LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
Data File : BG055966.D
Acq On : 14 Dec 2022 19:28
Operator : CG/JU
Sample : N6001-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-6M

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-BG121322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055966.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.399	14	19	30	rBB	75825	106499	14.55%	1.664%
2	5.409	357	361	366	rBB2	5435	7748	1.06%	0.121%
3	5.885	436	442	448	rBB	56551	85431	11.67%	1.335%
4	7.489	709	715	722	rBB	40852	67959	9.28%	1.062%
5	8.370	859	865	871	rBB	35742	56566	7.73%	0.884%
6	9.539	1057	1064	1071	rBB	65488	115882	15.83%	1.810%
7	11.202	1340	1347	1354	rBB	47597	82766	11.31%	1.293%
8	13.605	1749	1756	1763	rBB	271946	411061	56.16%	6.422%
9	14.980	1982	1990	1995	rBB	100516	155389	21.23%	2.427%
10	16.455	2234	2241	2248	rVB	327536	496744	67.87%	7.760%
11	17.712	2449	2455	2462	rBV	162000	240519	32.86%	3.757%
12	18.164	2527	2532	2540	rBV2	14746	23557	3.22%	0.368%
13	18.564	2596	2600	2604	rVB	6563	8425	1.15%	0.132%
14	19.351	2729	2734	2741	rVB	95801	123152	16.83%	1.924%
15	19.721	2791	2797	2801	rBV3	6381	8678	1.19%	0.136%
16	20.133	2863	2867	2872	rVB	16836	20569	2.81%	0.321%
17	20.286	2888	2893	2902	rBV	483074	731941	100.00%	11.434%
18	20.409	2908	2914	2919	rBV2	317074	566310	77.37%	8.847%
19	20.474	2919	2925	2928	rVV2	274451	472092	64.50%	7.375%
20	20.515	2928	2932	2936	rVV	201243	267264	36.51%	4.175%
21	20.603	2936	2947	2950	rVV4	240342	668543	91.34%	10.444%
22	20.673	2954	2959	2963	rVV	414331	526188	71.89%	8.220%
23	20.703	2963	2964	2966	rVV	29272	27907	3.81%	0.436%
24	20.738	2966	2970	2976	rVB	226719	273979	37.43%	4.280%
25	20.855	2987	2990	2992	rBV	9118	11845	1.62%	0.185%
26	21.202	3043	3049	3051	rBV4	7483	9268	1.27%	0.145%
27	21.608	3115	3118	3122	rVB4	6950	8863	1.21%	0.138%
28	21.807	3148	3152	3159	rVB	12230	17089	2.33%	0.267%
29	22.019	3181	3188	3195	rVV2	190501	330577	45.16%	5.164%
30	22.113	3199	3204	3207	rVV	22183	35252	4.82%	0.551%
31	22.183	3207	3216	3225	rVB4	40149	88292	12.06%	1.379%
32	25.515	3772	3783	3798	rVB2	119356	354891	48.49%	5.544%

Sum of corrected areas: 6401246

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
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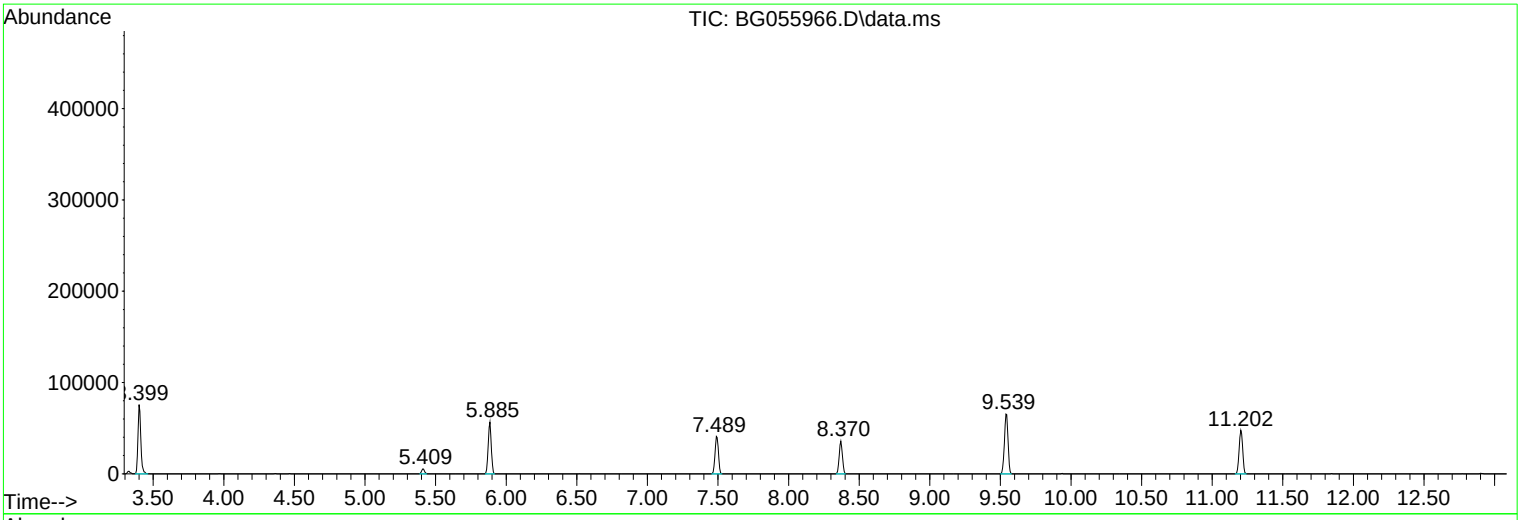
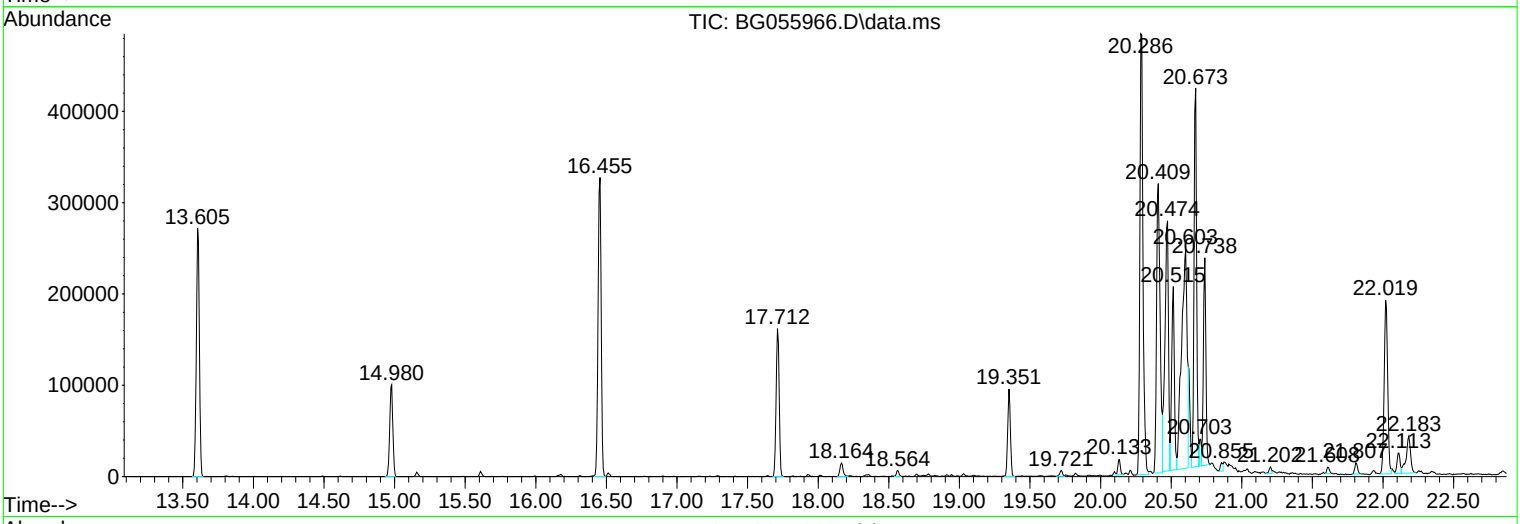
Acq On : 14 Dec 2022 19:28
Operator : CG/JU
Sample : N6001-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

