LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010521\
Data File : BG047869.D
Acq On : 5 Jan 2021 16:15
Operator : CG/JU
Sample : M1006-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : R-LA-21-5-WC

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-BG121720.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG047869.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.251	319	325	332	rBV	21329	36449	2.16%	0.382%
2	5.727	398	406	415	rBV	403421	644351	38.15%	6.758%
3	7.336	672	680	689	rBV	412044	712655	42.20%	7.474%
4	8.194	820	826	833	rBV	108215	186000	11.01%	1.951%
5	9.363	1016	1025	1033	rBV	262735	471385	27.91%	4.944%
6	11.020	1301	1307	1316	rBV	121619	231445	13.70%	2.427%
7	13.447	1712	1720	1728	rBV	636503	995392	58.94%	10.439%
8	14.099	1823	1831	1834	rBV3	11442	19284	1.14%	0.202%
9	14.146	1834	1839	1846	rVB4	11164	21740	1.29%	0.228%
10	14.258	1852	1858	1865	rBV	101380	140484	8.32%	1.473%
11	14.822	1947	1954	1962	rVB	194637	313311	18.55%	3.286%
12	16.297	2199	2205	2212	rBV	575092	868488	51.42%	9.108%
13	17.554	2413	2419	2426	rBV	256590	407995	24.16%	4.279%
14	20.139	2853	2859	2868	rBV	1259812	1688881	100.00%	17.712%
15	20.780	2957	2968	2972	rBV5	100983	233915	13.85%	2.453%
16	20.909	2988	2990	2996	rVB6	13564	22862	1.35%	0.240%
17	21.396	3068	3073	3077	rBV2	71965	137918	8.17%	1.446%
18	21.467	3077	3085	3090	rVV	148000	322354	19.09%	3.381%
19	21.532	3090	3096	3102	rVV	491541	734836	43.51%	7.707%
20	21.614	3106	3110	3115	rVB	27138	38009	2.25%	0.399%
21	21.831	3141	3147	3156	rVB	317254	568087	33.64%	5.958%
22	23.553	3431	3440	3445	rBV5	33872	81586	4.83%	0.856%
23	24.181	3543	3547	3555	rVB10	12562	27093	1.60%	0.284%
24	25.174	3707	3716	3729	rVB3	204392	612276	36.25%	6.421%
25	27.754	4149	4155	4157	rBV5	10125	18367	1.09%	0.193%

