LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
Data File : BG059773.D
Acq On : 20 Nov 2023 17:47
Operator : MA/JU
Sample : 05311-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-6

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: BG059773.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.823	407	414	423	rVB2	397626	648273	31.72%	5.237%
2	7.451	683	691	698	rBV	500097	841864	41.19%	6.800%
3	8.332	835	841	849	rVB	112718	198276	9.70%	1.602%
4	9.531	1036	1045	1051	rBV	331005	575384	28.15%	4.648%
5	11.176	1315	1325	1332	rBV	157158	292165	14.29%	2.360%
6	13.585	1727	1735	1741	rBV	1108613	1607382	78.64%	12.984%
7	13.790	1764	1770	1776	rVB7	17951	37132	1.82%	0.300%
8	14.272	1846	1852	1853	rBV3	14672	22580	1.10%	0.182%
9	14.960	1960	1969	1976	rBV2	305920	469856	22.99%	3.795%
10	16.446	2214	2222	2229	rBV	852084	1324012	64.77%	10.695%
11	17.527	2402	2406	2412	rVB7	17352	26710	1.31%	0.216%
12	17.709	2431	2437	2441	rBV2	390647	587046	28.72%	4.742%
13	17.750	2441	2444	2449	rVB	183477	265124	12.97%	2.142%
14	17.844	2454	2460	2468	rVB4	47235	86756	4.24%	0.701%
15	18.115	2503	2506	2512	rVB8	23796	36940	1.81%	0.298%
16	18.526	2571	2576	2580	rBV4	172265	234788	11.49%	1.897%
17	18.567	2581	2583	2588	rVV6	50850	81133	3.97%	0.655%
18	18.626	2588	2593	2598	rVV6	58272	85169	4.17%	0.688%
19	18.755	2612	2615	2616	rBV3	31713	30471	1.49%	0.246%
20	19.061	2665	2667	2674	rBV7	26749	49146	2.40%	0.397%
21	19.119	2674	2677	2682	rVB6	33981	40287	1.97%	0.325%
22	19.460	2732	2735	2738	rBV5	29428	43979	2.15%	0.355%
23	19.742	2778	2783	2787	rBV2	290416	404675	19.80%	3.269%
24	19.783	2787	2790	2794	rVB6	48691	64685	3.16%	0.523%
25	20.059	2835	2837	2838	rBV2	23824	22605	1.11%	0.183%
26	20.112	2841	2846	2851	rVB	187258	290173	14.20%	2.344%
27	20.289	2870	2876	2883	rVB	1549845	2044054	100.00%	16.511%
28	20.582	2923	2926	2933	rVB8	28745	54918	2.69%	0.444%
29	21.381	3060	3062	3067	rVB6	39822	50660	2.48%	0.409%
30	21.528	3083	3087	3089	rBV5	23093	39783	1.95%	0.321%
31	21.569	3091	3094	3099	rVB7	69130	119322	5.84%	0.964%
32	21.740	3119	3123	3131	rVB7	26549	56193	2.75%	0.454%
33	22.034	3165	3173	3179	rBV3	259848	591919	28.96%	4.781%
34	22.086	3179	3182	3189	rVB	90518	153975	7.53%	1.244%
35	23.444	3411	3413	3418	rBV6	19356	28578	1.40%	0.231%
36	24.454	3578	3585	3589	rBV3	70182	174729	8.55%	1.411%

LSC Area Percent Report

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Operator : MA/JU
Sample : 05311-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-6

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	25.441	3744	3753	3760	rBV3	55618	167270	8.18%	1.351%
38	25.618	3775	3783	3791	rVB	123653	349818	17.11%	2.826%
39	28.062	4197	4199	4203	rVV4	18920	22037	1.08%	0.178%
40	28.091	4203	4204	4211	rVB7	25740	40606	1.99%	0.328%
41	29.678	4471	4474	4476	rBV4	14884	21773	1.07%	0.176%
42	29.754	4483	4487	4492	rBV8	19141	40243	1.97%	0.325%
43	29.883	4507	4509	4514	rBV6	15310	23331	1.14%	0.188%
44	32.028	4870	4874	4877	rBV6	22080	33859	1.66%	0.274%

