LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059886.D
Acq On : 25 Nov 2023 11:15
Operator : MA/JU
Sample : 05366-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P-14(10-15)

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-BG111623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059886.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.811	403	412	421	rBV	419273	688976	39.81%	6.949%
2	6.928	595	602	608	rBV	179366	283873	16.40%	2.863%
3	7.439	682	689	698	rBV	472341	768185	44.39%	7.748%
4	8.314	832	838	845	rBV2	114418	200018	11.56%	2.017%
5	8.496	864	869	877	rVB4	22783	35929	2.08%	0.362%
6	9.513	1035	1042	1053	rBV2	299151	530849	30.68%	5.354%
7	11.164	1317	1323	1330	rBV	164260	300277	17.35%	3.029%
8	11.211	1330	1331	1339	rVB6	13670	20956	1.21%	0.211%
9	13.567	1725	1732	1739	rVB	839632	1283128	74.15%	12.942%
10	13.772	1762	1767	1774	rVB5	15647	29491	1.70%	0.297%
11	14.125	1819	1827	1832	rVB10	12250	30326	1.75%	0.306%
12	14.618	1907	1911	1916	rBV3	46874	69002	3.99%	0.696%
13	14.906	1957	1960	1961	rBV3	17218	18006	1.04%	0.182%
14	14.948	1962	1967	1975	rVB2	269714	414968	23.98%	4.185%
15	15.993	2136	2145	2149	rVB3	11101	22856	1.32%	0.231%
16	16.434	2213	2220	2229	rVB	678819	1048612	60.60%	10.576%
17	17.697	2429	2435	2440	rBV	338884	508994	29.41%	5.134%
18	17.738	2440	2442	2447	rVV2	36262	46121	2.67%	0.465%
19	17.797	2447	2452	2454	rVV4	11287	20251	1.17%	0.204%
20	17.826	2454	2457	2461	rVB2	11467	17985	1.04%	0.181%
21	18.150	2509	2512	2518	rVB	18694	21724	1.26%	0.219%
22	18.508	2566	2573	2578	rBV2	71254	110430	6.38%	1.114%
23	18.761	2608	2616	2620	rBV8	17398	45551	2.63%	0.459%
24	19.460	2731	2735	2738	rBV	48407	59138	3.42%	0.596%
25	19.736	2777	2782	2785	rBV2	29899	38945	2.25%	0.393%
26	19.771	2785	2788	2791	rVB4	20266	24814	1.43%	0.250%
27	19.906	2808	2811	2814	rBV3	26352	30459	1.76%	0.307%
28	20.100	2839	2844	2848	rVB	28547	42166	2.44%	0.425%
29	20.271	2866	2873	2880	rVB	1357339	1730518	100.00%	17.454%
30	20.412	2892	2897	2902	rVB3	57078	78844	4.56%	0.795%
31	20.735	2946	2952	2955	rBV7	26210	50101	2.90%	0.505%
32	20.805	2959	2964	2970	rVB5	67146	108863	6.29%	1.098%
33	21.005	2994	2998	3002	rVB6	26417	35070	2.03%	0.354%
34	21.064	3005	3008	3011	rBV5	18573	22746	1.31%	0.229%
35	21.563	3085	3093	3103	rBV5	46730	149663	8.65%	1.509%
36	21.898	3146	3150	3156	rVB9	72149	114013	6.59%	1.150%

LSC Area Percent Report

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Misc :
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Instrument :
BNA_G
ClientSampleId :
P-14(10-15)

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-BG111623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	22.016	3164	3170	3177	rVB	230375	411549	23.78%	4.151%
38	23.561	3427	3433	3436	rBV7	17788	32764	1.89%	0.330%
39	23.749	3459	3465	3473	rVB7	20758	54045	3.12%	0.545%
40	25.588	3768	3778	3789	rVB3	133522	414616	23.96%	4.182%

Sum of corrected areas: 9914822

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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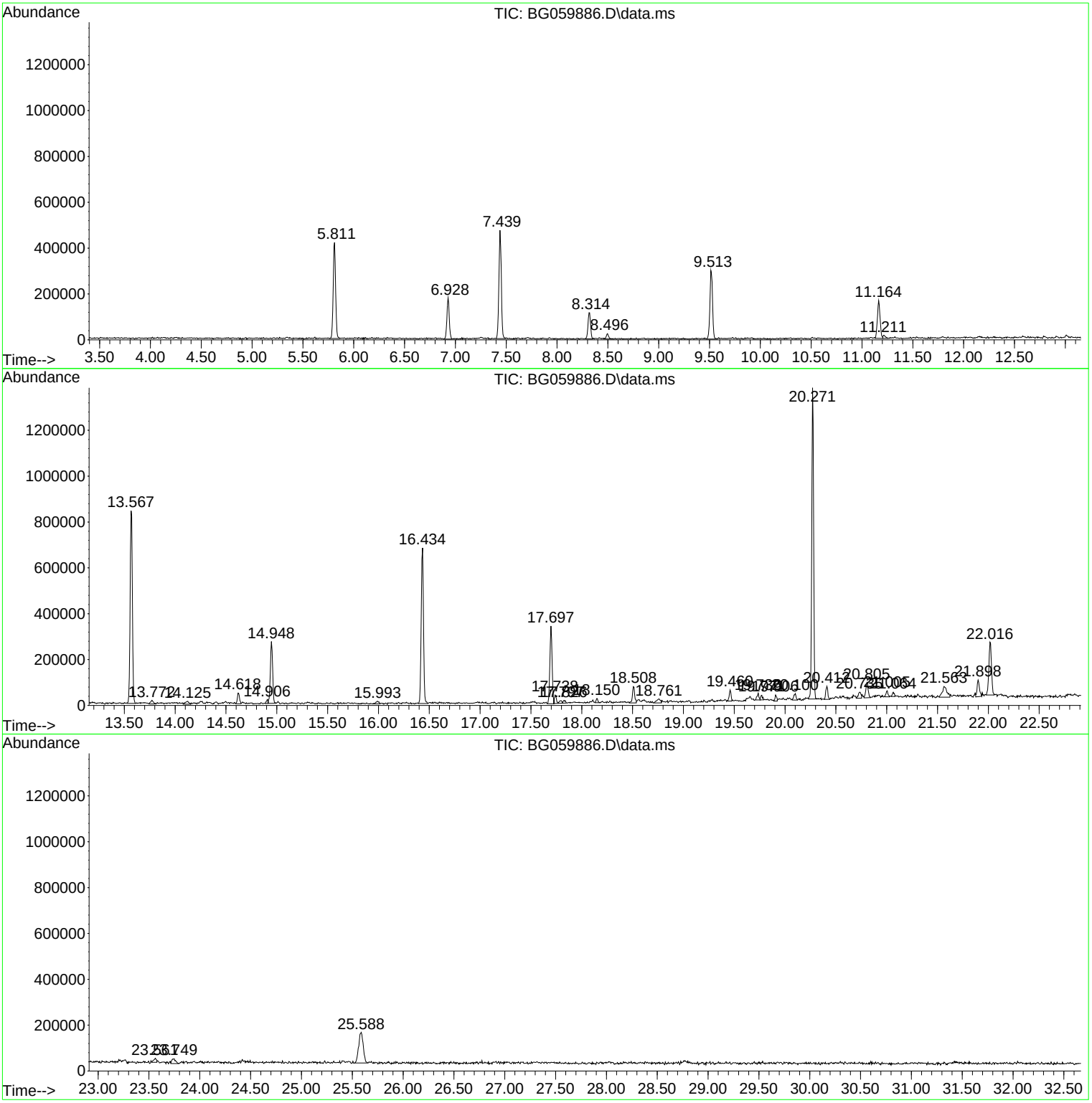
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059886.D
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Sample : 05366-02
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Instrument :
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ClientSampleId :
P-14(10-15)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

