LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042021\
Data File : BG048809.D
Acq On : 21 Apr 2021 00:55
Operator : CG/JU
Sample : M2026-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-15

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-BG041421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048809.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.342	335	341	348	rVB3	27999	45653	2.77%	0.630%
2	5.606	379	386	396	rVB	165633	258093	15.67%	3.561%
3	7.222	655	661	673	rVB2	120105	214042	13.00%	2.953%
4	8.062	797	804	815	rVB2	70331	126129	7.66%	1.740%
5	9.173	987	993	996	rBV3	15713	24002	1.46%	0.331%
6	9.232	996	1003	1015	rVB	283372	503732	30.59%	6.950%
7	9.590	1057	1064	1069	rBV2	44908	83867	5.09%	1.157%
8	10.889	1277	1285	1292	rBV	89977	167537	10.17%	2.312%
9	12.222	1508	1512	1517	rVB2	18174	27243	1.65%	0.376%
10	13.339	1696	1702	1708	rVB	724500	1087349	66.03%	15.002%
11	14.161	1837	1842	1848	rBV	45282	65712	3.99%	0.907%
12	14.719	1931	1937	1943	rBV2	146855	235481	14.30%	3.249%
13	15.918	2137	2141	2145	rVB2	13779	22208	1.35%	0.306%
14	16.053	2159	2164	2169	rBV5	10129	16625	1.01%	0.229%
15	16.218	2185	2192	2199	rBV	655185	1020807	61.99%	14.084%
16	16.406	2218	2224	2231	rBV	34857	63635	3.86%	0.878%
17	16.735	2275	2280	2284	rBV	42616	59307	3.60%	0.818%
18	17.475	2400	2406	2412	rBV	220136	335092	20.35%	4.623%
19	18.362	2553	2557	2564	rBV4	62848	99650	6.05%	1.375%
20	19.631	2769	2773	2778	rBV7	19939	34426	2.09%	0.475%
21	19.860	2809	2812	2816	rBV4	31048	41906	2.54%	0.578%
22	19.901	2816	2819	2827	rVB2	21664	34873	2.12%	0.481%
23	20.090	2845	2851	2857	rVB	1274802	1646822	100.00%	22.721%
24	20.865	2980	2983	2989	rVB7	15496	23948	1.45%	0.330%
25	21.394	3069	3073	3082	rVV3	79048	133892	8.13%	1.847%
26	21.776	3131	3138	3144	rVB2	225205	372075	22.59%	5.134%
27	22.598	3272	3278	3286	rVB3	39853	81003	4.92%	1.118%
28	23.268	3387	3392	3403	rVB10	21094	54302	3.30%	0.749%
29	25.107	3695	3705	3715	rVB	125388	368449	22.37%	5.084%