Sum of corrected areas: 12379679

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Misc :
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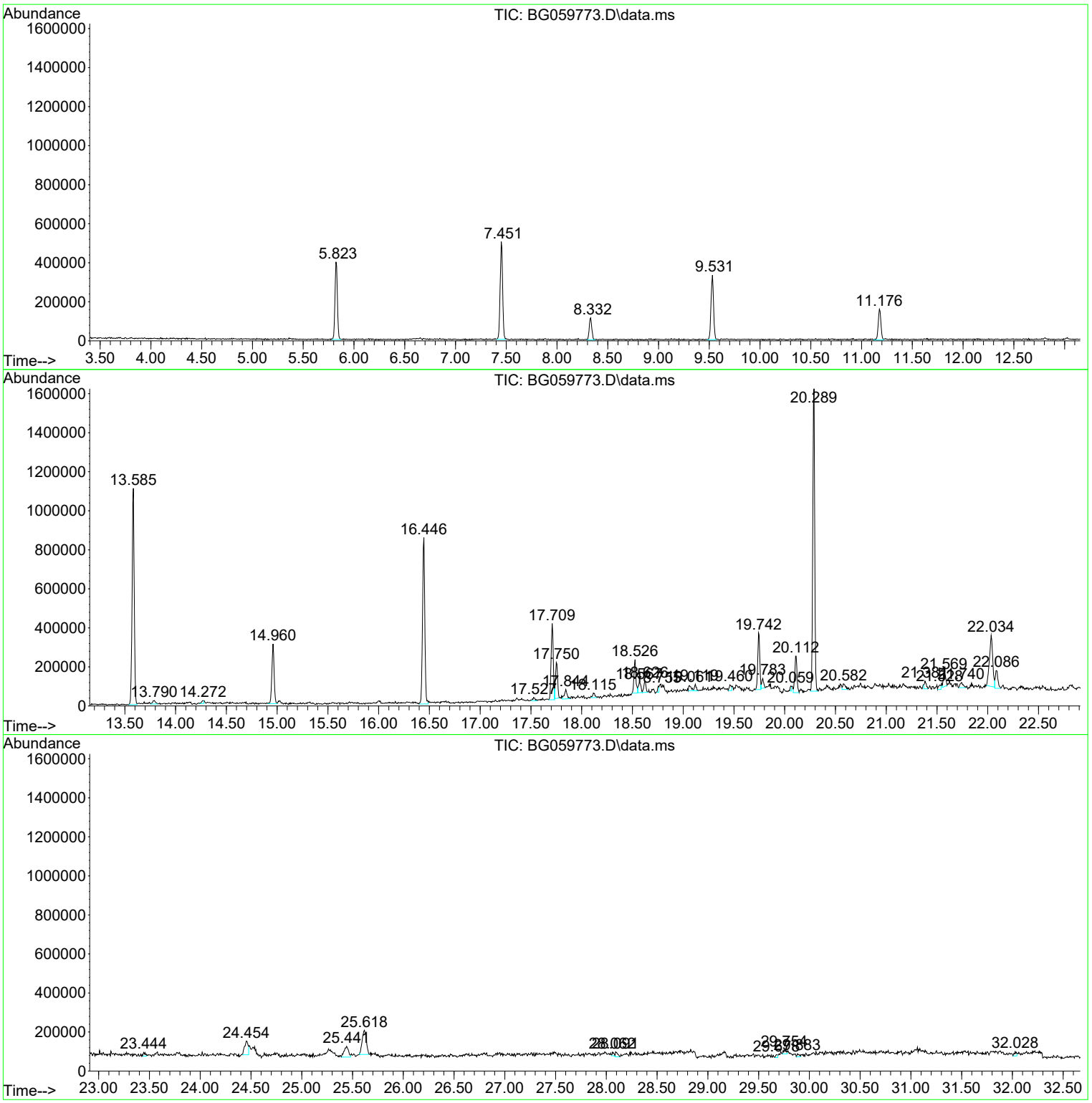
Instrument :
BNA_G
ClientSampleId :
TP-6

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\BG112023\
Data File : BG059773.D
Acq On : 20 Nov 2023 17:47
Operator : MA/JU
Sample : 05311-16
Misc :
ALS Vial : 7 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