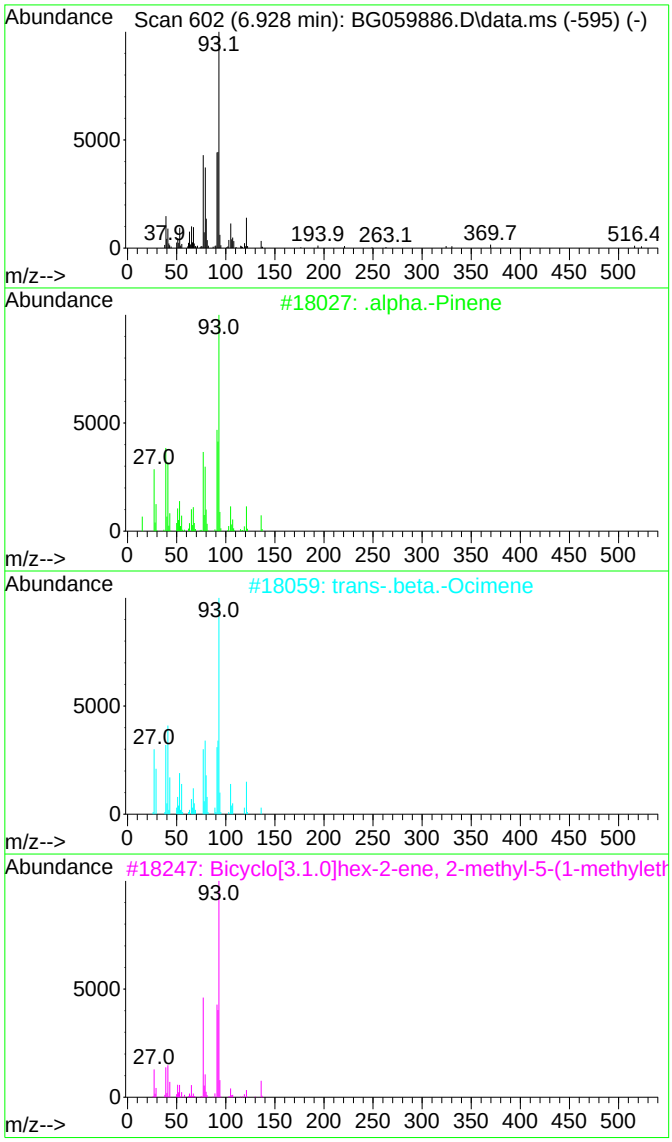
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

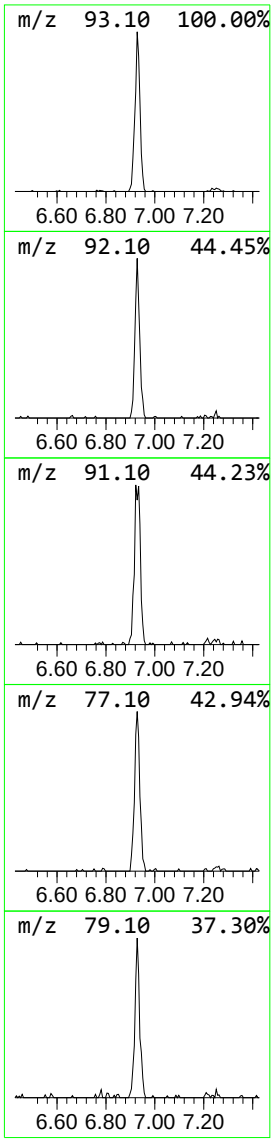
****

Peak Number 1 .alpha.-Pinene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.928	28.38 ng	283873	1,4-Dichlorobenzene-d4	8.314

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	94
2	trans-.beta.-Ocimene	136	C10H16	003779-61-1	68
3	Bicyclo[3.1.0]hex-2-ene, 2-methy...	136	C10H16	002867-05-2	64
4	1,3,7-Octatriene, 3,7-dimethyl-	136	C10H16	000502-99-8	64
5	Bicyclo[3.1.0]hexane, 4-methylen...	136	C10H16	003387-41-5	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059886.D
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Operator : MA/JU
Sample : 05366-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P-14(10-15)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

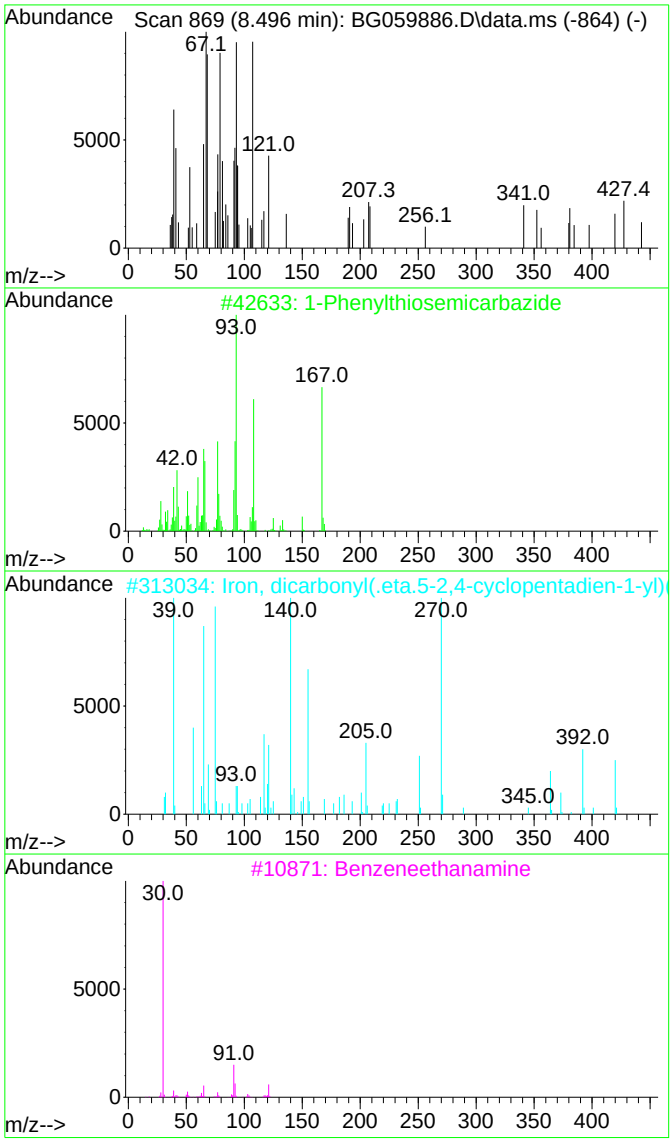
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