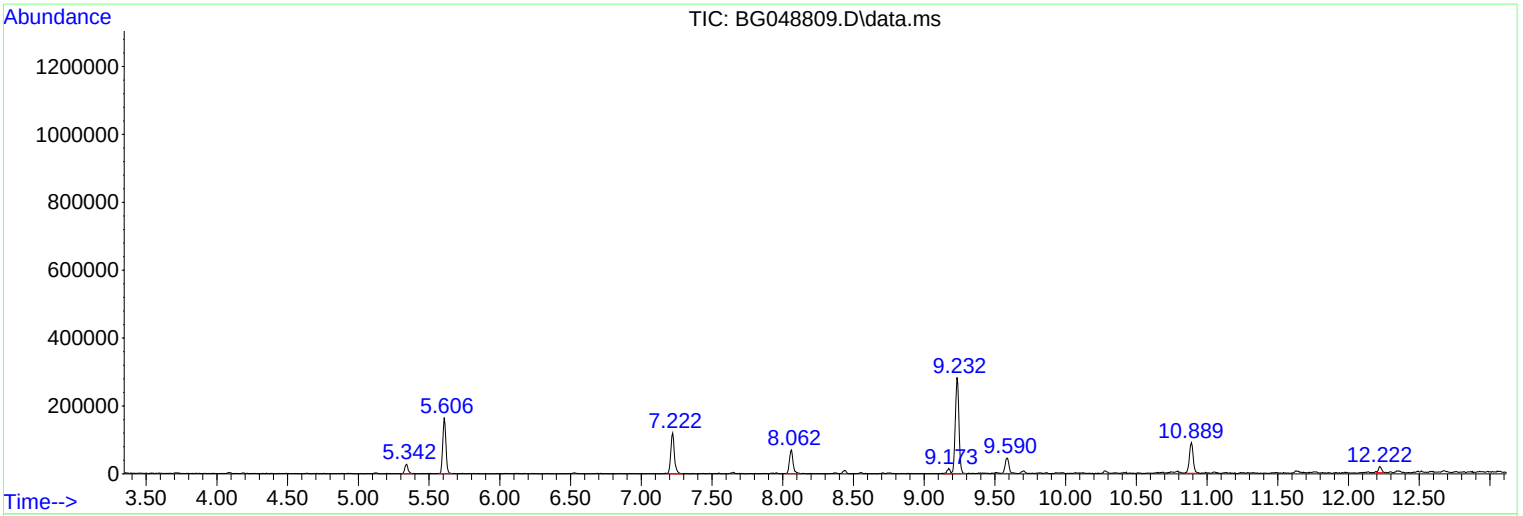
Sum of corrected areas: 7247860

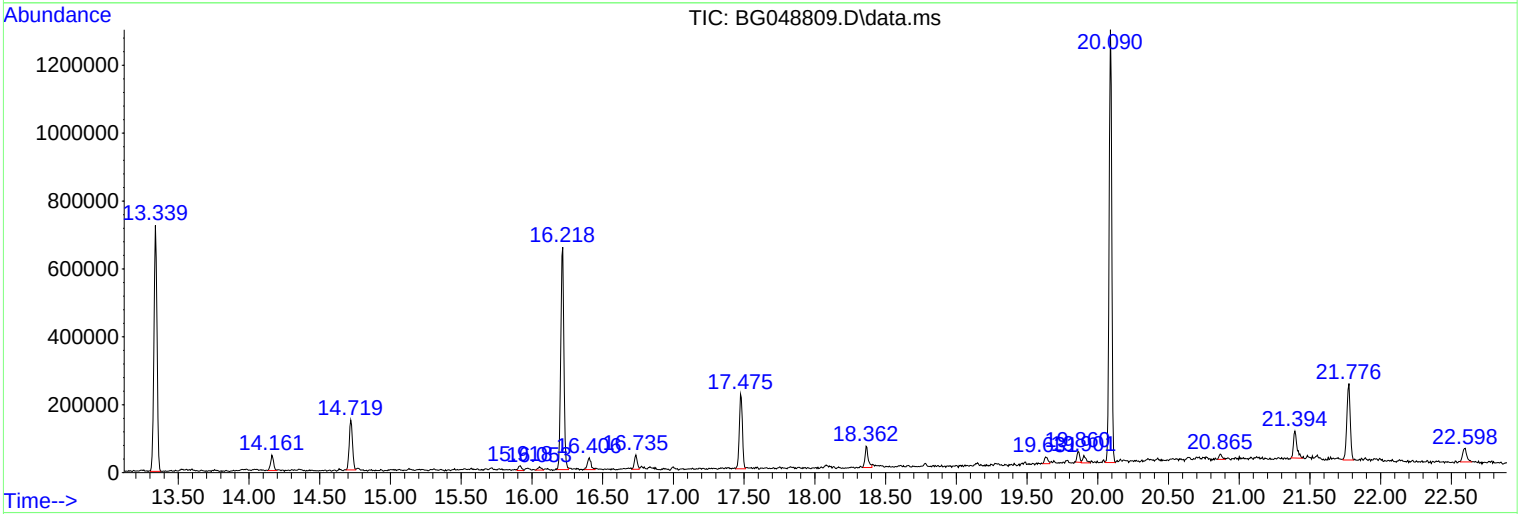
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042021\
Data File : BG048809.D
Acq On : 21 Apr 2021 00:55
Operator : CG/JU
Sample : M2026-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

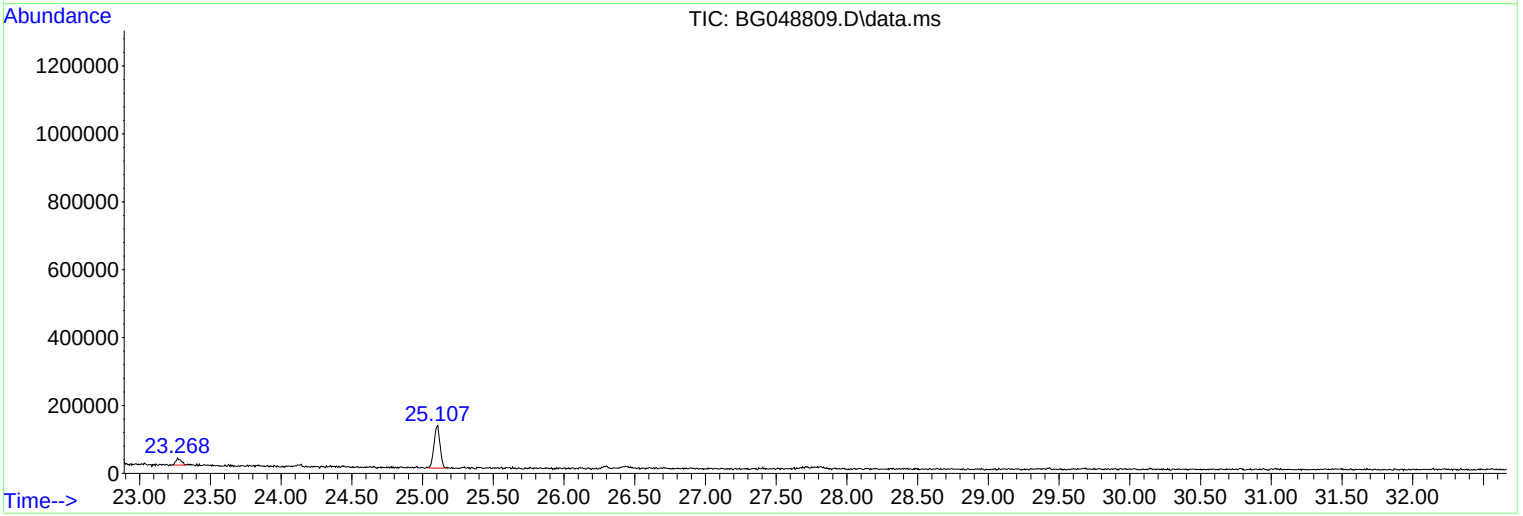
Instrument :
BNA_G
ClientSampleId :
PZ-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.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\BG042021\
Data File : BG048809.D
Acq On : 21 Apr 2021 00:55
Operator : CG/JU
Sample : M2026-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-15

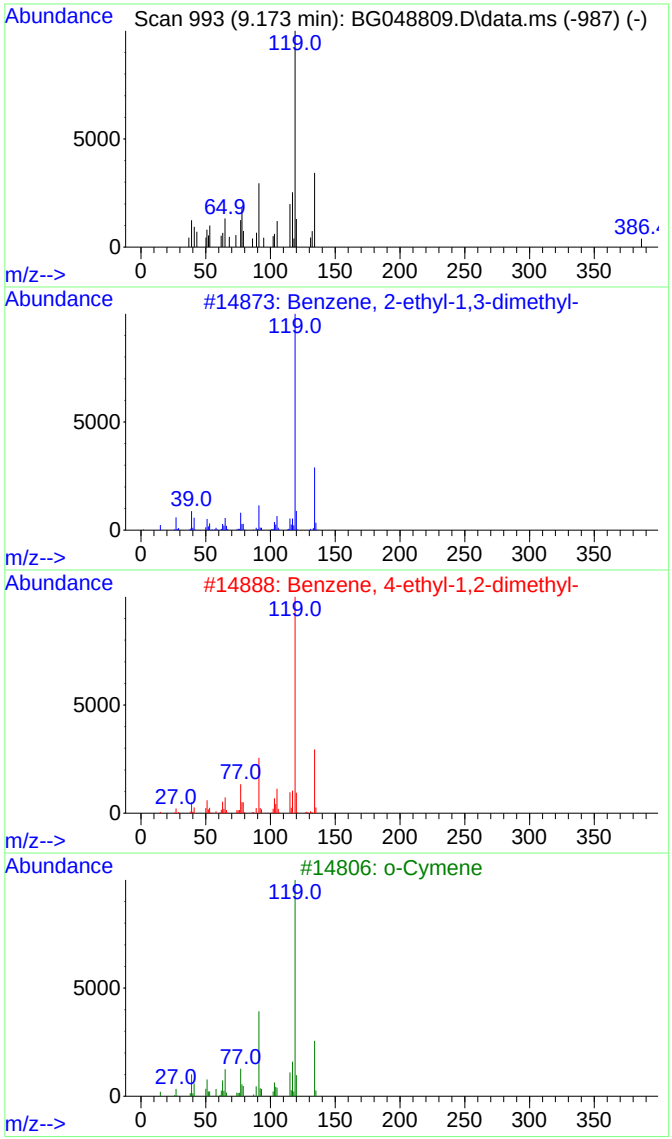
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

