LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
Data File : BG059852.D
Acq On : 23 Nov 2023 14:40
Operator : MA/JU
Sample : 05485-01
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-14-STOCKPILE-BIN-5

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: BG059852.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.367	331	337	343	rBV2	52544	89653	2.40%	0.513%
2	5.831	409	416	423	rBV	608839	953795	25.54%	5.458%
3	7.459	686	693	702	rBV	781784	1330944	35.64%	7.616%
4	8.334	834	842	850	rBV2	177243	303995	8.14%	1.740%
5	9.533	1040	1046	1055	rVB2	624896	1106469	29.63%	6.332%
6	11.184	1321	1327	1335	rBV	227767	420671	11.26%	2.407%
7	12.811	1599	1604	1609	rBV2	36108	58044	1.55%	0.332%
8	13.023	1633	1640	1645	rBV5	29841	57266	1.53%	0.328%
9	13.587	1729	1736	1743	rBV	2137899	3171075	84.91%	18.146%
10	14.274	1847	1853	1859	rBV5	43981	77496	2.08%	0.443%
11	14.327	1859	1862	1868	rVB5	22022	42971	1.15%	0.246%
12	14.962	1964	1970	1976	rBV2	363618	568386	15.22%	3.253%
13	15.561	2065	2072	2075	rBV6	21042	42083	1.13%	0.241%
14	16.008	2144	2148	2156	rVB3	37697	71390	1.91%	0.409%
15	16.448	2216	2223	2230	rBV	1599172	2367373	63.39%	13.547%
16	17.535	2405	2408	2414	rVB7	25859	44455	1.19%	0.254%
17	17.717	2433	2439	2443	rBV	429239	687206	18.40%	3.933%
18	17.759	2443	2446	2452	rVB2	146258	211725	5.67%	1.212%
19	18.299	2533	2538	2541	rBV7	36954	57140	1.53%	0.327%
20	18.528	2573	2577	2581	rBV3	119476	150905	4.04%	0.864%
21	18.581	2583	2586	2590	rVV2	59122	91815	2.46%	0.525%
22	18.628	2591	2594	2597	rVB2	67208	87738	2.35%	0.502%
23	18.775	2614	2619	2622	rBV7	47379	95072	2.55%	0.544%
24	19.186	2686	2689	2692	rBV5	27984	40702	1.09%	0.233%
25	19.351	2715	2717	2722	rVB6	35769	37416	1.00%	0.214%
26	19.480	2735	2739	2741	rBV4	40605	50341	1.35%	0.288%
27	19.750	2781	2785	2789	rVB	180676	222010	5.94%	1.270%
28	20.115	2843	2847	2853	rVB	185663	268234	7.18%	1.535%
29	20.291	2872	2877	2882	rBV	3078040	3734623	100.00%	21.371%
30	22.048	3169	3176	3180	rVB2	307411	578232	15.48%	3.309%
31	25.638	3781	3787	3795	rVB3	176350	455647	12.20%	2.607%