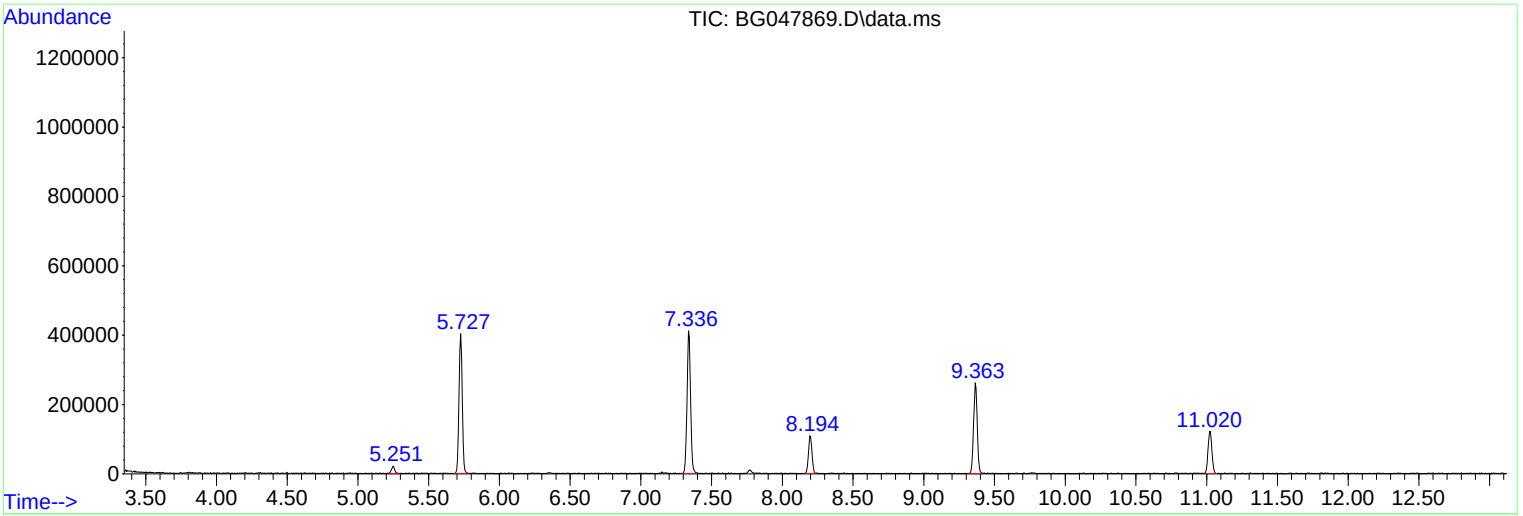
Sum of corrected areas: 9535163

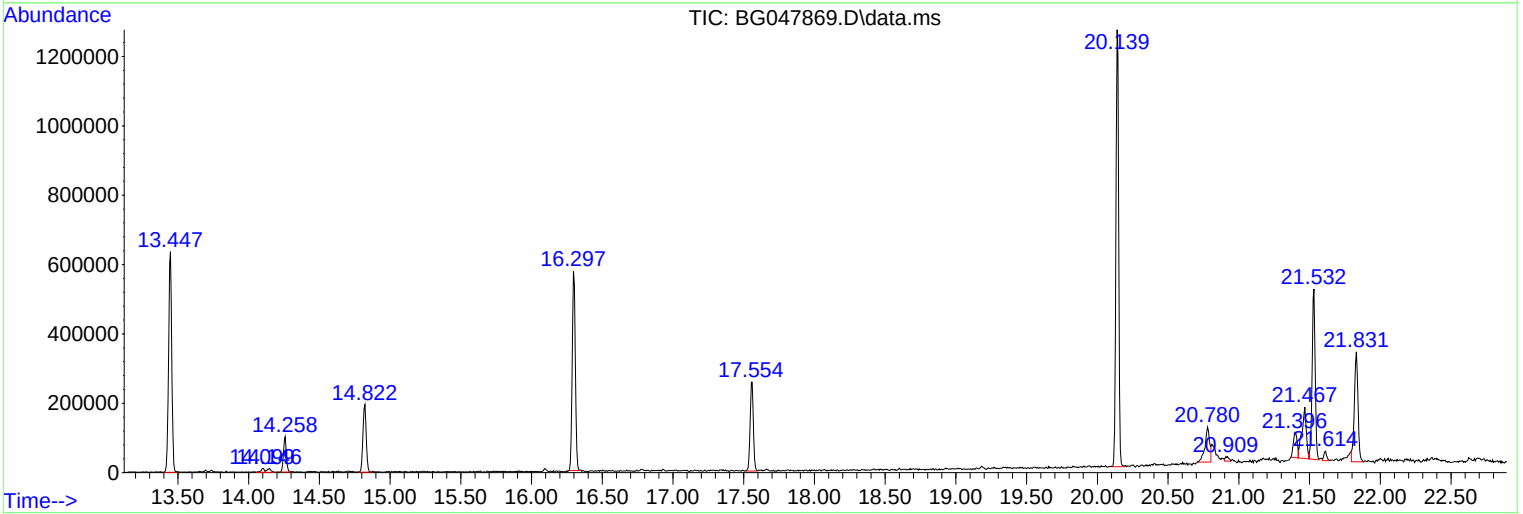
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010521\
Data File : BG047869.D
Acq On : 5 Jan 2021 16:15
Operator : CG/JU
Sample : M1006-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