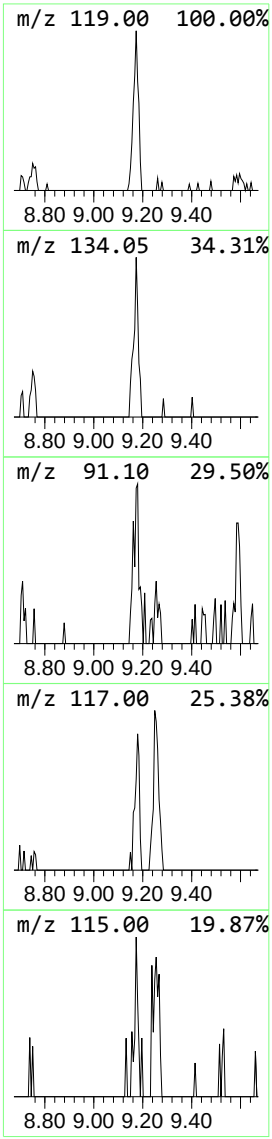
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 2-ethyl-1,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.173	3.81 ng	24002	1,4-Dichlorobenzene-d4	8.062

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	64
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	64
3	o-Cymene	134	C10H14	000527-84-4	64
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	64
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042021\
Data File : BG048809.D
Acq On : 21 Apr 2021 00:55
Operator : CG/JU
Sample : M2026-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PZ-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

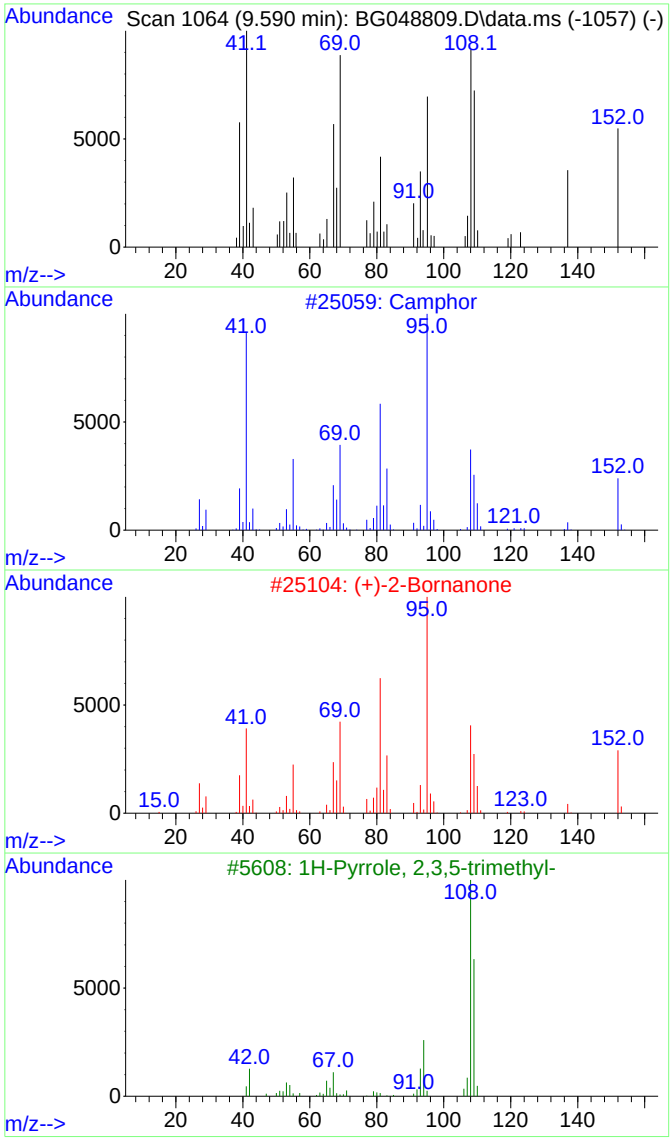
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

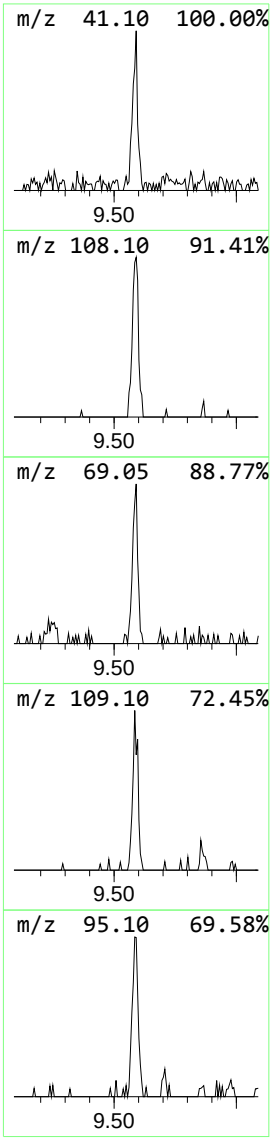
****

Peak Number 3 Camphor Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.590	10.01 ng	83867	Naphthalene-d8	10.889

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Camphor	152	C10H16O	000076-22-2	59
2	(+)-2-Bornanone	152	C10H16O	000464-49-3	59
3	1H-Pyrrole, 2,3,5-trimethyl-	109	C7H11N	002199-41-9	30
4	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	22
5	1,2,3,1',2',3'-Hexamethyl-bicycl...	218	C16H26	051999-35-0	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042021\
Data File : BG048809.D
Acq On : 21 Apr 2021 00:55
Operator : CG/JU
Sample : M2026-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PZ-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