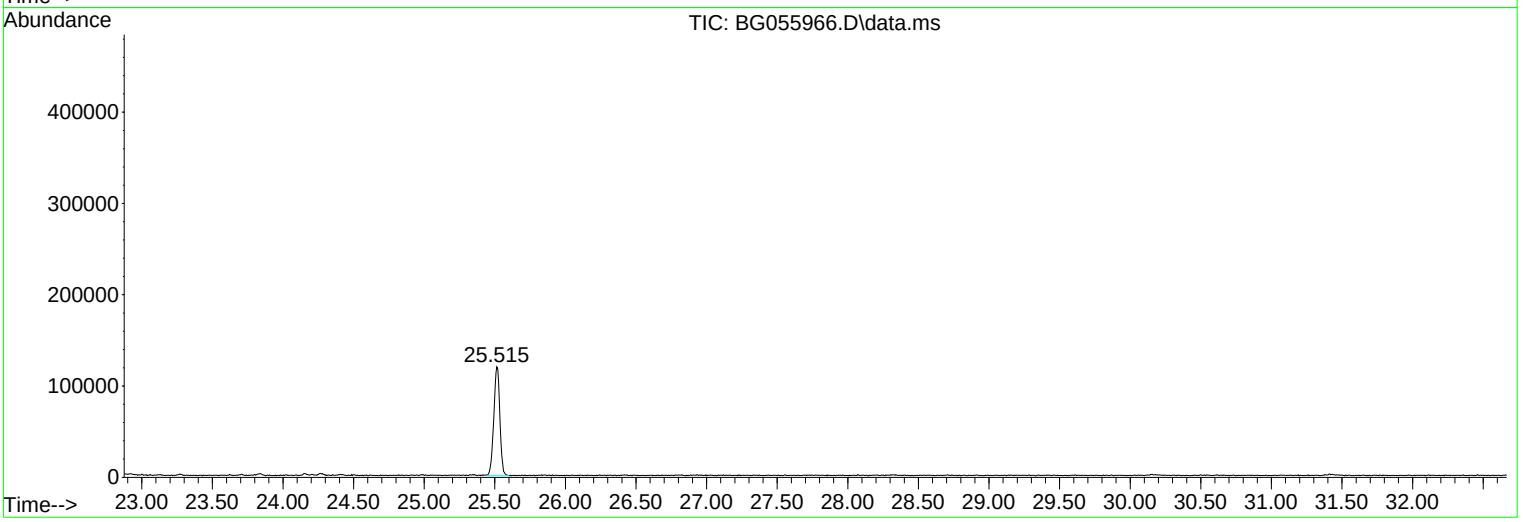
Instrument :
BNA_G
ClientSampleId :
MW-6M

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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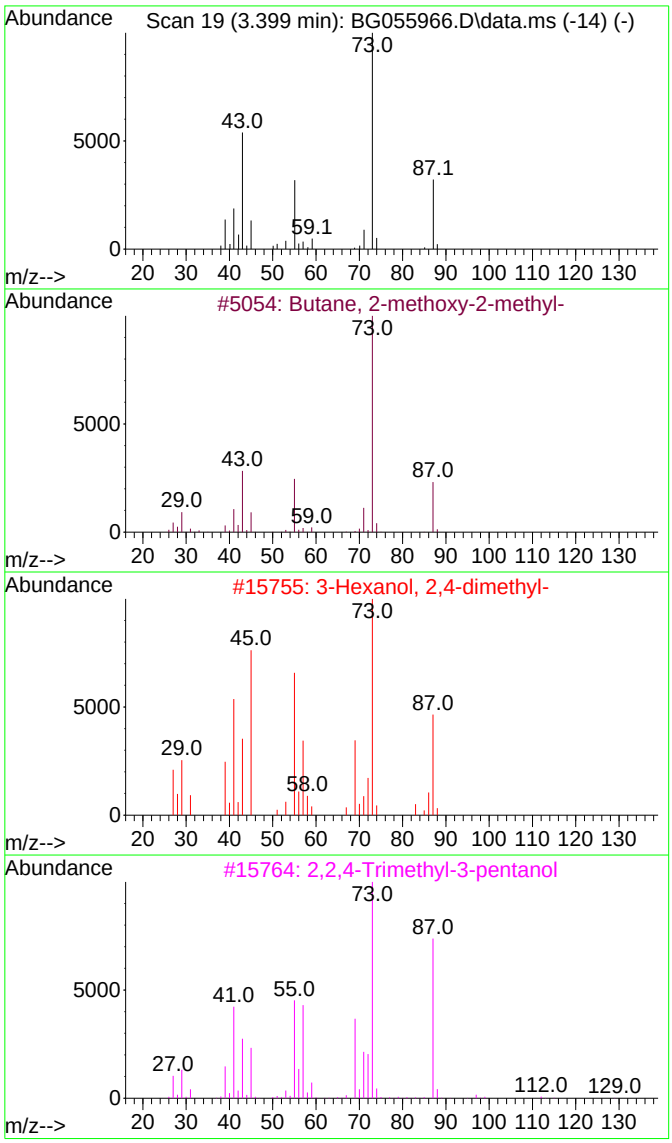
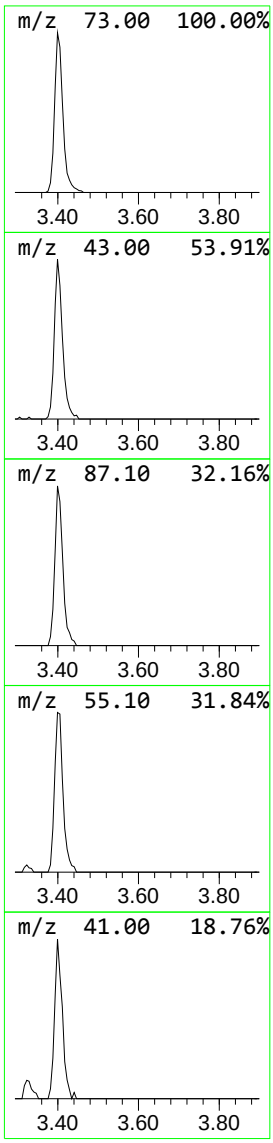
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.399	37.65 ng	106499	1,4-Dichlorobenzene-d4	8.370