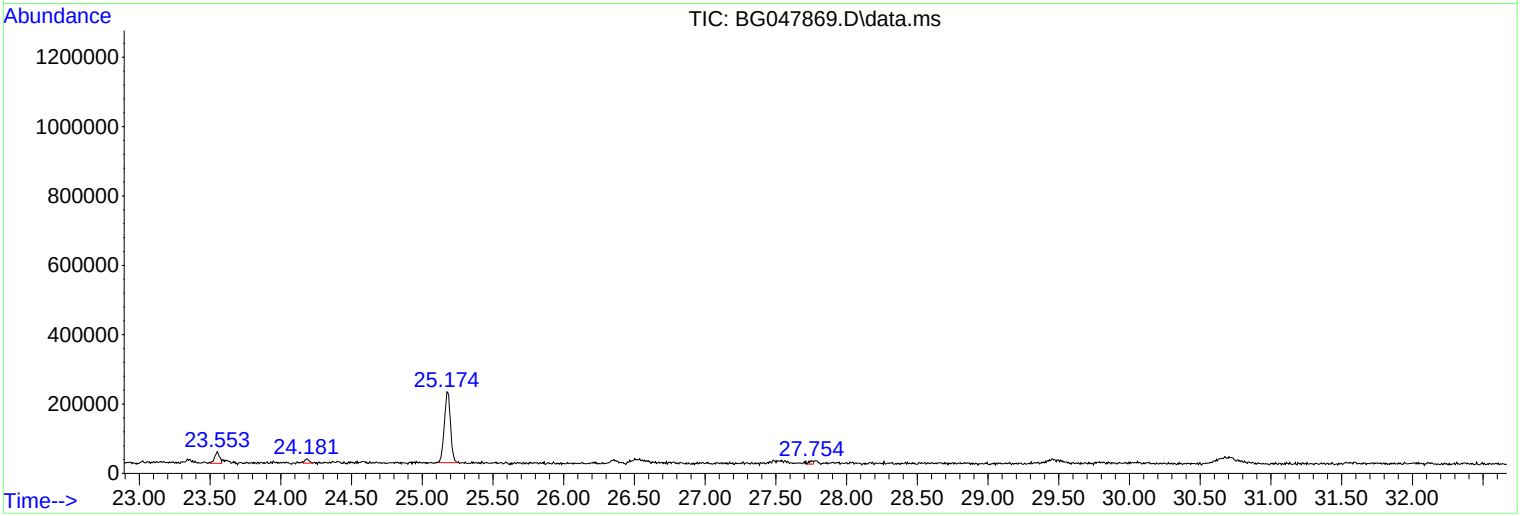
Instrument :
BNA_G
ClientSampleId :
R-LA-21-5-WC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.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\BG010521\
Data File : BG047869.D
Acq On : 5 Jan 2021 16:15
Operator : CG/JU
Sample : M1006-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
R-LA-21-5-WC

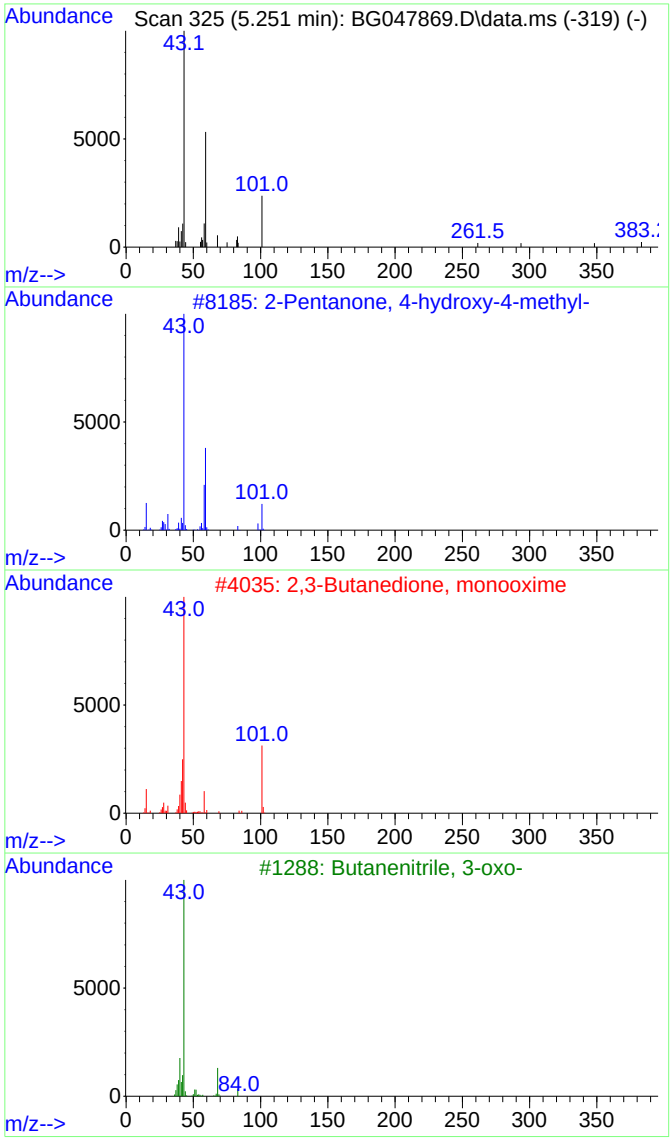
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