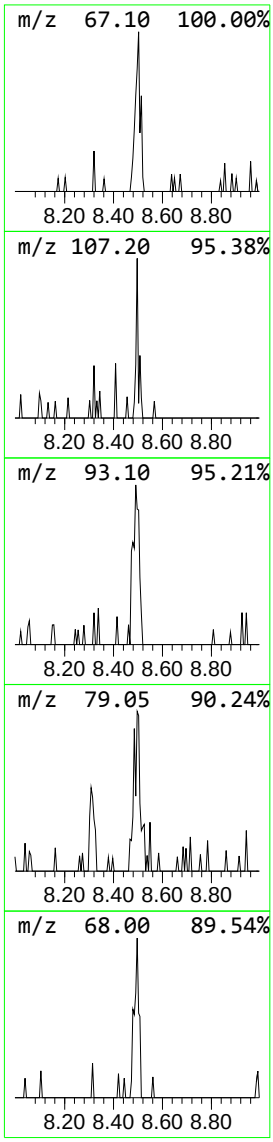
****

Peak Number 2 unknown8.496 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.496	3.59 ng	35929	1,4-Dichlorobenzene-d4	8.314

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenylthiosemicarbazide	167	C7H9N3S	000645-48-7	23
2	Iron, dicarbonyl(.eta.5-2,4-cycl...	420	C13H5F9FeO2	012215-33-7	12
3	Benzeneethanamine	121	C8H11N	000064-04-0	9
4	Pyrimidine-2,4,6-trione, hexahyd...	352	C19H16N2O5	314041-26-4	9
5	Diphenyl N,N'-(ethylenebis(oxy-p...	568	C34H36N2O6	005508-93-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059886.D
Acq On : 25 Nov 2023 11:15
Operator : MA/JU
Sample : 05366-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P-14(10-15)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

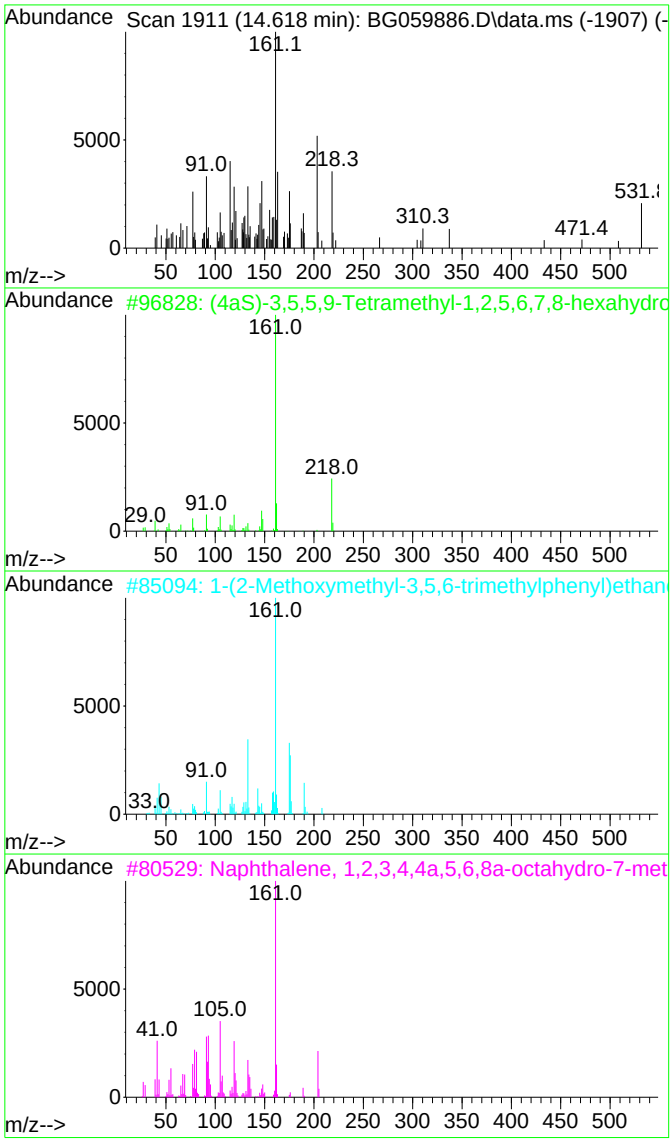
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

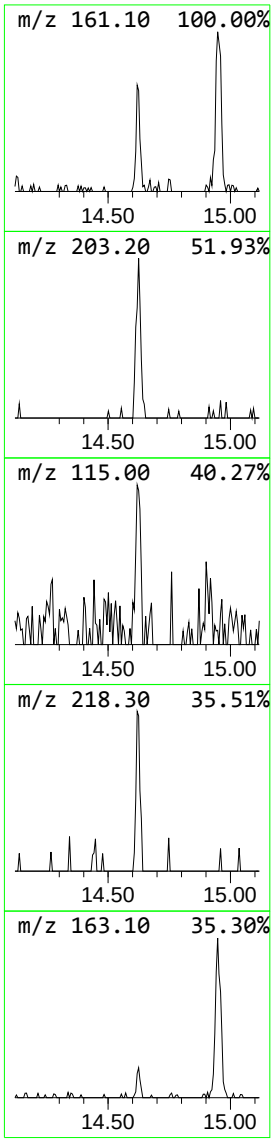
****

Peak Number 3 unknown14.618 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.618	3.33 ng	69002	Acenaphthene-d10	14.948

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(4aS)-3,5,5,9-Tetramethyl-1,2,5,...	218	C15H22O	064825-84-9	41
2	1-(2-Methoxymethyl-3,5,6-trimeth...	208	C13H20O2	1000202-04-5	38
3	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	039029-41-9	30
4	2-(3-Pyridyl)piperidine, N-penta...	308	C13H13F5N2O	1000449-82-1	30
5	Benzene, 2-methyl-1,4-bis(1-meth...	176	C13H20	058502-85-5	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
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Sample : 05366-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P-14(10-15)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