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	36
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
4	2-Pentanol, acetate	130	C7H14O2	000626-38-0	23
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17





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Data File : BG055966.D
Acq On : 14 Dec 2022 19:28
Operator : CG/JU
Sample : N6001-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
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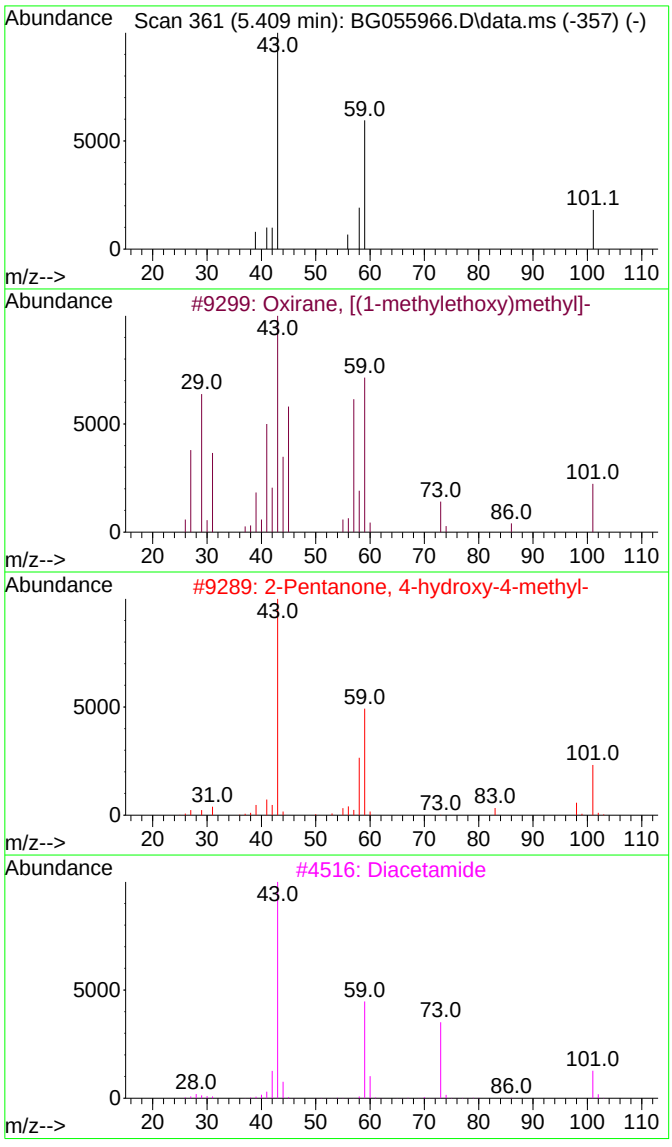
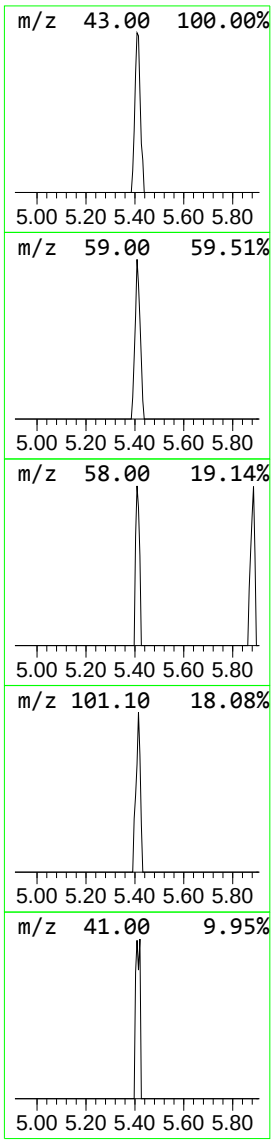
****

Peak Number 2 unknown5.409 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.409	2.74 ng	7748	1,4-Dichlorobenzene-d4	8.370

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	43
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
3	Diacetamide	101	C4H7NO2	000625-77-4	7
4	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	5
5	Acetone	58	C3H6O	000067-64-1	5





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Sample : N6001-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-6M

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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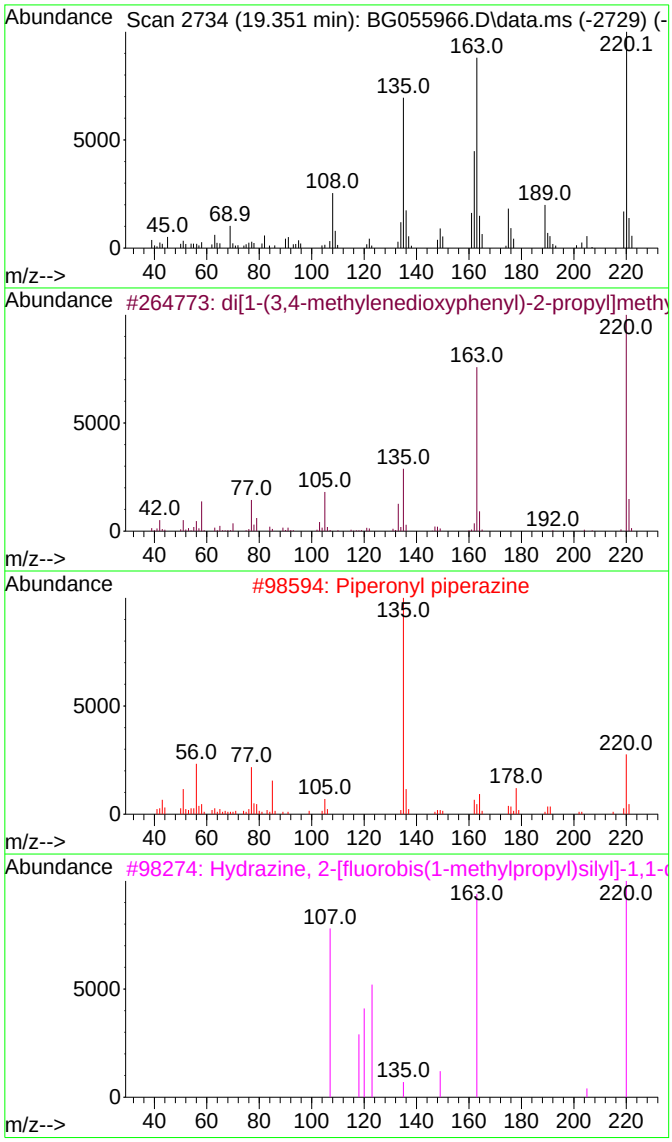
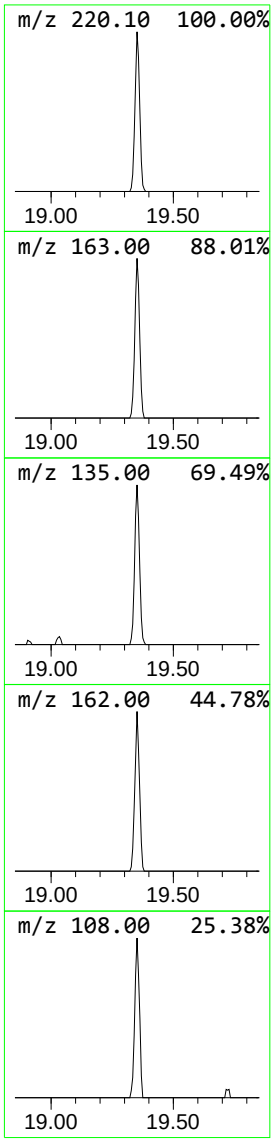
****