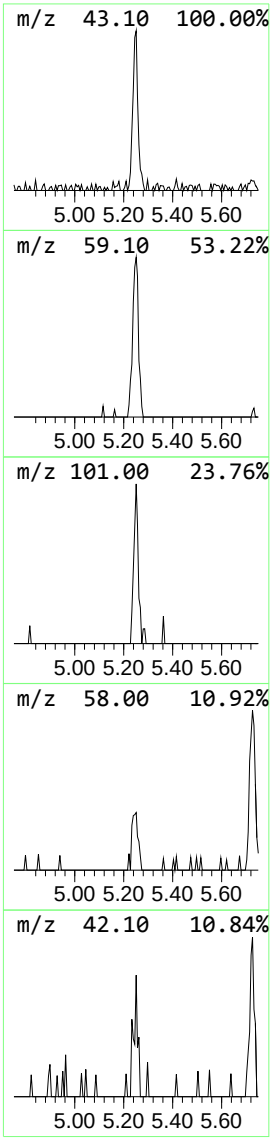
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.251	3.92 ng	36449	1,4-Dichlorobenzene-d4	8.200

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	Butanenitrile, 3-oxo-	83	C4H5NO	1000337-73-7	14
4	Butane	58	C4H10	000106-97-8	12
5	Propylamine	59	C3H9N	000107-10-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010521\
Data File : BG047869.D
Acq On : 5 Jan 2021 16:15
Operator : CG/JU
Sample : M1006-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : R-LA-21-5-WC

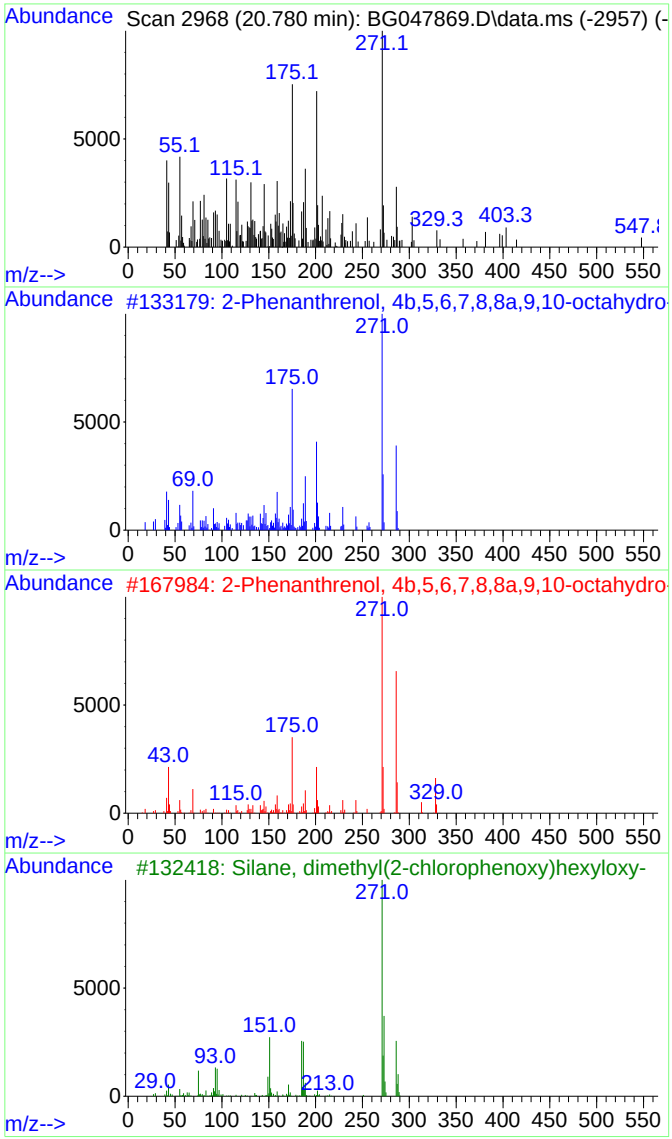
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

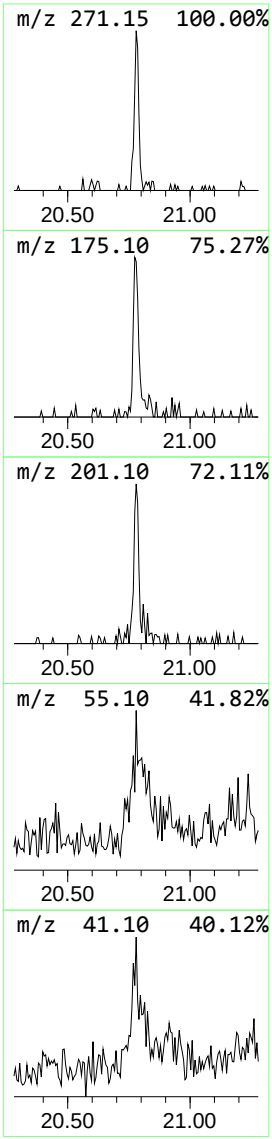
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.779	8.24 ng	233915	Chrysene-d12	21.831