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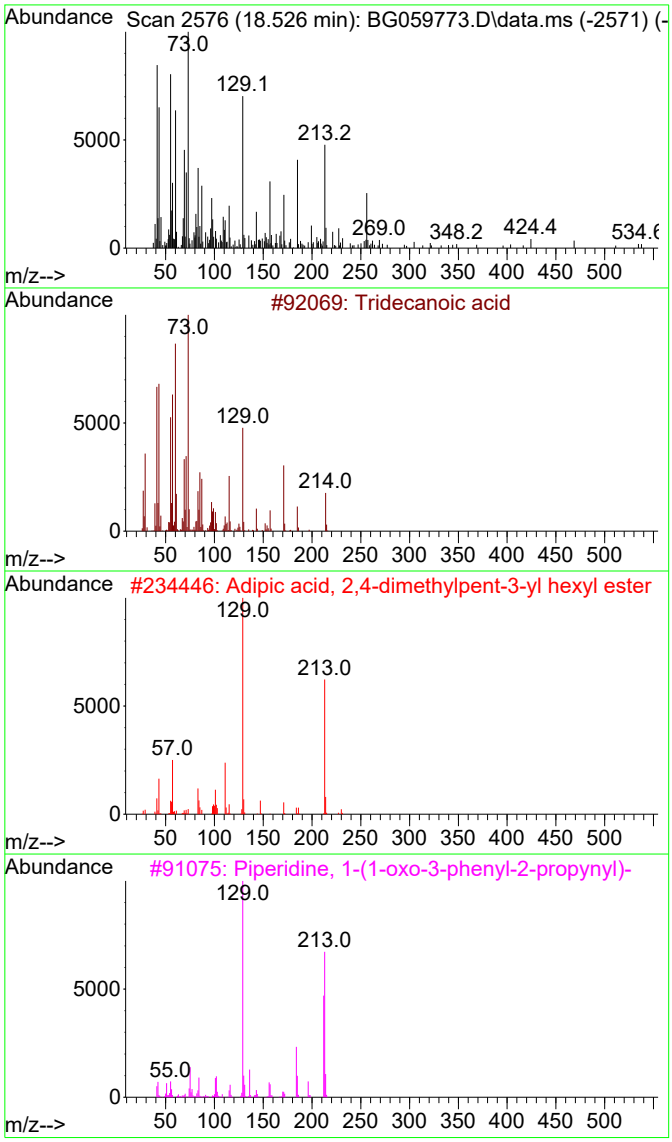
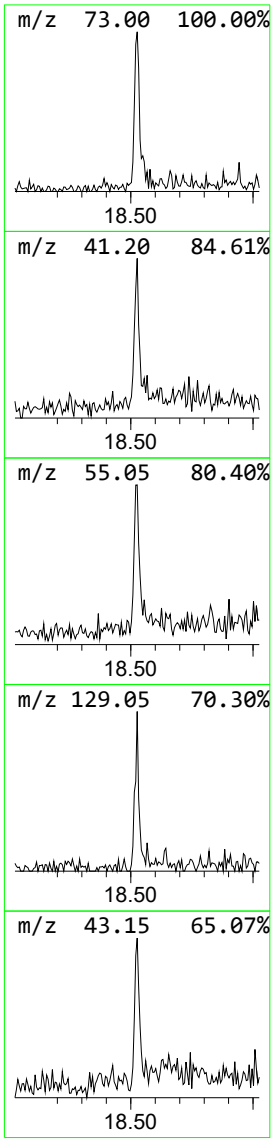
Peak Number 1 unknown18.526 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.526	8.00 ng	234788	Phenanthrene-d10	17.709

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	38
2	Adipic acid, 2,4-dimethylpent-3-...	328	C19H36O4	1000353-52-3	30
3	Piperidine, 1-(1-oxo-3-phenyl-2-...	213	C14H15NO	014143-92-1	30
4	3,7-Dimethyl-8-oxo-1,5-dioxa-spi...	256	C13H20O5	1000193-79-8	27
5	Hexanedioic acid, dihexyl ester	314	C18H34O4	000110-33-8	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
Data File : BG059773.D
Acq On : 20 Nov 2023 17:47
Operator : MA/JU
Sample : 05311-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-6

