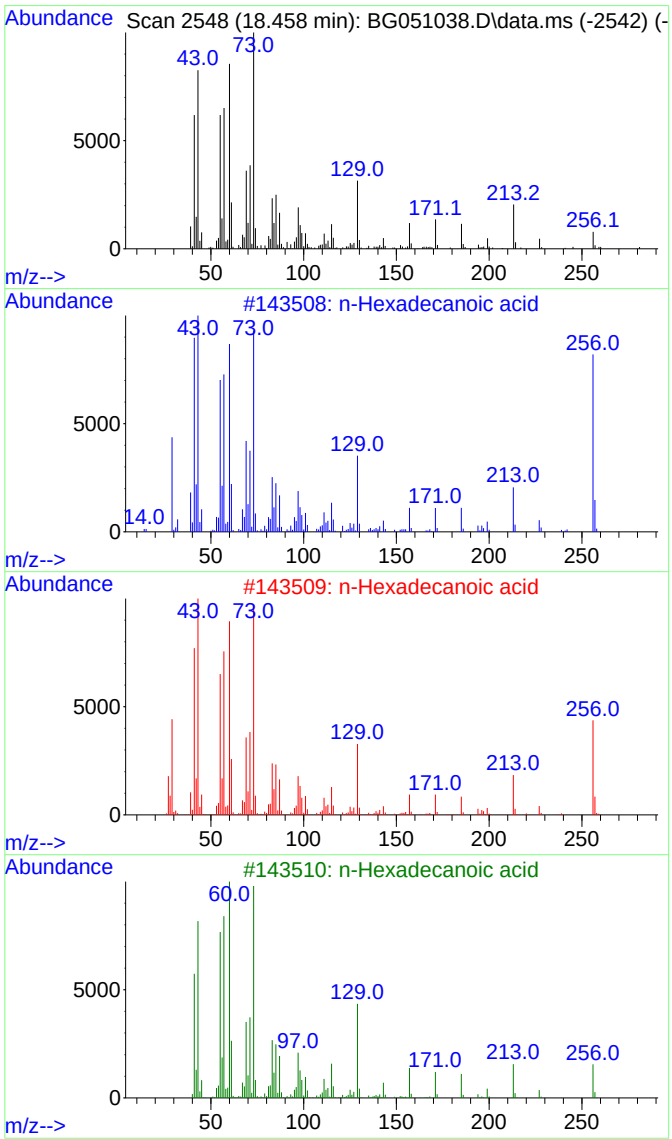
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

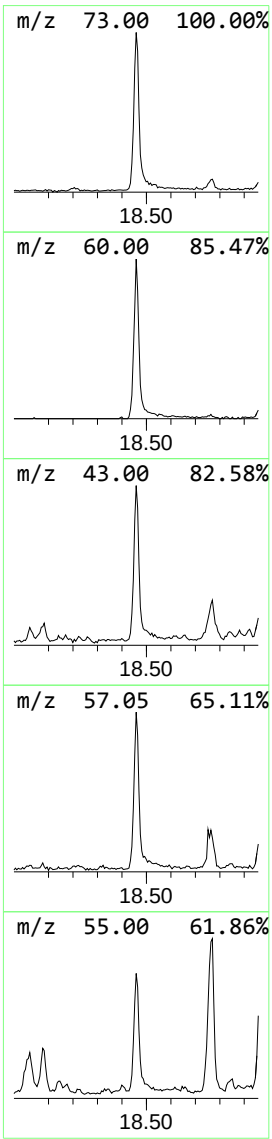
****

Peak Number 19 n-Hexadecanoic acid Concentration Rank 25

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.458	14.73 ng/ul	467716	Phenanthrene-d10	17.594

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	81





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Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

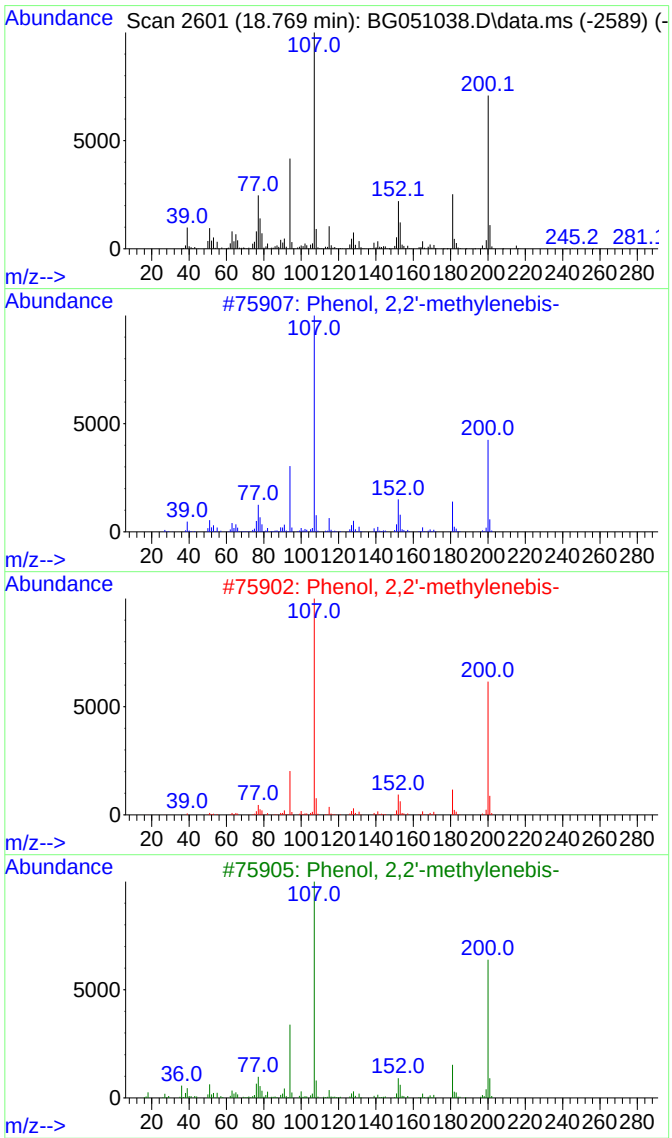
Quant Title :

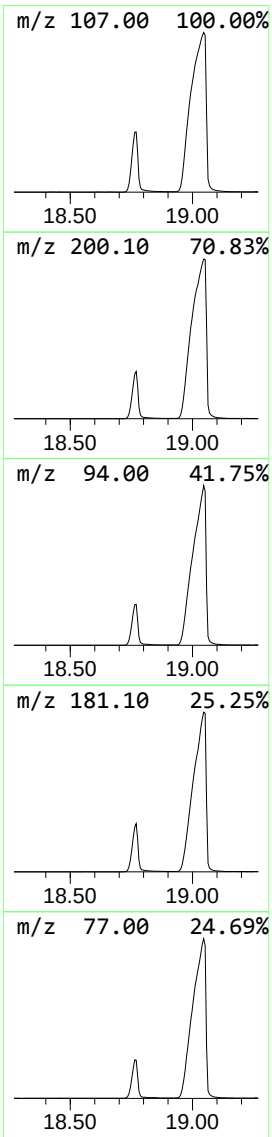
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 Phenol, 2-[(4-hydroxyphenyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.769	194.55 ng/ul	6178410	Phenanthrene-d10	17.594

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,2'-methylenebis-	200	C13H12O2	002467-02-9	97
2	Phenol, 2,2'-methylenebis-	200	C13H12O2	002467-02-9	95
3	Phenol, 2,2'-methylenebis-	200	C13H12O2	002467-02-9	95
4	Phenol, 2-[(4-hydroxyphenyl)meth...	200	C13H12O2	002467-03-0	90
5	Phenol, 2-[(4-hydroxyphenyl)meth...	200	C13H12O2	002467-03-0	87





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Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

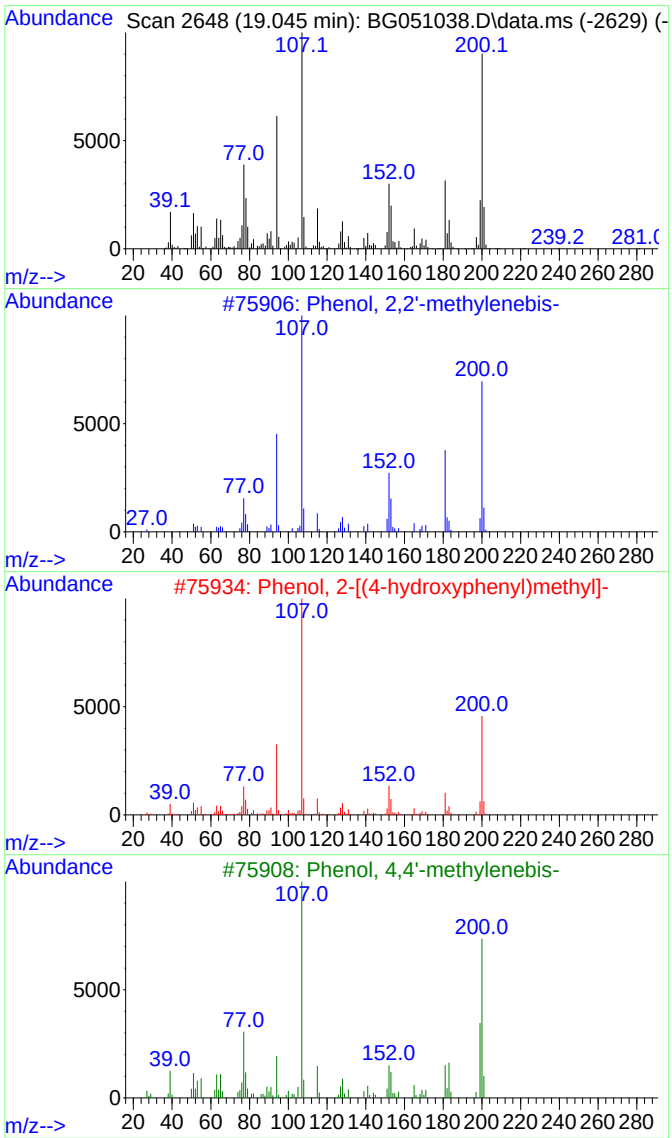
Quant Title :