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	93
2	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	64
3	Silane, dimethyl(2-chlorophenoxy...	286	C14H23ClO2Si	1000347-07-3	41
4	Quinuclidin-3-one, 2-(4-dimethyl...	271	C16H21N3O	1000266-14-6	38
5	Silane, dimethyl(2-chloro-5-meth...	286	C14H23ClO2Si	1000347-54-6	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010521\
Data File : BG047869.D
Acq On : 5 Jan 2021 16:15
Operator : CG/JU
Sample : M1006-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : R-LA-21-5-WC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

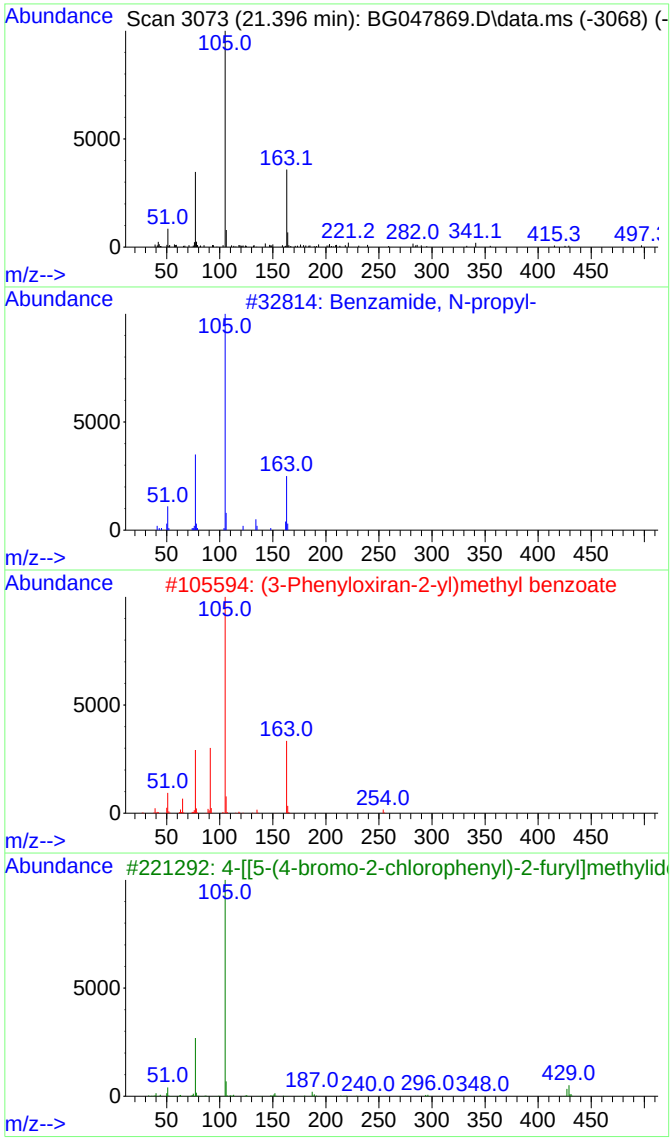
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

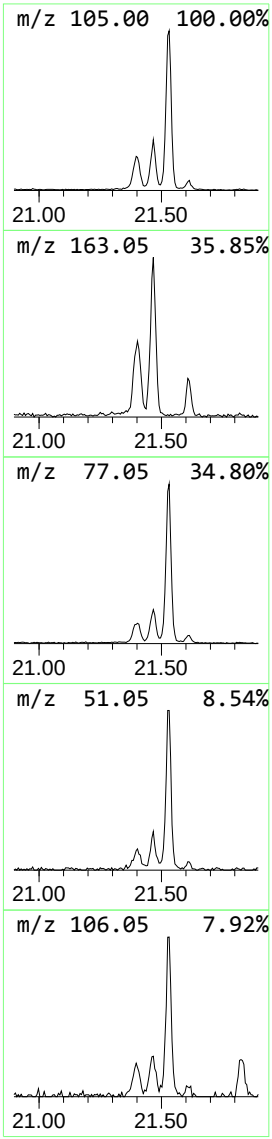
****

Peak Number 3 Benzamide, N-propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.396	4.86 ng	137918	Chrysene-d12	21.831