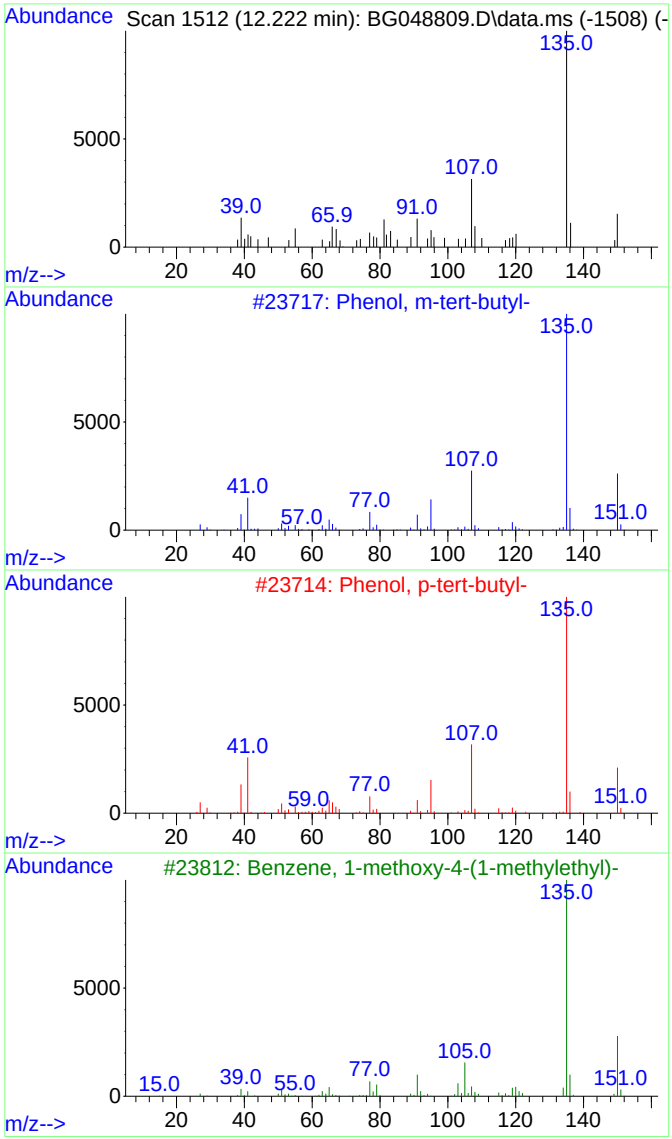
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

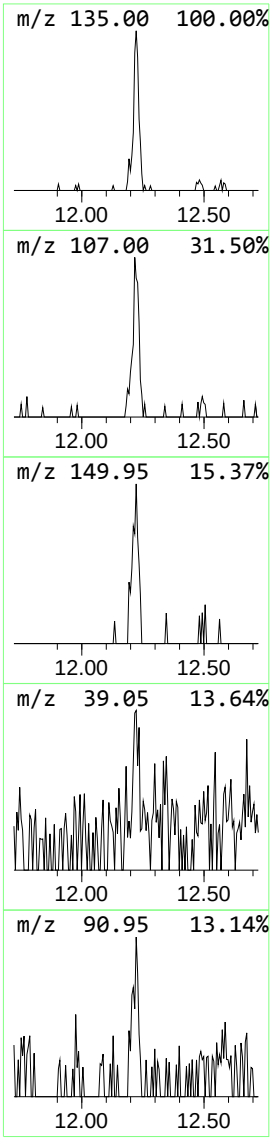
****

Peak Number 4 Phenol, m-tert-butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.222	3.25 ng	27243	Naphthalene-d8	10.889

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	64
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	64
3	Benzene, 1-methoxy-4-(1-methylet...	150	C10H14O	004132-48-3	53
4	ortho-Methoxyacetophenone	150	C9H10O2	000579-74-8	50
5	Benzenamine, 2,4,6-trimethyl-	135	C9H13N	000088-05-1	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042021\
Data File : BG048809.D
Acq On : 21 Apr 2021 00:55
Operator : CG/JU
Sample : M2026-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PZ-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

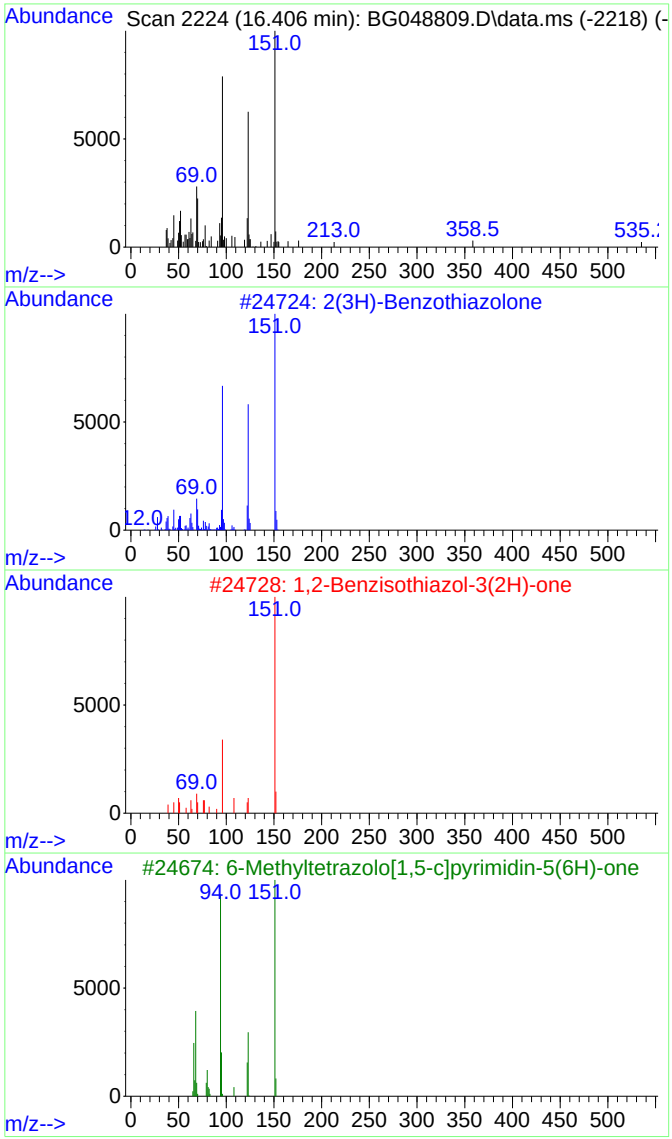
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

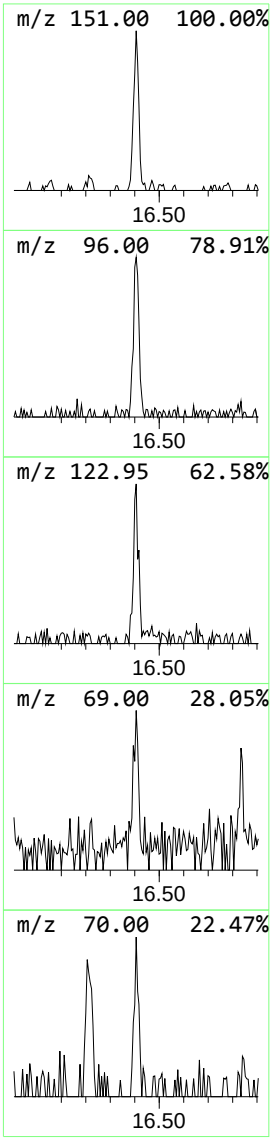
****

Peak Number 5 2(3H)-Benzothiazolone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.406	3.80 ng	63635	Phenanthrene-d10	17.475