Peak Number 3 unknown19.351 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.351	10.24 ng	123152	Phenanthrene-d10	17.712

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	di[1-(3,4-methylenedioxyphenyl)-...	355	C21H25NO4	1000378-88-6	47
2	Piperonyl piperazine	220	C12H16N2O2	032231-06-4	43
3	Hydrazine, 2-[fluorobis(1-methyl...	220	C10H25FN2Si	066436-26-8	38
4	8-Fluoro-4-hydroxyquinoline	163	C9H6FNO	063010-71-9	38
5	4-Oxa-3,5-diazatetracyclo[11.4.0...	220	C14H8N2O	000236-07-7	30





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Instrument :
BNA_G
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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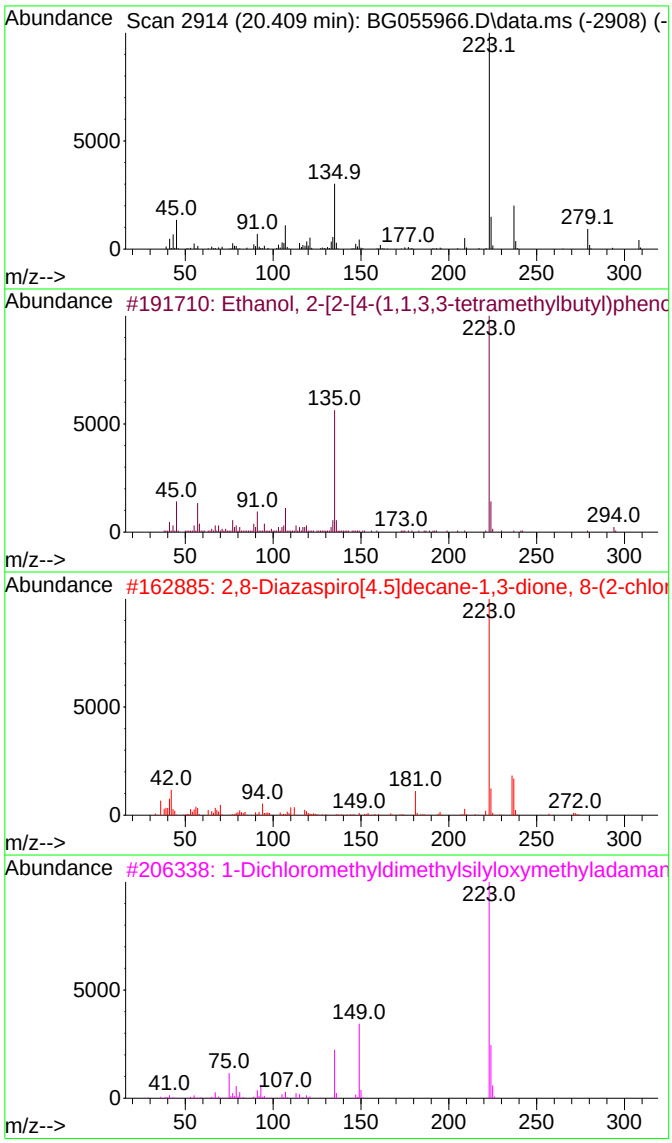
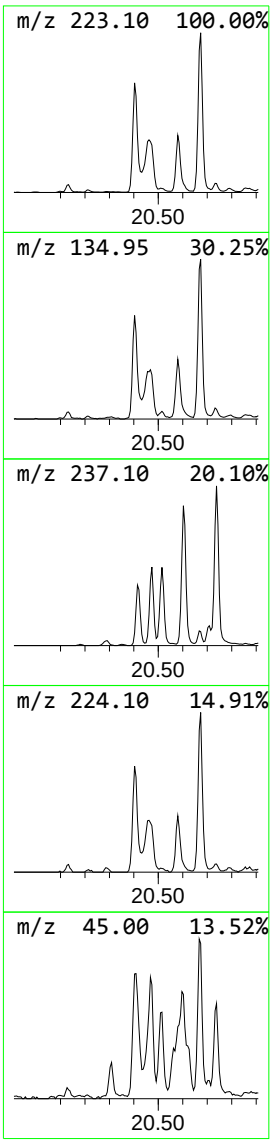
****
Peak Number 4 Ethanol, 2-[2-[4-(1,1,3,3-t... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.409	34.26 ng	566310	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	53
2	2,8-Diazaspiro[4.5]decane-1,3-di...	272	C13H21ClN2O2	132168-96-8	53
3	1-Dichloromethyldimethylsilyloxy...	306	C14H24Cl2OSi	1000283-10-5	38
4	Mono-4-methylpentan-2-yl phthala...	364	C20H32O4Si	1000373-88-2	37
5	Silane, dimethyldi(hex-4-yn-3-yl...	252	C14H24O2Si	1000347-92-8	33





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Operator : CG/JU
Sample : N6001-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-6M

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

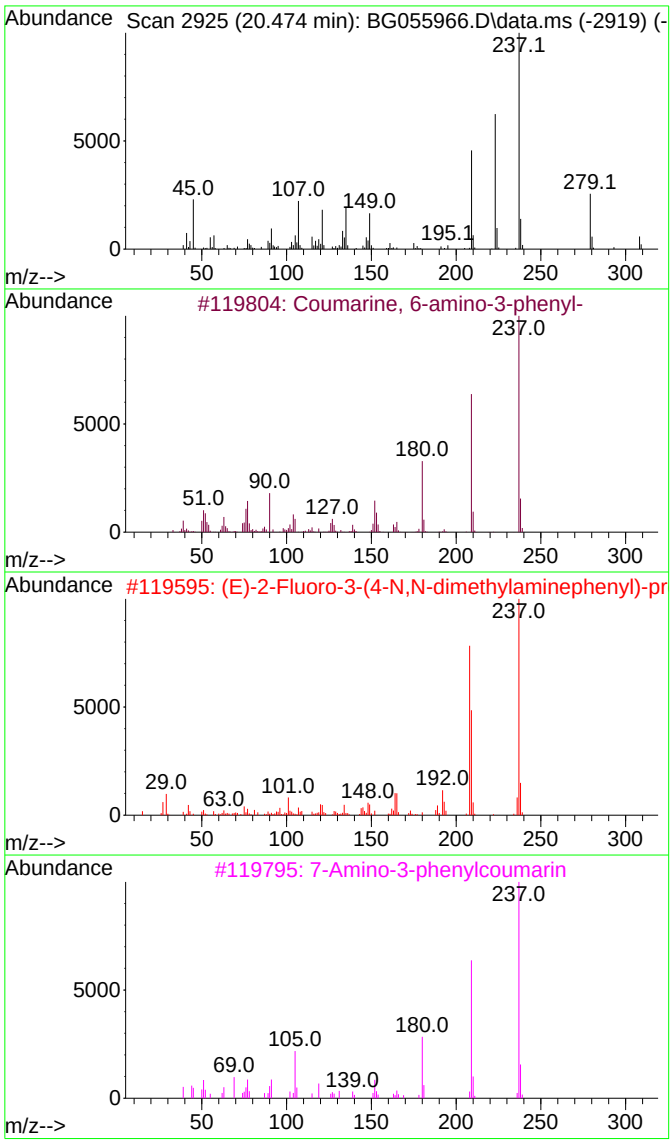
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