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	59
2	(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	59
3	4-[[5-(4-bromo-2-chlorophenyl)-2...	427	C20H11BrClNO3	282539-13-3	43
4	1-Benzoyl-2-trichloroacetylhydra...	280	C9H7Cl3N2O2	090273-66-8	43
5	1H-Indole, 1-benzoyl-	221	C15H11NO	001496-76-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010521\
Data File : BG047869.D
Acq On : 5 Jan 2021 16:15
Operator : CG/JU
Sample : M1006-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
R-LA-21-5-WC

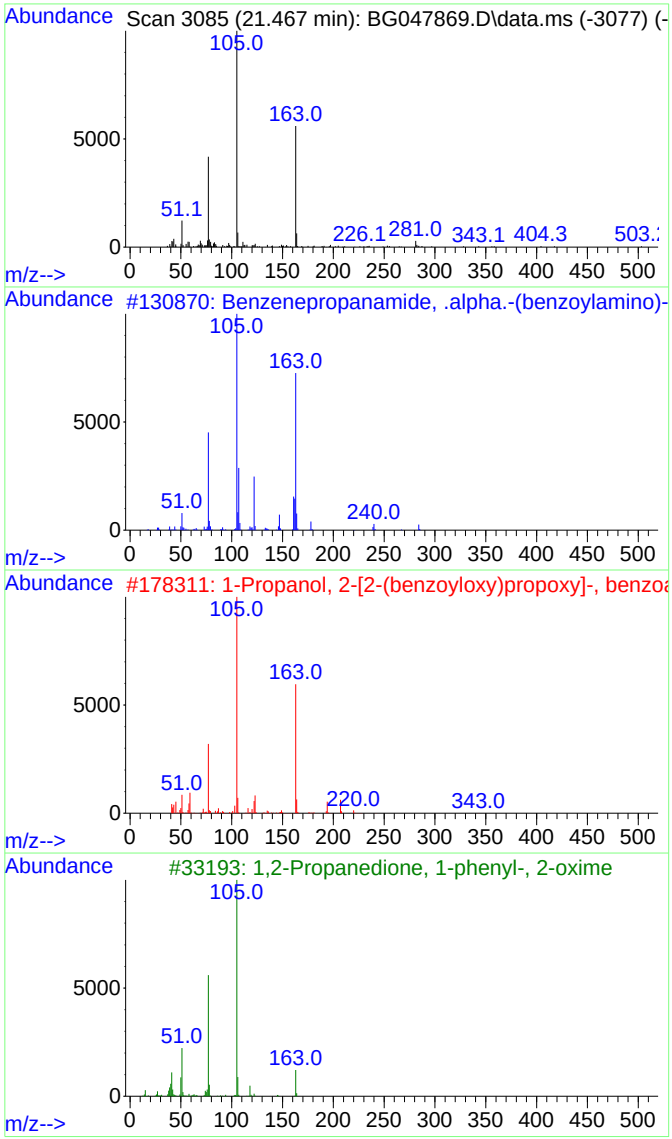
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

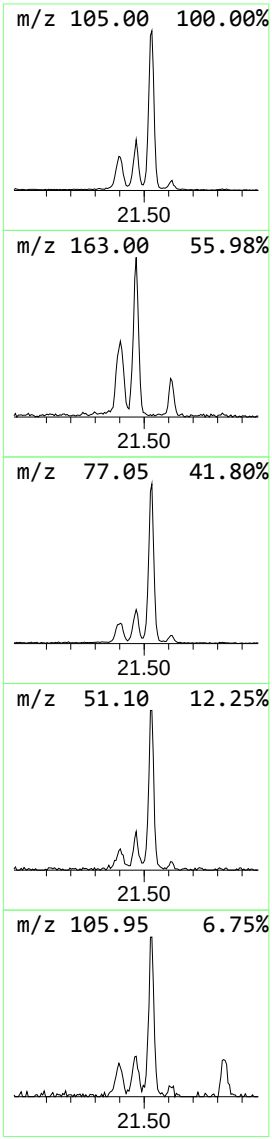
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzenepropanamide, .alpha.... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.467	11.35 ng	322354	Chrysene-d12	21.831

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	78
2	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	78
3	1,2-Propanedione, 1-phenyl-, 2-o...	163	C9H9NO2	000119-51-7	72
4	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	56
5	1,2,3-Propanetriol, tribenzoate	404	C24H20O6	000614-33-5	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010521\
Data File : BG047869.D
Acq On : 5 Jan 2021 16:15
Operator : CG/JU
Sample : M1006-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : R-LA-21-5-WC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

