LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041221\
Data File : BG048669.D
Acq On : 12 Apr 2021 20:35
Operator : CG/JU
Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-115RR

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\8270-BG033021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048669.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.643	385	392	399	rBV	274915	451474	26.46%	3.966%
2	7.247	659	665	675	rBV	187201	355116	20.81%	3.120%
3	8.088	798	808	815	rBV	100383	177164	10.38%	1.556%
4	8.469	866	873	877	rBV	25655	43156	2.53%	0.379%
5	9.263	1001	1008	1015	rBV	290680	531384	31.14%	4.668%
6	9.521	1045	1052	1060	rBV	64548	108903	6.38%	0.957%
7	9.715	1079	1085	1092	rVB4	12527	23791	1.39%	0.209%
8	10.079	1140	1147	1153	rBV	84713	137977	8.09%	1.212%
9	10.214	1166	1170	1175	rVB6	12181	20400	1.20%	0.179%
10	10.385	1195	1199	1207	rBV2	47409	81248	4.76%	0.714%
11	10.825	1270	1274	1280	rVB3	21499	36032	2.11%	0.317%
12	10.919	1283	1290	1294	rVV	124526	225103	13.19%	1.978%
13	10.966	1294	1298	1305	rVV2	54303	99962	5.86%	0.878%
14	11.055	1307	1313	1320	rVB3	31676	55383	3.25%	0.487%
15	11.190	1328	1336	1343	rBV7	15697	41504	2.43%	0.365%
16	12.306	1522	1526	1532	rVB9	10004	18970	1.11%	0.167%
17	12.629	1574	1581	1588	rBV2	97868	182226	10.68%	1.601%
18	12.776	1602	1606	1613	rBV8	20816	45856	2.69%	0.403%
19	12.888	1621	1625	1631	rVB8	18955	36924	2.16%	0.324%
20	13.035	1646	1650	1656	rBV8	17169	33218	1.95%	0.292%
21	13.229	1678	1683	1688	rBV2	30565	59018	3.46%	0.518%
22	13.364	1699	1706	1713	rVB	748305	1119713	65.62%	9.837%
23	13.505	1726	1730	1732	rBV5	15401	23793	1.39%	0.209%
24	13.851	1785	1789	1793	rVB6	28693	42478	2.49%	0.373%
25	13.892	1793	1796	1801	rVB7	15659	20798	1.22%	0.183%
26	14.186	1841	1846	1850	rBV	76841	107488	6.30%	0.944%
27	14.568	1899	1911	1917	rBV2	67439	177768	10.42%	1.562%
28	14.744	1935	1941	1947	rVB2	189286	316380	18.54%	2.779%
29	15.244	2023	2026	2032	rVB	27584	42152	2.47%	0.370%
30	15.479	2062	2066	2070	rVB4	20331	33624	1.97%	0.295%
31	16.237	2189	2195	2202	rVB	670673	1024222	60.03%	8.998%
32	16.354	2211	2215	2218	rBV6	33366	45443	2.66%	0.399%
33	16.390	2218	2221	2228	rVB5	31344	61235	3.59%	0.538%
34	16.519	2232	2243	2254	rBV	573977	1398899	81.98%	12.290%
35	17.500	2405	2410	2414	rBV	236831	347420	20.36%	3.052%
36	18.393	2557	2562	2570	rBV2	195220	294050	17.23%	2.583%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041221\
Data File : BG048669.D
Acq On : 12 Apr 2021 20:35
Operator : CG/JU
Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-115RR

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\8270-BG033021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.298	2712	2716	2723	rVB	136694	212866	12.48%	1.870%
38	19.656	2773	2777	2781	rBV6	84164	110730	6.49%	0.973%
39	20.109	2849	2854	2860	rBV	1318728	1706308	100.00%	14.990%
40	21.419	3073	3077	3084	rVB2	112670	181329	10.63%	1.593%
41	21.795	3136	3141	3148	rVB2	219158	367232	21.52%	3.226%
42	23.487	3422	3429	3440	rVB2	252462	595011	34.87%	5.227%
43	25.144	3704	3711	3721	rVB3	130941	389003	22.80%	3.417%

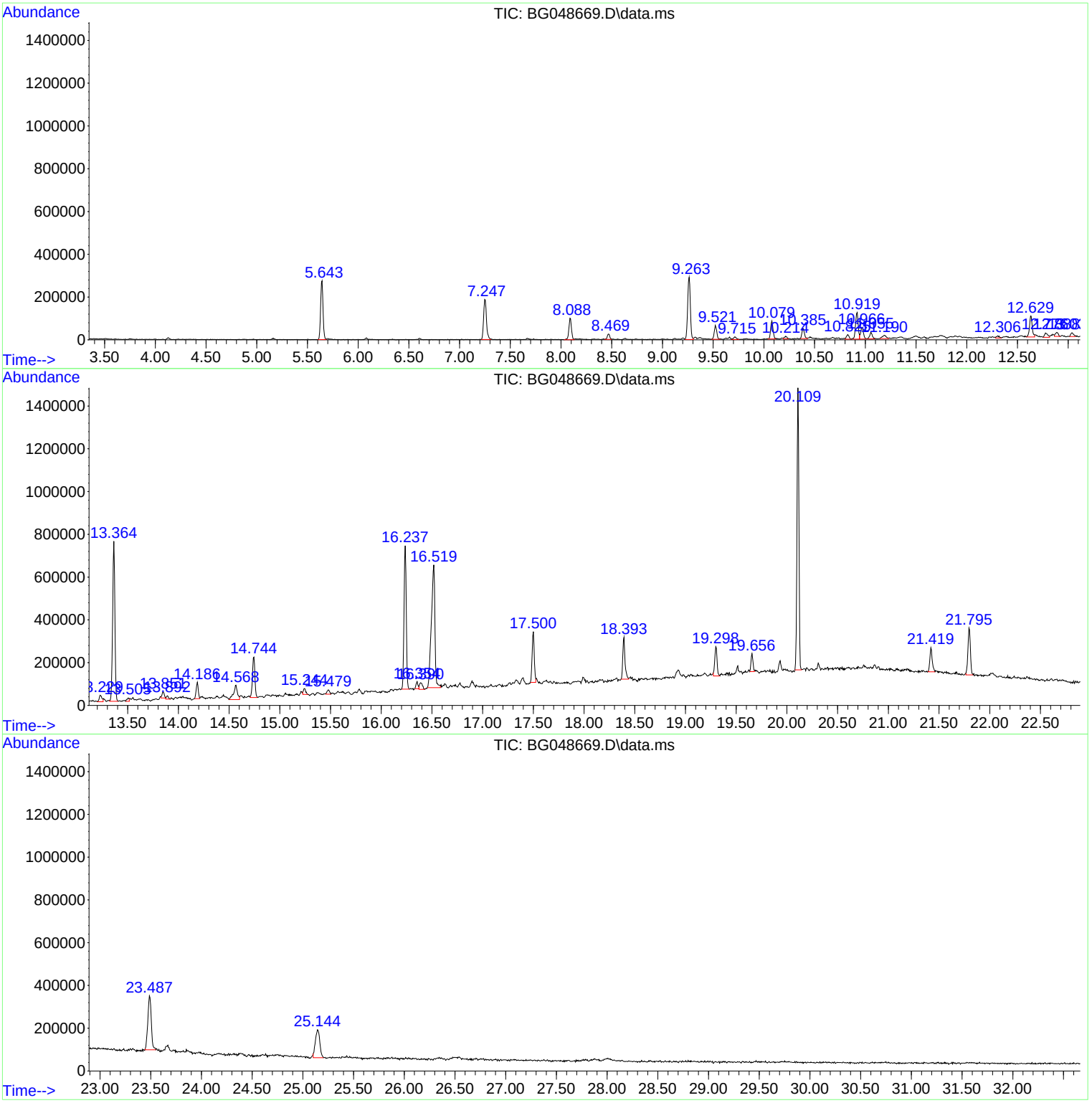
Sum of corrected areas: 11382751

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041221\
Data File : BG048669.D
Acq On : 12 Apr 2021 20:35
Operator : CG/JU
Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041221\
Data File : BG048669.D
Acq On : 12 Apr 2021 20:35
Operator : CG/JU
Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-115RR

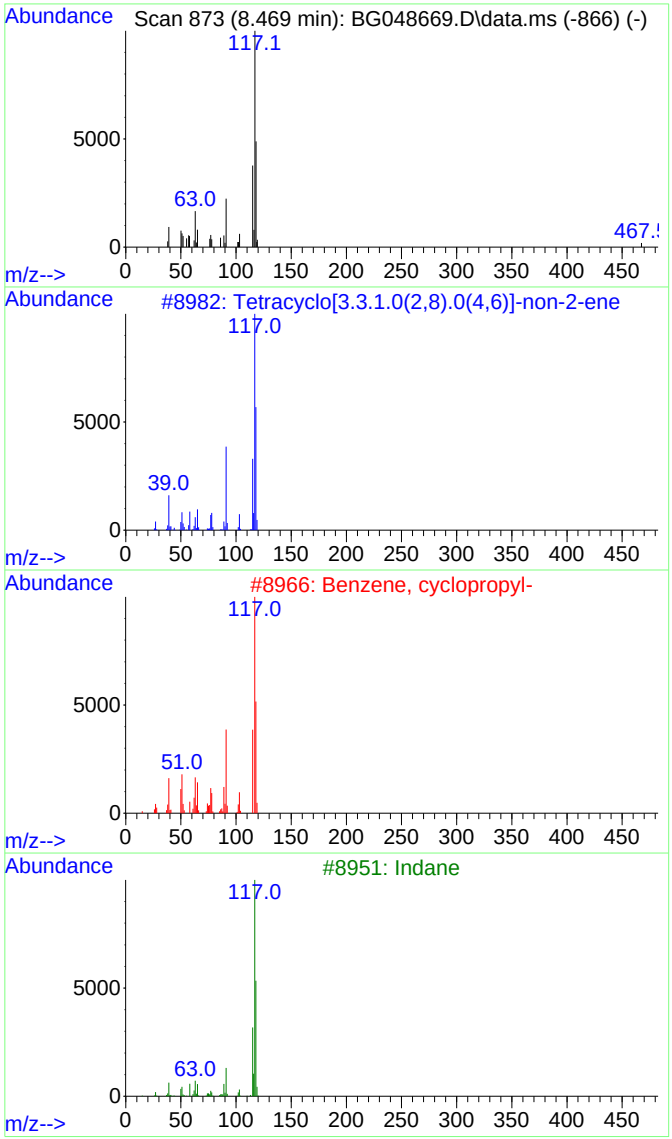
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

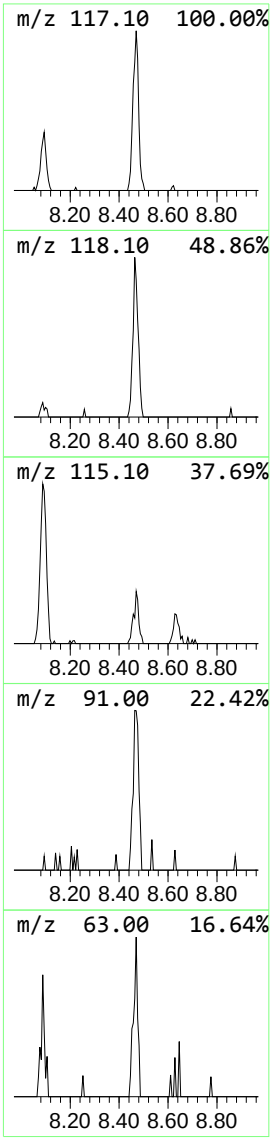
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Tetracyclo[3.3.1.0(2,8).0(4... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.469	4.87 ng	43156	1,4-Dichlorobenzene-d4	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	81
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
3	Indane	118	C9H10	000496-11-7	74
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	74
5	Deltacyclene	118	C9H10	007785-10-6	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041221\
Data File : BG048669.D
Acq On : 12 Apr 2021 20:35
Operator : CG/JU
Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