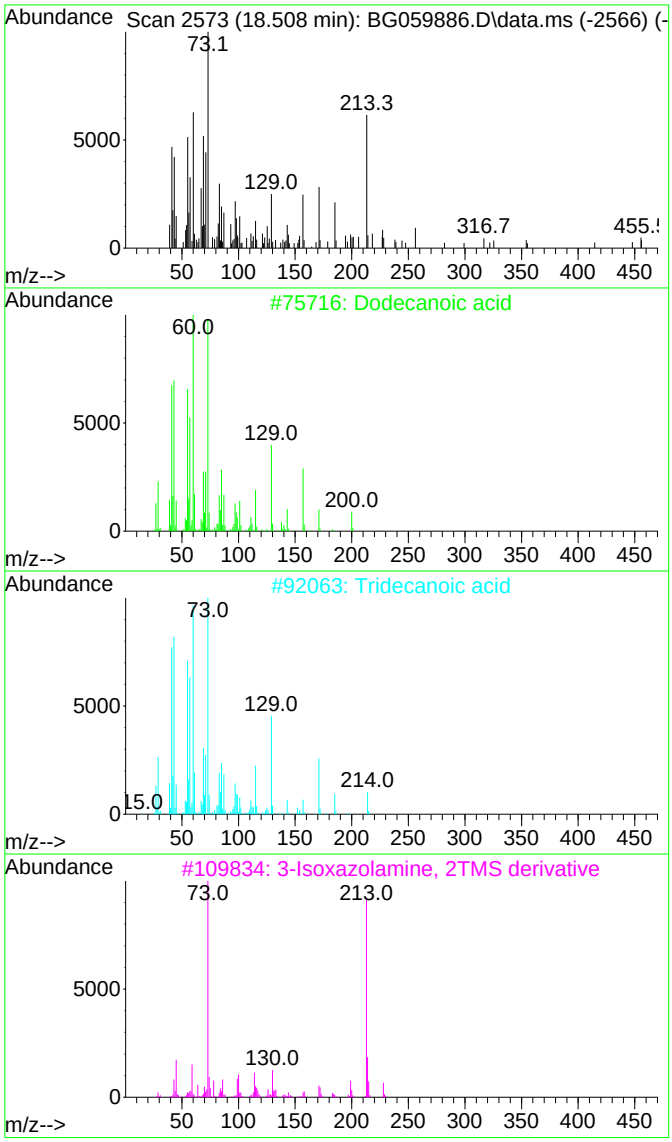
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

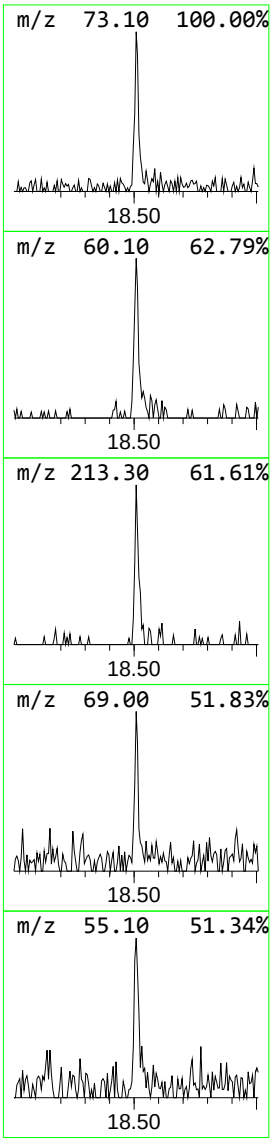
****

Peak Number 4 unknown18.508 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.508	4.34 ng	110430	Phenanthrene-d10	17.697

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	41
2	Tridecanoic acid	214	C13H26O2	000638-53-9	35
3	3-Isoxazolamine, 2TMS derivative	228	C9H20N2OSi2	1010478-88-5	25
4	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	14
5	Malonic acid, 2,4-dimethylpent-3...	328	C19H36O4	1000349-01-5	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P-14(10-15)

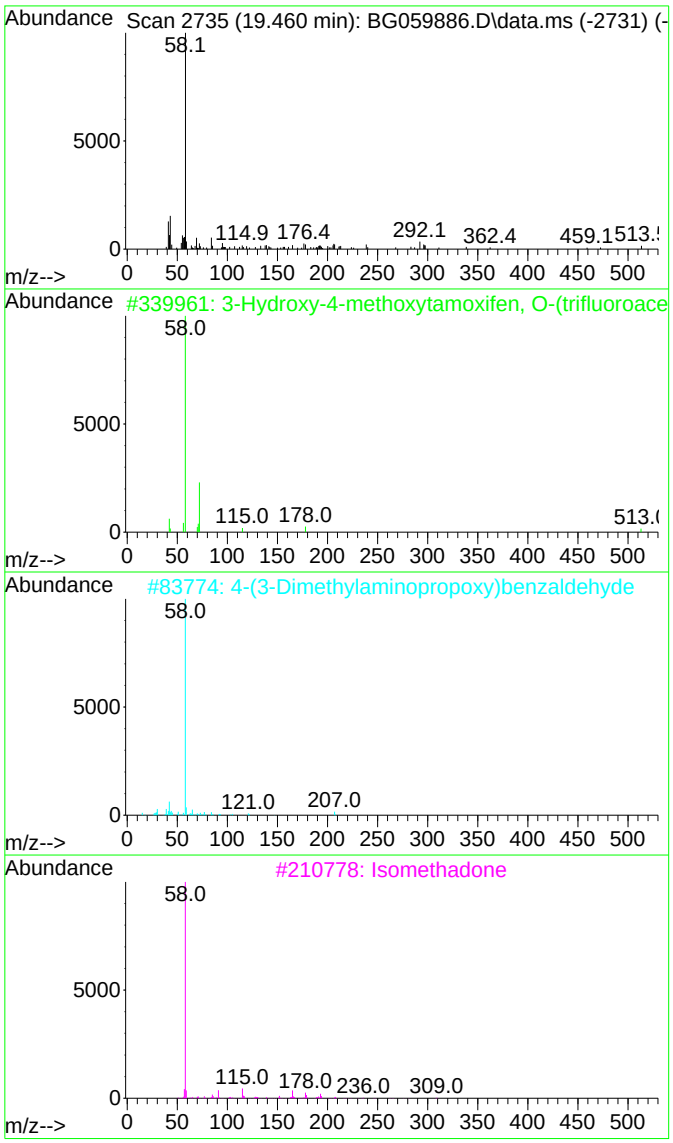
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