Sum of corrected areas: 17474872

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
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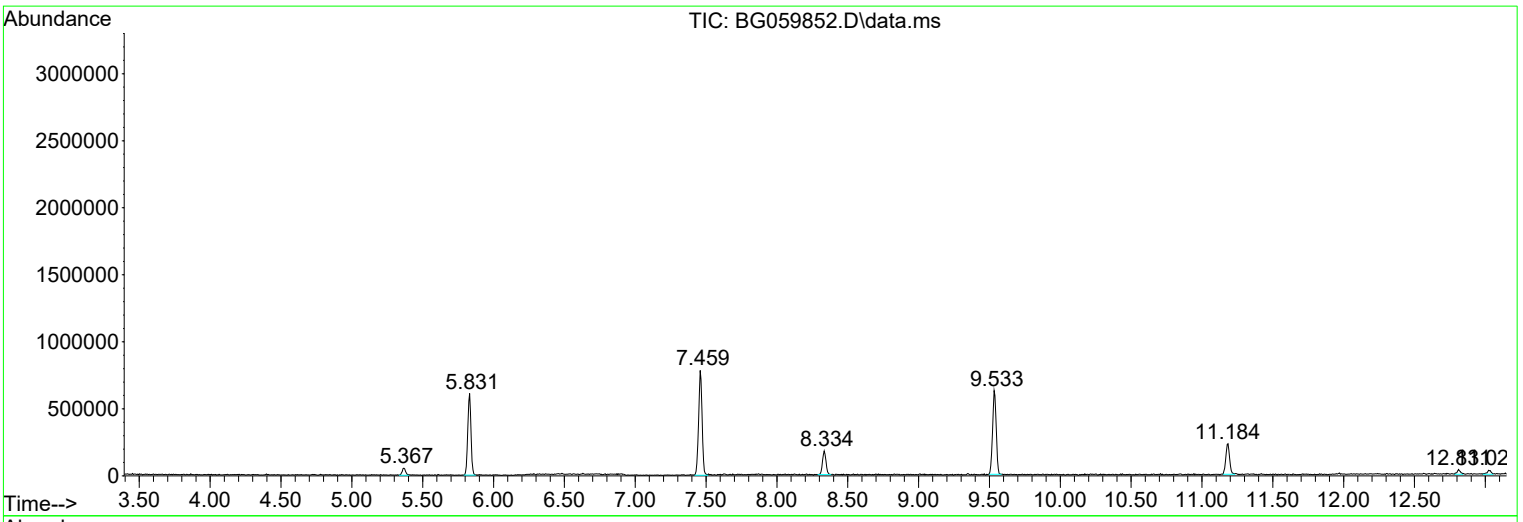
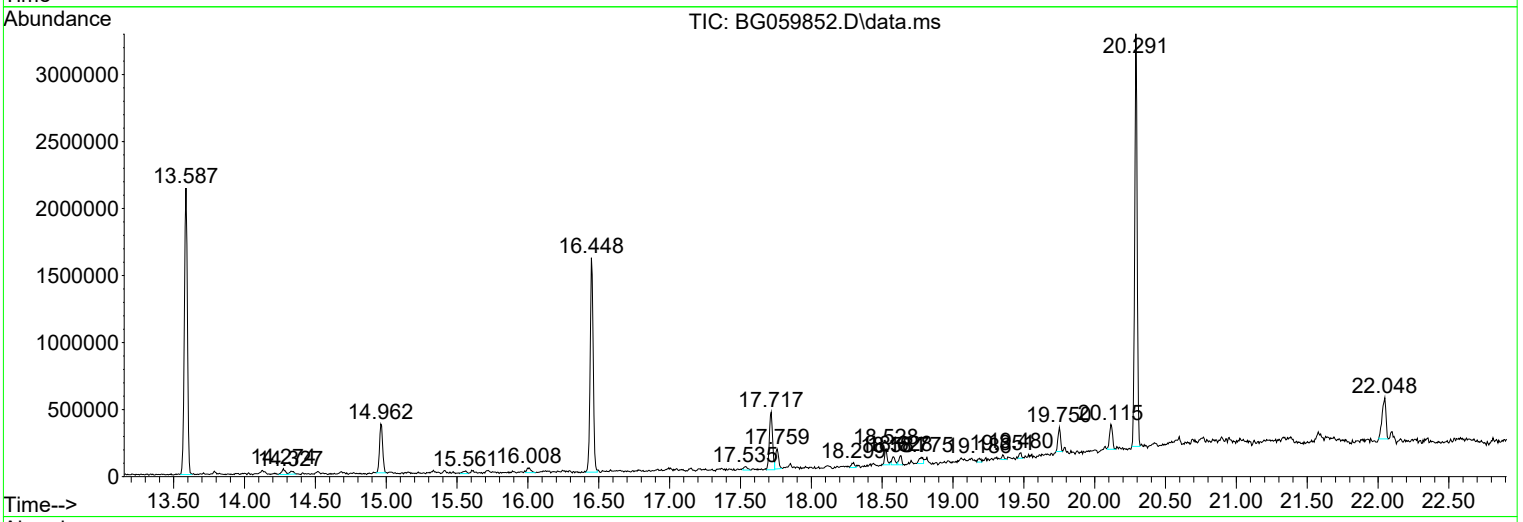
Misc :
ALS Vial : 34 Sample Multiplier: 1

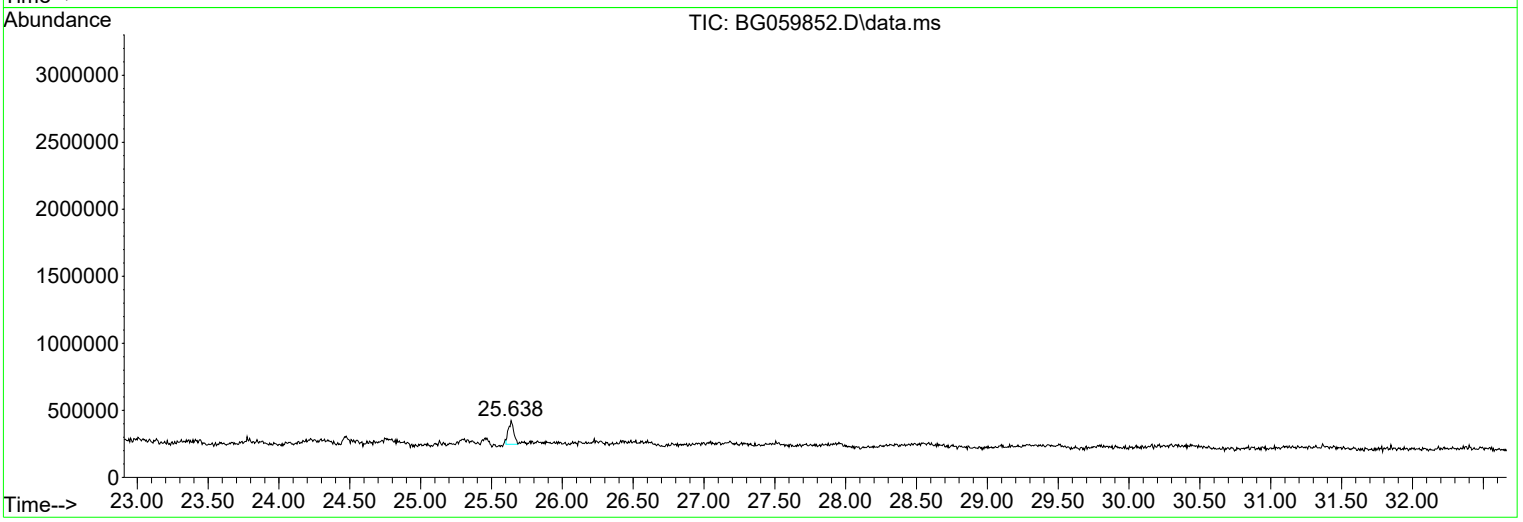
Instrument :
BNA_G
ClientSampleId :
AU-14-STOCKPILE-BIN-5