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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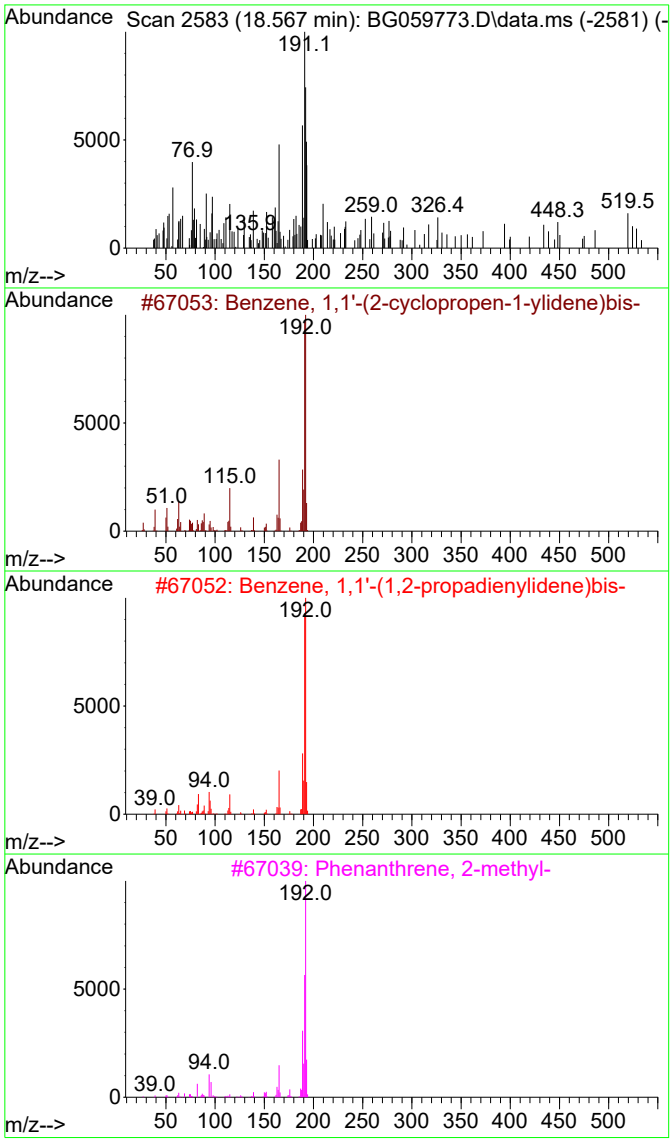
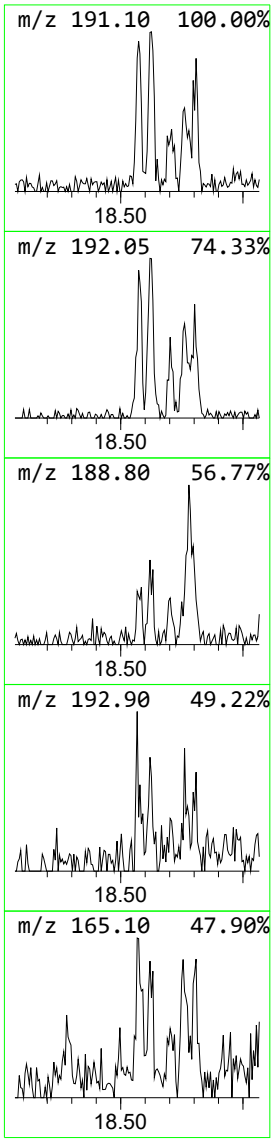
Peak Number 2 unknown18.567 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.567	2.76 ng	81133	Phenanthrene-d10	17.709

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(2-cyclopropen-1-y...	192	C15H12	022825-21-4	43
2	Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	38
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	30
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	30
5	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
Data File : BG059773.D
Acq On : 20 Nov 2023 17:47
Operator : MA/JU
Sample : 05311-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-6