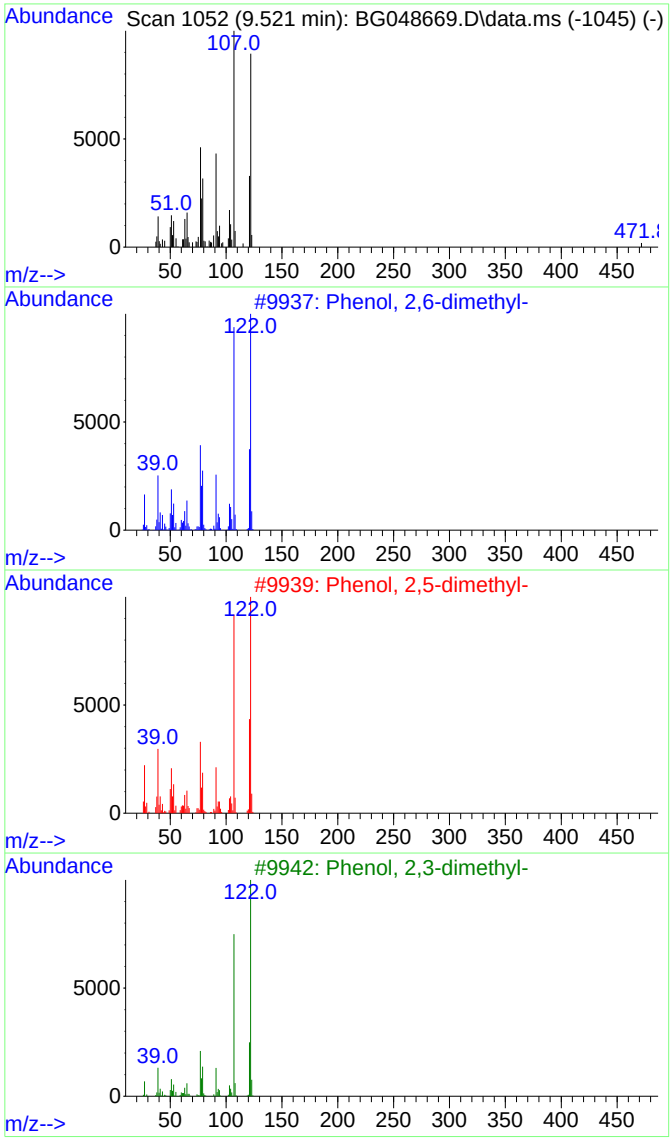
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

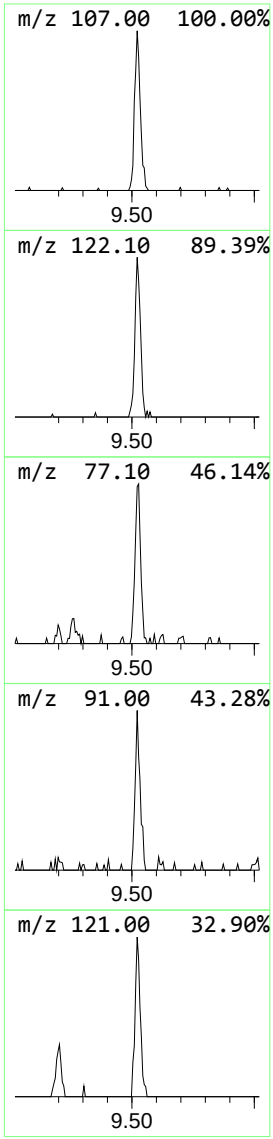
****

Peak Number 2 Phenol, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.521	9.68 ng	108903	Naphthalene-d8	10.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-dimethyl-	122	C8H10O	000576-26-1	95
2	Phenol, 2,5-dimethyl-	122	C8H10O	000095-87-4	90
3	Phenol, 2,3-dimethyl-	122	C8H10O	000526-75-0	86
4	Phenol, 3,5-dimethyl-	122	C8H10O	000108-68-9	83
5	Formic acid, 2,3-dimethylphenyl ...	150	C9H10O2	1000368-91-7	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041221\
Data File : BG048669.D
Acq On : 12 Apr 2021 20:35
Operator : CG/JU
Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

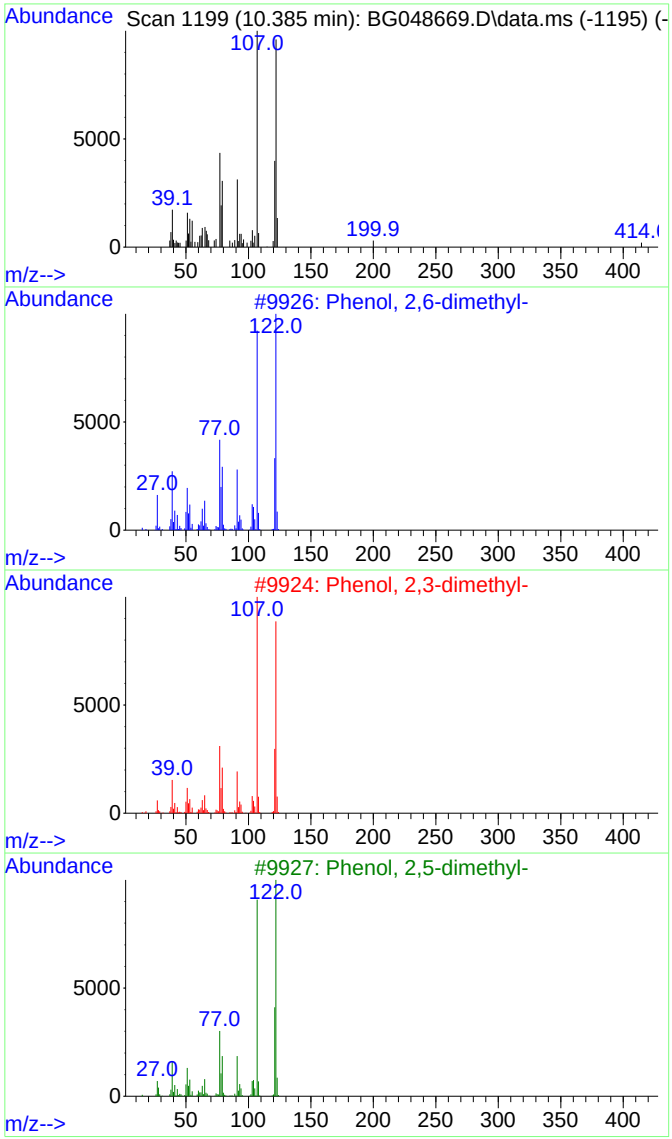
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

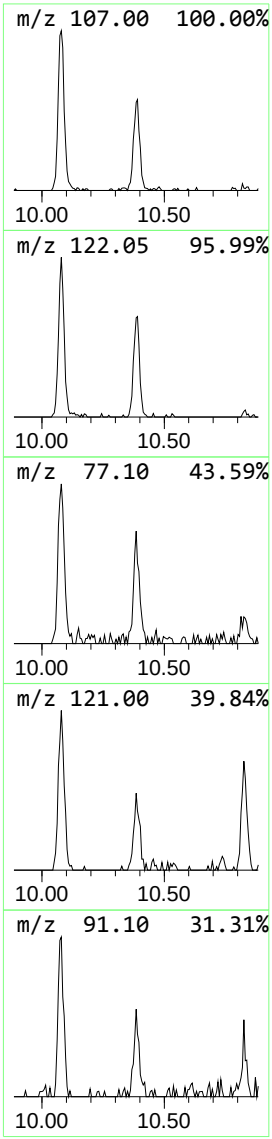
****

Peak Number 3 Phenol, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.385	7.22 ng	81248	Naphthalene-d8	10.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-dimethyl-	122	C8H10O	000576-26-1	94
2	Phenol, 2,3-dimethyl-	122	C8H10O	000526-75-0	91
3	Phenol, 2,5-dimethyl-	122	C8H10O	000095-87-4	91
4	Phenol, 3,4-dimethyl-	122	C8H10O	000095-65-8	90
5	Phenol, 3,5-dimethyl-	122	C8H10O	000108-68-9	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041221\
Data File : BG048669.D
Acq On : 12 Apr 2021 20:35
Operator : CG/JU
Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

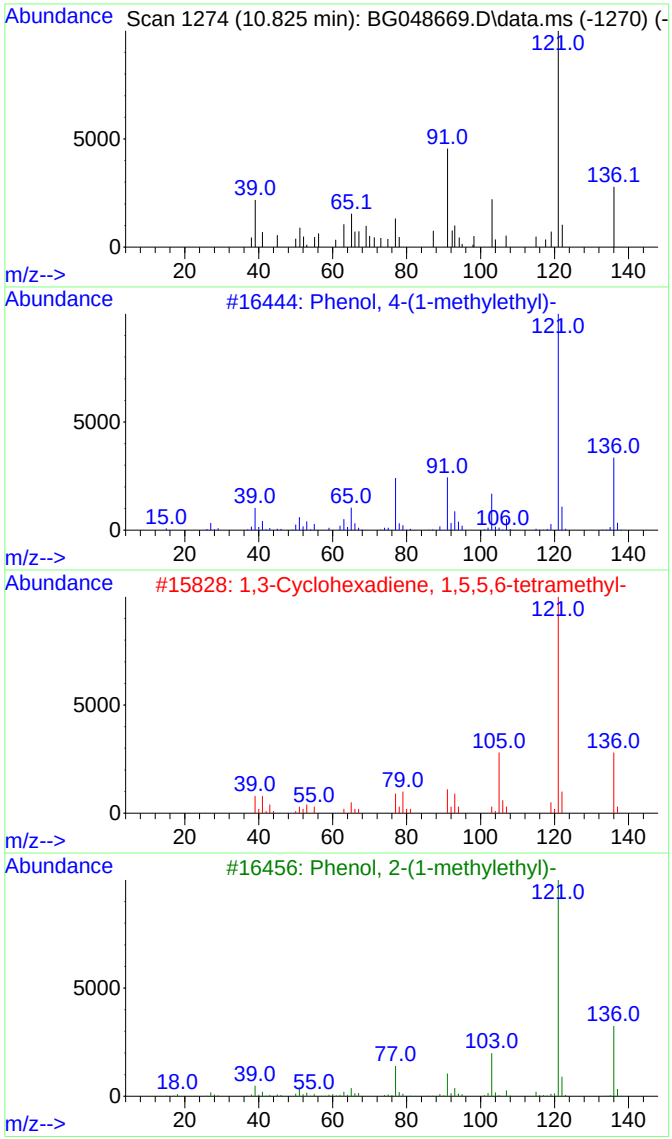
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