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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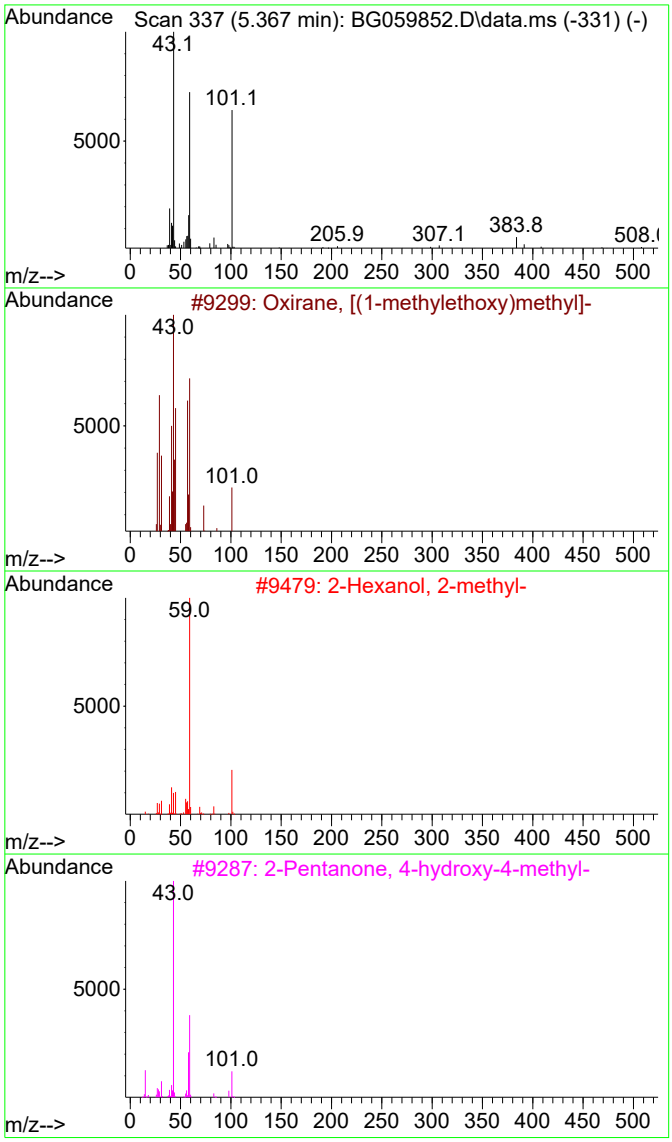
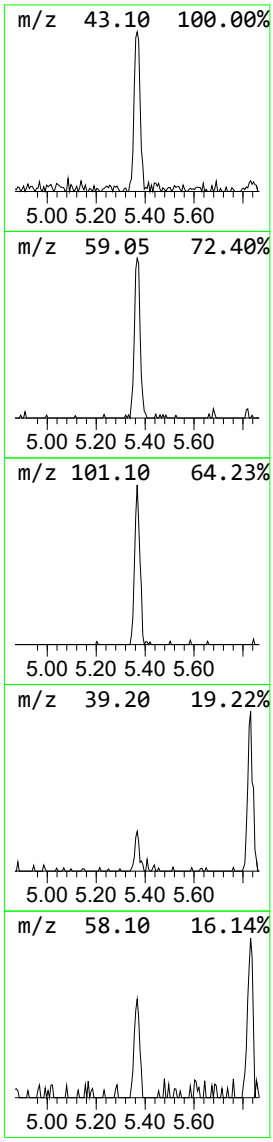
****
Peak Number 1 Oxirane, [(1-methylethoxy)m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.367	5.90 ng	89653	1,4-Dichlorobenzene-d4	8.334

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	45
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
4	2-Pentanol, 2,3-dimethyl-	116	C7H16O	004911-70-0	45
5	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	27