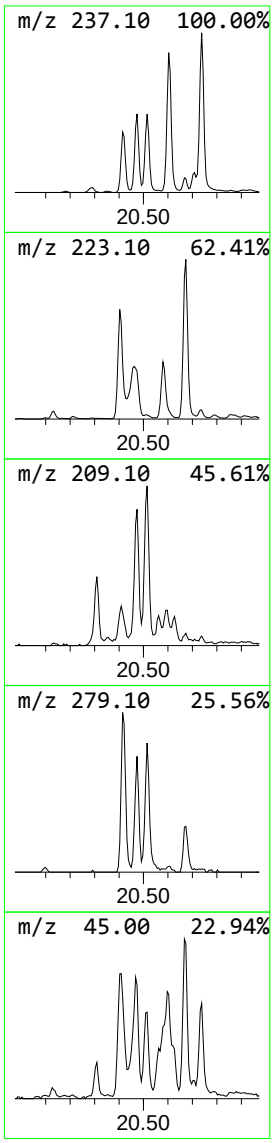
****

Peak Number 5 unknown20.474 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.474	28.56 ng	472092	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Coumarine, 6-amino-3-phenyl-	237	C15H11NO2	021408-16-2	38
2	(E)-2-Fluoro-3-(4-N,N-dimethylam...	237	C13H16FNO2	110915-65-6	38
3	7-Amino-3-phenylcoumarin	237	C15H11NO2	004108-61-6	38
4	3'-(Trifluoromethyl)[1,1'-biphen...	279	C15H12F3NO	1000512-87-1	35
5	Pyrazolo[1,5-a]pyrimidine, 5,6-d...	279	C18H21N3	1010273-96-0	35





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Data File : BG055966.D
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-6M

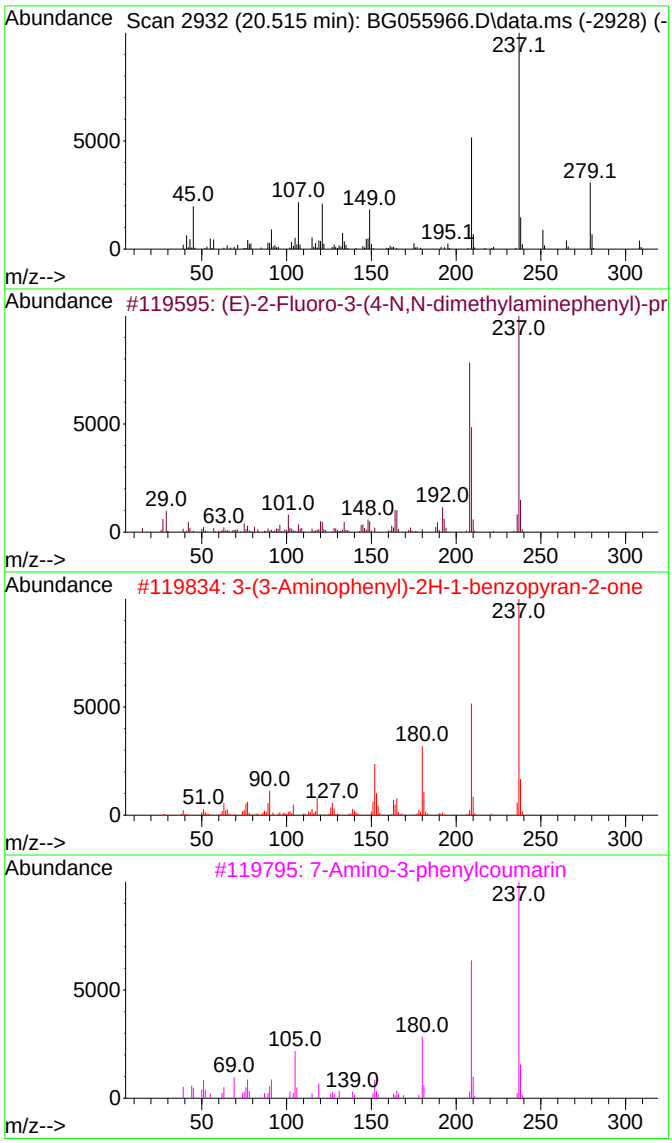
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