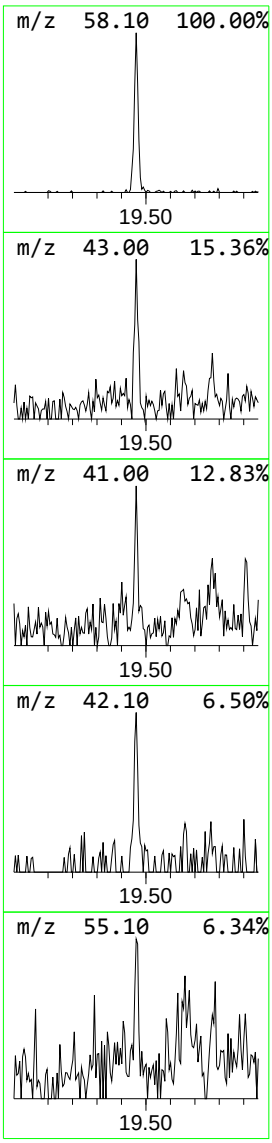
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3-Hydroxy-4-methoxytamoxife... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.460	2.32 ng	59138	Phenanthrene-d10	17.697

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hydroxy-4-methoxytamoxifen, O-...	513	C29H30F3NO4	1000445-51-7	59
2	4-(3-Dimethylaminopropoxy)benzal...	207	C12H17NO2	026934-35-0	59
3	Isomethadone	309	C21H27NO	000466-40-0	59
4	Amitriptylinoxide	293	C20H23NO	004317-14-0	59
5	2-Amino-2-methyl-1-(pyrrolidin-1...	156	C8H16N2O	1000459-38-4	59





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Instrument :
BNA_G
ClientSampleId :
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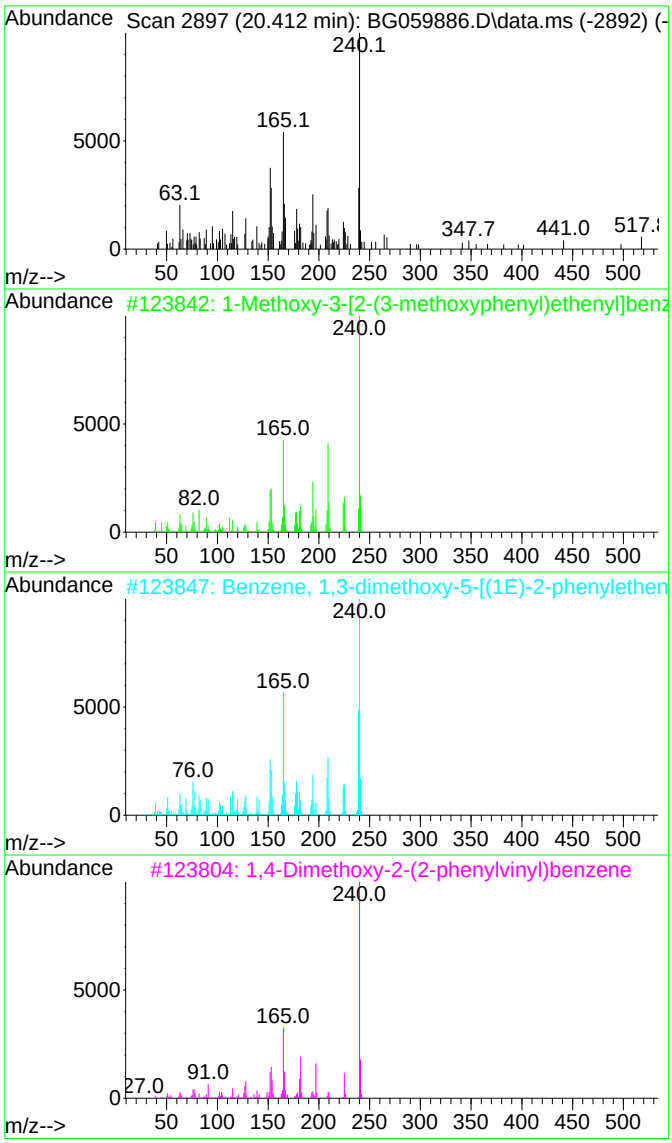
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

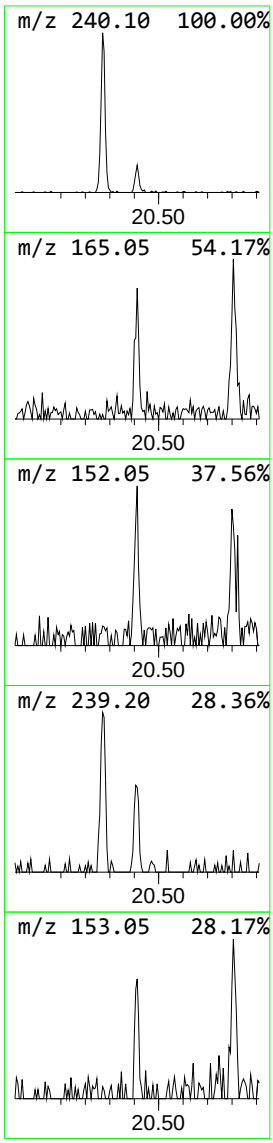
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Methoxy-3-[2-(3-methoxyph... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.412	3.83 ng	78844	Chrysene-d12	22.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methoxy-3-[2-(3-methoxyphenyl)...	240	C16H16O2	006325-63-9	68
2	Benzene, 1,3-dimethoxy-5-[(1E)-2...	240	C16H16O2	021956-56-9	62
3	1,4-Dimethoxy-2-(2-phenylvinyl)b...	240	C16H16O2	021889-09-8	49
4	Benzene, 1,1'-(1,2-ethenediyl)bi...	240	C16H16O2	004705-34-4	49
5	Benzenamine, 4-[2-(4-nitrophenyl...	240	C14H12N2O2	004629-58-7	46