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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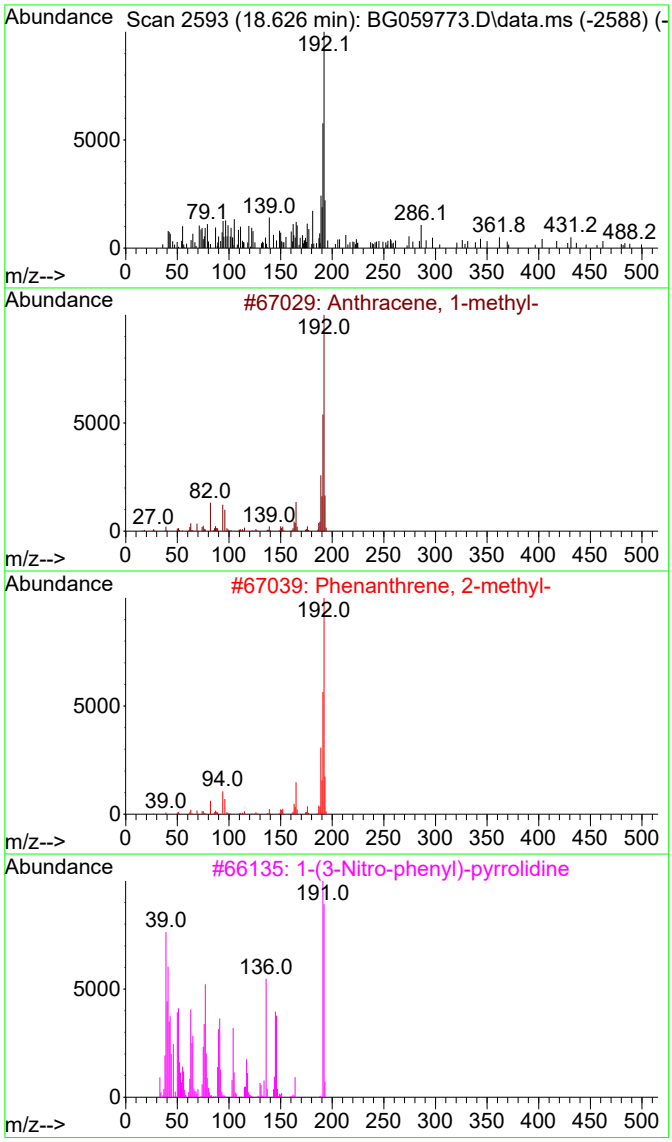
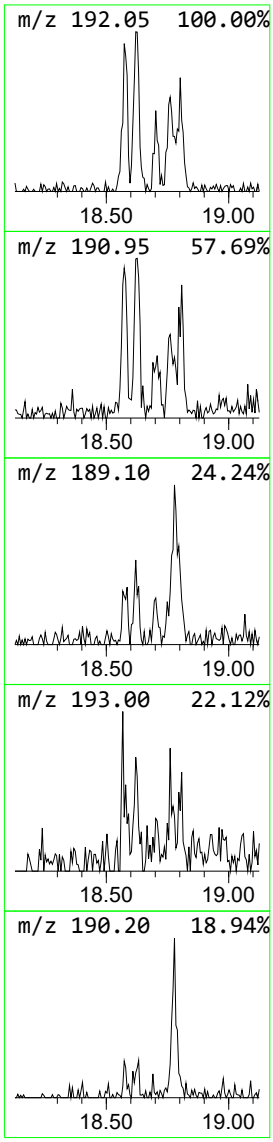
Peak Number 3 Anthracene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.626	2.90 ng	85169	Phenanthrene-d10	17.709

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	70
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	70
3	1-(3-Nitro-phenyl)-pyrrolidine	192	C10H12N2O2	1000300-34-7	60
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	58
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	58





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Instrument :
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