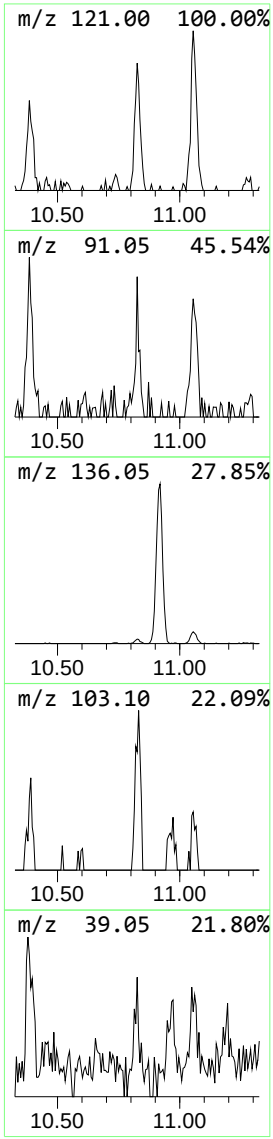
****

Peak Number 4 Phenol, 4-(1-methylethyl)- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.826	3.20 ng	36032	Naphthalene-d8	10.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1-methylethyl)-	136	C9H12O	000099-89-8	80
2	1,3-Cyclohexadiene, 1,5,5,6-tetr...	136	C10H16	000514-94-3	72
3	Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	72
4	1,3-Cyclohexadiene, 1,2,6,6-tetr...	136	C10H16	000514-96-5	64
5	Phenol, 2-ethyl-5-methyl-	136	C9H12O	001687-61-2	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041221\
Data File : BG048669.D
Acq On : 12 Apr 2021 20:35
Operator : CG/JU
Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

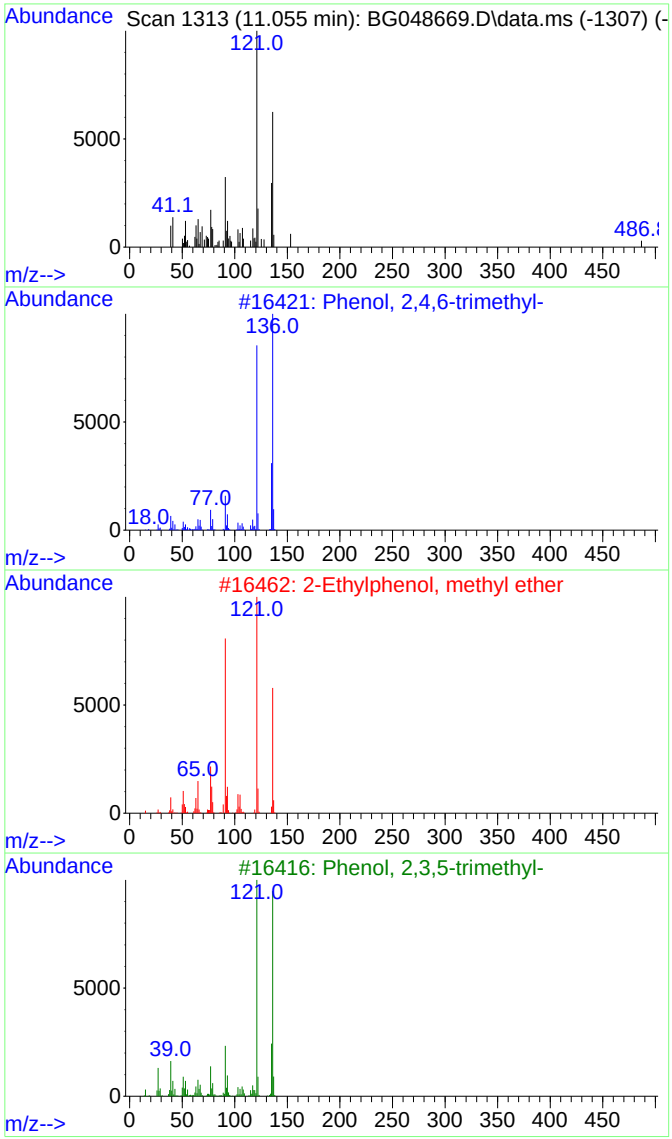
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

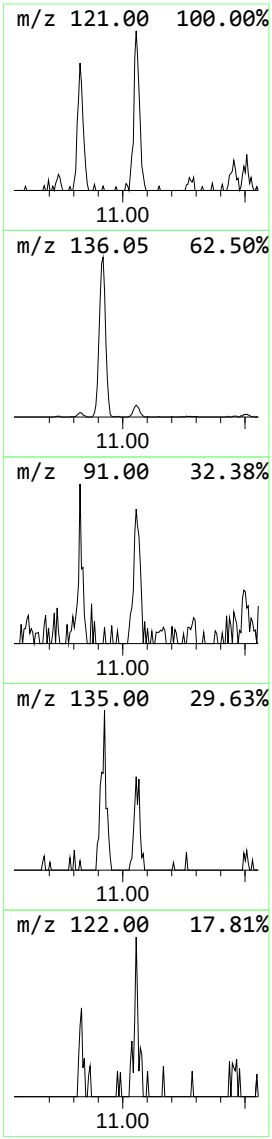
****

Peak Number 5 Phenol, 2,4,6-trimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.055	4.92 ng	55383	Naphthalene-d8	10.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4,6-trimethyl-	136	C9H12O	000527-60-6	93
2	2-Ethylphenol, methyl ether	136	C9H12O	1000333-44-2	89
3	Phenol, 2,3,5-trimethyl-	136	C9H12O	000697-82-5	87
4	3,4-Dimethylanisole	136	C9H12O	004685-47-6	87
5	Phenol, 2,3,6-trimethyl-	136	C9H12O	002416-94-6	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041221\
Data File : BG048669.D
Acq On : 12 Apr 2021 20:35
Operator : CG/JU
Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

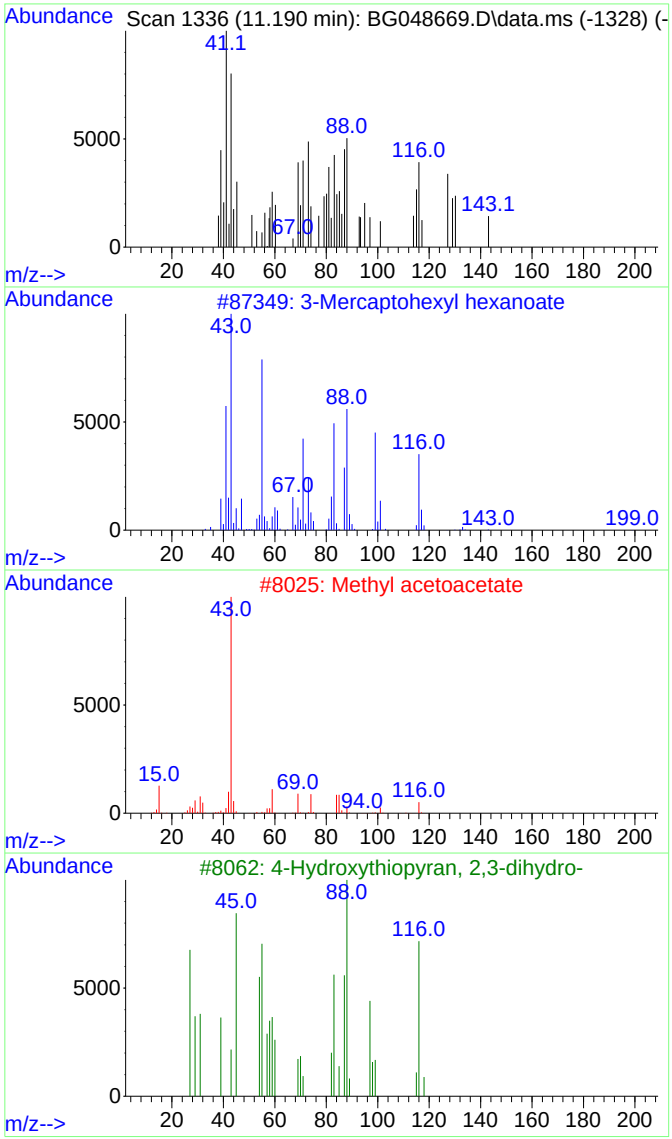
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

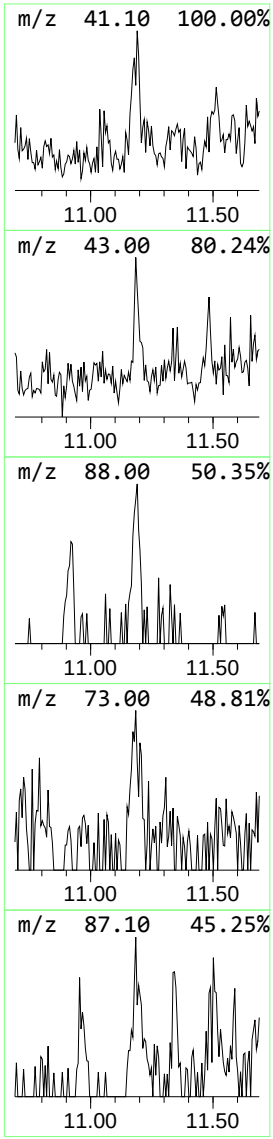
****

Peak Number 6 unknown11.190 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.190	3.69 ng	41504	Naphthalene-d8	10.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Mercaptohexyl hexanoate	232	C12H24O2S	136954-22-8	30
2	Methyl acetoacetate	116	C5H8O3	000105-45-3	22
3	4-Hydroxythiopyran, 2,3-dihydro-	116	C5H8OS	120627-18-1	16
4	3-Mercaptohexyl acetate	176	C8H16O2S	136954-20-6	16
5	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041221\
Data File : BG048669.D
Acq On : 12 Apr 2021 20:35
Operator : CG/JU
Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

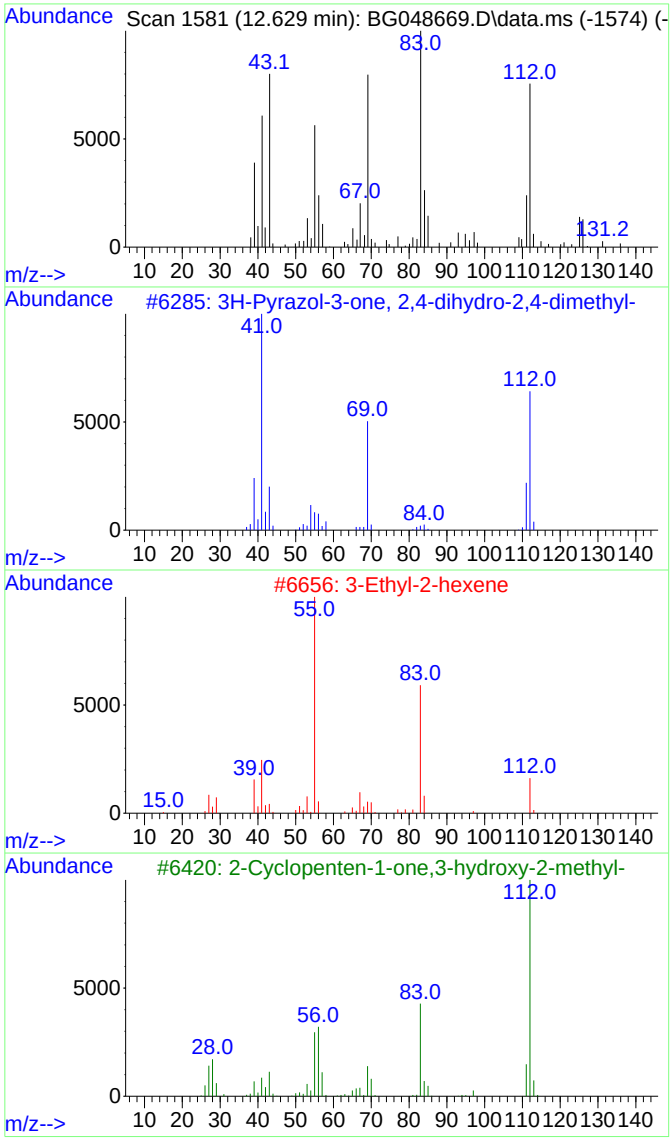
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