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Sample : 05485-01
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ALS Vial : 34 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
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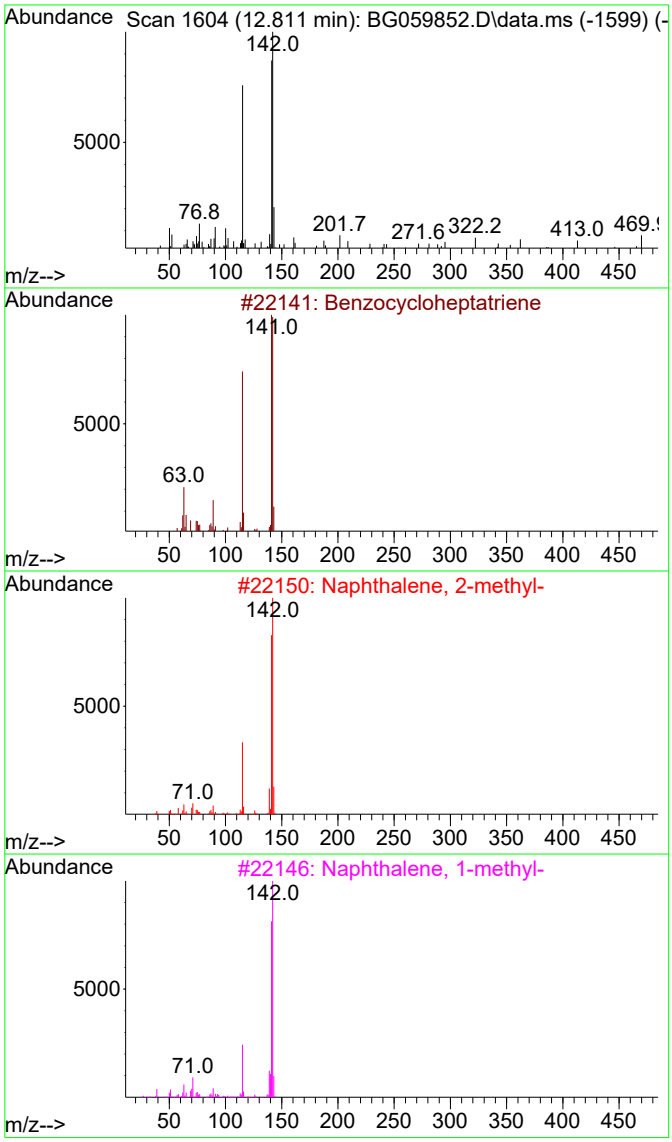
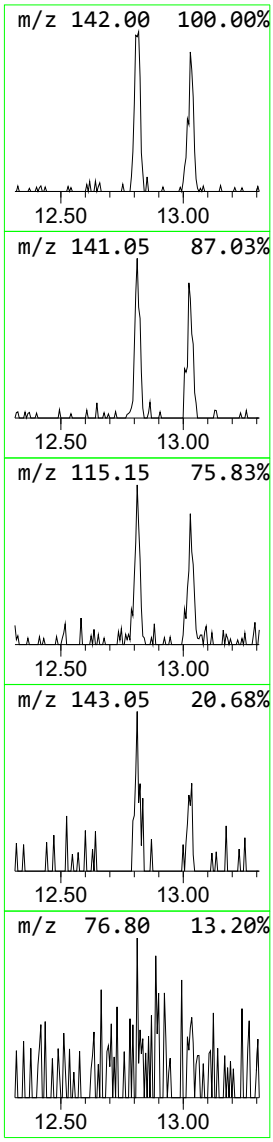
****

Peak Number 2 Benzocycloheptatriene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.811	2.76 ng	58044	Naphthalene-d8	11.178

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzocycloheptatriene	142	C11H10	000264-09-5	87
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	83
3	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	83
4	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	80
5	Benzaldehyde, 3-methoxy-4-(1-nap...	292	C19H16O3	1000338-37-2	22





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Acq On : 23 Nov 2023 14:40
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Sample : 05485-01
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-14-STOCKPILE-BIN-5

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

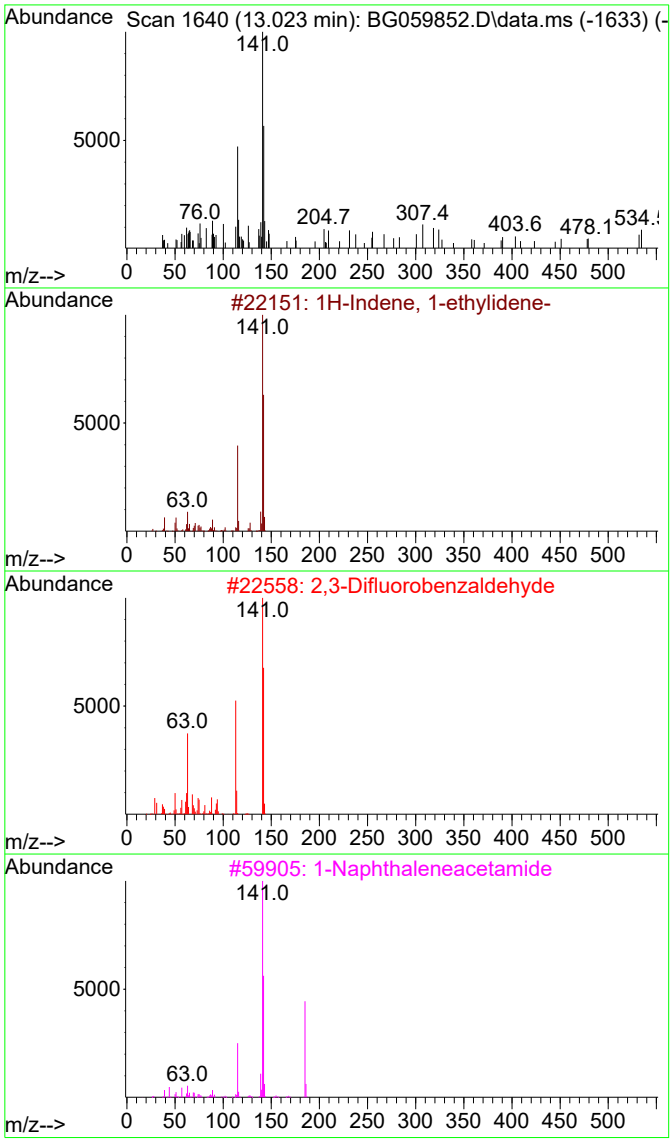
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