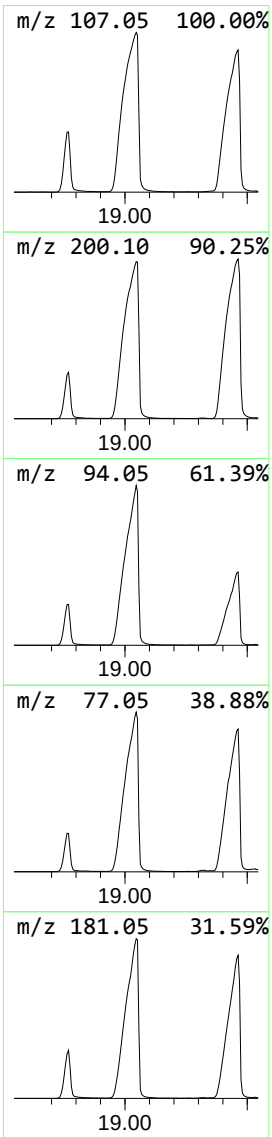
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 21 Phenol, 2,2'-methylenebis- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.045	1670.82 ng/ul	53060500	Phenanthrene-d10	17.594

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,2'-methylenebis-	200	C13H12O2	002467-02-9	89
2	Phenol, 2-[(4-hydroxyphenyl)meth...	200	C13H12O2	002467-03-0	83
3	Phenol, 4,4'-methylenebis-	200	C13H12O2	000620-92-8	76
4	Phenol, 2-[(4-hydroxyphenyl)meth...	200	C13H12O2	002467-03-0	70
5	Phenol, 2,2'-methylenebis-	200	C13H12O2	002467-02-9	60





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Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

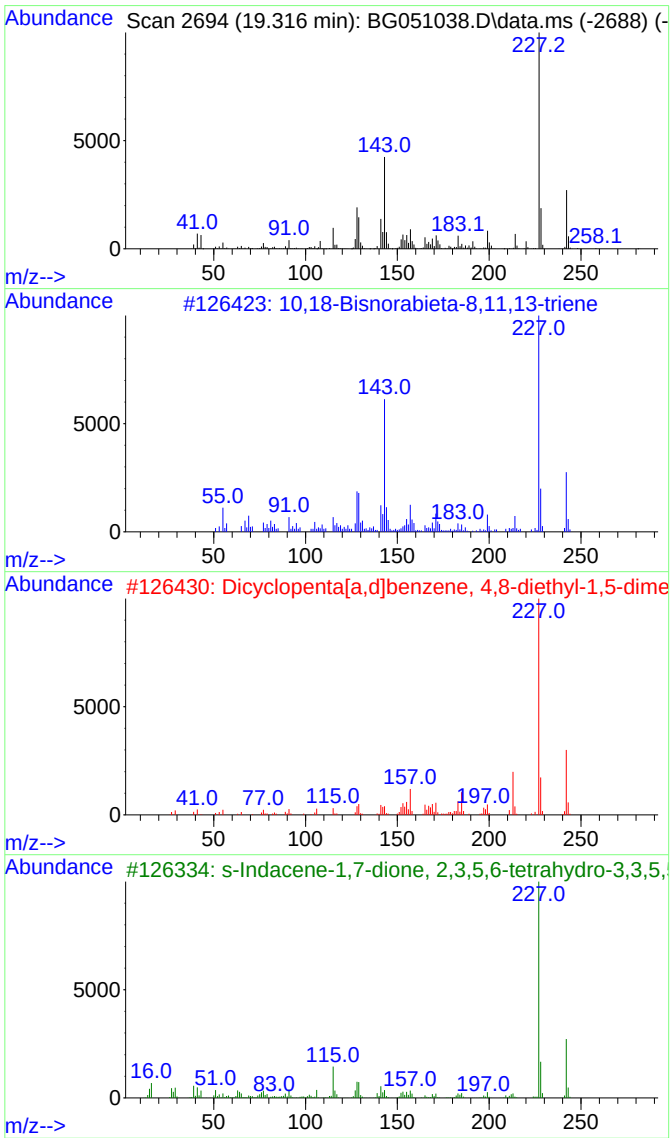
Quant Title :

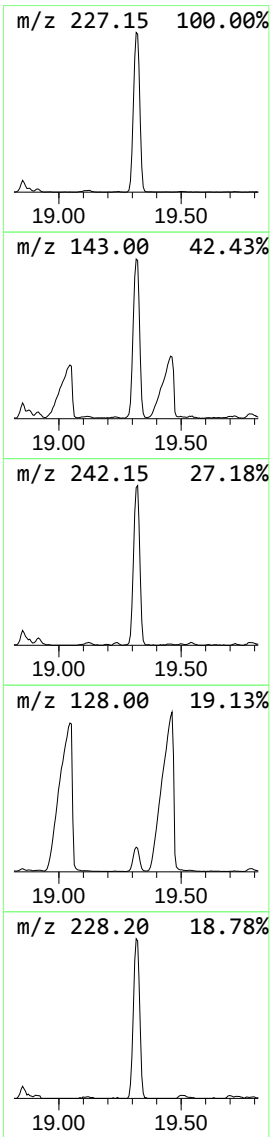
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 22 10,18-Bisnorabieta-8,11,13-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.316	52.75 ng/ul	1675200	Phenanthrene-d10	17.594

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,18-Bisnorabieta-8,11,13-triene	242	C18H26	032624-67-2	93
2	Dicyclopenta[a,d]benzene, 4,8-di...	242	C18H26	1000156-41-6	60
3	s-Indacene-1,7-dione, 2,3,5,6-te...	242	C16H18O2	055591-17-8	49
4	Lapachol	242	C15H14O3	000084-79-7	49
5	1,4-Naphthalenedione, 2-hydroxy-...	242	C15H14O3	004042-39-1	46





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Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

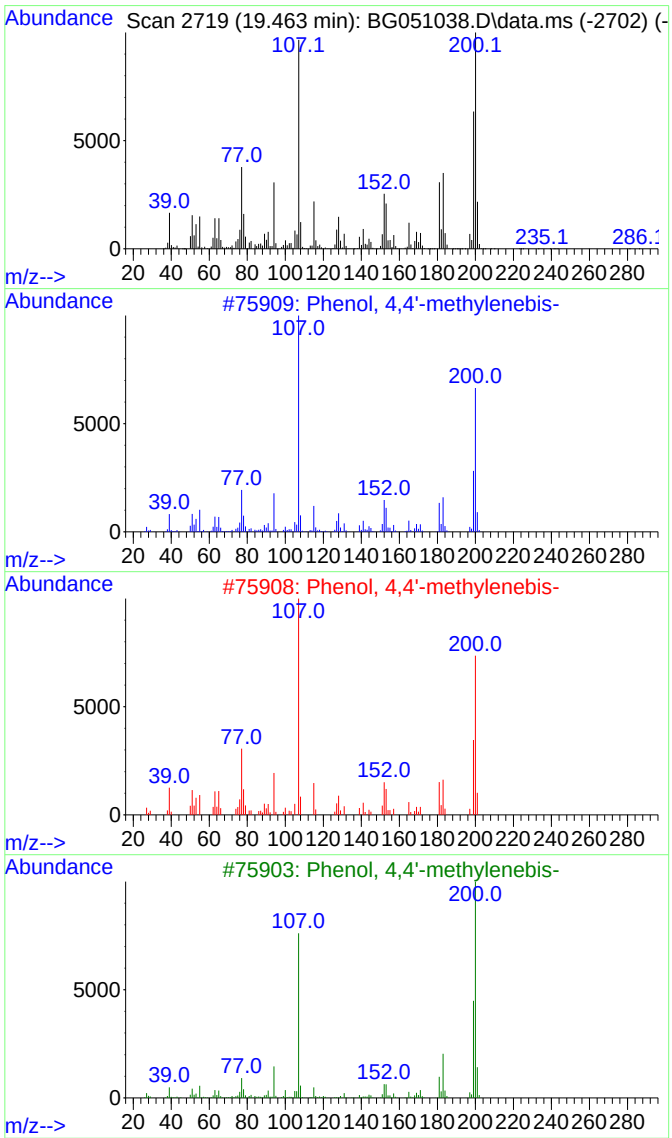
Quant Title :

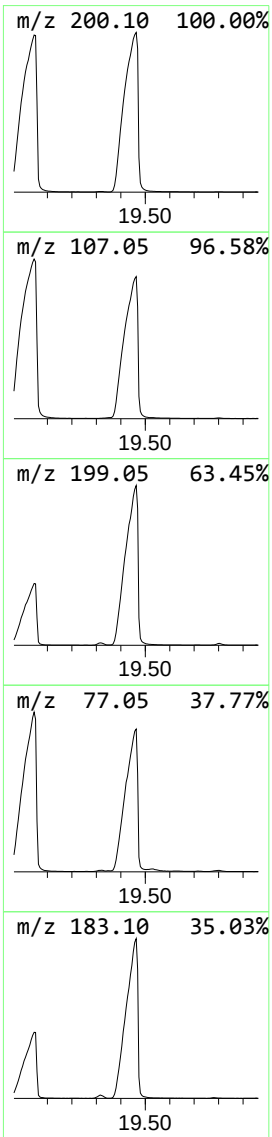
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 23 Phenol, 4,4'-methylenebis- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.463	1546.58 ng/ul	49115000	Phenanthrene-d10	17.594

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-methylenebis-	200	C13H12O2	000620-92-8	93
2	Phenol, 4,4'-methylenebis-	200	C13H12O2	000620-92-8	91
3	Phenol, 4,4'-methylenebis-	200	C13H12O2	000620-92-8	74
4	Phenol, 2-[(4-hydroxyphenyl)meth...	200	C13H12O2	002467-03-0	58
5	Phenol, 2,2'-methylenebis-	200	C13H12O2	002467-02-9	55





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Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