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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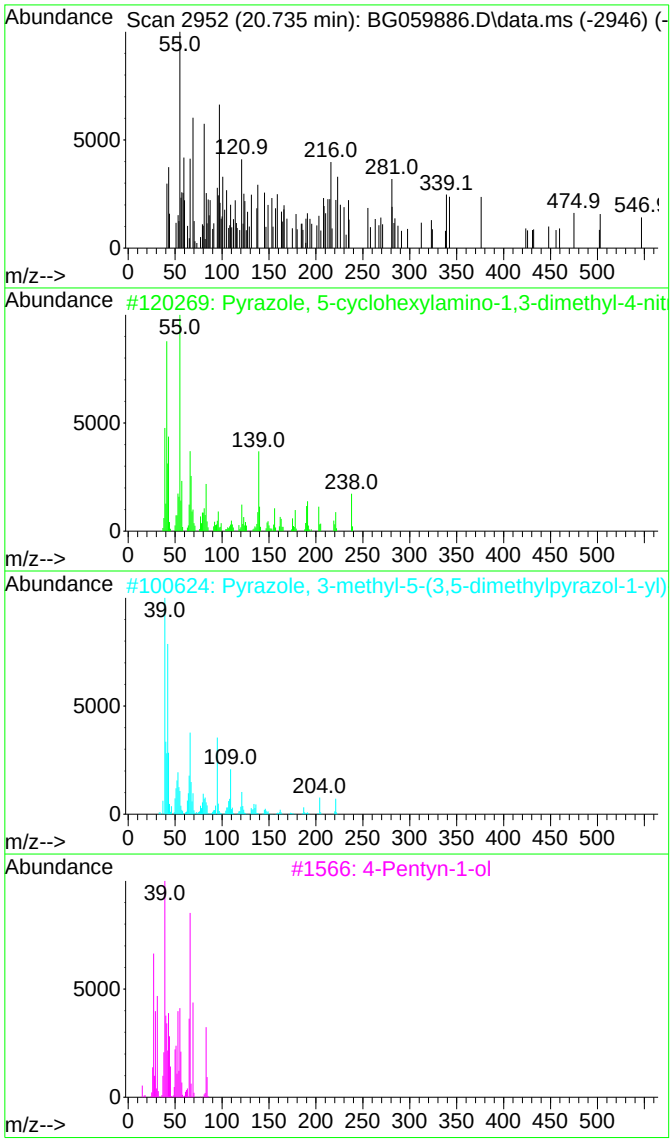
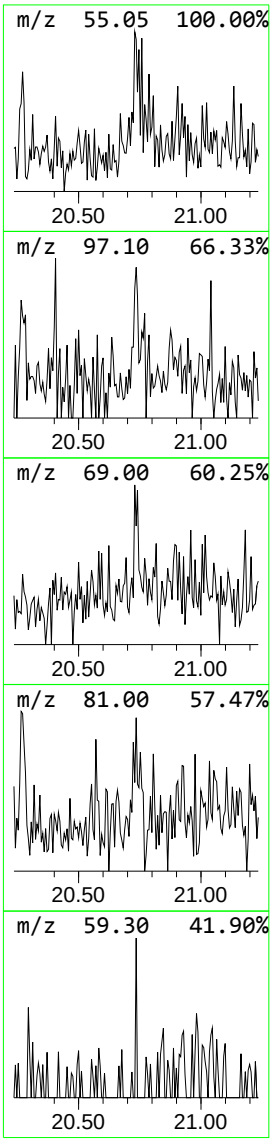
****

Peak Number 8 unknown20.735 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.735	2.43 ng	50101	Chrysene-d12	22.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrazole, 5-cyclohexylamino-1,3-...	238	C11H18N4O2	1000263-20-2	32
2	Pyrazole, 3-methyl-5-(3,5-dimeth...	221	C9H11N5O2	1000263-78-5	32
3	4-Pentyn-1-ol	84	C5H8O	005390-04-5	32
4	1,1-Cyclopropanedicarboxylic aci...	212	C11H16O4	007686-78-4	23
5	Bicyclo[2.2.1]heptan-2-one, 7,7-...	138	C9H14O	000514-15-8	23