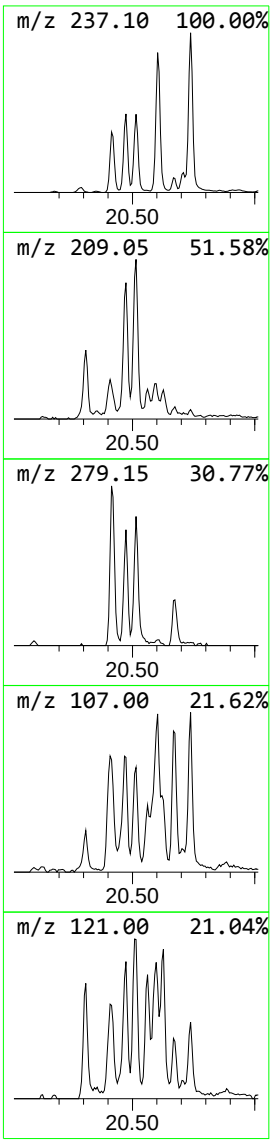
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (E)-2-Fluoro-3-(4-N,N-dimet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.515	16.17 ng	267264	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-2-Fluoro-3-(4-N,N-dimethylam...	237	C13H16FNO2	110915-65-6	58
2	3-(3-Aminophenyl)-2H-1-benzopyra...	237	C15H11NO2	292644-31-6	53
3	7-Amino-3-phenylcoumarin	237	C15H11NO2	004108-61-6	53
4	Pyrazolo[1,5-a]pyrimidine, 5,6-d...	279	C18H21N3	1010273-96-0	52
5	3'-(Trifluoromethyl)[1,1'-biphen...	279	C15H12F3NO	1000512-87-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
Data File : BG055966.D
Acq On : 14 Dec 2022 19:28
Operator : CG/JU
Sample : N6001-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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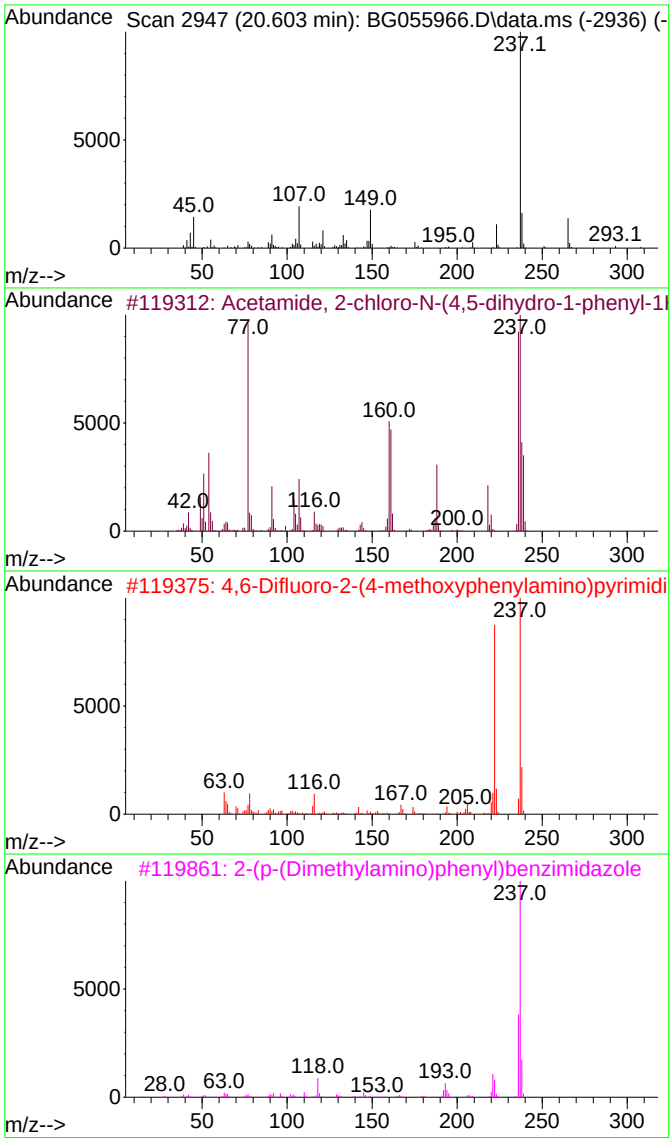
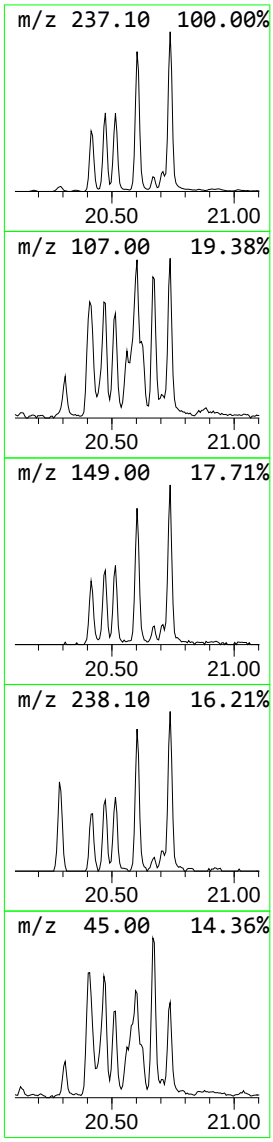
****
Peak Number 7 Acetamide, 2-chloro-N-(4,5-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.603	40.45 ng	668543	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, 2-chloro-N-(4,5-dihyd...	237	C11H12ClN3O	1000337-23-3	53
2	4,6-Difluoro-2-(4-methoxyphenyla...	237	C11H9F2N3O	1010070-53-0	50
3	2-(p-(Dimethylamino)phenyl)benzi...	237	C15H15N3	002562-71-2	47
4	Pyrido[2,3-d]pyrimidin-5(8H)-one...	237	C14H11N3O	161465-98-1	47
5	1-Phenyl-3-(2-pyridyl)-5-pyrazolone	237	C14H11N3O	021683-60-3	43





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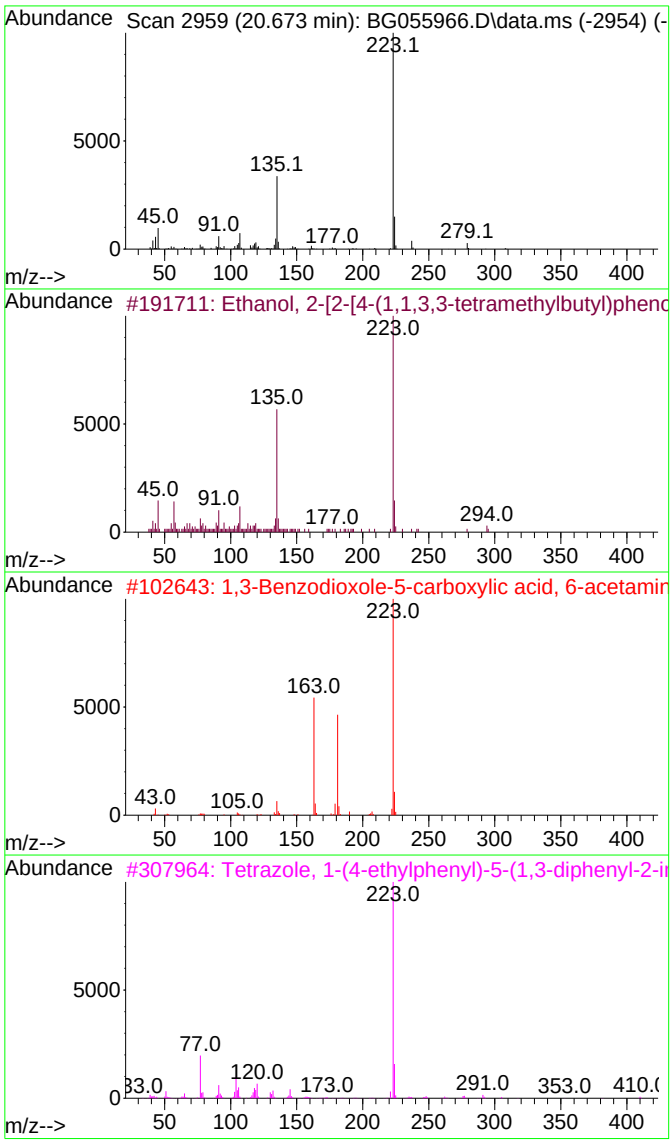
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

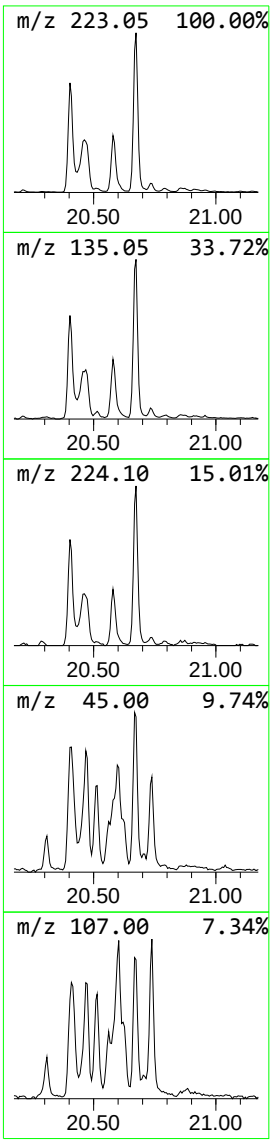
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1,3-Benzodioxole-5-carboxyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.673	31.83 ng	526188	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	56
2	1,3-Benzodioxole-5-carboxylic ac...	223	C10H9NO5	099185-29-2	50
3	Tetrazole, 1-(4-ethylphenyl)-5-(...	410	C25H26N6	125038-06-4	47
4	Imidazolidine, 1,3-diphenyl-2-pr...	266	C18H22N2	055320-82-6	40
5	Ethyl 3-[3-amino-5-methoxyphenyl...	223	C12H17NO3	1010213-27-3	40