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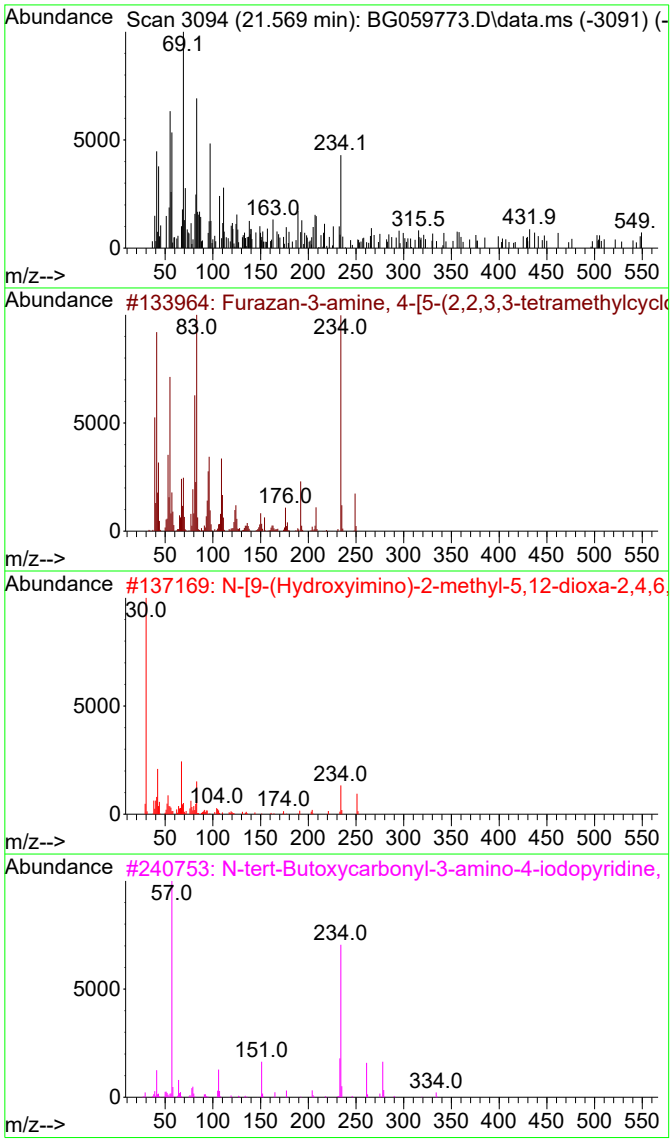
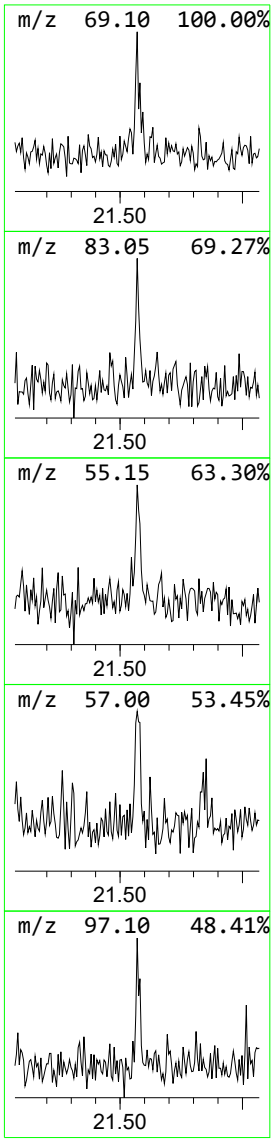
Peak Number 4 unknown21.569 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.569	4.03 ng	119322	Chrysene-d12	22.040

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furazan-3-amine, 4-[5-(2,2,3,3-t...	249	C11H15N5O2	1000274-02-9	17
2	N-[9-(Hydroxyimino)-2-methyl-5,1...	251	C7H5N7O4	1000436-04-1	17
3	N-tert-Butoxycarbonyl-3-amino-4-...	334	C11H15IN2O2	1258873-50-5	9
4	Decanoic acid, 10,10'-diselenodi-	502	C20H38O4Se2	022686-34-6	4
5	5-(2,5-Difluorophenyl)-[1,2,5]ox...	234	C10H4F2N4O	1000487-13-4	4





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Misc :
ALS Vial : 7 Sample Multiplier: 1