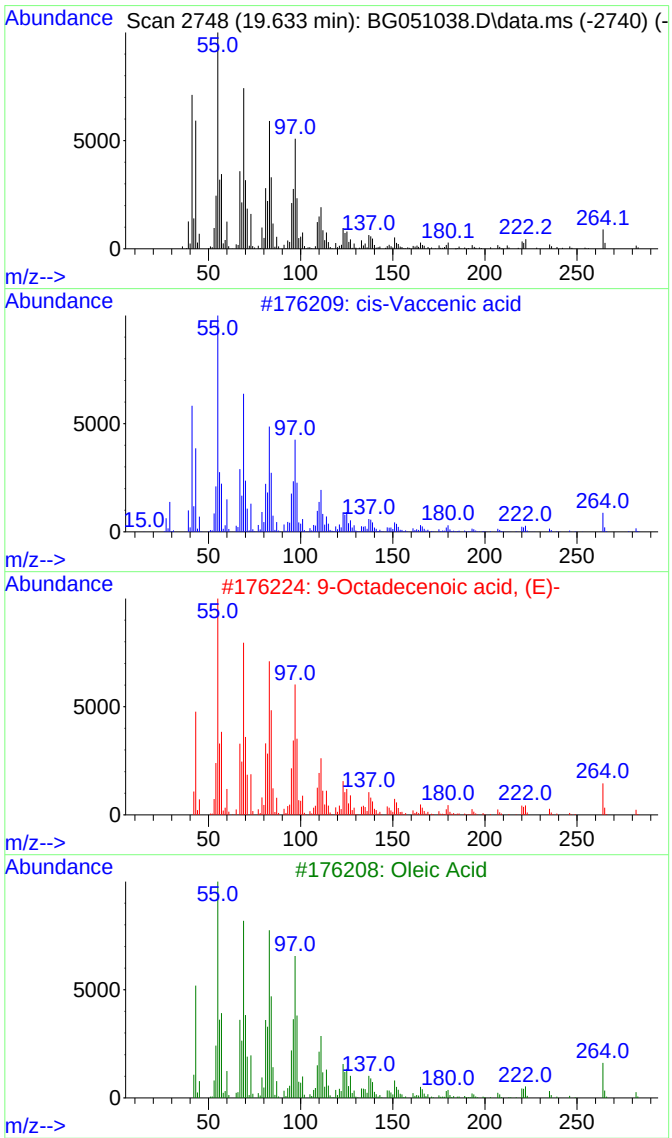
Quant Title :

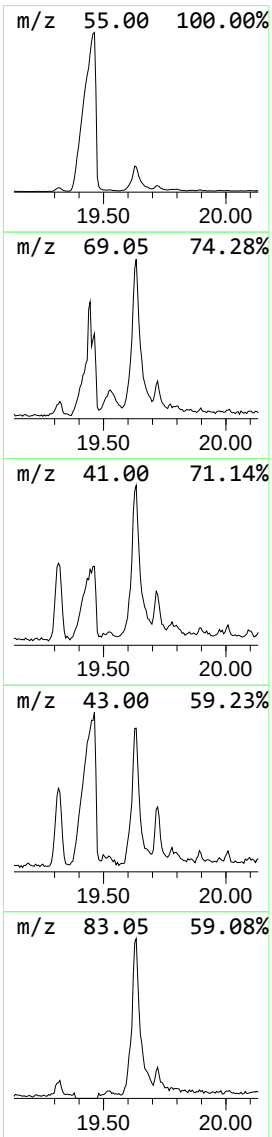
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 25 cis-Vaccenic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.633	32.28 ng/ul	1025140	Phenanthrene-d10	17.594

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Vaccenic acid	282	C18H34O2	000506-17-2	99
2	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	99
3	Oleic Acid	282	C18H34O2	000112-80-1	99
4	6-Octadecenoic acid	282	C18H34O2	1000336-66-8	99
5	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	97





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Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

Quant Title :

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

****

Peak Number 26 Octadecanoic acid Concentration Rank 34

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.721	9.43 ng/ul	299431	Phenanthrene-d10	17.594

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Octadecanoic acid	284	C18H36O2	000057-11-4	95
3	Octadecanoic acid	284	C18H36O2	000057-11-4	92
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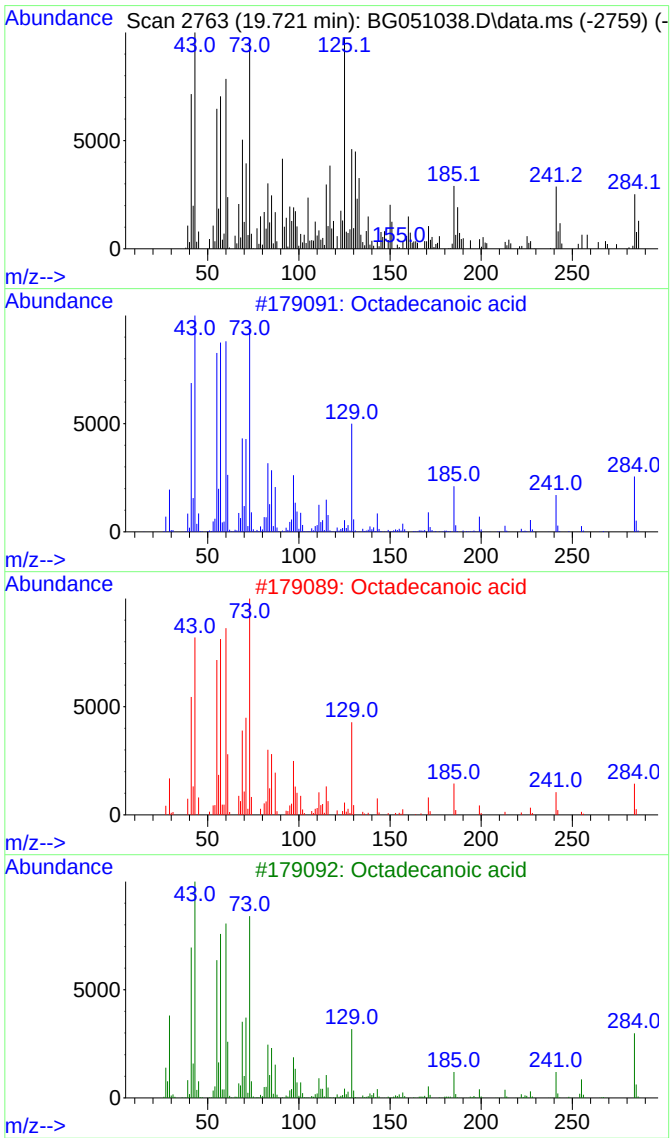

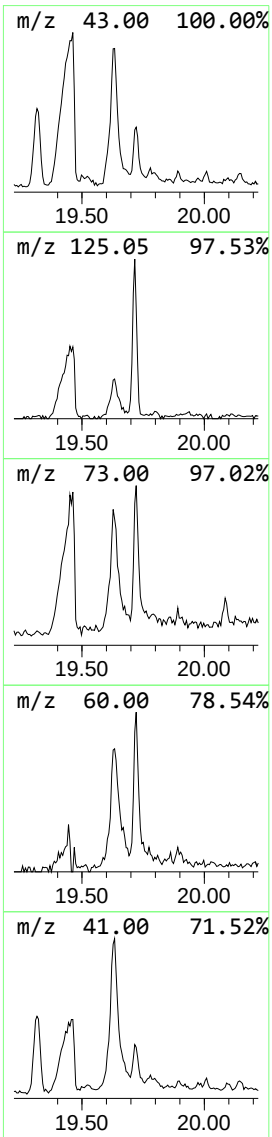

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Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

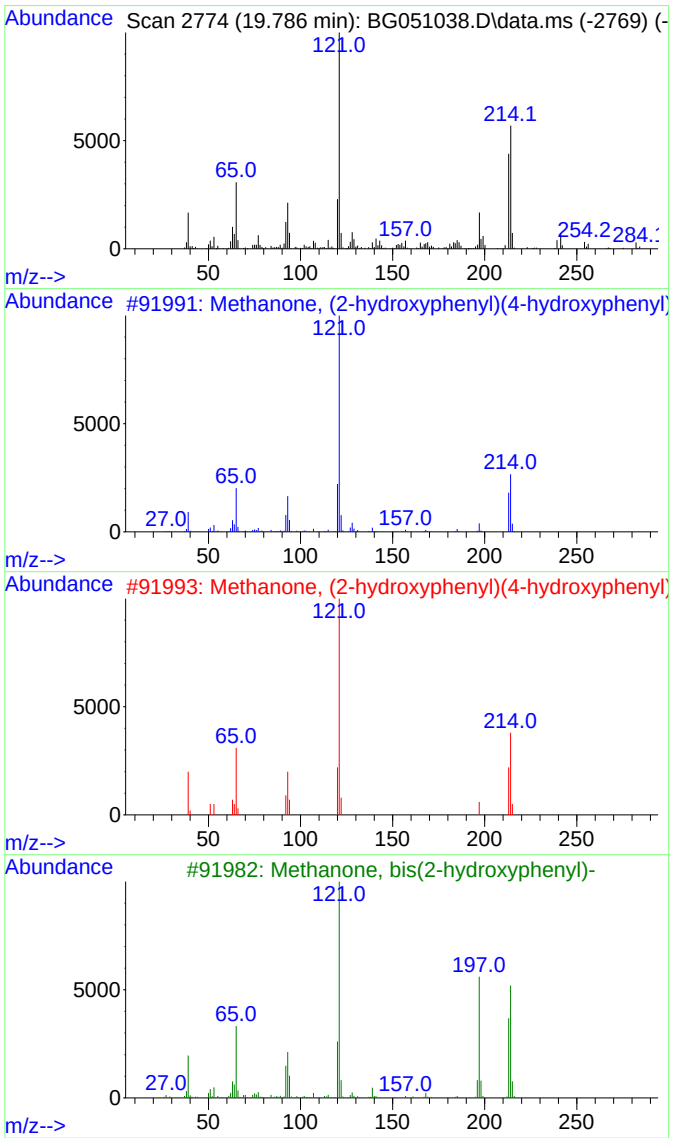
Quant Title :

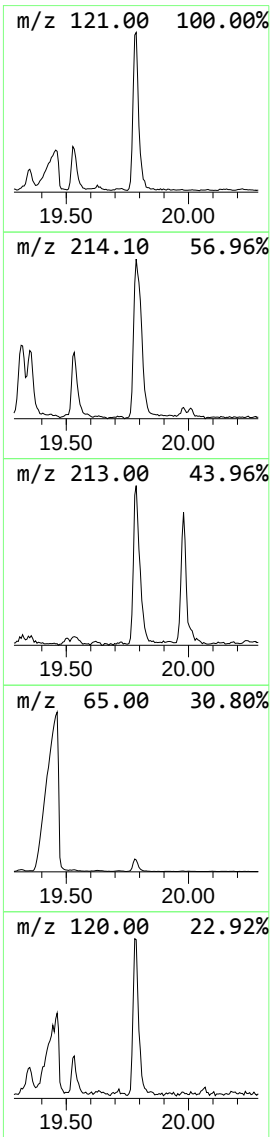
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 27 Methanone, (2-hydroxyphenyl... Concentration Rank 21

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.786	20.34 ng/ul	671443	Chrysene-d12	21.895

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (2-hydroxyphenyl)(4-h...	214	C13H10O3	000606-12-2	95
2	Methanone, (2-hydroxyphenyl)(4-h...	214	C13H10O3	000606-12-2	94
3	Methanone, bis(2-hydroxyphenyl)-	214	C13H10O3	000835-11-0	87
4	4,4'-Dihydroxybenzophenone	214	C13H10O3	000611-99-4	70
5	4,4'-Dihydroxybenzophenone	214	C13H10O3	000611-99-4	64