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	86
2	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	59
3	6-Methyltetrazolo[1,5-c]pyrimidi...	151	C5H5N5O	144877-40-7	38
4	1H-Isoindole-1,3(2H)-dione, 3a,4...	151	C8H9NO2	001469-48-3	27
5	2(1H)-Pyrimidinone	96	C4H4N2O	000557-01-7	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042021\
Data File : BG048809.D
Acq On : 21 Apr 2021 00:55
Operator : CG/JU
Sample : M2026-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

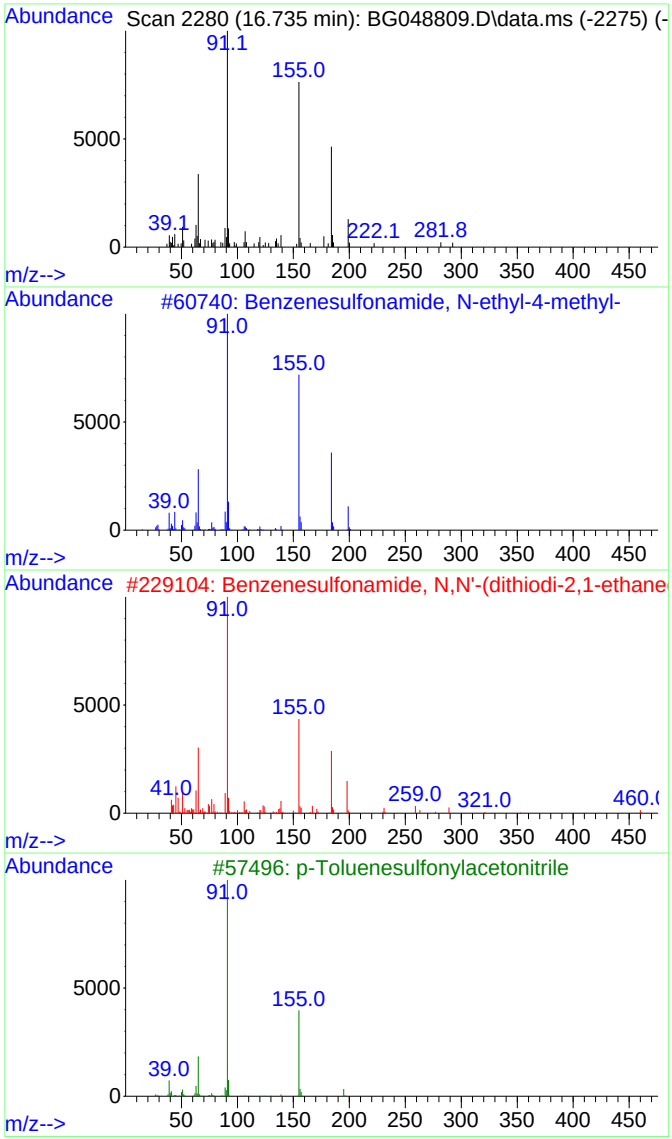
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

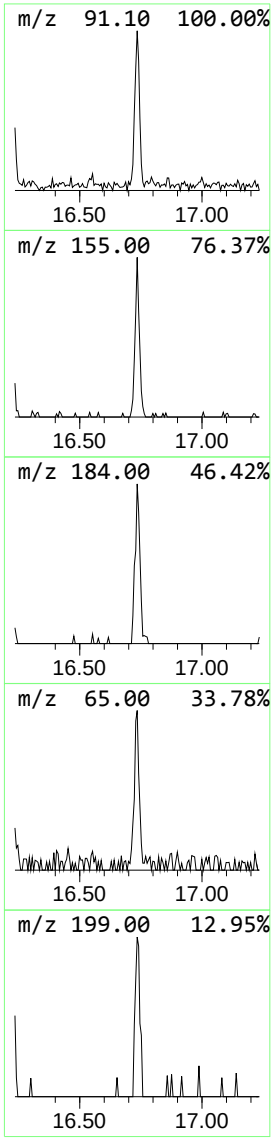
****

Peak Number 6 Benzenesulfonamide, N-ethyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.735	3.54 ng	59307	Phenanthrene-d10	17.475

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	87
2	Benzenesulfonamide, N,N'-(dithio...	460	C18H24N2O4S4	023516-74-7	47
3	p-Toluenesulfonylacetonitrile	195	C9H9NO2S	005697-44-9	43
4	Carbamic acid, methyl[(4-methylp...	243	C10H13NO4S	032258-50-7	43
5	N-(4H-1,2,4-Triazol-4-yl)-p-tolu...	238	C9H10N4O2S	032585-76-5	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042021\
Data File : BG048809.D
Acq On : 21 Apr 2021 00:55
Operator : CG/JU
Sample : M2026-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

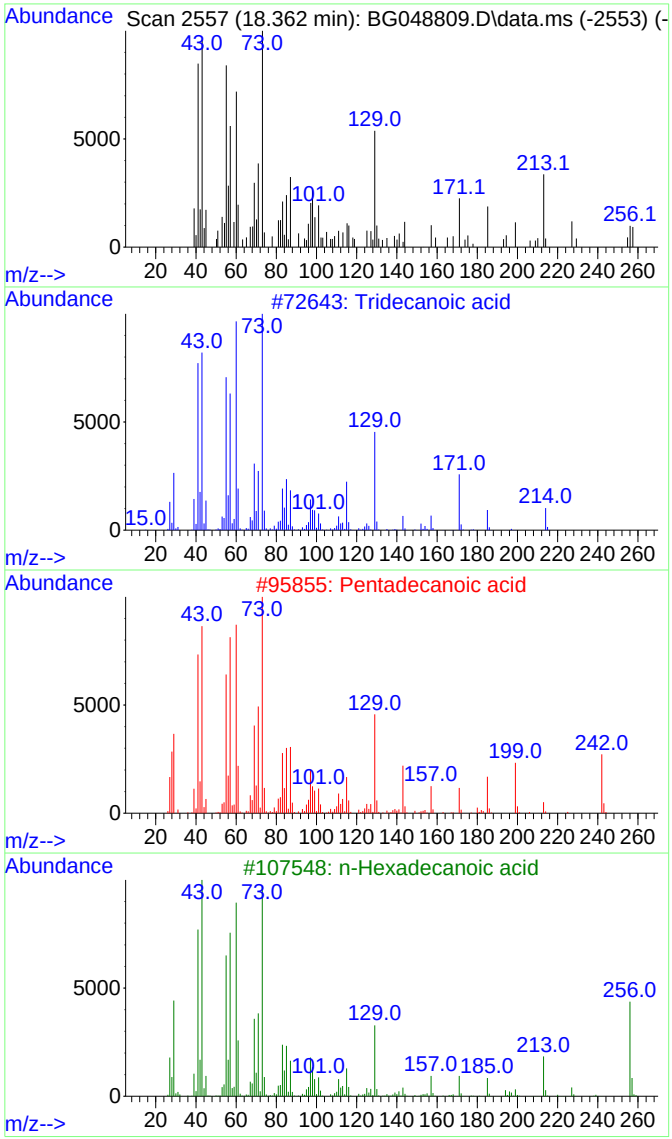
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