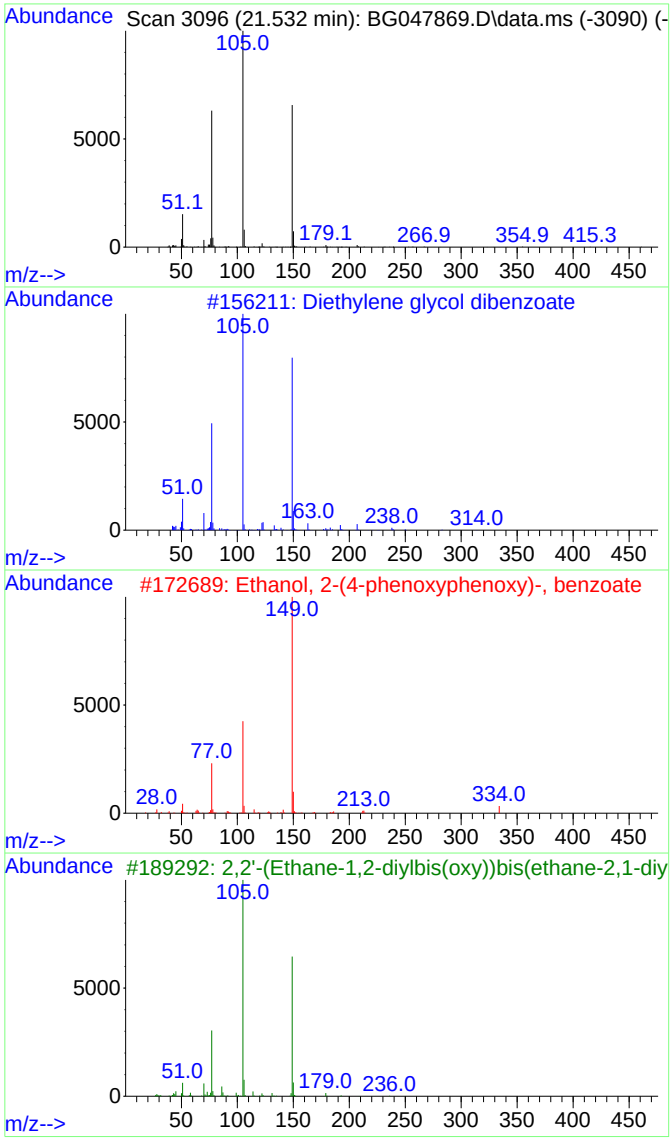
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

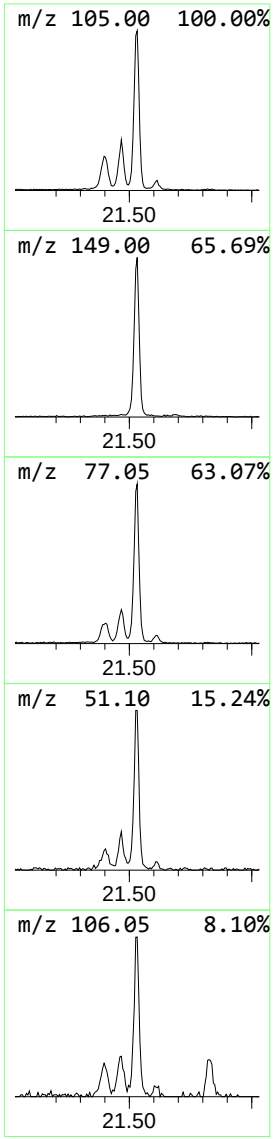
****

Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.532	25.87 ng	734836	Chrysene-d12	21.831

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	83
2	Ethanol, 2-(4-phenoxyphenoxy)-, ...	334	C21H18O4	055191-59-8	83
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	74
4	1-Triazene, 3,3-dimethyl-1-phenyl-	149	C8H11N3	007227-91-0	58
5	Benzoic acid, (4-nitrophenyl)-me...	269	C14H11N3O3	028123-77-5	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010521\
Data File : BG047869.D
Acq On : 5 Jan 2021 16:15
Operator : CG/JU
Sample : M1006-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
R-LA-21-5-WC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