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Data File : BG051038.D
Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

Quant Title :

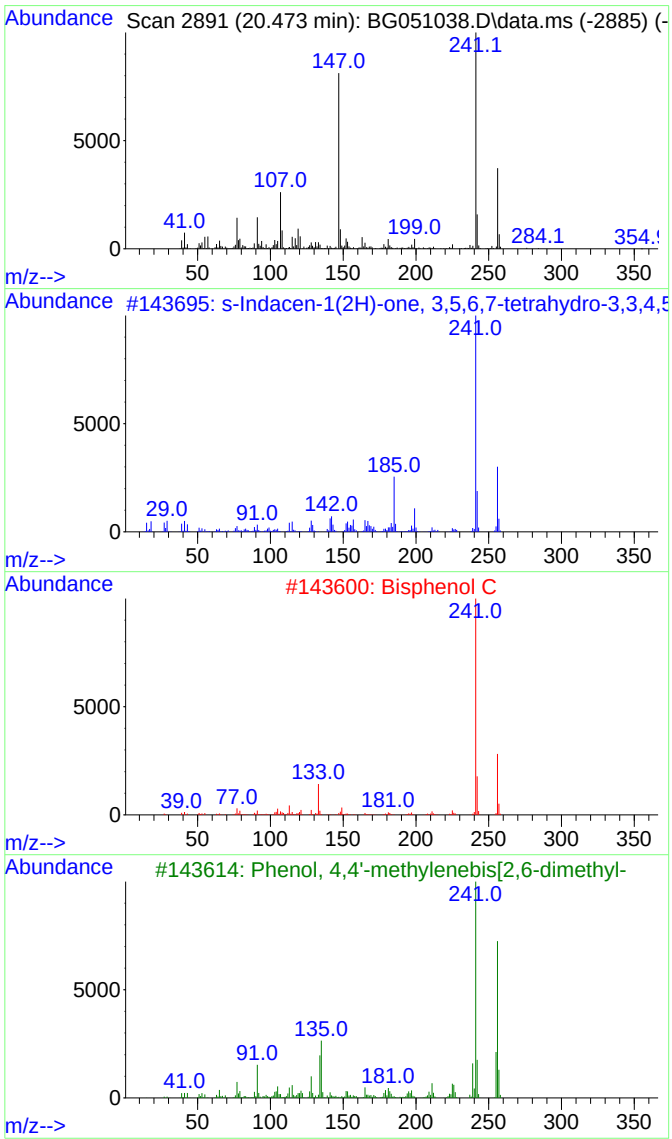
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

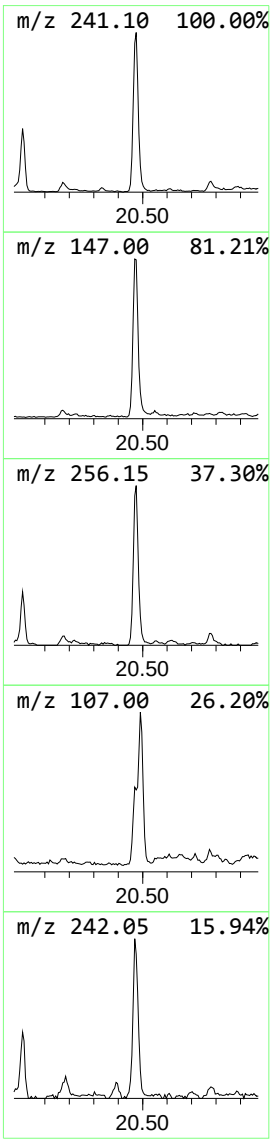
****

Peak Number 30 unknown-02 Concentration Rank 23

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.473	17.99 ng/ul	594055	Chrysene-d12	21.895

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	s-Indacen-1(2H)-one, 3,5,6,7-tet...	256	C18H24O	038754-94-8	45
2	Bisphenol C	256	C17H20O2	000079-97-0	43
3	Phenol, 4,4'-methylenebis[2,6-di...	256	C17H20O2	005384-21-4	38
4	4b,8-Dimethyl-2-isopropylphenant...	256	C19H28	1000197-14-1	35
5	1,2-Dihydro-5,6-acenaphthylenedi...	256	C15H20N2Si	1000497-03-6	35





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Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

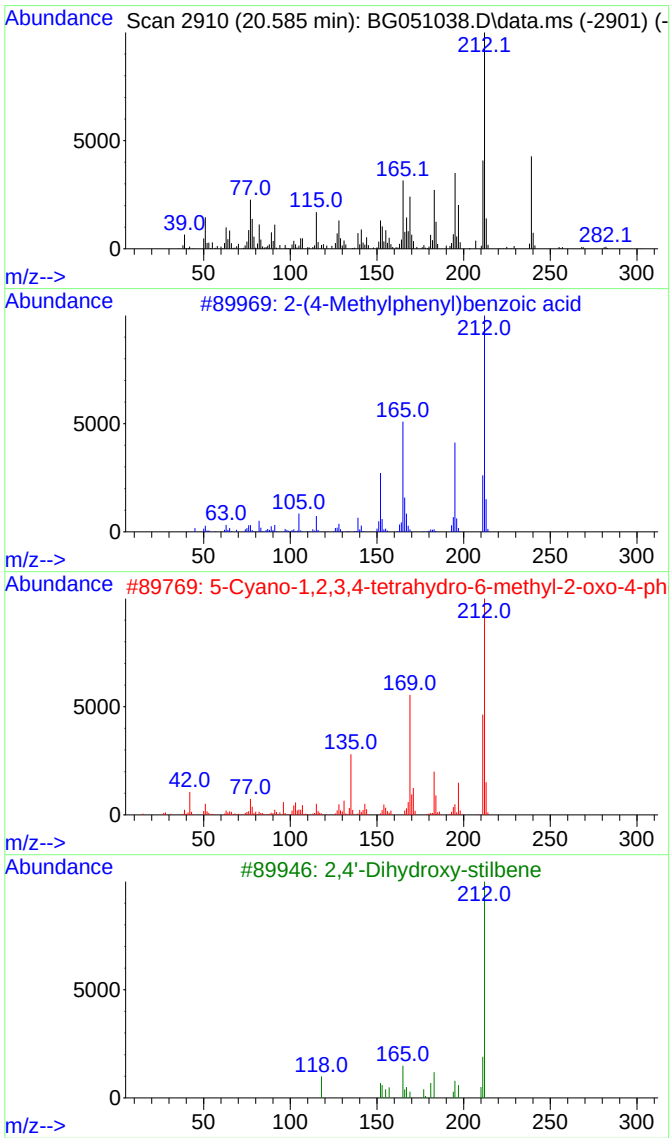
Quant Title :

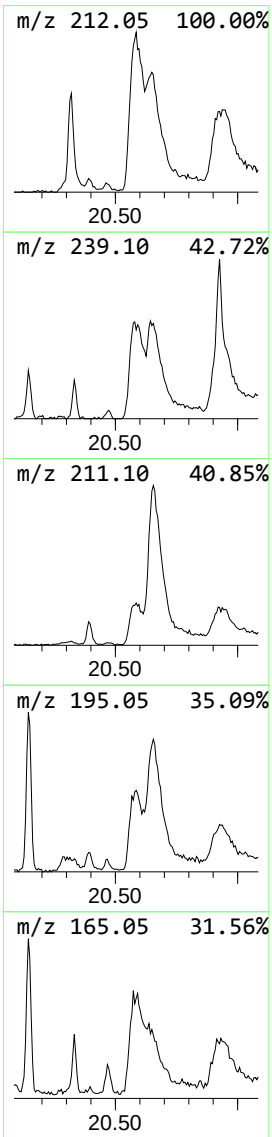
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 31 2-(4-Methylphenyl)benzoic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.585	20.72 ng/ul	683994	Chrysene-d12	21.895

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Methylphenyl)benzoic acid	212	C14H12O2	1000305-27-8	50
2	5-Cyano-1,2,3,4-tetrahydro-6-met...	212	C13H12N2O	027036-92-6	49
3	2,4'-Dihydroxy-stilbene	212	C14H12O2	1000147-73-5	49
4	1,7-Dimethyldibenzothiophene	212	C14H12S	089816-53-5	46
5	Harmine	212	C13H12N2O	000442-51-3	46





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Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

Quant Title :

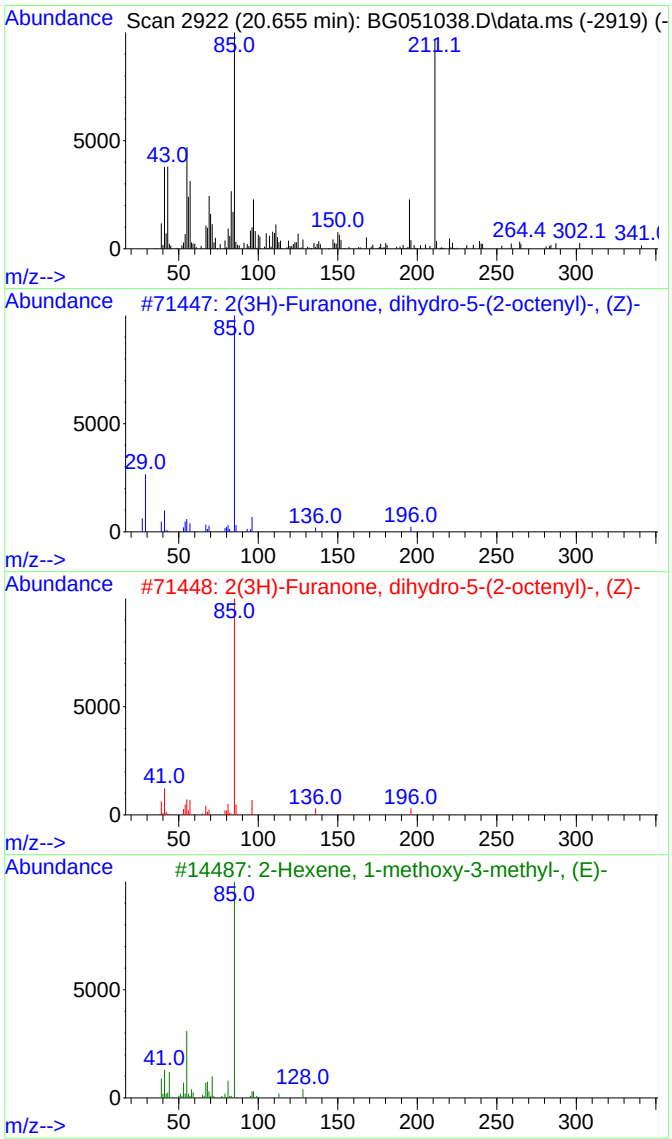
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