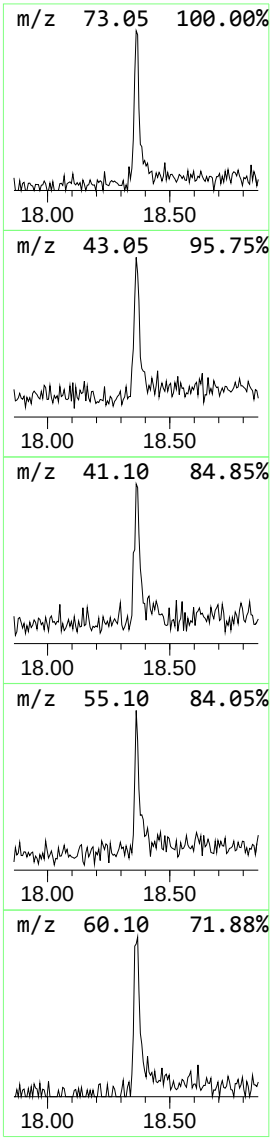
****

Peak Number 7 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.362	5.95 ng	99650	Phenanthrene-d10	17.475

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	76
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49
4	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	27
5	1,2,3-Thiadiazole-4-carboxylic a...	144	C3H4N4OS	004100-18-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042021\
Data File : BG048809.D
Acq On : 21 Apr 2021 00:55
Operator : CG/JU
Sample : M2026-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PZ-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

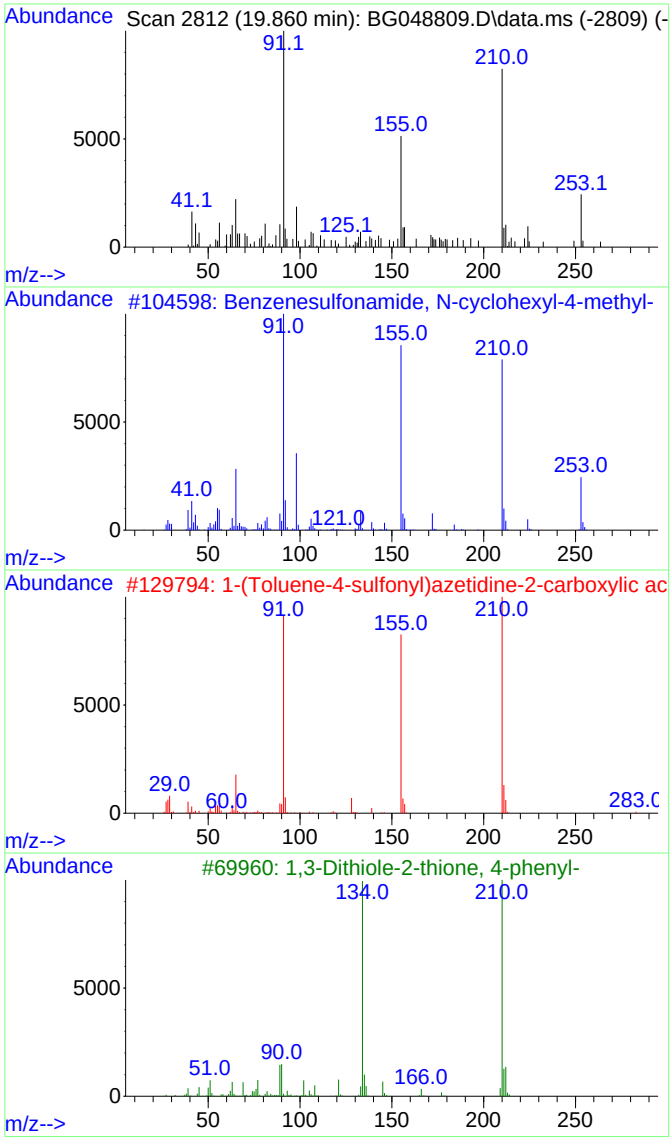
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

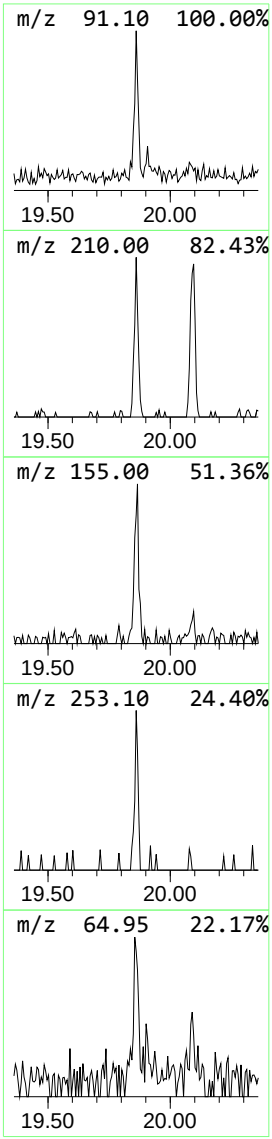
****

Peak Number 8 Benzenesulfonamide, N-cyclo... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.860	2.25 ng	41906	Chrysene-d12	21.776

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N-cyclohexyl...	253	C13H19NO2S	000080-30-8	58
2	1-(Toluene-4-sulfonyl)azetidine-...	283	C13H17NO4S	1000185-95-4	53
3	1,3-Dithiole-2-thione, 4-phenyl-	210	C9H6S3	002314-61-6	35
4	1H-Purin-6-amine, N-phenyl-	211	C11H9N5	001210-66-8	35
5	4-Methoxy-2-nitrophenyl isothioc...	210	C8H6N2O3S	023165-60-8	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042021\
Data File : BG048809.D
Acq On : 21 Apr 2021 00:55
Operator : CG/JU
Sample : M2026-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-15