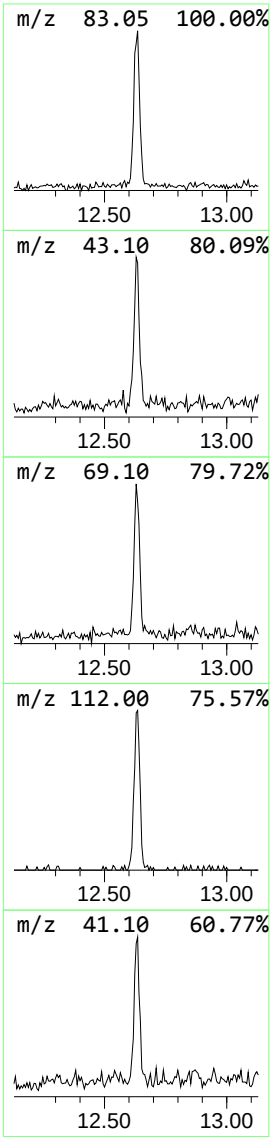
****

Peak Number 7 unknown12.629 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.629	16.19 ng	182226	Naphthalene-d8	10.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-Pyrazol-3-one, 2,4-dihydro-2,...	112	C5H8N2O	003310-38-1	46
2	3-Ethyl-2-hexene	112	C8H16	000620-00-8	43
3	2-Cyclopenten-1-one,3-hydroxy-2-...	112	C6H8O2	005870-63-3	27
4	2-Pentene, 3-methyl-, (E)-	84	C6H12	000616-12-6	25
5	1-Pentene, 3-ethyl-2-methyl-	112	C8H16	019780-66-6	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041221\
Data File : BG048669.D
Acq On : 12 Apr 2021 20:35
Operator : CG/JU
Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

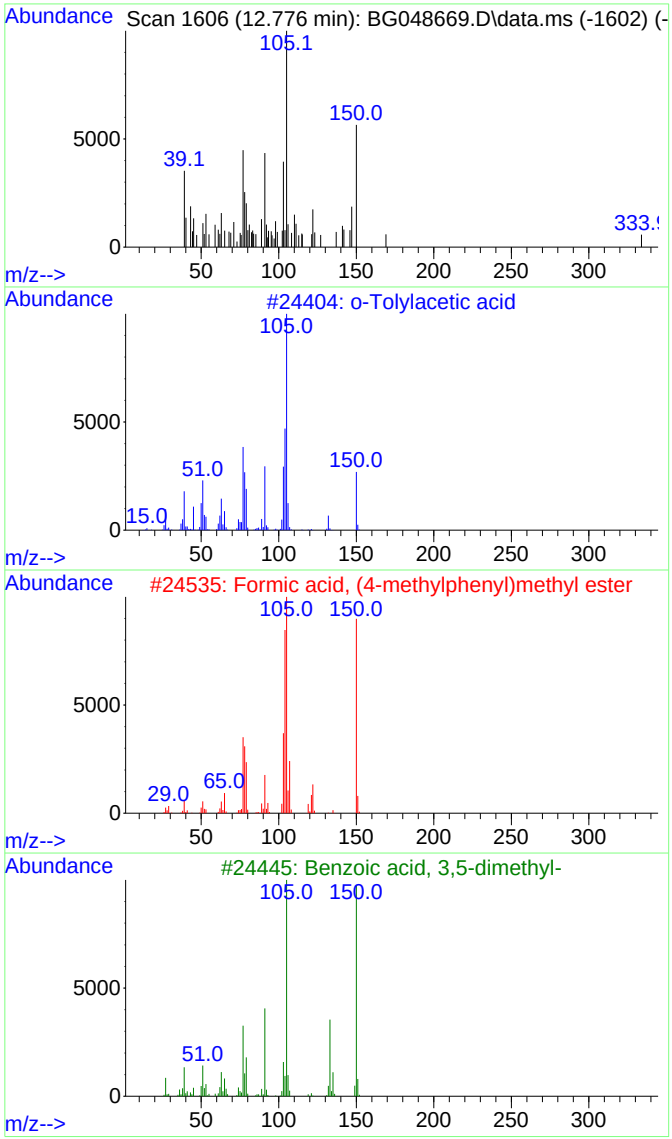
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

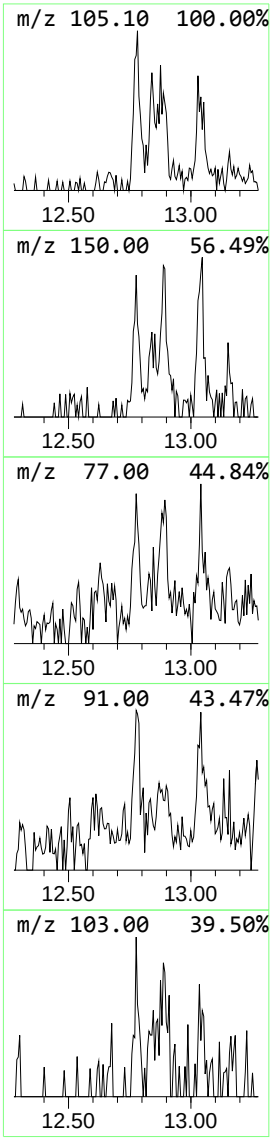
****

Peak Number 8 o-Tolylacetic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.776	4.07 ng	45856	Naphthalene-d8	10.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Tolylacetic acid	150	C9H10O2	000644-36-0	52
2	Formic acid, (4-methylphenyl)met...	150	C9H10O2	1000368-93-7	46
3	Benzoic acid, 3,5-dimethyl-	150	C9H10O2	000499-06-9	43
4	4-Ethylbenzoic acid	150	C9H10O2	000619-64-7	43
5	Benzamide, 2-(methylamino)-	150	C8H10N2O	007505-81-9	35





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Data File : BG048669.D
Acq On : 12 Apr 2021 20:35
Operator : CG/JU
Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-115RR

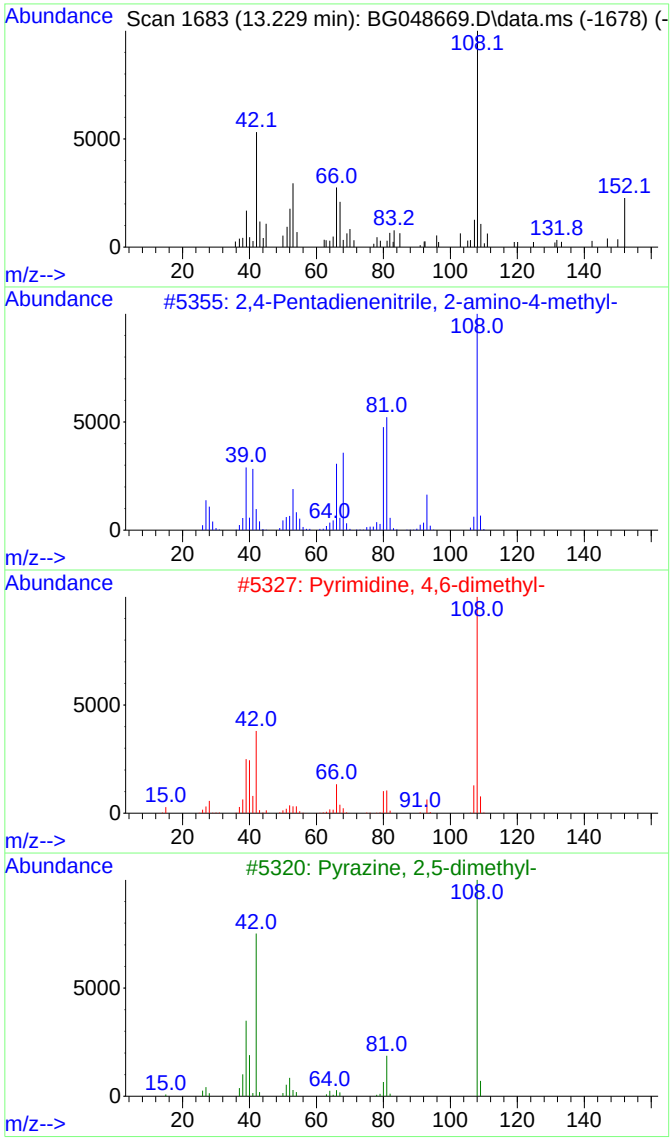
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

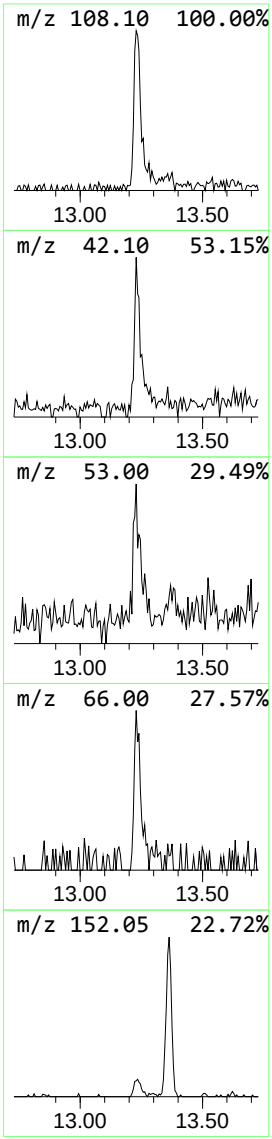
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 2,4-Pentadienenitrile, 2-am... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.229	3.73 ng	59018	Acenaphthene-d10	14.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Pentadienenitrile, 2-amino-4...	108	C6H8N2	1000196-09-3	50
2	Pyrimidine, 4,6-dimethyl-	108	C6H8N2	001558-17-4	38
3	Pyrazine, 2,5-dimethyl-	108	C6H8N2	000123-32-0	35
4	2-Pyridinamine, 3-methyl-	108	C6H8N2	001603-40-3	27
5	1,3-Benzenediamine	108	C6H8N2	000108-45-2	22





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Operator : CG/JU
Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