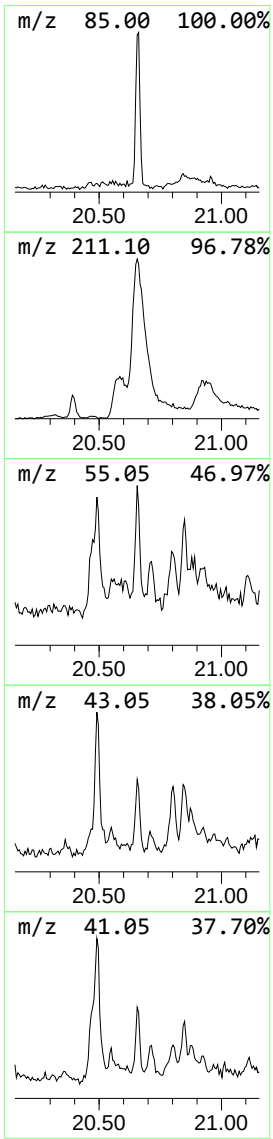
****

Peak Number 32 unknown-03 Concentration Rank 27

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.655	13.71 ng/ul	452610	Chrysene-d12	21.895

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, dihydro-5-(2-oct...	196	C12H20O2	018679-18-0	27
2	2(3H)-Furanone, dihydro-5-(2-oct...	196	C12H20O2	018679-18-0	27
3	2-Hexene, 1-methoxy-3-methyl-, (E)-	128	C8H16O	056052-84-7	25
4	1-Dodecanamine, N-methyl-N-nitroso-	228	C13H28N2O	055090-44-3	25
5	4,6,6-Trimethyl-bicyclo[3.1.1]he...	154	C10H18O	007316-84-9	25





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Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

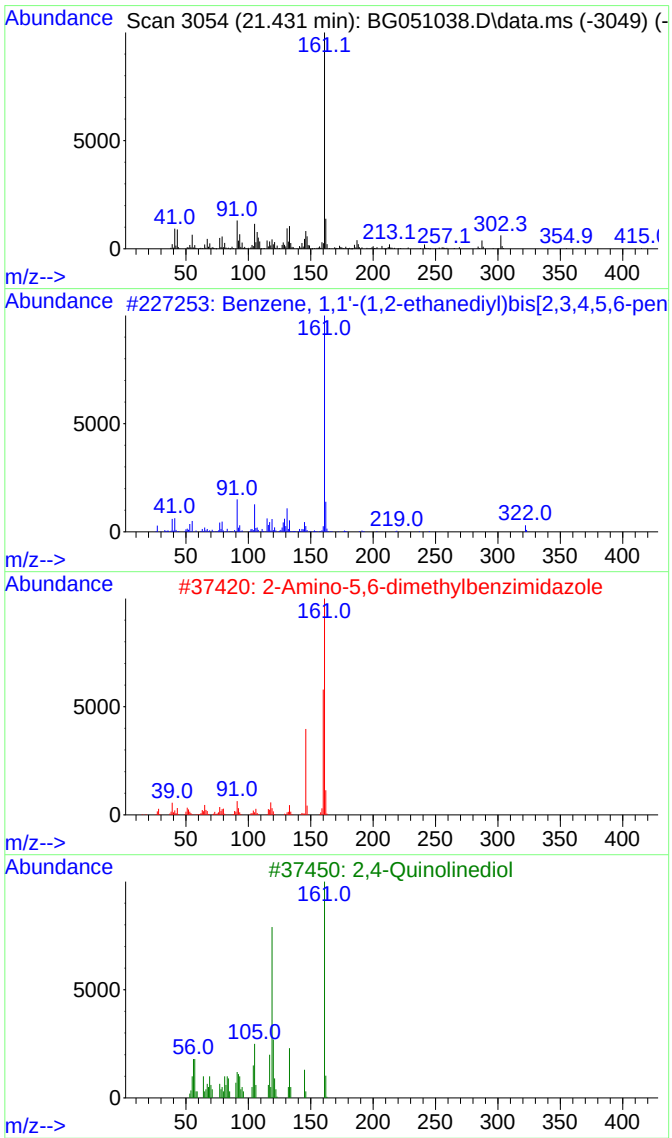
Quant Title :

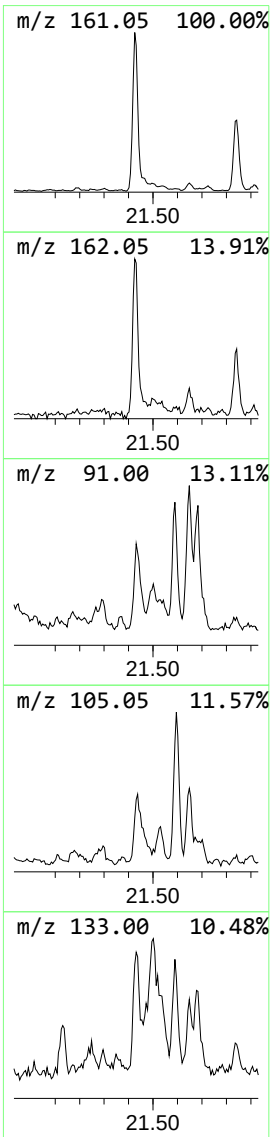
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 37 Benzene, 1,1'-(1,2-ethanedi... Concentration Rank 28

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.431	13.30 ng/ul	439230	Chrysene-d12	21.895

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,2-ethanediyl)bi...	322	C24H34	052145-28-5	72
2	2-Amino-5,6-dimethylbenzimidazole	161	C9H11N3	029096-75-1	64
3	2,4-Quinolinediol	161	C9H7NO2	000086-95-3	64
4	1-(Allyldimethylsilyl)-4-vinylbe...	202	C13H18Si	018052-72-7	64
5	2H-1-Benzopyran-2-one, 6-amino-	161	C9H7NO2	014415-44-2	64





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Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

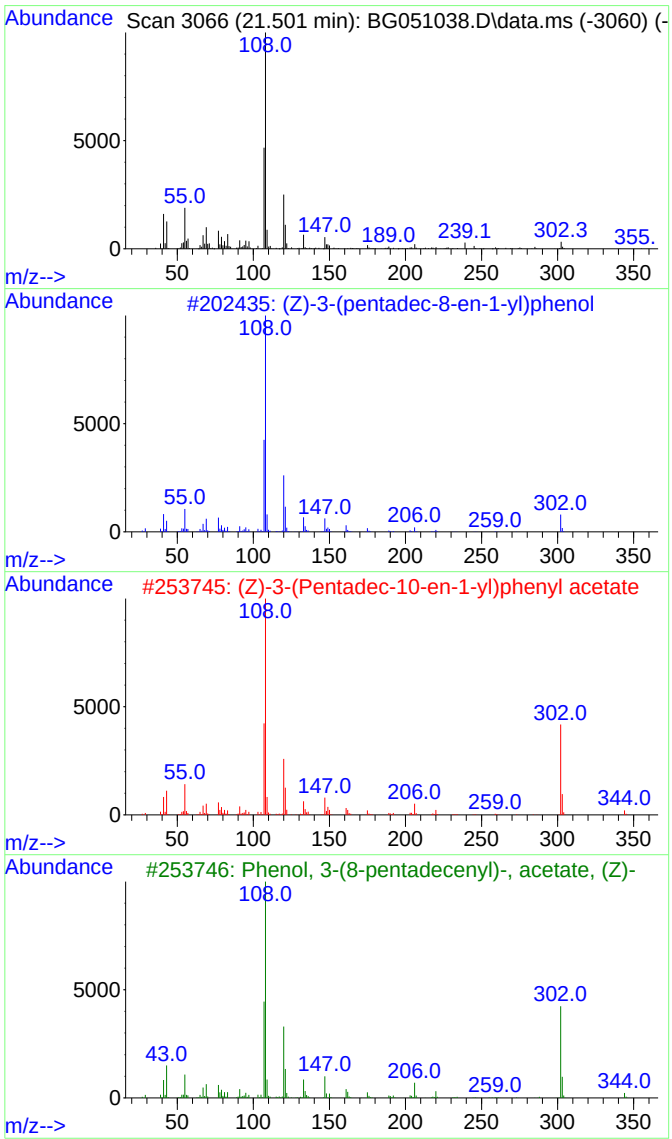
Quant Title :

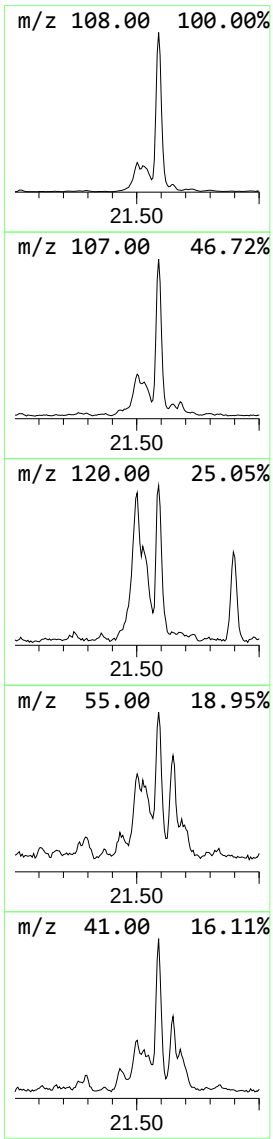
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 38 (Z)-3-(pentadec-8-en-1-yl)p... Concentration Rank 29

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.501	12.44 ng/ul	410606	Chrysene-d12	21.895

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-3-(pentadec-8-en-1-yl)phenol	302	C21H34O	000501-26-8	97
2	(Z)-3-(Pentadec-10-en-1-yl)pheny...	344	C23H36O2	1000478-00-3	83
3	Phenol, 3-(8-pentadecenyl)-, ace...	344	C23H36O2	111047-34-8	83
4	Acetic acid, 4-methylphenyl ester	150	C9H10O2	000140-39-6	58
5	Carbamic acid, methyl-, 3-methyl...	165	C9H11NO2	001129-41-5	53





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Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