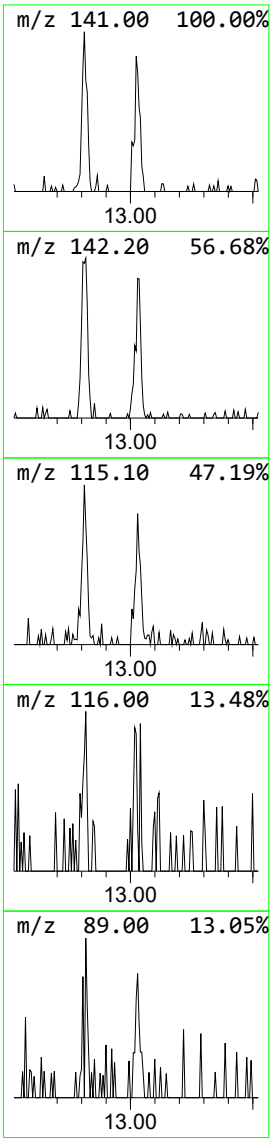
****

Peak Number 3 1H-Indene, 1-ethylidene- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.023	2.72 ng	57266	Naphthalene-d8	11.178

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	53
2	2,3-Difluorobenzaldehyde	142	C7H4F2O	002646-91-5	47
3	1-Naphthaleneacetamide	185	C12H11NO	000086-86-2	47
4	3,5-Difluorobenzaldehyde	142	C7H4F2O	032085-88-4	47
5	4-(2,4-Difluorobenzoyl)-3-phenyl...	301	C16H9F2NO3	1000434-45-5	47





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Data File : BG059852.D
Acq On : 23 Nov 2023 14:40
Operator : MA/JU
Sample : 05485-01
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-14-STOCKPILE-BIN-5

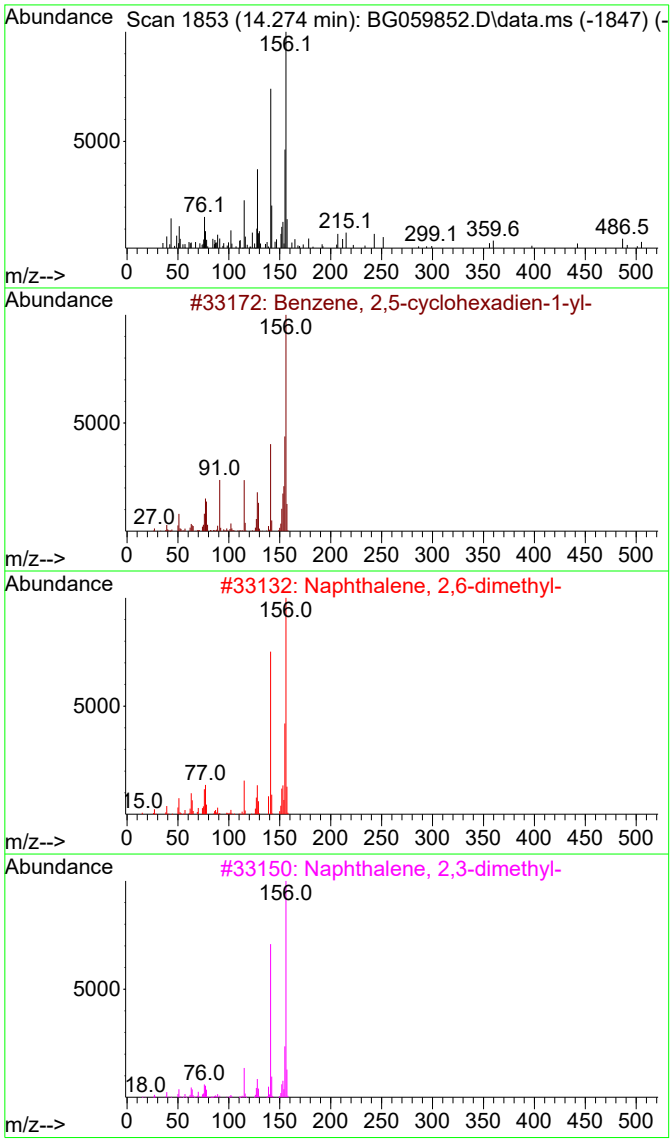
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