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BNA_G
ClientSampleId :
P-14(10-15)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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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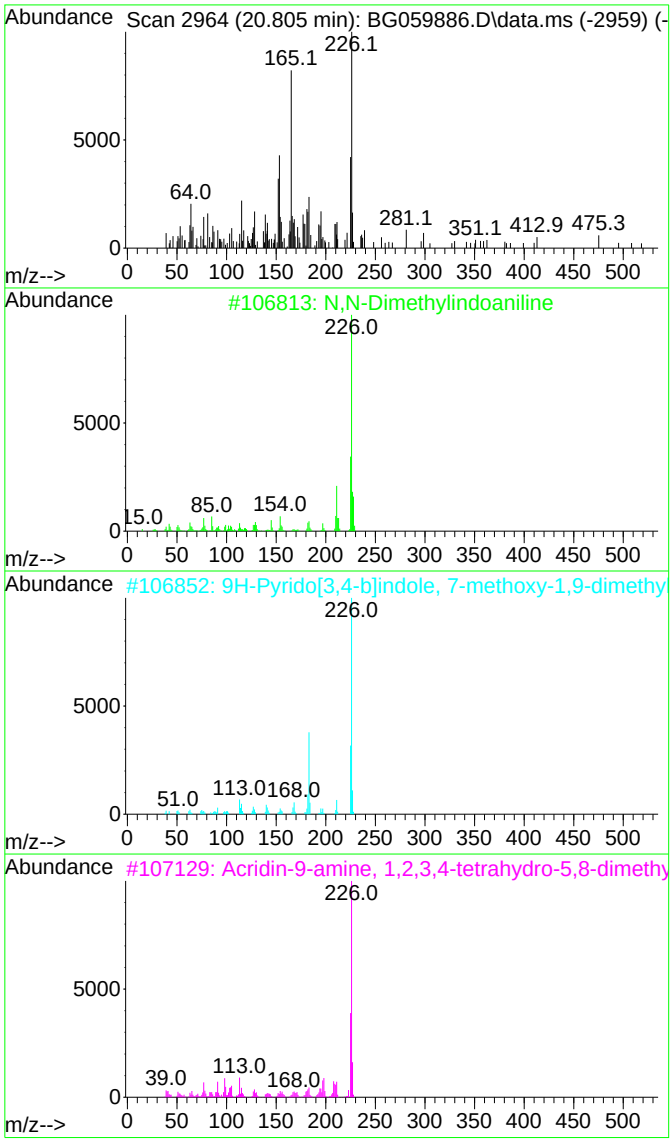
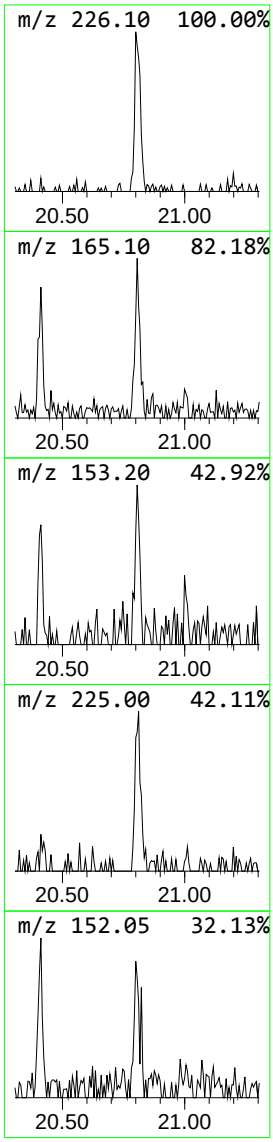
Peak Number 9 unknown20.805 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.805	5.29 ng	108863	Chrysene-d12	22.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N,N-Dimethylindoaniline	226	C14H14N2O	002150-58-5	41
2	9H-Pyrido[3,4-b]indole, 7-methox...	226	C14H14N2O	143502-37-8	38
3	Acridin-9-amine, 1,2,3,4-tetrahy...	226	C15H18N2	297758-19-1	38
4	Acridin-9-amine, 1,2,3,4-tetrahy...	226	C15H18N2	1000300-57-6	30
5	9H-Xanthen-9-one, 2-methoxy-	226	C14H10O3	001214-20-6	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059886.D
Acq On : 25 Nov 2023 11:15
Operator : MA/JU
Sample : 05366-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P-14(10-15)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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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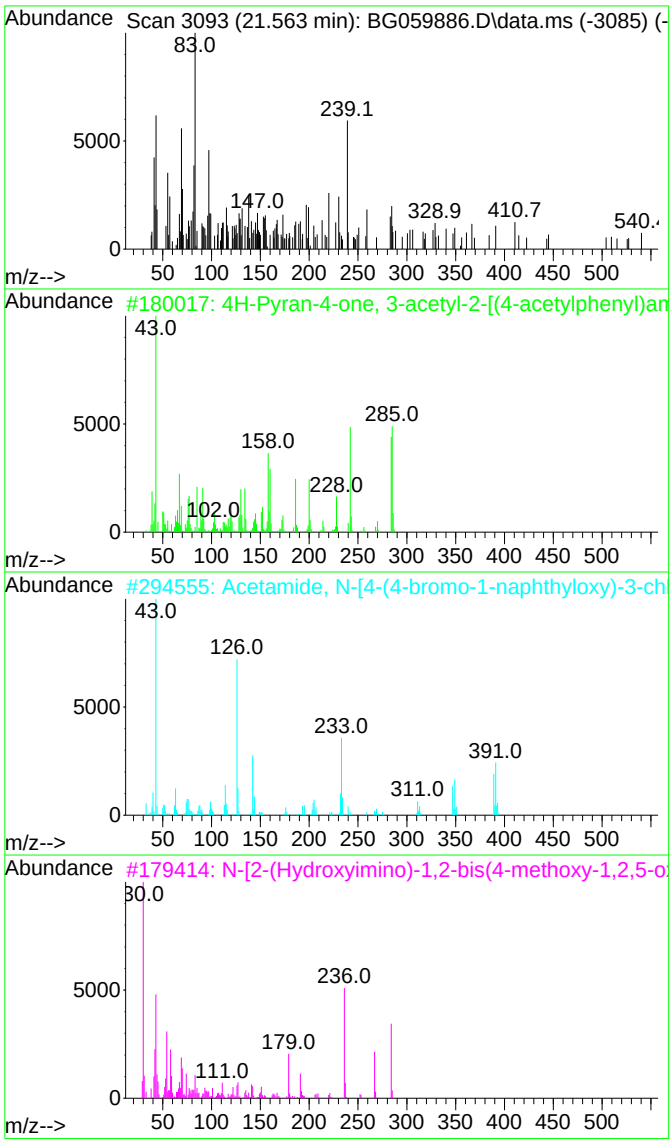
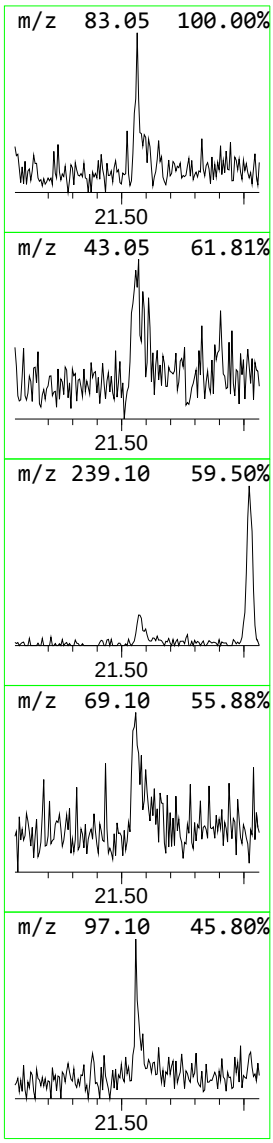
Peak Number 10 unknown21.563 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.563	7.27 ng	149663	Chrysene-d12	22.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Pyran-4-one, 3-acetyl-2-[(4-a...	285	C16H15NO4	1000350-41-2	10
2	Acetamide, N-[4-(4-bromo-1-napht...	389	C18H13BrClNO2	1000274-06-2	10
3	N-[2-(Hydroxyimino)-1,2-bis(4-me...	284	C8H8N6O6	1000443-58-5	9
4	.alpha.-[4-(Adamantyl-1)phenyl]p...	284	C19H24O2	1000140-75-3	9
5	Carbonic acid, monoamide, N-(2-p...	375	C24H41NO2	1000490-72-4	9





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Operator : MA/JU
Sample : 05366-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P-14(10-15)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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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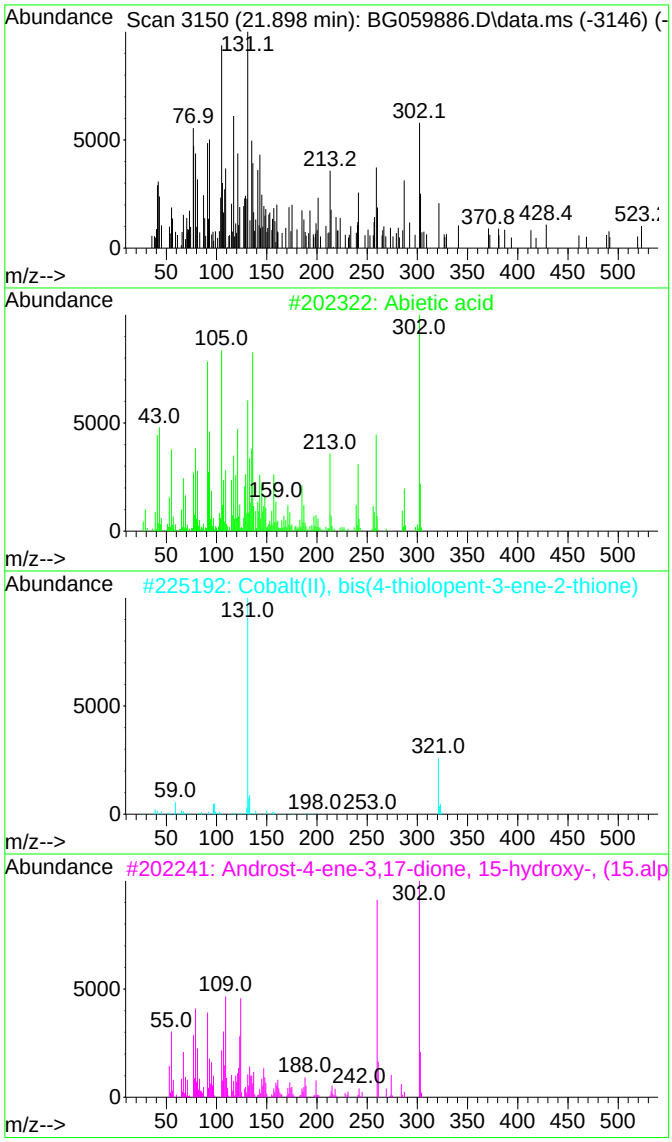
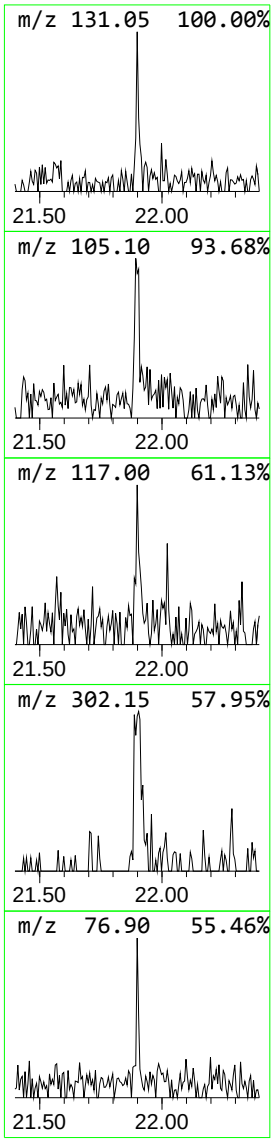
Peak Number 11 unknown21.898 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.898	5.54 ng	114013	Chrysene-d12	22.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Abietic acid	302	C20H30O2	000514-10-3	37
2	Cobalt(II), bis(4-thiolopent-3-e...	321	C10H14CoS4	1000164-51-2	22
3	Androst-4-ene-3,17-dione, 15-hyd...	302	C19H26O3	000566-08-5	15
4	1,5-Diaminonaphthalene, 2TMS der...	302	C16H26N2Si2	033285-89-1	10
5	Benzaldehyde hydrazone,4-methoxy...	302	C15H18N4O3	052421-35-9	10