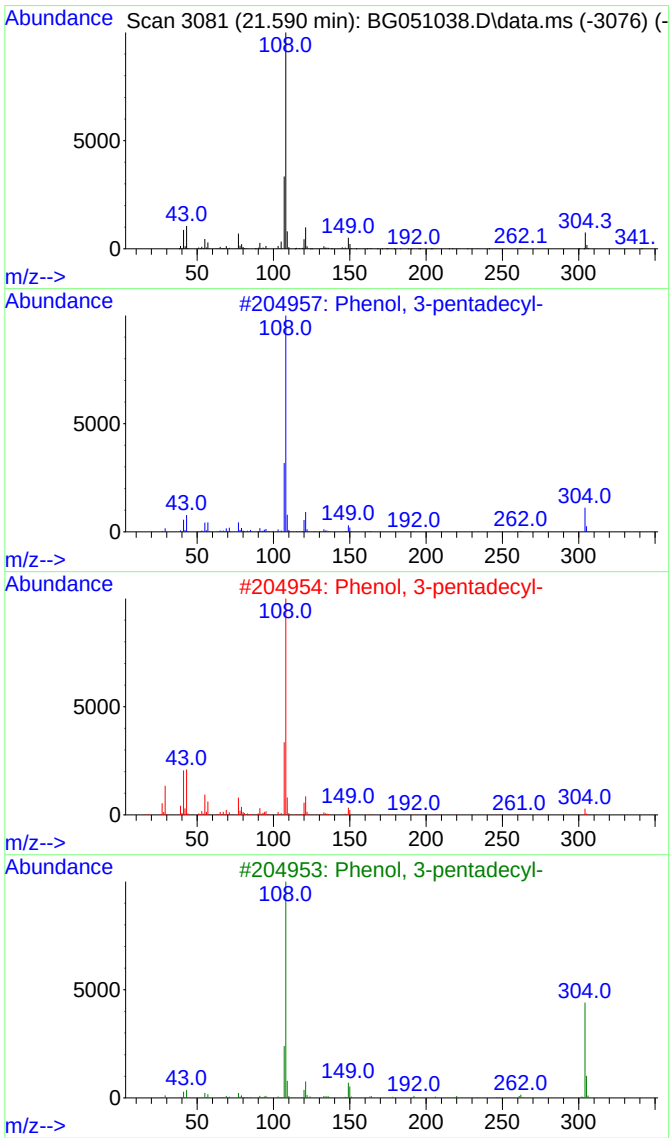
Quant Title :

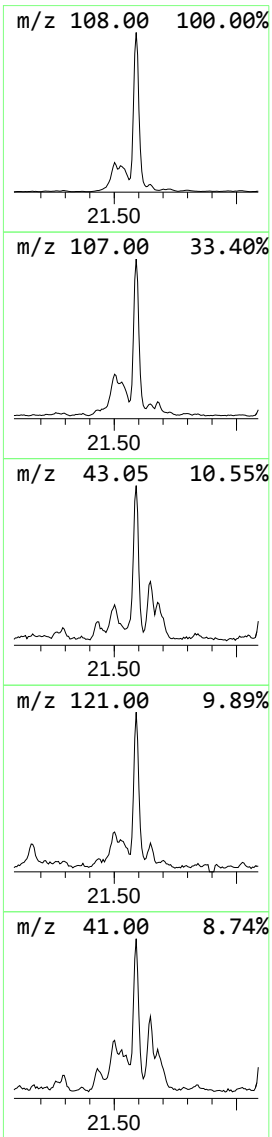
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 39 Phenol, 3-pentadecyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.590	39.36 ng/ul	1299500	Chrysene-d12	21.895

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-pentadecyl-	304	C21H36O	000501-24-6	97
2	Phenol, 3-pentadecyl-	304	C21H36O	000501-24-6	94
3	Phenol, 3-pentadecyl-	304	C21H36O	000501-24-6	91
4	3-Pentadecylphenyl acetate	346	C23H38O2	052122-74-4	90
5	Phenol, 3-undecyl-	248	C17H28O	020056-72-8	86





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Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

Quant Title :

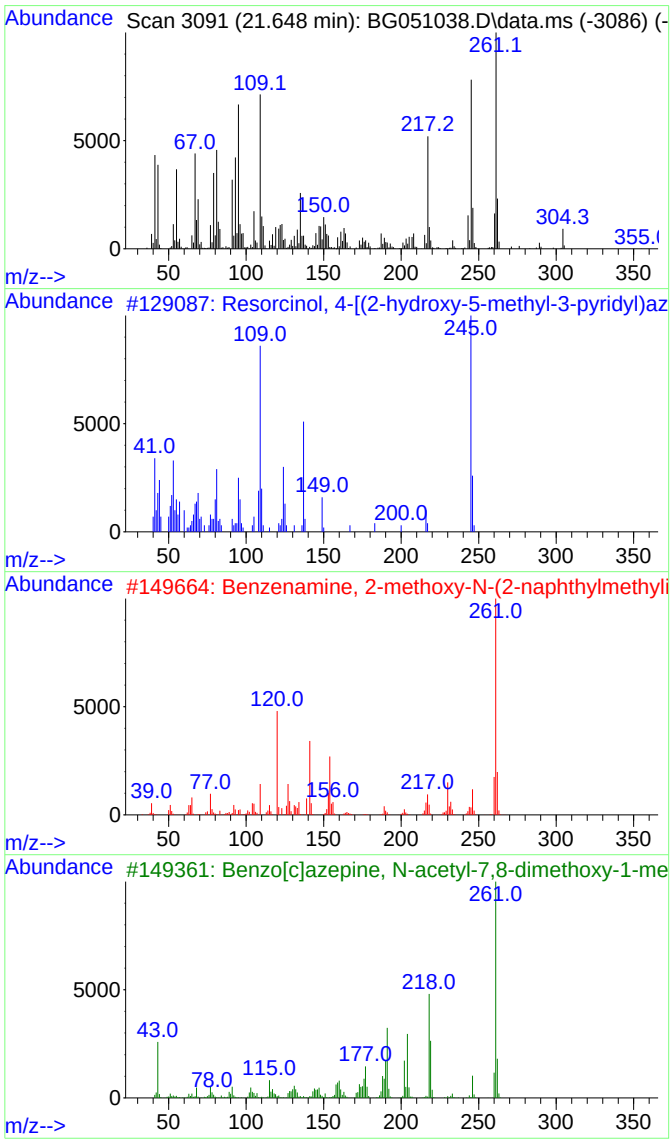
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

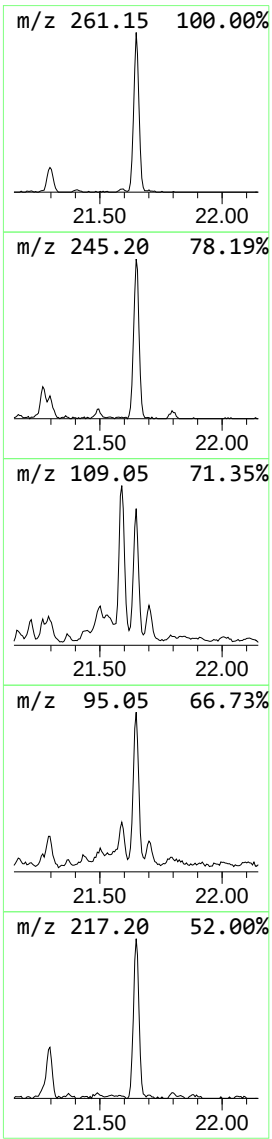
****

Peak Number 40 unknown-04 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.648	24.00 ng/ul	792445	Chrysene-d12	21.895

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Resorcinol, 4-[(2-hydroxy-5-meth...	245	C12H11N3O3	021269-88-5	30
2	Benzenamine, 2-methoxy-N-(2-naph...	261	C18H15NO	059374-36-6	30
3	Benzo[c]azepine, N-acetyl-7,8-di...	261	C15H19NO3	113193-86-5	22
4	[1]Benzothieno[2,3-d]pyrimidine-...	245	C12H11N3OS	1000338-12-8	22
5	Phenylthioacetamide, N-(2-fluoro...	261	C14H12FNOS	1000308-15-8	20





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Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

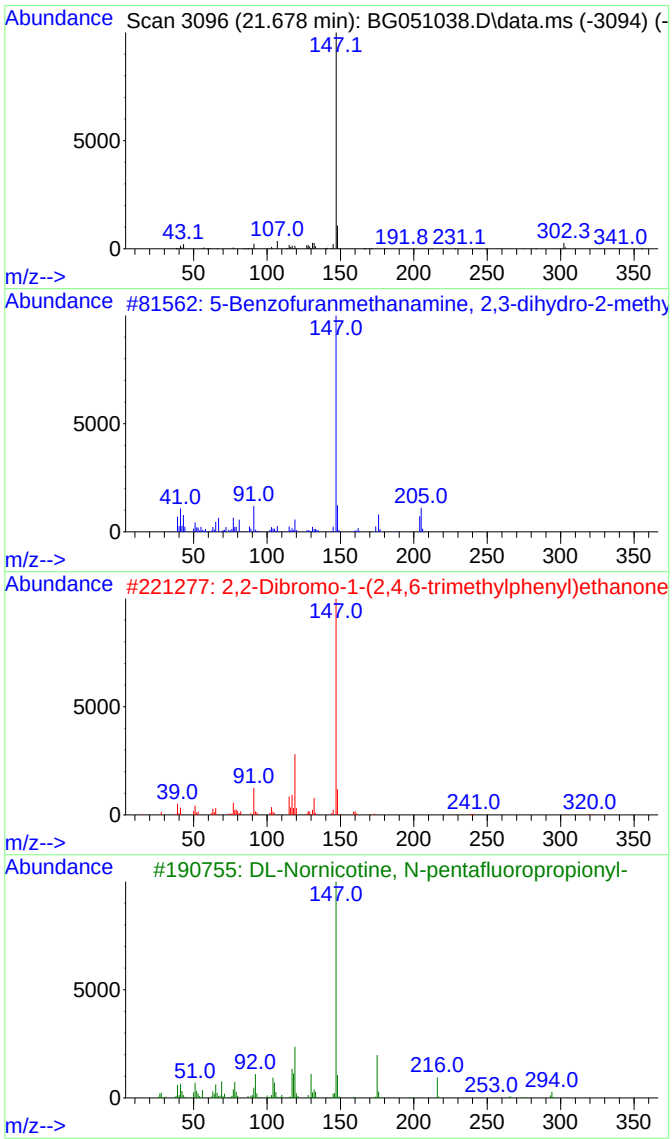
Quant Title :