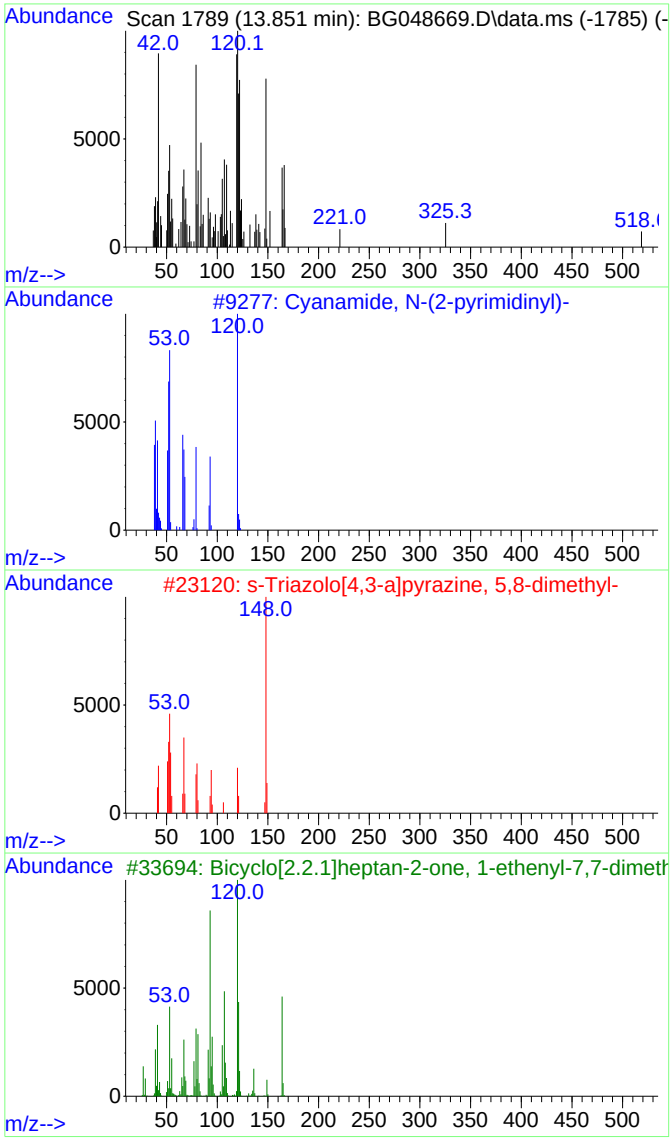
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

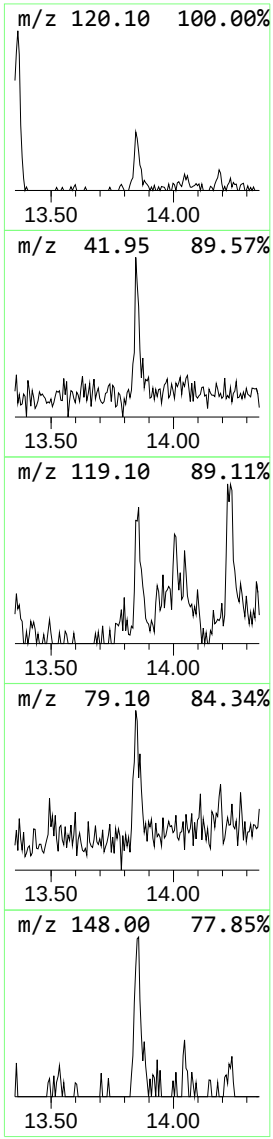
****

Peak Number 10 unknown13.851 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	2.69 ng	42478	Acenaphthene-d10	14.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyanamide, N-(2-pyrimidinyl)-	120	C5H4N4	1000362-57-6	41
2	s-Triazolo[4,3-a]pyrazine, 5,8-d...	148	C7H8N4	019848-77-2	38
3	Bicyclo[2.2.1]heptan-2-one, 1-et...	164	C11H16O	001782-96-3	16
4	1,5-Dioxaspiro[5.5]undec-2-en-4-...	318	C20H30O3	1000155-15-0	12
5	Pyrazine, 3,5-dimethyl-2-propyl-	150	C9H14N2	032350-16-6	12





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Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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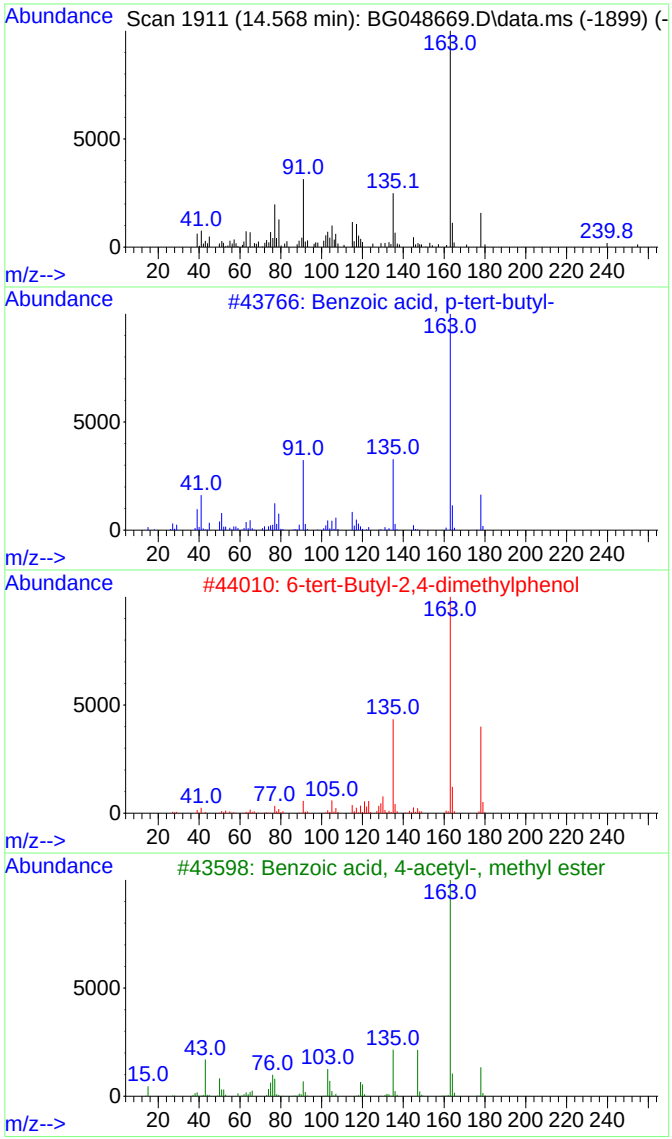
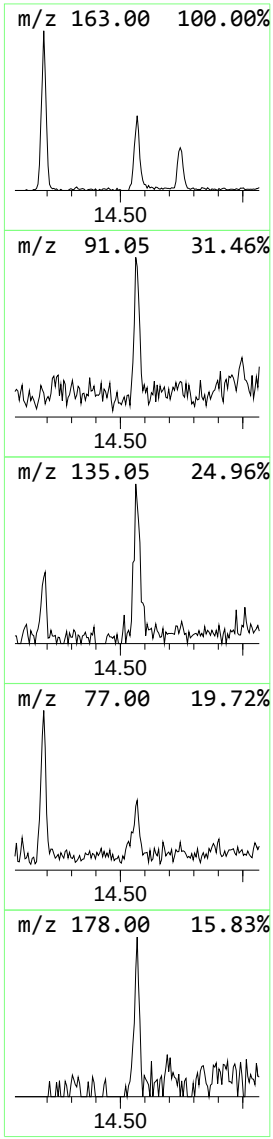
Peak Number 11 Benzoic acid, p-tert-butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.568	11.24 ng	177768	Acenaphthene-d10	14.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	80
2	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	64
3	Benzoic acid, 4-acetyl-, methyl ...	178	C10H10O3	003609-53-8	53
4	1,4-Cyclohexadiene, 3,3,6,6-tetr...	192	C14H24	078578-89-9	53
5	Propofol	178	C12H18O	002078-54-8	52





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Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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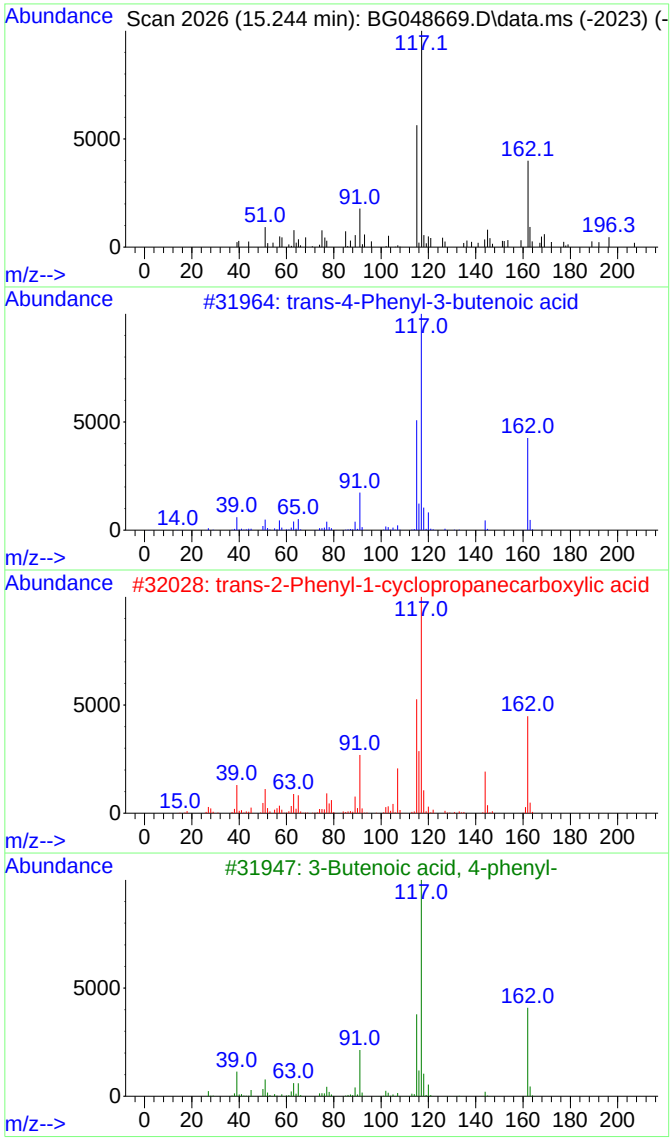
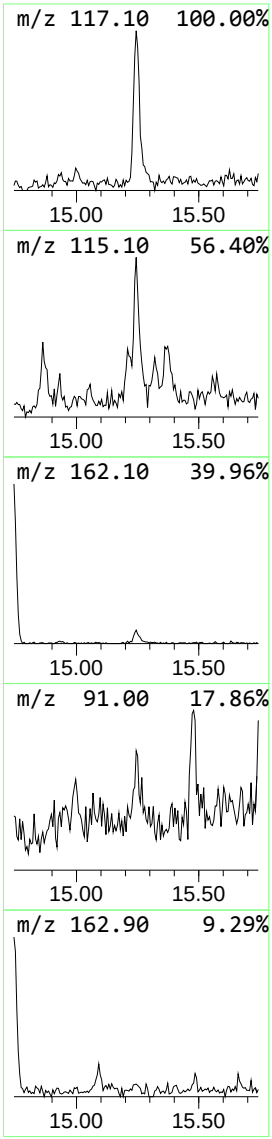
Peak Number 12 trans-4-Phenyl-3-butenoic acid Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.244	2.66 ng	42152	Acenaphthene-d10	14.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-4-Phenyl-3-butenoic acid	162	C10H10O2	001914-58-5	56
2	trans-2-Phenyl-1-cyclopropanecar...	162	C10H10O2	000939-90-2	56
3	3-Butenoic acid, 4-phenyl-	162	C10H10O2	002243-53-0	45
4	1H-Indene-5-carboxylic acid, 2,3...	162	C10H10O2	1000337-61-3	45
5	3-Bromo-1-phenyl-1-propene	196	C9H9Br	004392-24-9	40