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Data File : BG059886.D
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Operator : MA/JU
Sample : 05366-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P-14(10-15)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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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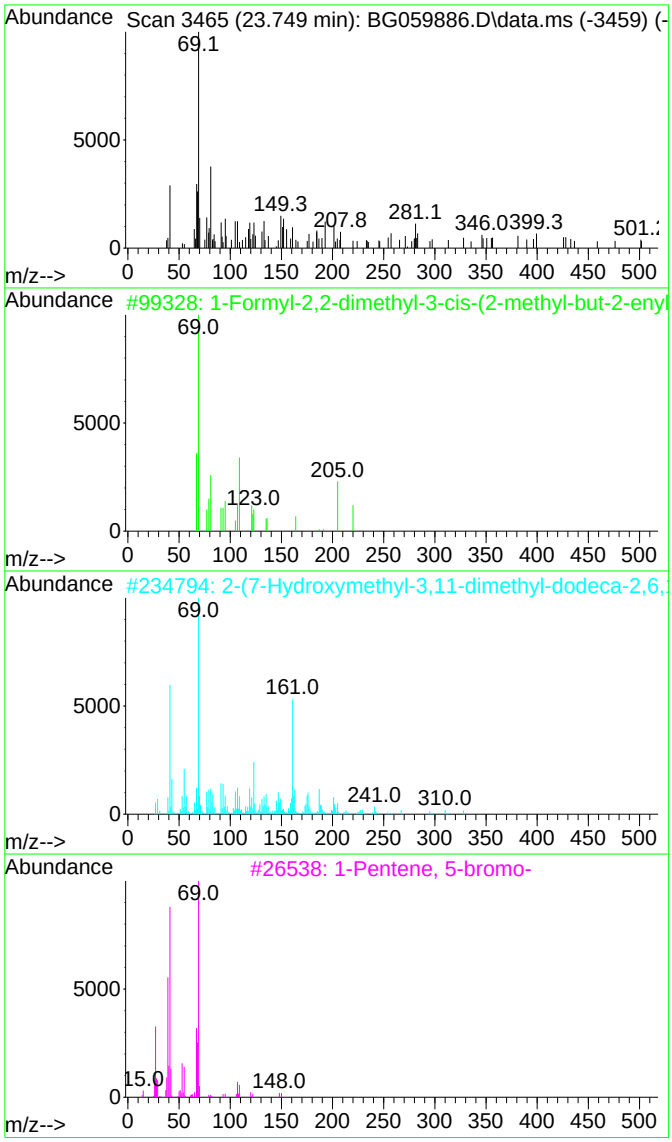
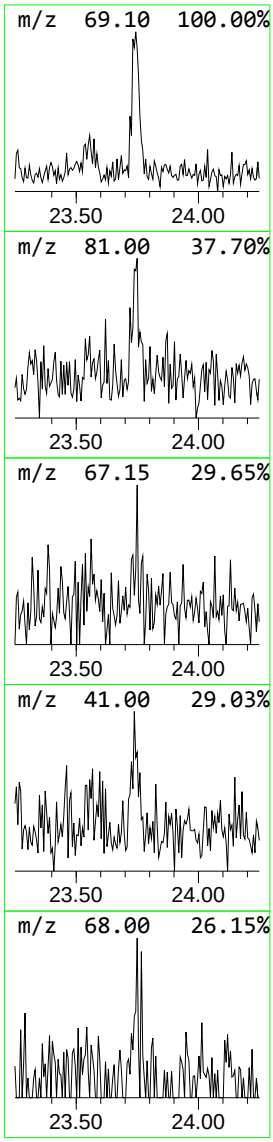
Peak Number 12 unknown23.749 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.749	2.63 ng	54045	Chrysene-d12	22.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Formyl-2,2-dimethyl-3-cis-(2-m...	220	C15H24O	1000144-10-0	47
2	2-(7-Hydroxymethyl-3,11-dimethyl...	328	C21H28O3	1000189-16-4	47
3	1-Pentene, 5-bromo-	148	C5H9Br	001119-51-3	47
4	(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	38
5	1-(1,1,2,3,3,3-Hexafluoropropyl)...	277	C7H5F6N3O2	307929-62-0	38





Tentatively Identified Compound (LSC) summary

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Data File : BG059886.D
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BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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
.alpha.-Pinene	6.928	28.4	ng	283873	1	8.314	200018	20.0
unknown8.496	8.496	3.6	ng	35929	1	8.314	200018	20.0
unknown14.618	14.618	3.3	ng	69002	3	14.948	414968	20.0
unknown18.508	18.508	4.3	ng	110430	4	17.697	508994	20.0
3-Hydroxy-4-met...	19.460	2.3	ng	59138	4	17.697	508994	20.0
1-Methoxy-3-[2-...	20.412	3.8	ng	78844	5	22.016	411549	20.0
unknown20.735	20.735	2.4	ng	50101	5	22.016	411549	20.0
unknown20.805	20.805	5.3	ng	108863	5	22.016	411549	20.0
unknown21.563	21.563	7.3	ng	149663	5	22.016	411549	20.0
unknown21.898	21.898	5.5	ng	114013	5	22.016	411549	20.0
unknown23.749	23.749	2.6	ng	54045	5	22.016	411549	20.0