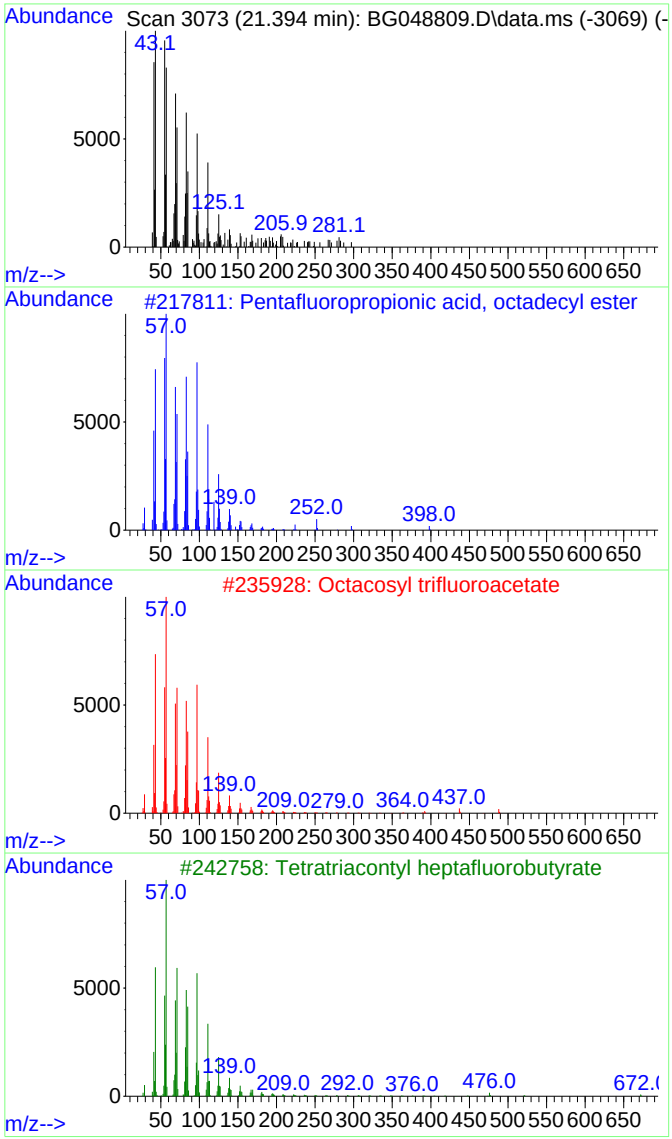
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

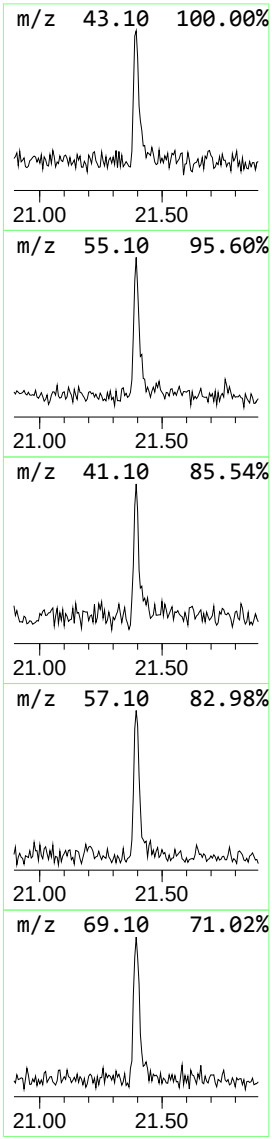
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.394	7.20 ng	133892	Chrysene-d12	21.776

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	87
2	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87
3	Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	83
4	Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	83
5	Octatriacontyl trifluoroacetate	647	C40H77F3O2	1000351-88-7	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042021\
Data File : BG048809.D
Acq On : 21 Apr 2021 00:55
Operator : CG/JU
Sample : M2026-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-15

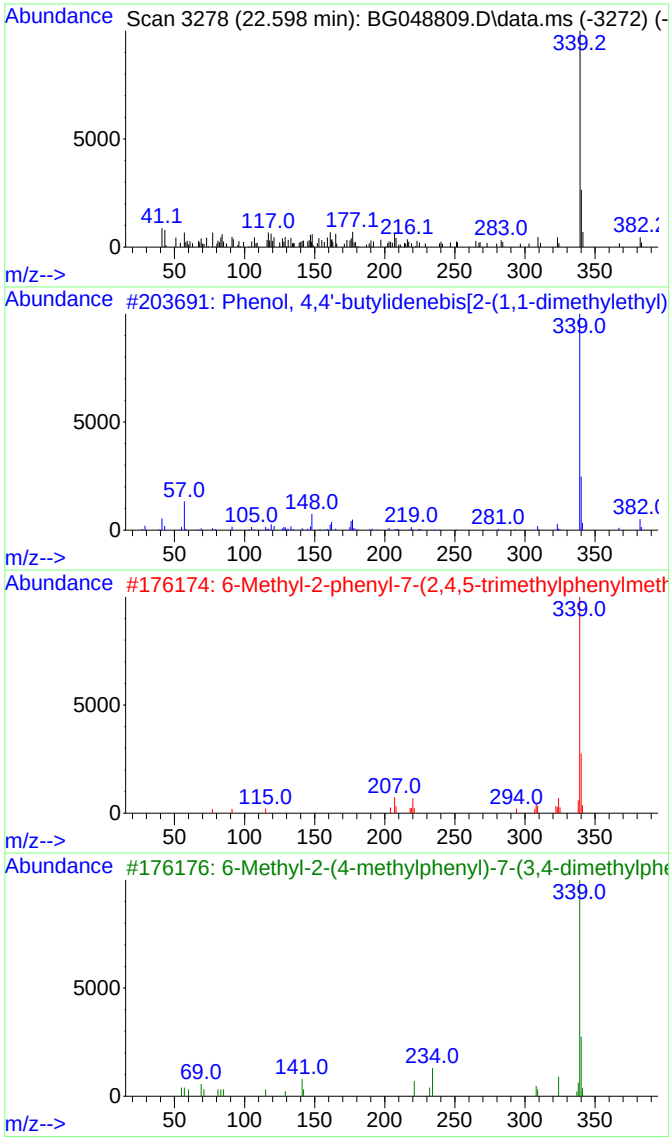
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