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Operator : CG/JU
Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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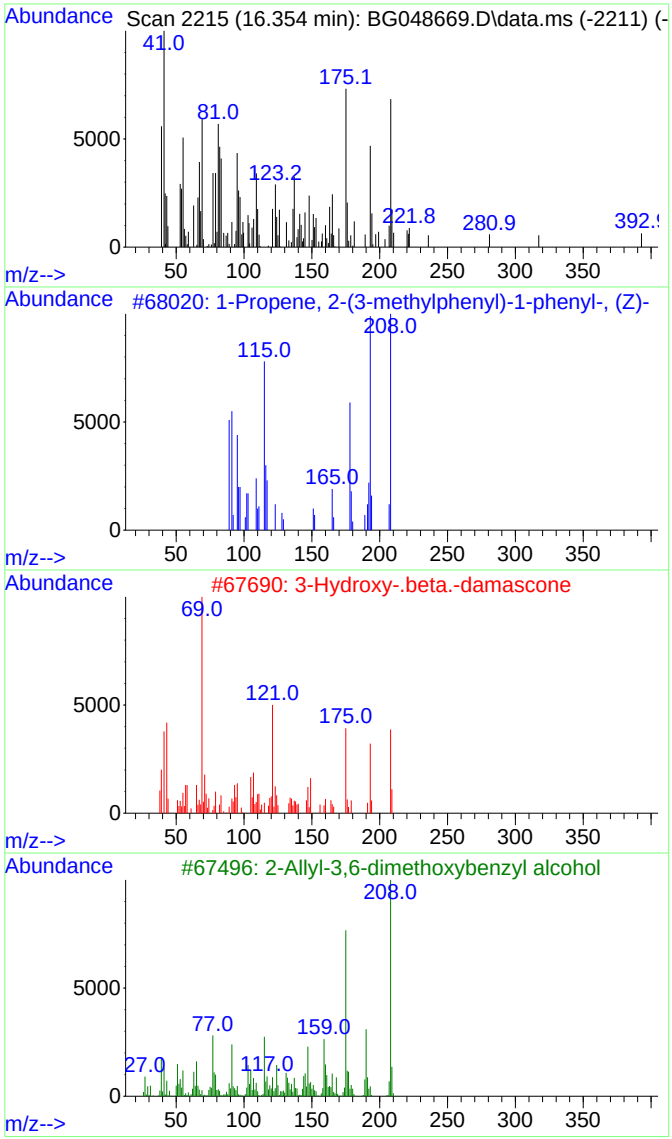
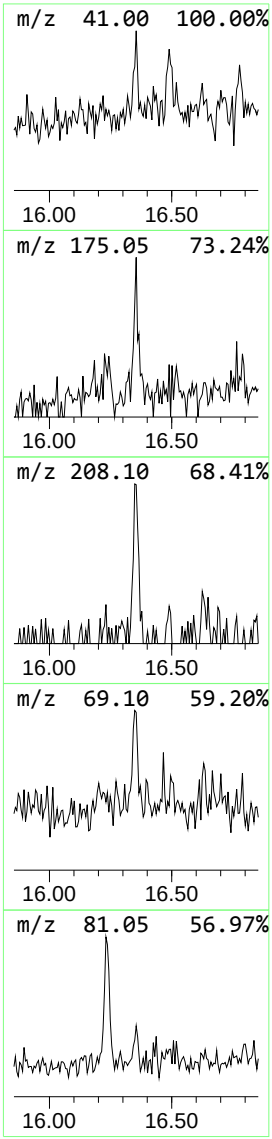
Peak Number 13 unknown16.354 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.354	2.62 ng	45443	Phenanthrene-d10	17.500

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-(3-methylphenyl)-1-...	208	C16H16	1000138-72-6	46
2	3-Hydroxy-.beta.-damascone	208	C13H20O2	102488-09-5	27
3	2-Allyl-3,6-dimethoxybenzyl alcohol	208	C12H16O3	154051-49-7	22
4	Coumarin, 7,8-dihydro-7-hydroxy-...	208	C10H8O5	1000263-13-6	18
5	Cycloheptene, 1,2-dimethyl-	124	C9H16	020053-89-8	18





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Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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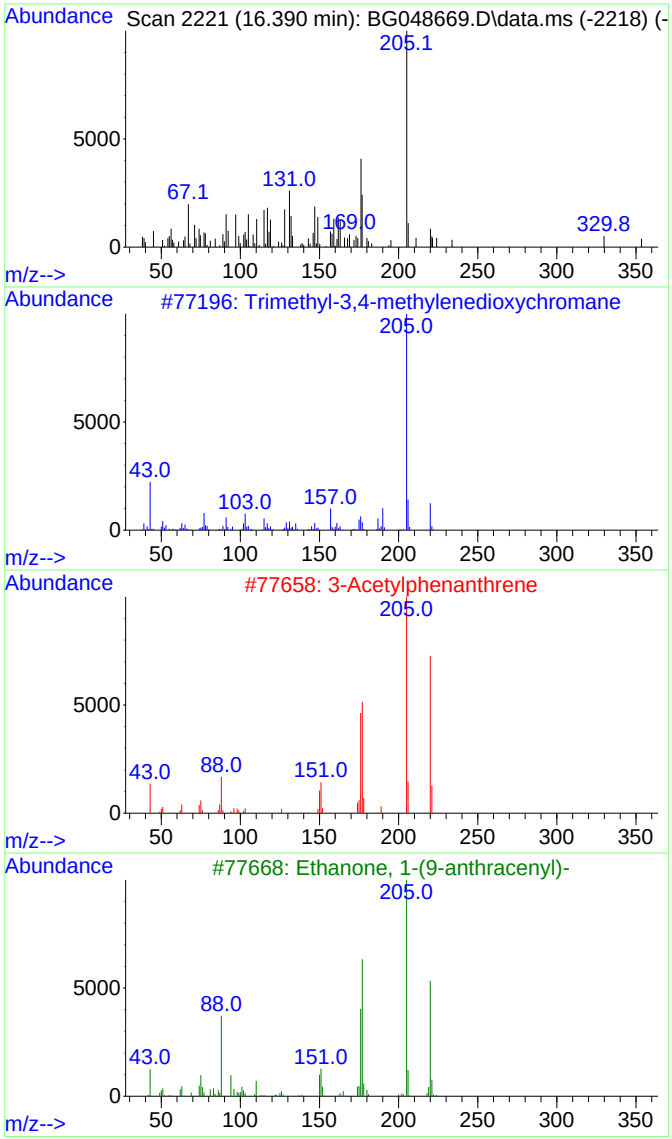
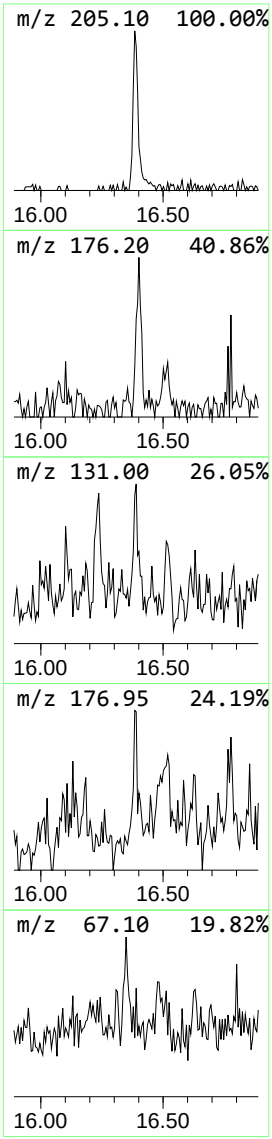
Peak Number 14 unknown16.390 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.390	3.53 ng	61235	Phenanthrene-d10	17.500

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trimethyl-3,4-methylenedioxychro...	220	C13H16O3	1000378-97-7	43
2	3-Acetylphenanthrene	220	C16H12O	002039-76-1	42
3	Ethanone, 1-(9-anthracenyl)-	220	C16H12O	000784-04-3	42
4	Xylazine	220	C12H16N2S	007361-61-7	40
5	2-Methyl-6-methoxy-7-hydroxy-8-p...	290	C17H26N2O2	1000254-76-0	40





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Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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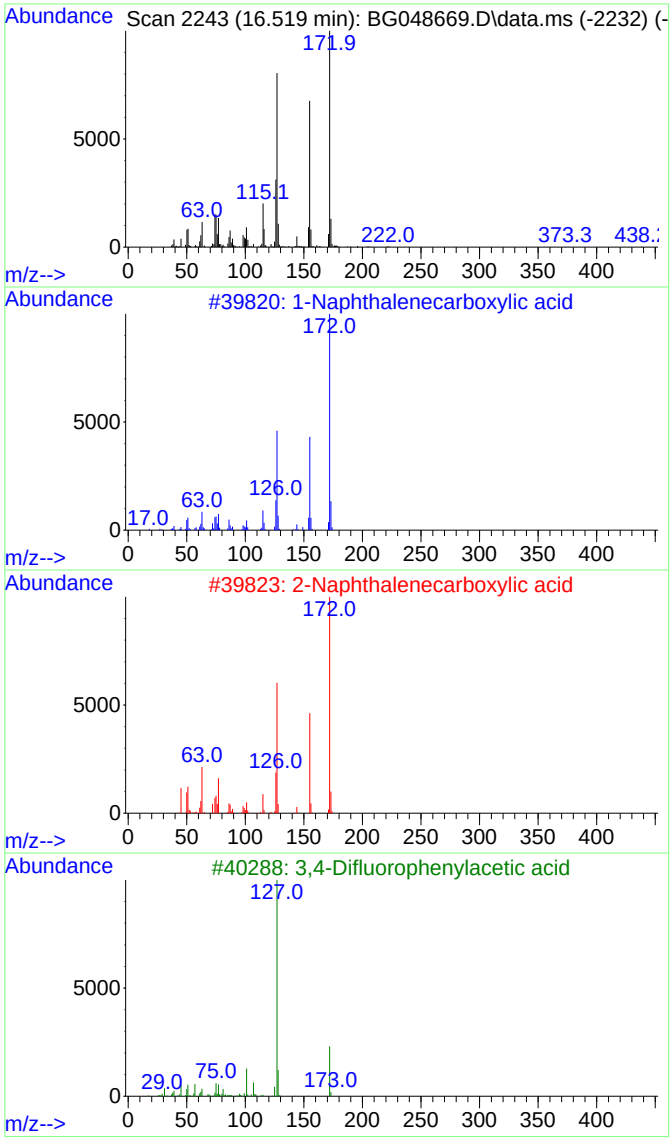
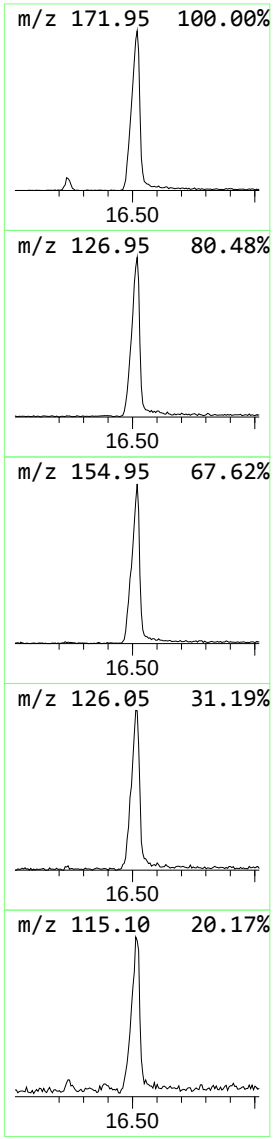
Peak Number 15 1-Naphthalenecarboxylic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.519	80.53 ng	1398900	Phenanthrene-d10	17.500