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Acq On : 14 Dec 2022 19:28
Operator : CG/JU
Sample : N6001-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-6M

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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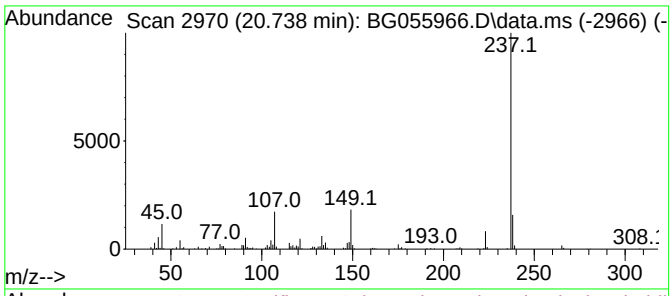
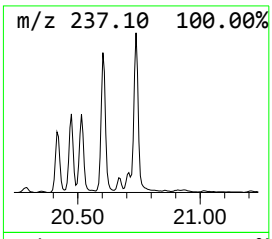
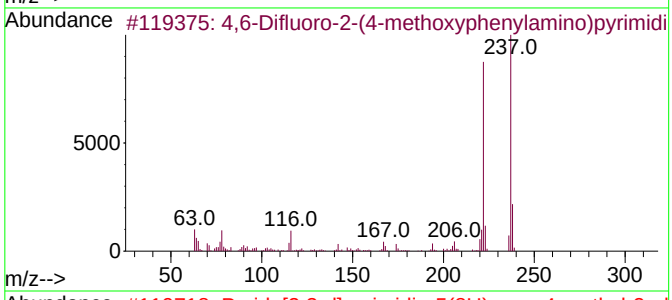
****
Peak Number 9 4,6-Difluoro-2-(4-methoxyph... Concentration Rank 6

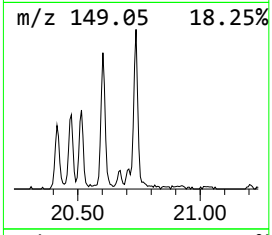
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.738	16.58 ng	273979	Chrysene-d12	22.019

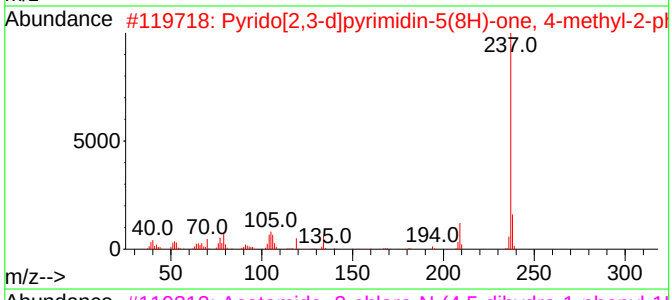
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,6-Difluoro-2-(4-methoxyphenyla...	237	C11H9F2N3O	1010070-53-0	53
2	Pyrido[2,3-d]pyrimidin-5(8H)-one...	237	C14H11N3O	161465-98-1	50
3	Acetamide, 2-chloro-N-(4,5-dihyd...	237	C11H12ClN3O	1000337-23-3	42
4	2-[3-(2H-1,2,3-Benzotriazol-2-yl...	323	C18H17N3O3	096478-09-0	40
5	1-Phenyl-3-(2-pyridyl)-5-pyrazolone	237	C14H11N3O	021683-60-3	40

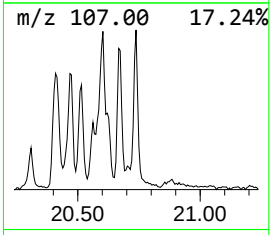


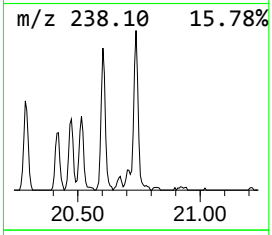


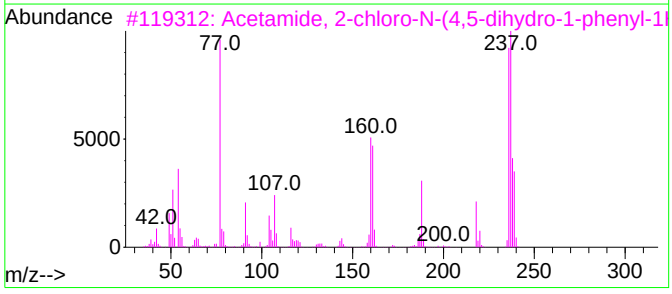


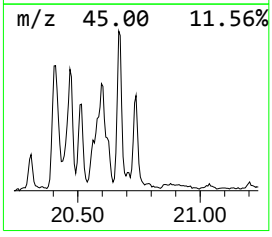












Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
Data File : BG055966.D
Acq On : 14 Dec 2022 19:28
Operator : CG/JU
Sample : N6001-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-6M

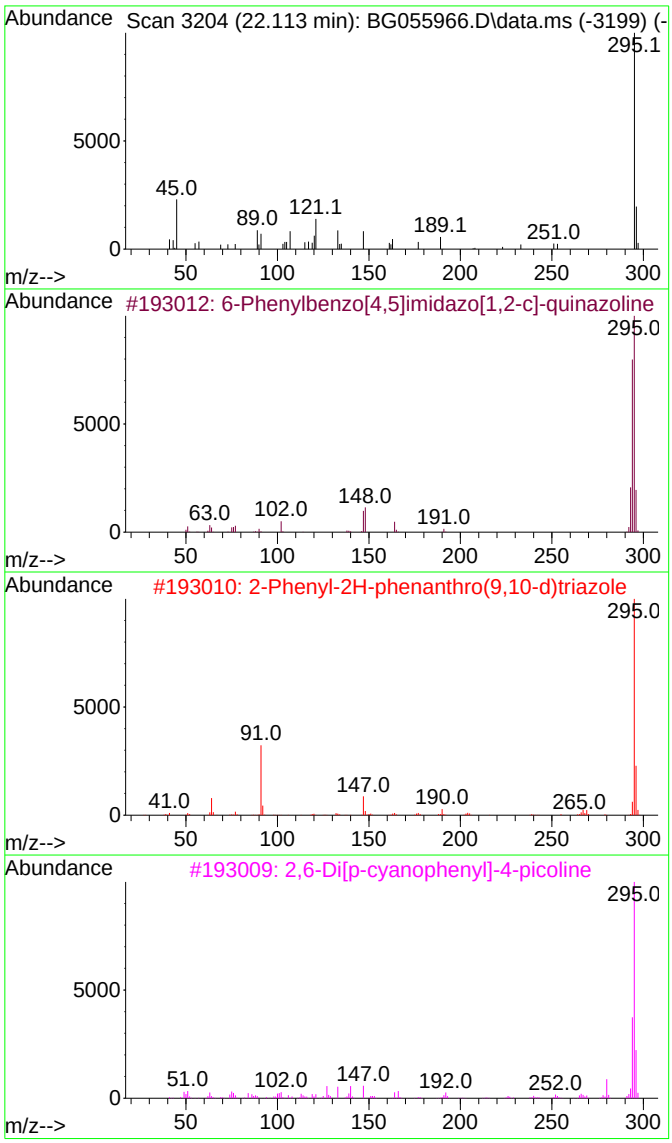
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