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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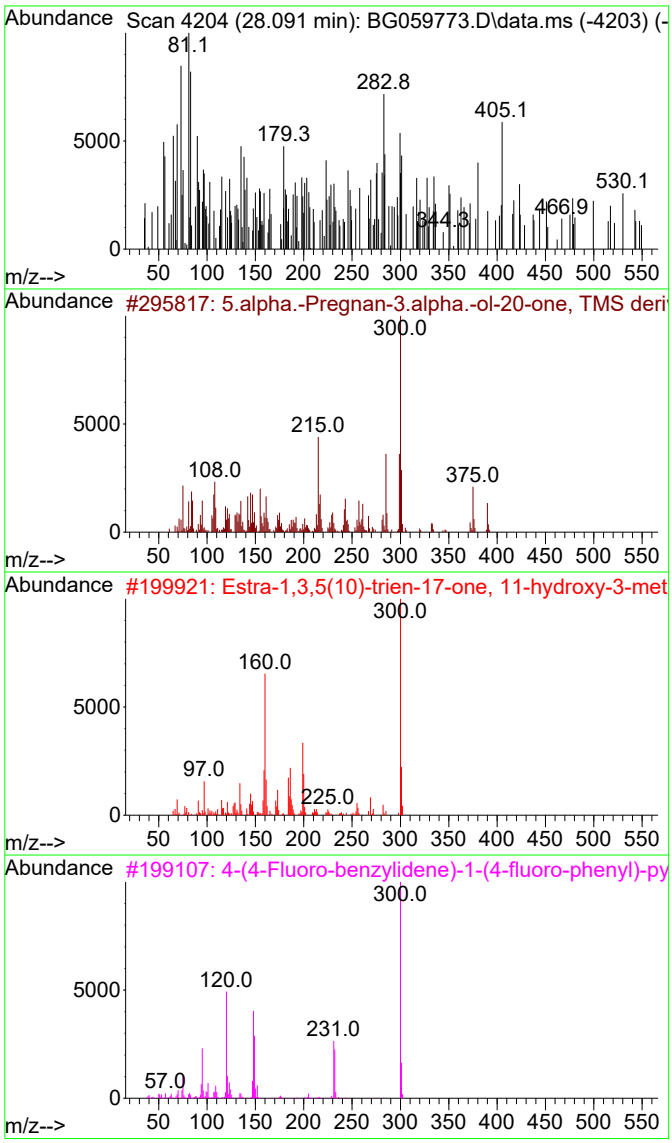
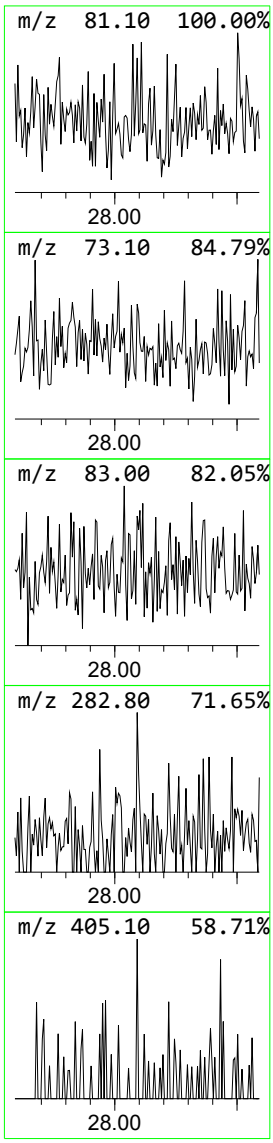
Peak Number 5 unknown28.091 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.091	2.32 ng	40606	Perylene-d12	25.612

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5.alpha.-Pregnan-3.alpha.-ol-20-...	390	C24H42O2Si	018880-80-3	14
2	Estra-1,3,5(10)-trien-17-one, 11...	300	C19H24O3	005210-12-8	14
3	4-(4-Fluoro-benzylidene)-1-(4-fl...	300	C16H10F2N2O2	343354-99-4	11
4	2-(6-Ethoxy-2-methylimino-4H-1-t...	317	C16H19N3O2S	1000311-55-1	11
5	Trimethylsilyl 6-bromopyrazolo[1...	313	C10H12BrN3O2Si	1000474-11-1	11





Tentatively Identified Compound (LSC) summary

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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
unknown18.526	18.526	8.0	ng	234788	4	17.709	587046	20.0
unknown18.567	18.567	2.8	ng	81133	4	17.709	587046	20.0
Anthracene, 1-m...	18.626	2.9	ng	85169	4	17.709	587046	20.0
unknown21.569	21.569	4.0	ng	119322	5	22.040	591919	20.0
unknown28.091	28.091	2.3	ng	40606	6	25.612	349818	20.0