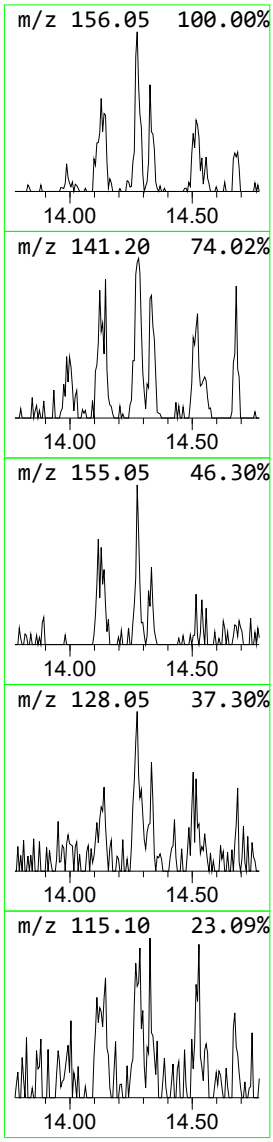
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 2,5-cyclohexadien-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.274	2.73 ng	77496	Acenaphthene-d10	14.962

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2,5-cyclohexadien-1-yl-	156	C12H12	004794-05-2	83
2	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	81
3	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	76
4	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	74
5	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
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ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-14-STOCKPILE-BIN-5

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

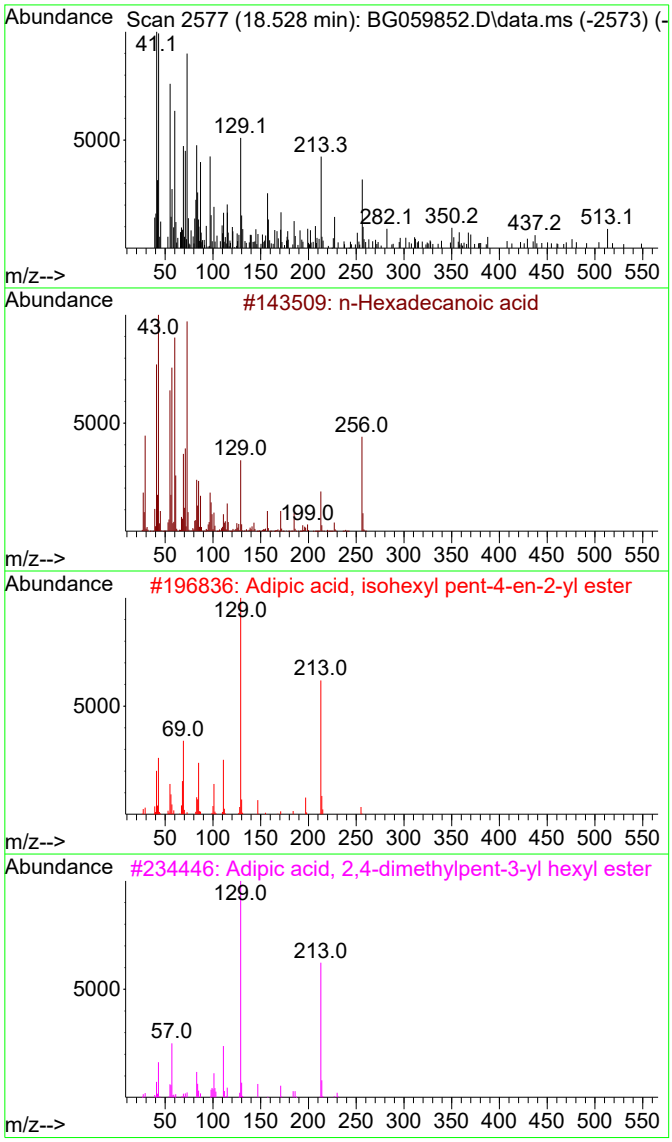
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

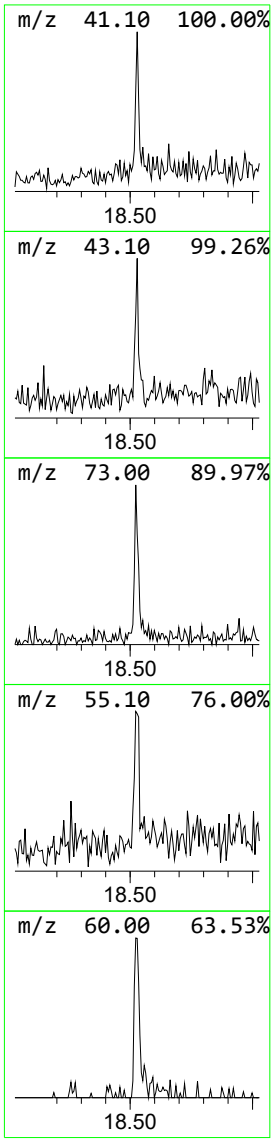
****

Peak Number 6 unknown18.528 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.528	4.39 ng	150905	Phenanthrene-d10	17.717

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	27
2	Adipic acid, isohexyl pent-4-en-...	298	C17H30O4	1000354-12-1	22
3	Adipic acid, 2,4-dimethylpent-3-...	328	C19H36O4	1000353-52-3	22
4	Adipic acid, 2-hexyl isohexyl ester	314	C18H34O4	1000353-71-2	22
5	Adipic acid, 3,3-dimethylbut-2-y...	314	C18H34O4	1000353-67-1	22