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenecarboxylic acid	172	C11H8O2	000086-55-5	95
2	2-Naphthalenecarboxylic acid	172	C11H8O2	000093-09-4	93
3	3,4-Difluorophenylacetic acid	172	C8H6F2O2	000658-93-5	58
4	1-Naphthalenecarbonyl chloride	190	C11H7ClO	000879-18-5	46
5	Naphthalene, 2-nitro-	173	C10H7NO2	000581-89-5	45





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Sample : M1966-04
Misc :
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Instrument : BNA_G
ClientSampleId : MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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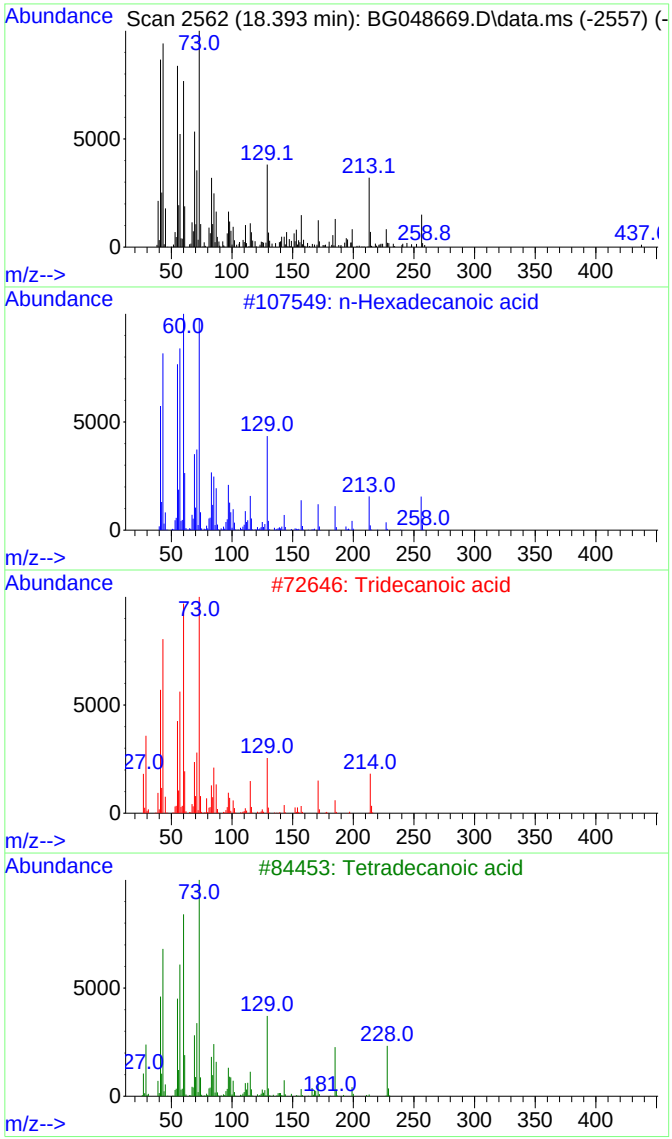
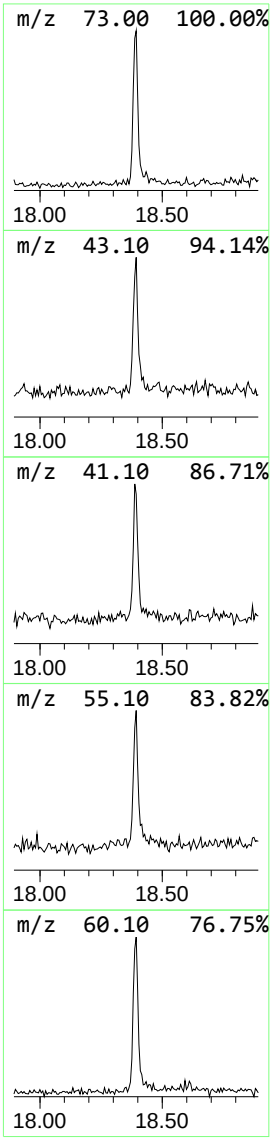
Peak Number 16 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.393	16.93 ng	294050	Phenanthrene-d10	17.500

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Octadecanoic acid	284	C18H36O2	000057-11-4	70
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	68





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Operator : CG/JU
Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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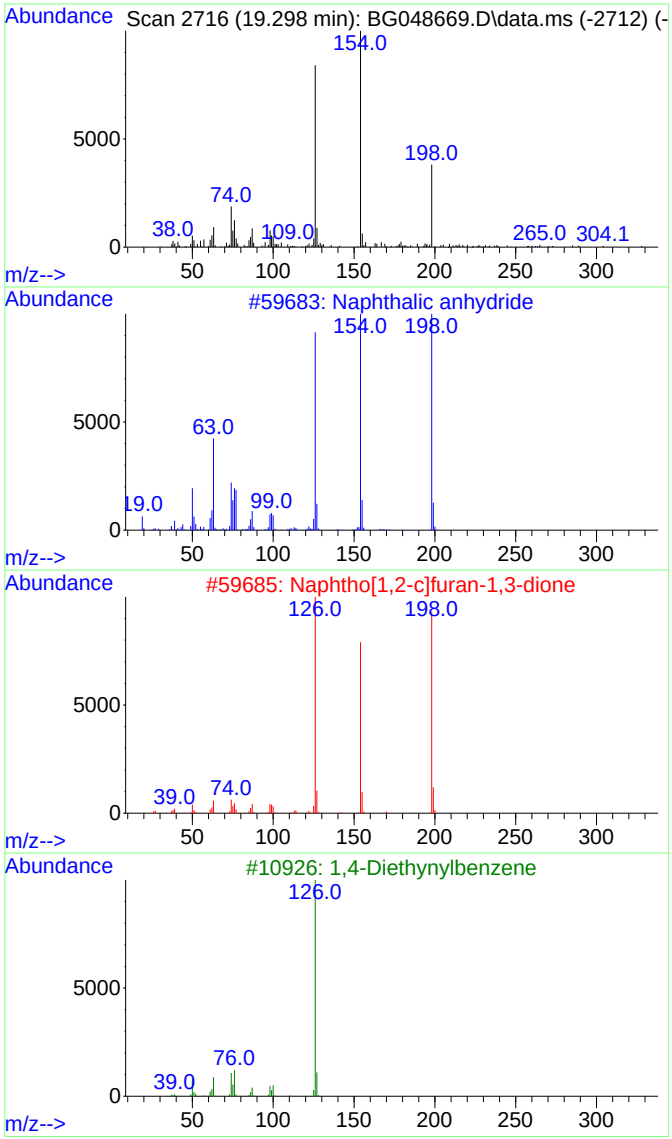
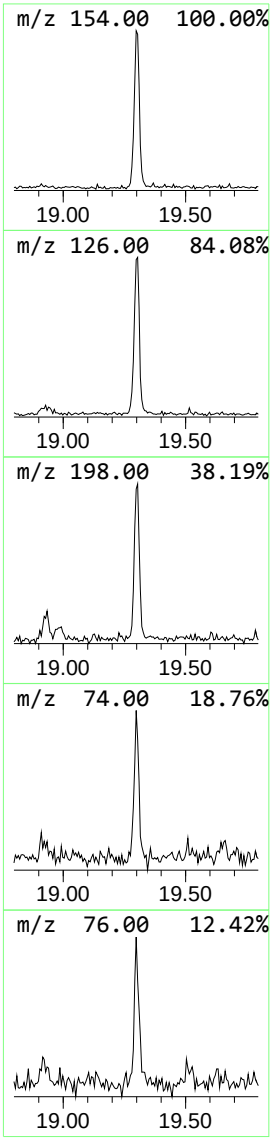
Peak Number 17 Naphthalic anhydride Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.298	12.25 ng	212866	Phenanthrene-d10	17.500

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalic anhydride	198	C12H6O3	000081-84-5	87
2	Naphtho[1,2-c]furan-1,3-dione	198	C12H6O3	005343-99-7	78
3	1,4-Diethynylbenzene	126	C10H6	000935-14-8	42
4	2,3-Naphthalenedicarboxylic acid	216	C12H8O4	002169-87-1	42
5	l-Valine, n-propargyloxycarbonyl...	409	C24H43NO4	1000323-31-7	22





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ClientSampleId : MW-115RR

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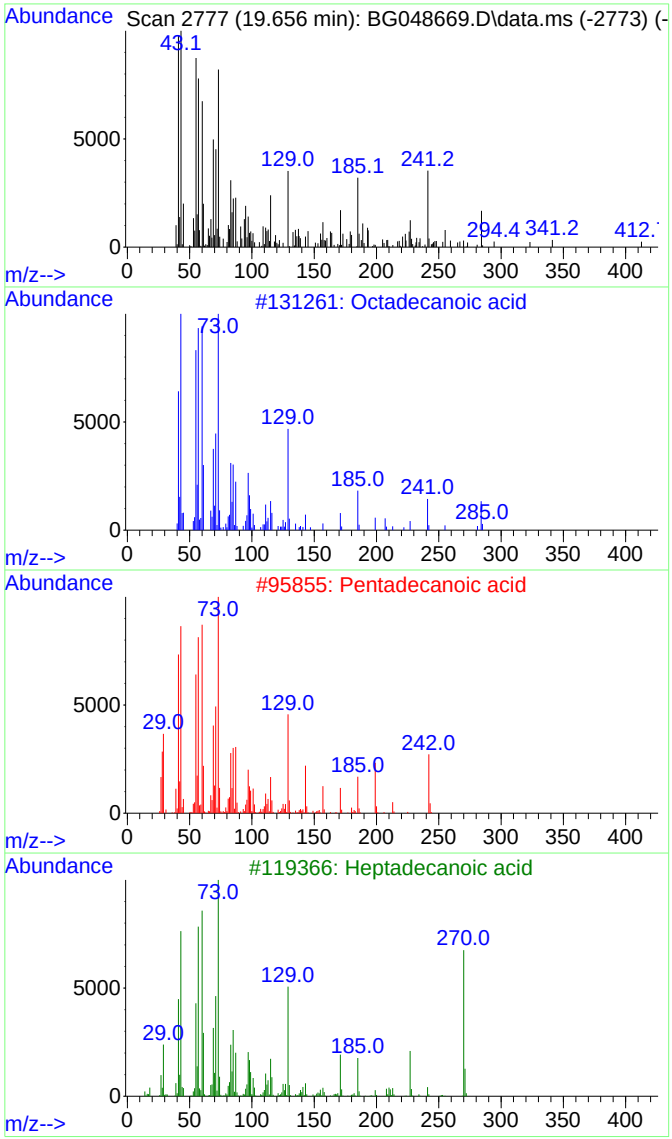
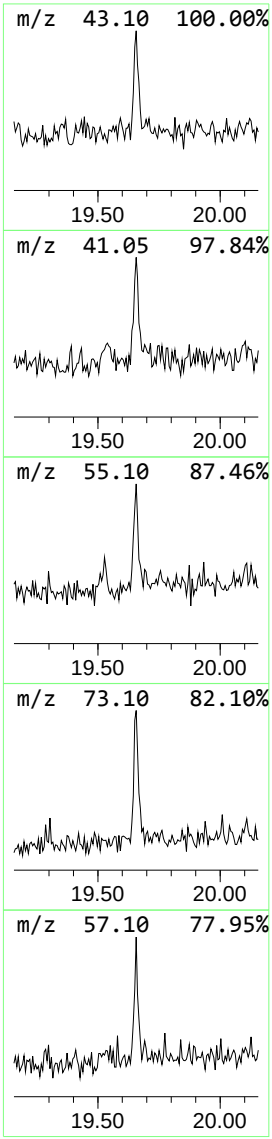
Peak Number 18 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.656	6.03 ng	110730	Chrysene-d12	21.795