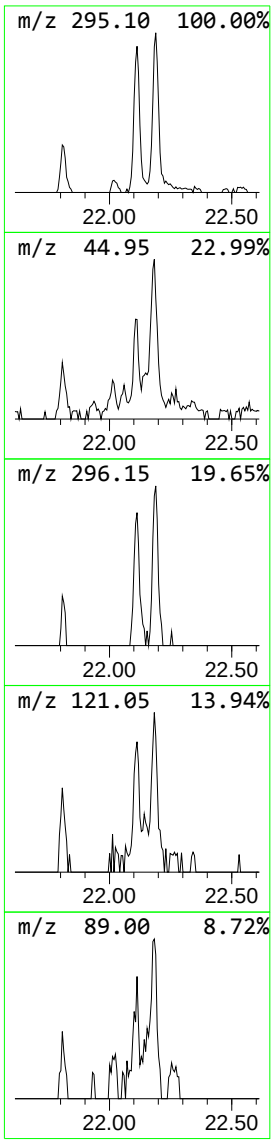
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 6-Phenylbenzo[4,5]imidazo[1... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.113	2.13 ng	35252	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Phenylbenzo[4,5]imidazo[1,2-c]...	295	C20H13N3	028381-92-2	64
2	2-Phenyl-2H-phenanthro(9,10-d)tr...	295	C20H13N3	000973-14-8	53
3	2,6-Di[p-cyanophenyl]-4-picoline	295	C20H13N3	1000212-46-7	53
4	N-[1,1'-Biphenyl]-4-yl-2-naphtha...	295	C22H17N	006336-92-1	53
5	3-Formyl-2-hydroxybenzoic acid, ...	310	C14H22O4Si2	1000497-41-3	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
Data File : BG055966.D
Acq On : 14 Dec 2022 19:28
Operator : CG/JU
Sample : N6001-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-6M

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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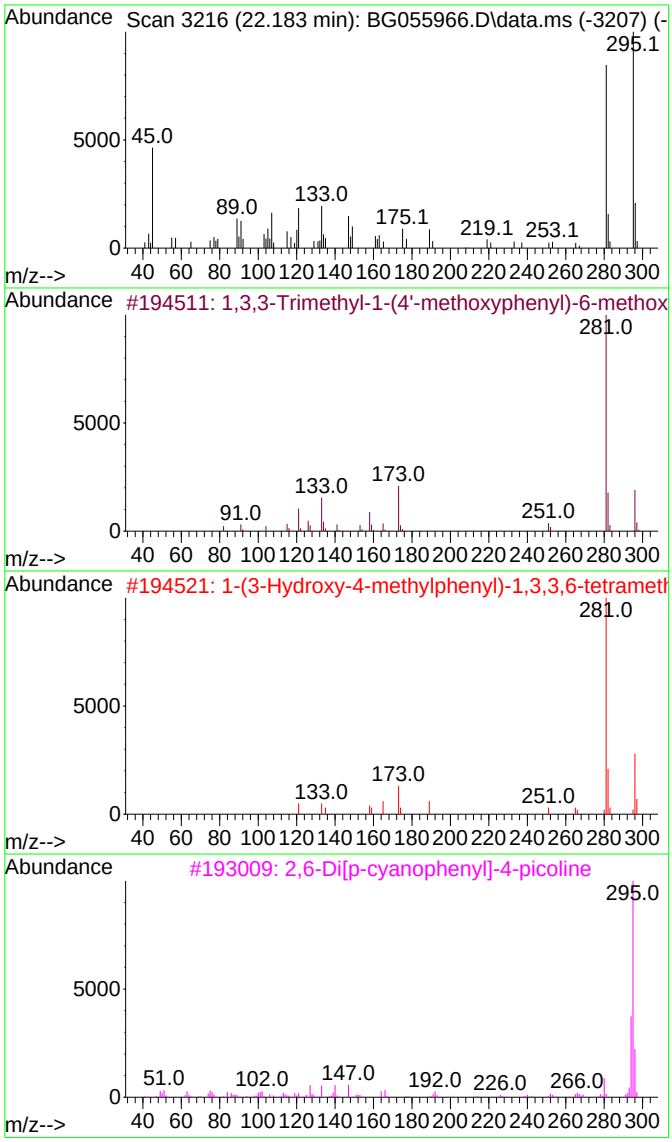
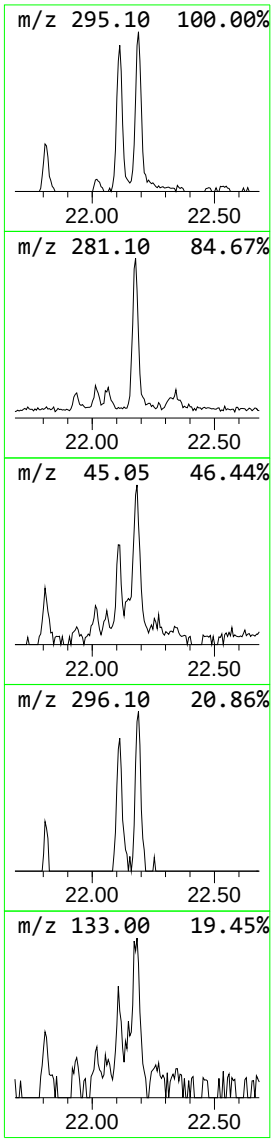
Peak Number 11 unknown22.183 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.183	5.34 ng	88292	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,3-Trimethyl-1-(4'-methoxyphe...	296	C20H24O2	108122-20-9	46
2	1-(3-Hydroxy-4-methylphenyl)-1,3...	296	C20H24O2	107535-11-5	43
3	2,6-Di[p-cyanophenyl]-4-picoline	295	C20H13N3	1000212-46-7	30
4	6-Phenylbenzo[4,5]imidazo[1,2-c]...	295	C20H13N3	028381-92-2	25
5	4-(5-Methyl-1H-benzimidazol-2-yl...	295	C17H21N3Si	1000485-94-2	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
Data File : BG055966.D
Acq On : 14 Dec 2022 19:28
Operator : CG/JU
Sample : N6001-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-6M

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.399	37.6	ng	106499	1	8.370	56566	20.0
unknown5.409	5.409	2.7	ng	7748	1	8.370	56566	20.0
unknown19.351	19.351	10.2	ng	123152	4	17.712	240519	20.0
Ethanol, 2-[2-[...	20.409	34.3	ng	566310	5	22.019	330577	20.0
unknown20.474	20.474	28.6	ng	472092	5	22.019	330577	20.0
(E)-2-Fluoro-3-...	20.515	16.2	ng	267264	5	22.019	330577	20.0
Acetamide, 2-ch...	20.603	40.5	ng	668543	5	22.019	330577	20.0
1,3-Benzodioxol...	20.673	31.8	ng	526188	5	22.019	330577	20.0
4,6-Difluoro-2-...	20.738	16.6	ng	273979	5	22.019	330577	20.0
6-Phenylbenzo[4...	22.113	2.1	ng	35252	5	22.019	330577	20.0
unknown22.183	22.183	5.3	ng	88292	5	22.019	330577	20.0