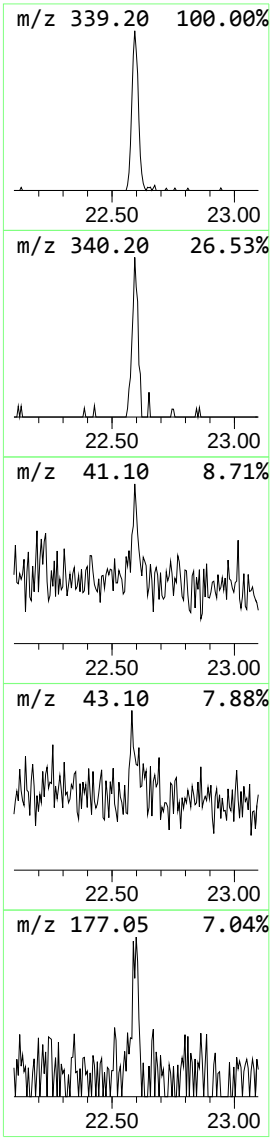
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phenol, 4,4'-butylidenebis[... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.598	4.35 ng	81003	Chrysene-d12	21.776

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-butylidenebis[2-(1,...	382	C26H38O2	000085-60-9	91
2	6-Methyl-2-phenyl-7-(2,4,5-trime...	339	C25H25N	064002-76-2	80
3	6-Methyl-2-(4-methylphenyl)-7-(3...	339	C25H25N	080193-44-8	72
4	4-(p-Methoxyphenyl)-2,6-di(2-pyr...	339	C22H17N3O	013104-56-8	64
5	2,7-Dibutoxy-fluoren-9-one oxime	339	C21H25NO3	1000318-21-2	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042021\
Data File : BG048809.D
Acq On : 21 Apr 2021 00:55
Operator : CG/JU
Sample : M2026-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

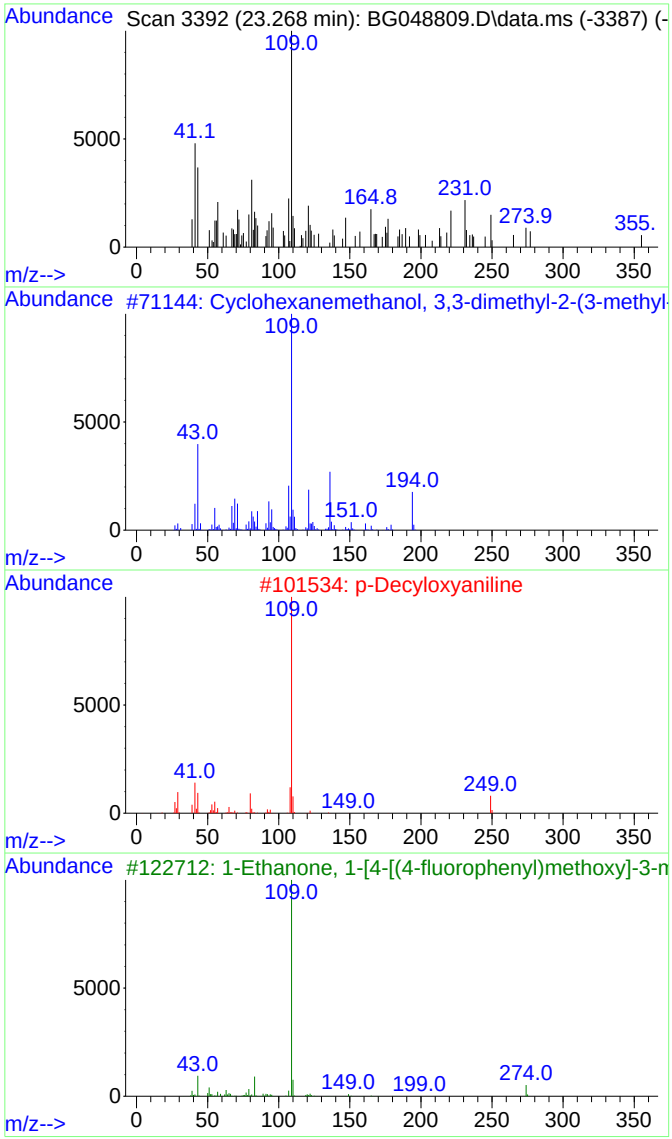
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

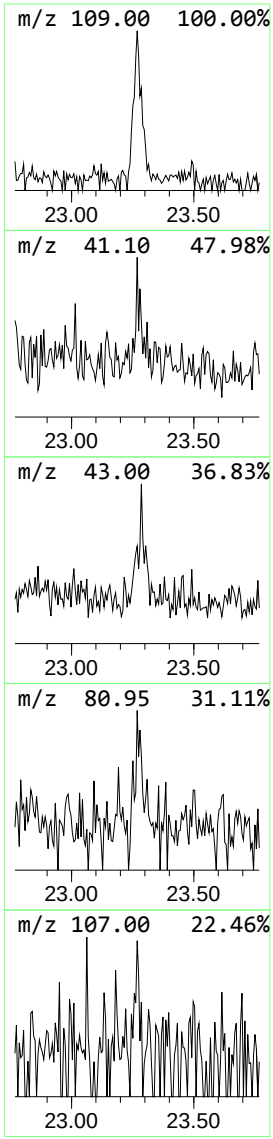
****

Peak Number 11 unknown23.268 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.268	2.92 ng	54302	Chrysene-d12	21.776

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, 3,3-dimethy...	212	C13H24O2	072541-28-7	47
2	p-Decyloxyaniline	249	C16H27NO	039905-47-0	43
3	1-Ethanone, 1-[4-[(4-fluoropheny...	274	C16H15FO3	1000338-31-4	43
4	Furane-3-carboxylic acid, 2-meth...	277	C14H12FNO4	351060-78-1	38
5	Trifluoroacetamide,(4-fluorobenzyl)	221	C9H7F4NO	170374-90-0	37





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042021\
Data File : BG048809.D
Acq On : 21 Apr 2021 00:55
Operator : CG/JU
Sample : M2026-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.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
Benzene, 2-ethy...	9.173	3.8	ng	24002	1	8.062	126129	20.0
Camphor	9.590	10.0	ng	83867	2	10.889	167537	20.0
Phenol, m-tert-...	12.222	3.3	ng	27243	2	10.889	167537	20.0
2(3H)-Benzothia...	16.406	3.8	ng	63635	4	17.475	335092	20.0
Benzenesulfonam...	16.735	3.5	ng	59307	4	17.475	335092	20.0
Tridecanoic acid	18.362	6.0	ng	99650	4	17.475	335092	20.0
Benzenesulfonam...	19.860	2.3	ng	41906	5	21.776	372075	20.0
Pentafluoroprop...	21.394	7.2	ng	133892	5	21.776	372075	20.0
Phenol, 4,4'-bu...	22.598	4.3	ng	81003	5	21.776	372075	20.0
unknown23.268	23.268	2.9	ng	54302	5	21.776	372075	20.0