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BNA_G
ClientSampleId :
AU-14-STOCKPILE-BIN-5

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

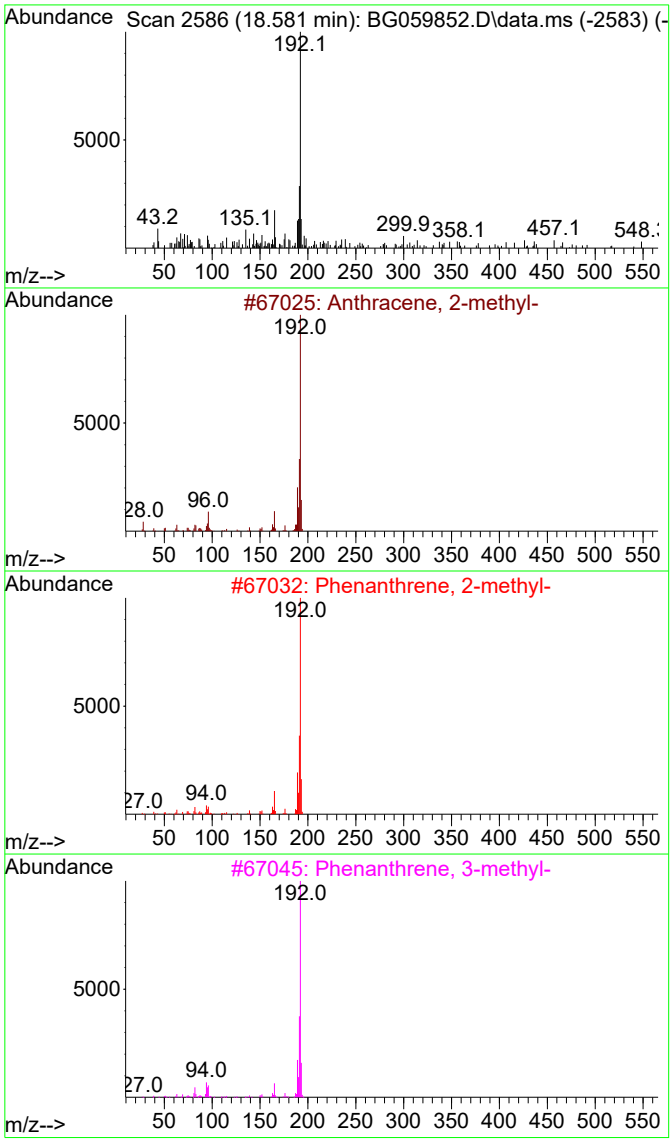
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

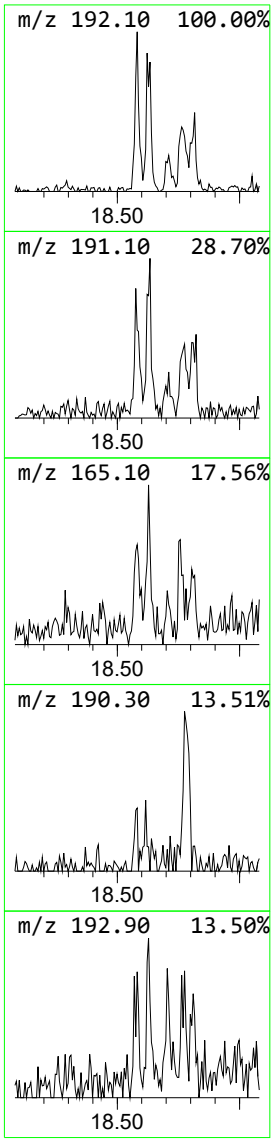
****

Peak Number 7 Anthracene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.581	2.67 ng	91815	Phenanthrene-d10	17.717

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	76
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	76
3	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	68
4	3,4-Methylenedioxycinnamic acid	192	C10H8O4	002373-80-0	64
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	64





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Operator : MA/JU
Sample : 05485-01
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-14-STOCKPILE-BIN-5