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	86
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	55
3	Heptadecanoic acid	270	C17H34O2	000506-12-7	53
4	.alpha.-D-Galactopyranoside, met...	306	C15H30O6	1000157-05-0	43
5	Undecanoic acid	186	C11H22O2	000112-37-8	27





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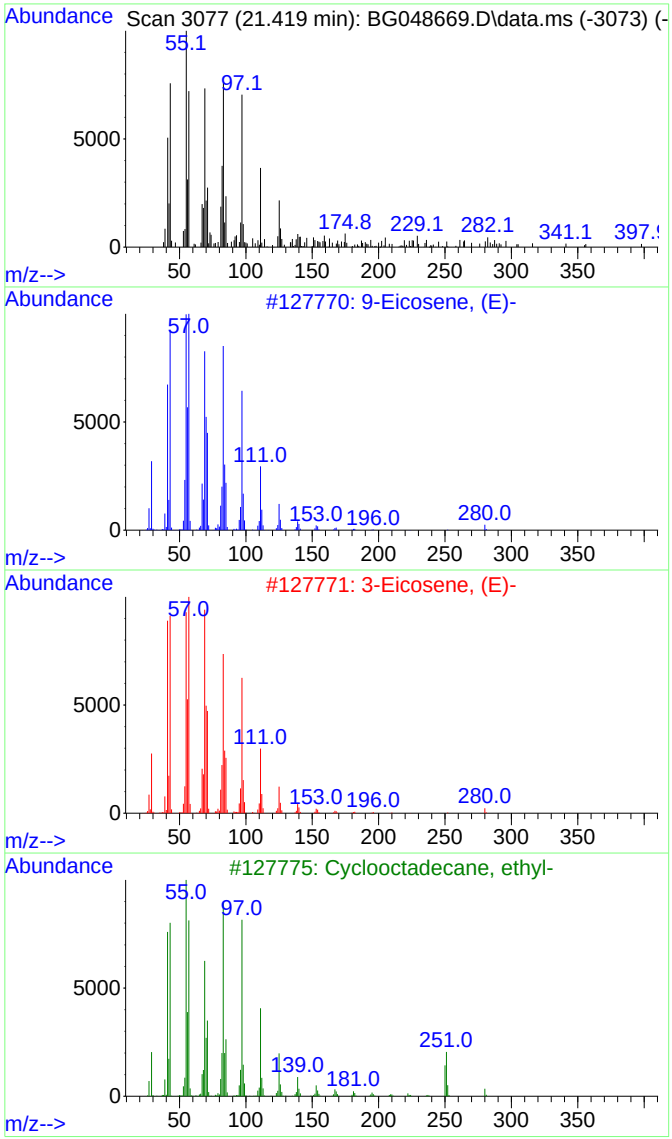
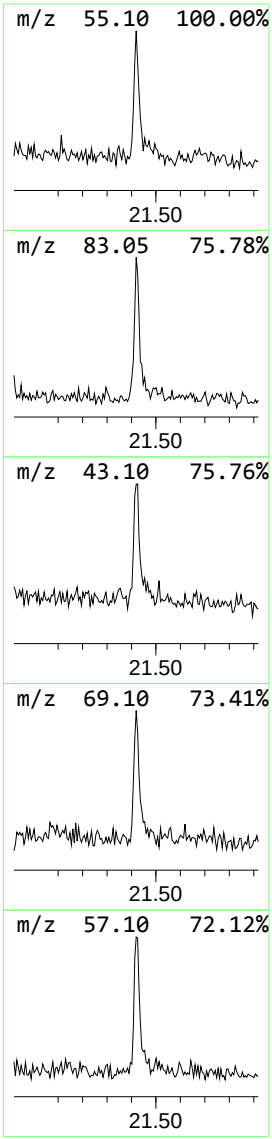
Peak Number 19 9-Eicosene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.419	9.88 ng	181329	Chrysene-d12	21.795

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Eicosene, (E)-	280	C20H40	074685-29-3	83
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	53
3	Cyclooctadecane, ethyl-	280	C20H40	1000151-22-5	53
4	Cyclopentane, (2-hexyloctyl)-	266	C19H38	055044-77-4	49
5	Cyclopentane, (2-methylpropyl)-	126	C9H18	003788-32-7	49





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Acq On : 12 Apr 2021 20:35
Operator : CG/JU
Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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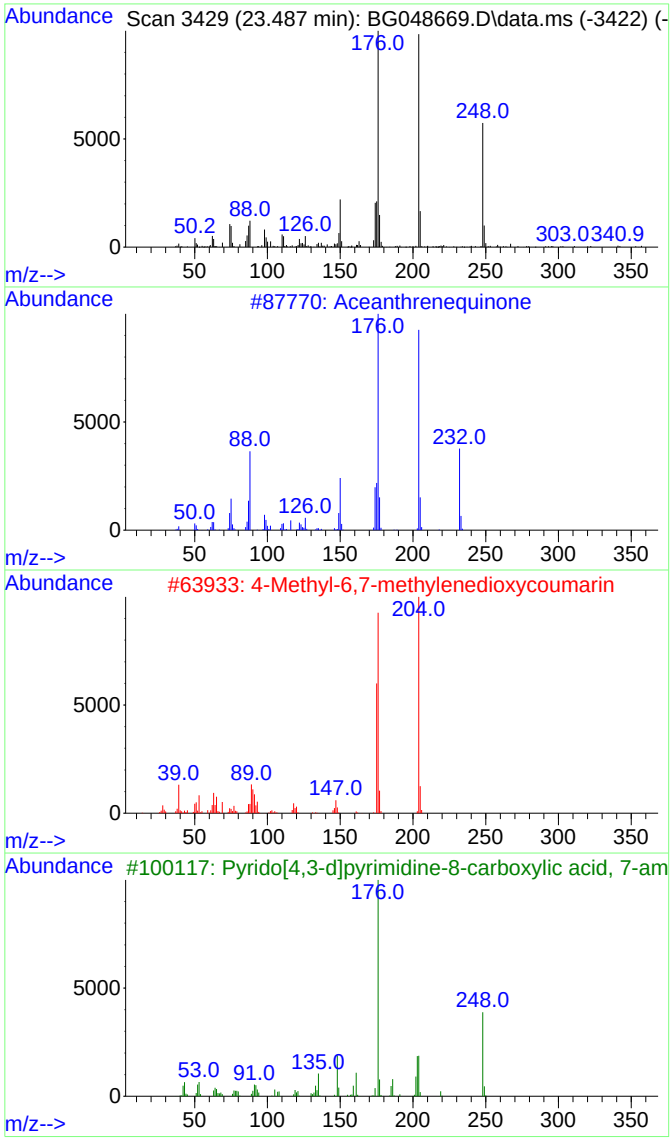
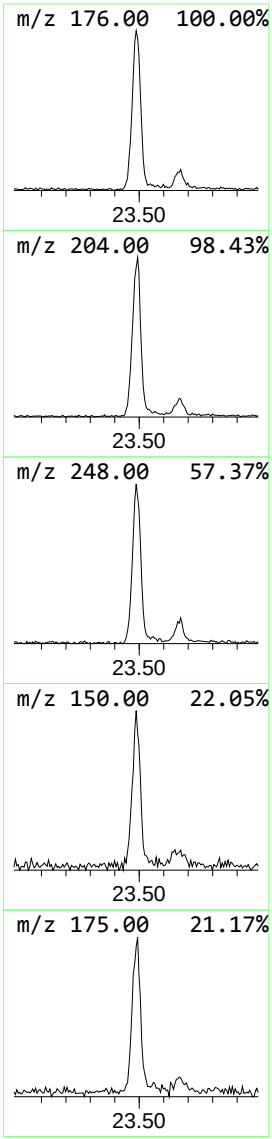
Peak Number 20 Aceanthrenequinone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.487	30.59 ng	595011	Perylene-d12	25.150

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aceanthrenequinone	232	C16H8O2	006373-11-1	74
2	4-Methyl-6,7-methylenedioxycoumarin	204	C11H8O4	015071-04-2	38
3	Pyrido[4,3-d]pyrimidine-8-carbox...	248	C11H12N4O3	1000350-96-4	38
4	Acephenanthrylene, 4,5-dihydro-	204	C16H12	006232-48-0	37
5	5-Thiazolecarboxylic acid, 2-ami...	248	C12H12N2O2S	064399-23-1	32





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041221\
Data File : BG048669.D
Acq On : 12 Apr 2021 20:35
Operator : CG/JU
Sample : M1966-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-115RR

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Tetracyclo[3.3....	8.469	4.9	ng	43156	1	8.088	177164	20.0
Phenol, 2,6-dim...	9.521	9.7	ng	108903	2	10.919	225103	20.0
Phenol, 2,3-dim...	10.385	7.2	ng	81248	2	10.919	225103	20.0
Phenol, 4-(1-me...	10.826	3.2	ng	36032	2	10.919	225103	20.0
Phenol, 2,4,6-t...	11.055	4.9	ng	55383	2	10.919	225103	20.0
unknown11.190	11.190	3.7	ng	41504	2	10.919	225103	20.0
unknown12.629	12.629	16.2	ng	182226	2	10.919	225103	20.0
o-Tolylacetic acid	12.776	4.1	ng	45856	2	10.919	225103	20.0
2,4-Pentadienen...	13.229	3.7	ng	59018	3	14.744	316380	20.0
unknown13.851	13.851	2.7	ng	42478	3	14.744	316380	20.0
Benzoic acid, p...	14.568	11.2	ng	177768	3	14.744	316380	20.0
trans-4-Phenyl-...	15.244	2.7	ng	42152	3	14.744	316380	20.0
unknown16.354	16.354	2.6	ng	45443	4	17.500	347420	20.0
unknown16.390	16.390	3.5	ng	61235	4	17.500	347420	20.0
1-Naphthaleneca...	16.519	80.5	ng	1398900	4	17.500	347420	20.0
n-Hexadecanoic ...	18.393	16.9	ng	294050	4	17.500	347420	20.0
Naphthalic anhy...	19.298	12.3	ng	212866	4	17.500	347420	20.0
Octadecanoic acid	19.656	6.0	ng	110730	5	21.795	367232	20.0
9-Eicosene, (E)-	21.419	9.9	ng	181329	5	21.795	367232	20.0
Aceanthrenequinone	23.487	30.6	ng	595011	6	25.150	389003	20.0