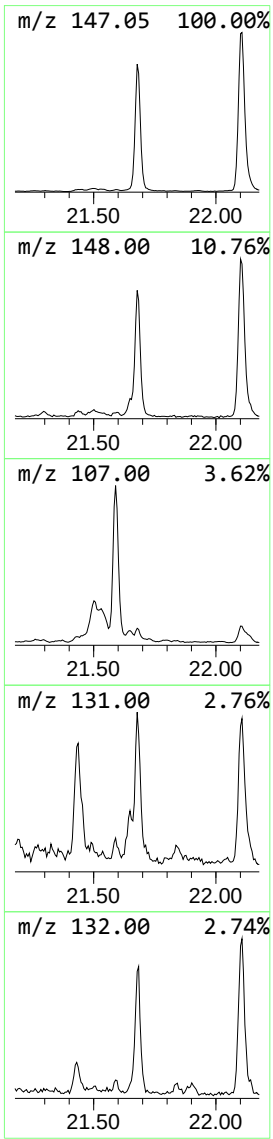
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 41 5-Benzofuranmethanamine, 2,... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.678	23.78 ng/ul	785216	Chrysene-d12	21.895

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Benzofuranmethanamine, 2,3-dih...	205	C13H19NO	1000351-55-3	64
2	2,2-Dibromo-1-(2,4,6-trimethylph...	318	C11H12Br2O	329349-15-7	56
3	DL-Nornicotine, N-pentafluoropro...	294	C12H11F5N2O	1000448-18-4	40
4	Benzene, 1-(1,1-dimethylethyl)-3...	162	C12H18	014411-56-4	40
5	1-Butanone, 2-chloro-3-methyl-1-...	238	C14H19ClO	055955-90-3	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111521\
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Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

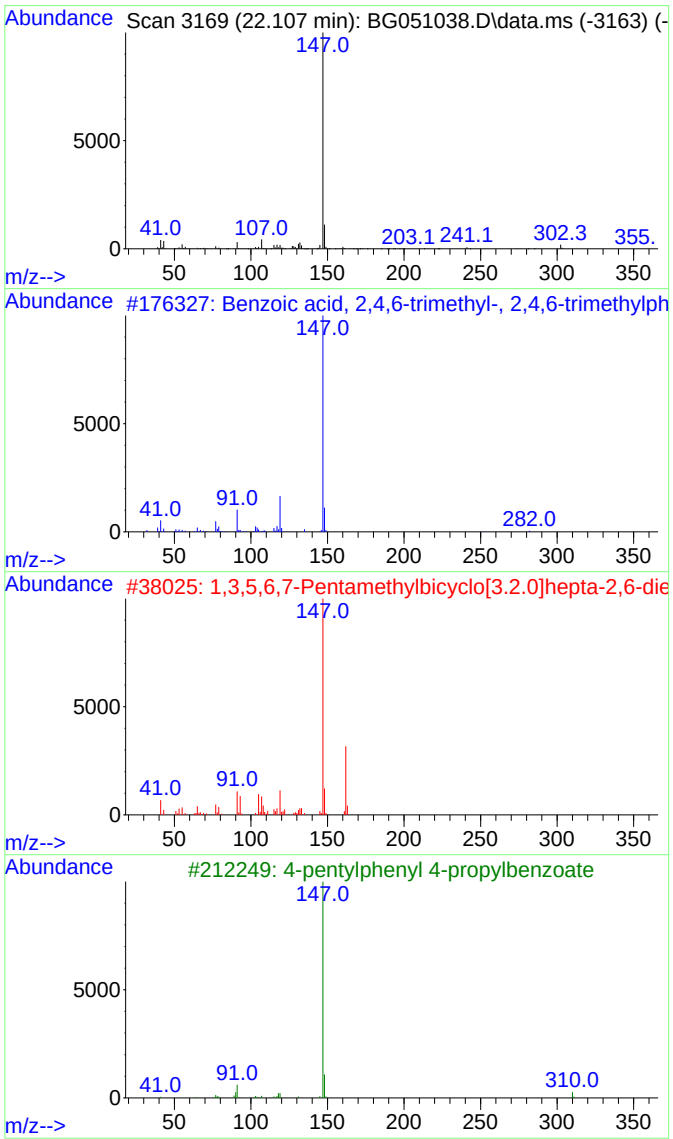
Quant Title :

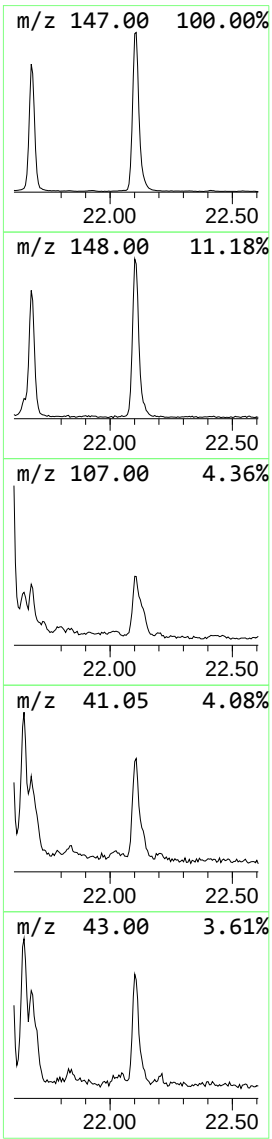
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 42 Benzoic acid, 2,4,6-trimeth... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.107	33.93 ng/ul	1120170	Chrysene-d12	21.895

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4,6-trimethyl-, ...	282	C19H22O2	001504-38-7	64
2	1,3,5,6,7-Pentamethylbicyclo[3.2...	162	C12H18	003099-00-1	64
3	4-pentylphenyl 4-propylbenzoate	310	C21H26O2	050649-60-0	50
4	5-Benzofuranmethanamine, 2,3-dih...	205	C13H19NO	1000351-55-3	43
5	Benzene, 1,1'-(1,1,10,10-tetrame...	406	C30H46	063934-83-8	40





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Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

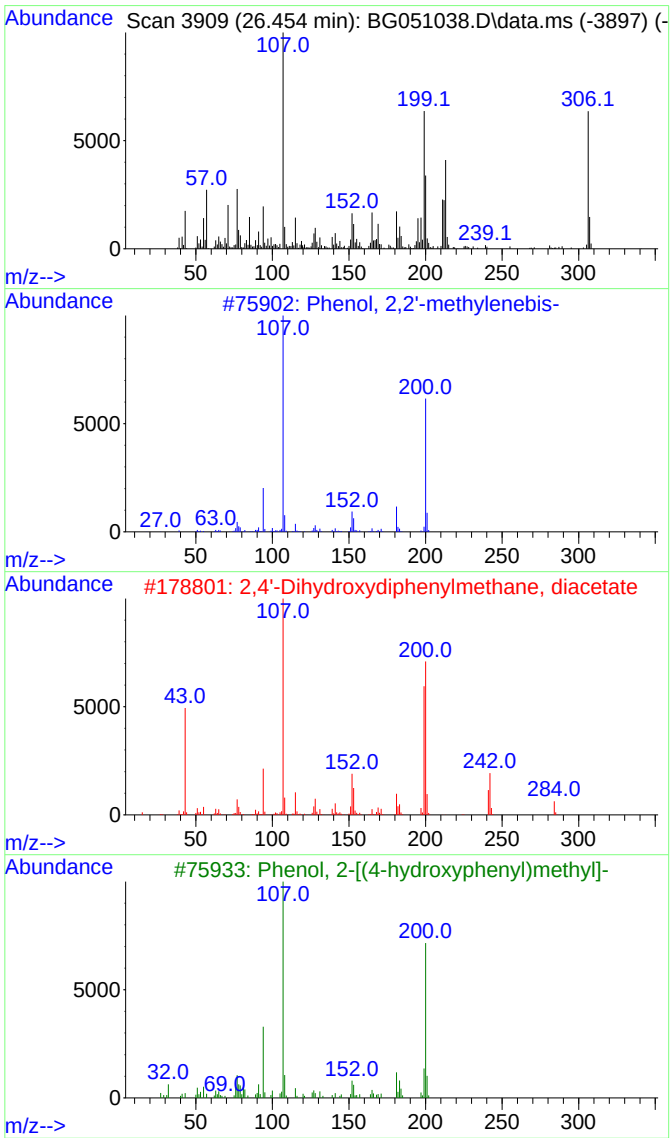
Quant Title :

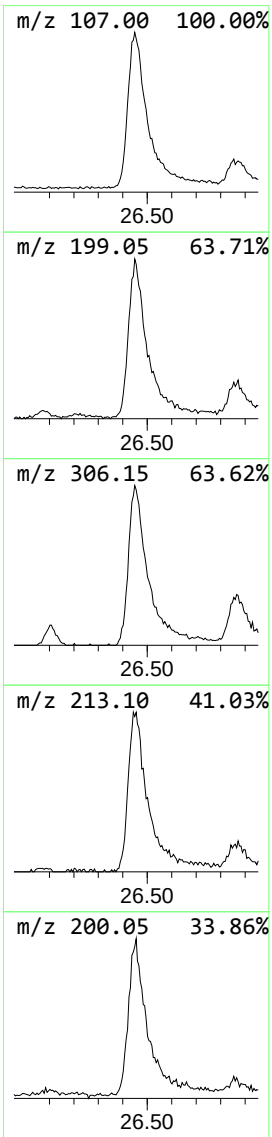
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 45 unknown-05 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.454	40.62 ng/ul	1364920	Perylene-d12	25.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,2'-methylenebis-	200	C13H12O2	002467-02-9	38
2	2,4'-Dihydroxydiphenylmethane, d...	284	C17H16O4	959033-36-4	35
3	Phenol, 2-[(4-hydroxyphenyl)meth...	200	C13H12O2	002467-03-0	30
4	2,2'-Methylenediphenol, acetate	242	C15H14O3	1000462-45-6	30
5	Phenol, 2,2'-methylenebis-	200	C13H12O2	002467-02-9	25





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Data File : BG051038.D
Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