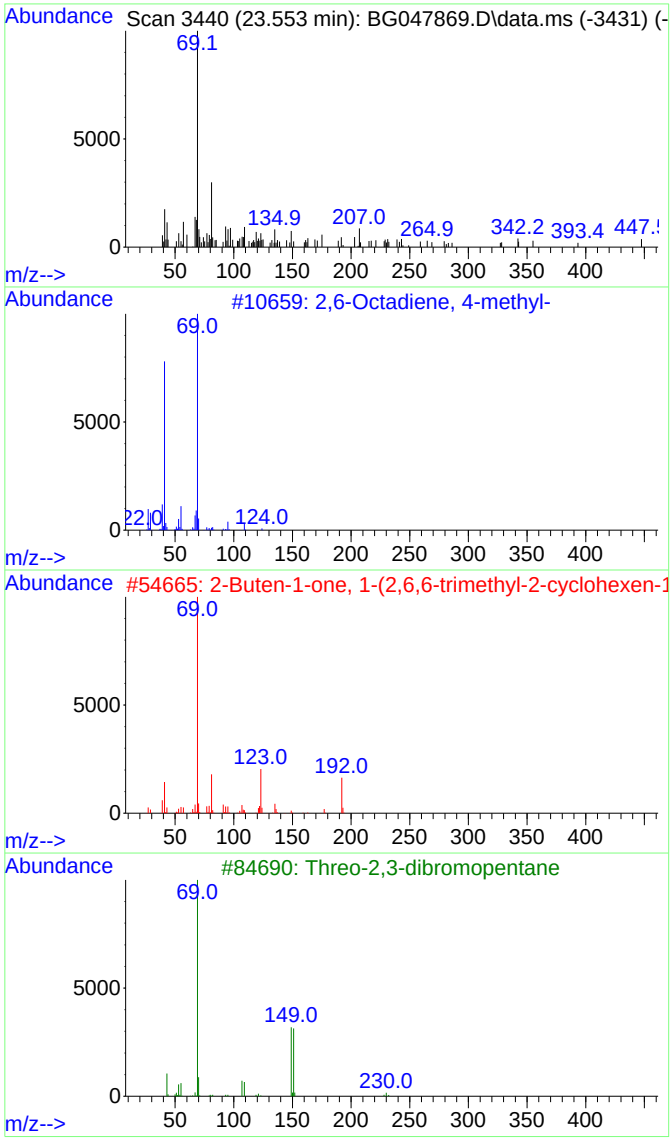
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

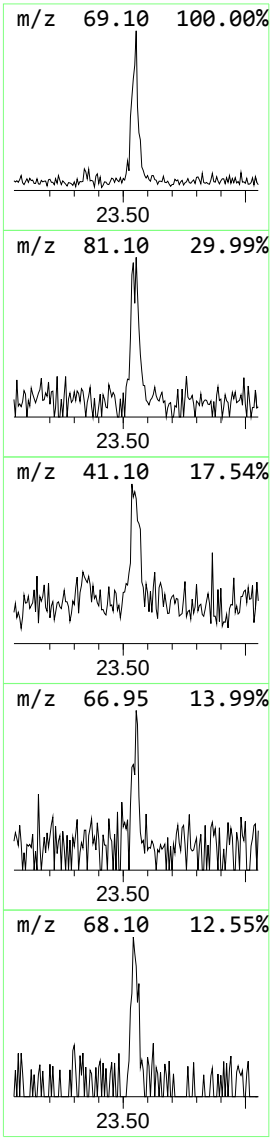
****

Peak Number 6 2,6-Octadiene, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.553	2.67 ng	81586	Perylene-d12	25.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	59
2	2-Buten-1-one, 1-(2,6,6-trimethy...	192	C13H20O	024720-09-0	59
3	Threo-2,3-dibromopentane	228	C5H10Br2	1000288-18-6	59
4	3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	58
5	Farnesol isomer a	222	C15H26O	1000108-92-4	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010521\
Data File : BG047869.D
Acq On : 5 Jan 2021 16:15
Operator : CG/JU
Sample : M1006-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : R-LA-21-5-WC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.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
2-Pentanone, 4-...	5.251	3.9	ng	36449	1	8.200	186000	20.0
2-Phenanthrenol...	20.779	8.2	ng	233915	5	21.831	568087	20.0
Benzamide, N-pr...	21.396	4.9	ng	137918	5	21.831	568087	20.0
Benzenepropanam...	21.467	11.4	ng	322354	5	21.831	568087	20.0
Diethylene glyc...	21.532	25.9	ng	734836	5	21.831	568087	20.0
2,6-Octadiene, ...	23.553	2.7	ng	81586	6	25.180	612276	20.0