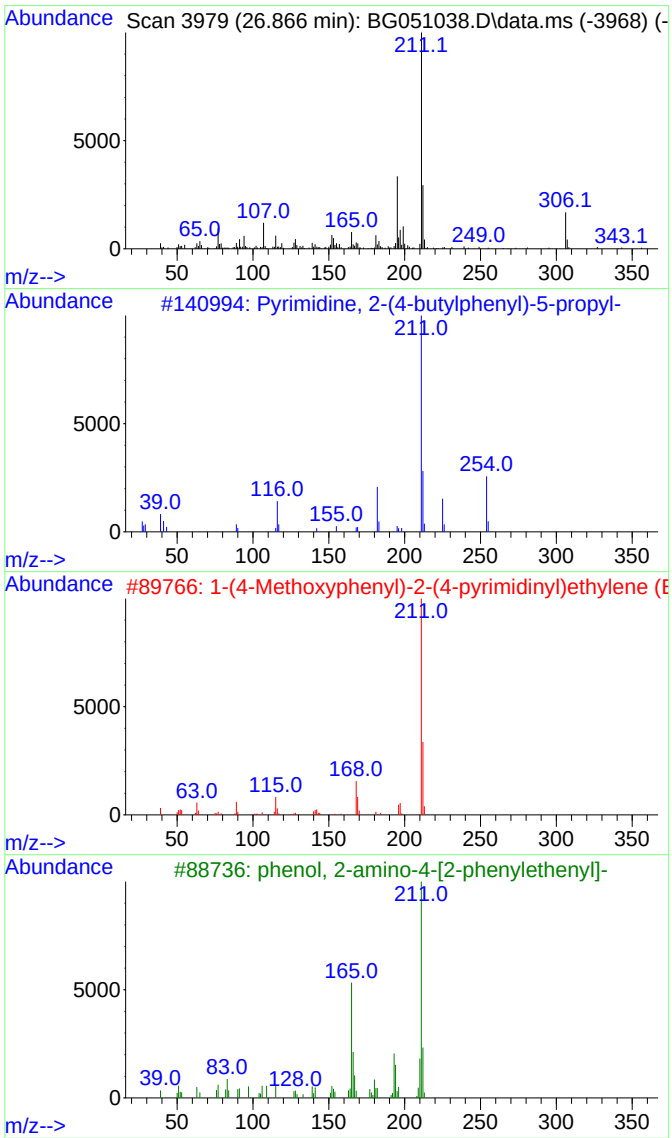
Quant Title :

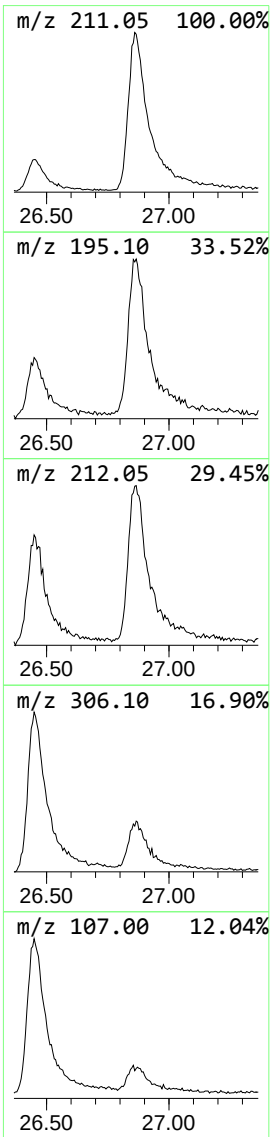
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 46 Pyrimidine, 2-(4-butylpheny... Concentration Rank 22

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.866	20.17 ng/ul	677747	Perylene-d12	25.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrimidine, 2-(4-butylphenyl)-5-...	254	C17H22N2	123740-94-3	50
2	1-(4-Methoxyphenyl)-2-(4-pyrimid...	212	C13H12N2O	163011-00-5	50
3	phenol, 2-amino-4-[2-phenylethen...	211	C14H13NO	1000396-15-8	47
4	5-Methyl-4-[(4-methylphenoxy)met...	318	C17H22O4Si	1000478-80-3	38
5	[1,1'-Biphenyl]-2-ol, 3-(1,1-dim...	226	C16H18O	002416-98-0	38





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Data File : BG051038.D
Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

Quant Title :

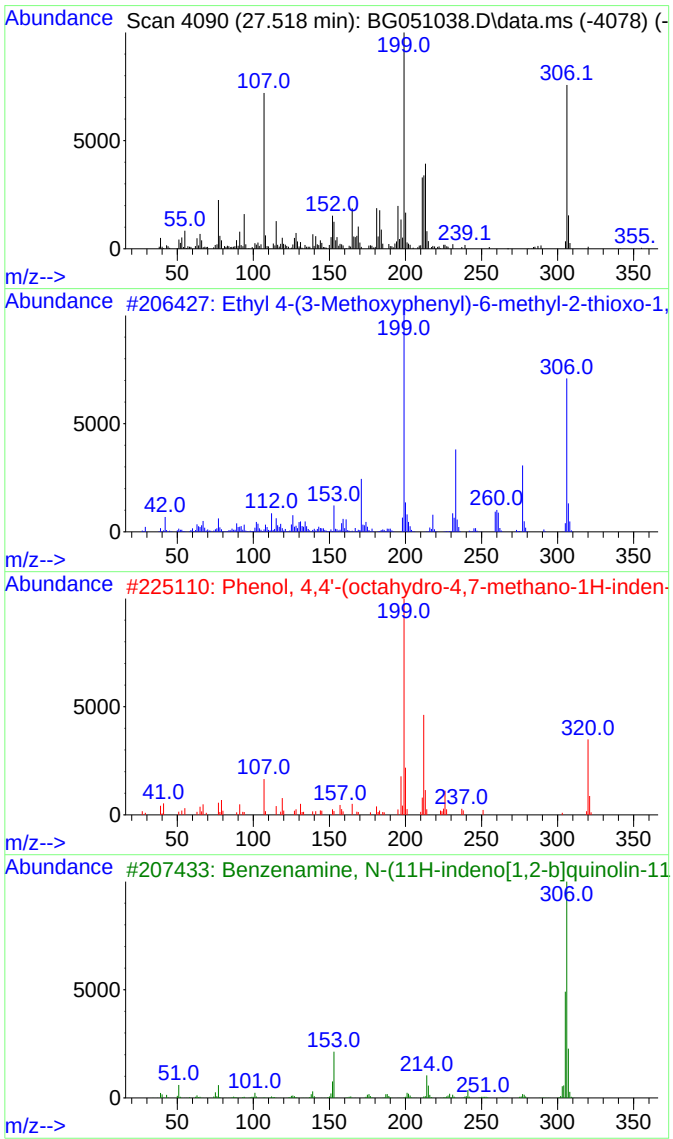
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

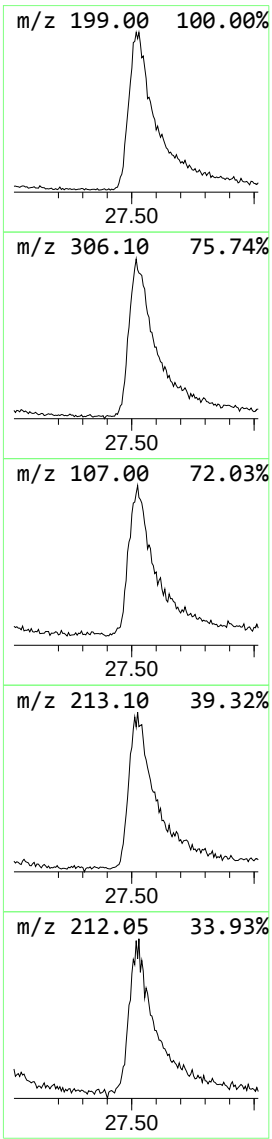
****

Peak Number 47 unknown-06 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.518	37.29 ng/ul	1253310	Perylene-d12	25.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl 4-(3-Methoxyphenyl)-6-meth...	306	C15H18N2O3S	292871-43-3	46
2	Phenol, 4,4'-(octahydro-4,7-meth...	320	C22H24O2	001943-97-1	41
3	Benzenamine, N-(11H-indeno[1,2-b...	306	C22H14N2	085635-73-0	35
4	Diphenyl(p-carboxyphenyl) phosphine	306	C19H15O2P	002129-31-9	35
5	4,4'-Ethylidenediphenol	214	C14H14O2	002081-08-5	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111521\
Data File : BG051038.D
Acq On : 15 Nov 2021 11:51
Operator : CG/JU
Sample : M4615-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0V04

Quant Title :

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	6.854	13.7	ng/ul	171181	1	8.240	249258	20.0
1,3,5-Triazine,...	7.741	218.0	ng/ul	2717200	1	8.240	249258	20.0
Benzaldehyde, 2...	8.769	98.6	ng/ul	1229190	1	8.240	249258	20.0
Benzeneacetonit...	10.973	16.5	ng/ul	347009	2	11.055	420119	20.0
Benzenamine, N,...	11.619	176.8	ng/ul	3714910	2	11.055	420119	20.0
Methenamine	11.842	847.9	ng/ul	17810000	2	11.055	420119	20.0
Hydroquinone	12.048	245.1	ng/ul	5149000	2	11.055	420119	20.0
Phenol, p-tert-...	12.389	68.5	ng/ul	1439270	2	11.055	420119	20.0
Benzaldehyde, 4...	13.241	129.1	ng/ul	3630400	3	14.850	562434	20.0
Benzenamine, N,...	13.546	103.8	ng/ul	2920510	3	14.850	562434	20.0
n-Hexadecanoic ...	18.458	14.7	ng/ul	467716	4	17.594	635145	20.0
Phenol, 2-[(4-h...	18.769	194.6	ng/ul	6178410	4	17.594	635145	20.0
Phenol, 2,2'-me...	19.045	1670.8	ng/ul	53060500	4	17.594	635145	20.0
10,18-Bisnorabi...	19.316	52.8	ng/ul	1675200	4	17.594	635145	20.0
Phenol, 4,4'-me...	19.463	1546.6	ng/ul	49115000	4	17.594	635145	20.0
cis-Vaccenic acid	19.633	32.3	ng/ul	1025140	4	17.594	635145	20.0
Octadecanoic acid	19.721	9.4	ng/ul	299431	4	17.594	635145	20.0
Methanone, (2-h...	19.786	20.3	ng/ul	671443	5	21.895	660375	20.0
unknown-02	20.473	18.0	ng/ul	594055	5	21.895	660375	20.0
2-(4-Methylphen...	20.585	20.7	ng/ul	683994	5	21.895	660375	20.0
unknown-03	20.655	13.7	ng/ul	452610	5	21.895	660375	20.0
Benzene, 1,1'-(...	21.431	13.3	ng/ul	439230	5	21.895	660375	20.0
(Z)-3-(pentadec...	21.501	12.4	ng/ul	410606	5	21.895	660375	20.0
Phenol, 3-penta...	21.590	39.4	ng/ul	1299500	5	21.895	660375	20.0
unknown-04	21.648	24.0	ng/ul	792445	5	21.895	660375	20.0
5-Benzofuranmet...	21.678	23.8	ng/ul	785216	5	21.895	660375	20.0
Benzoic acid, 2...	22.107	33.9	ng/ul	1120170	5	21.895	660375	20.0
unknown-05	26.454	40.6	ng/ul	1364920	6	25.309	672107	20.0
Pyrimidine, 2-(...	26.866	20.2	ng/ul	677747	6	25.309	672107	20.0
unknown-06	27.518	37.3	ng/ul	1253310	6	25.309	672107	20.0