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

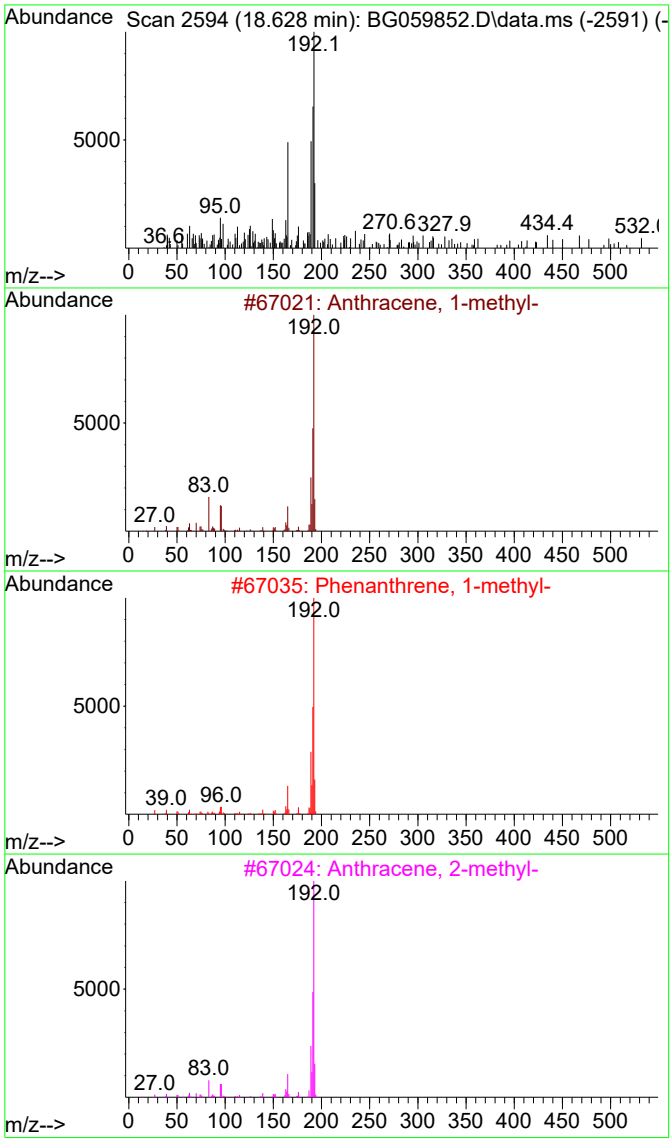
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

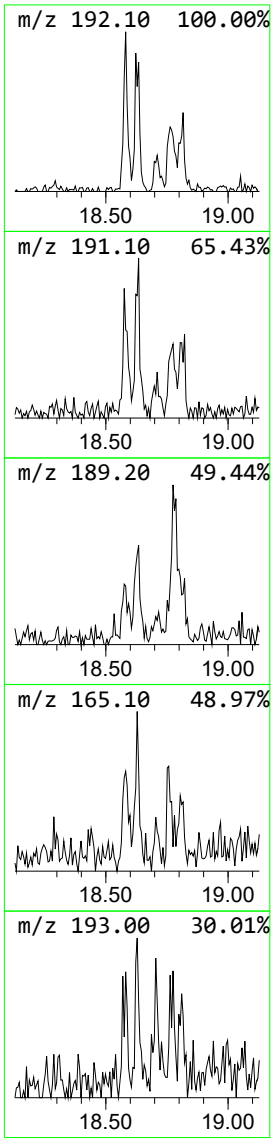
****

Peak Number 8 Anthracene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.628	2.55 ng	87738	Phenanthrene-d10	17.717

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	70
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	70
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	70
4	Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	62
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	62





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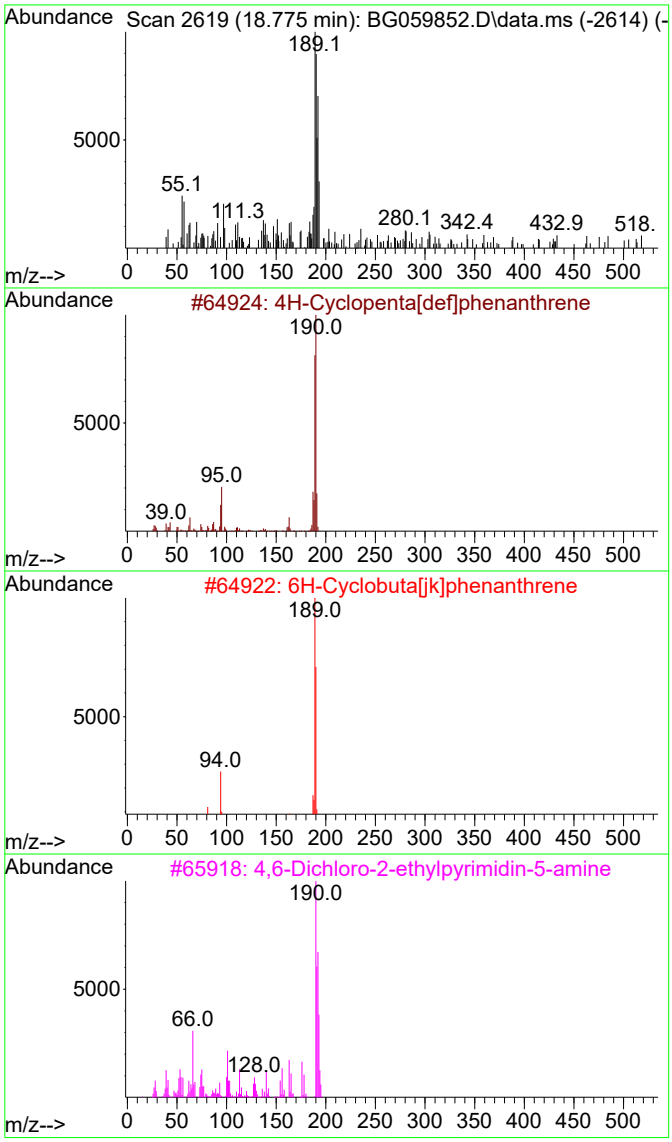
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

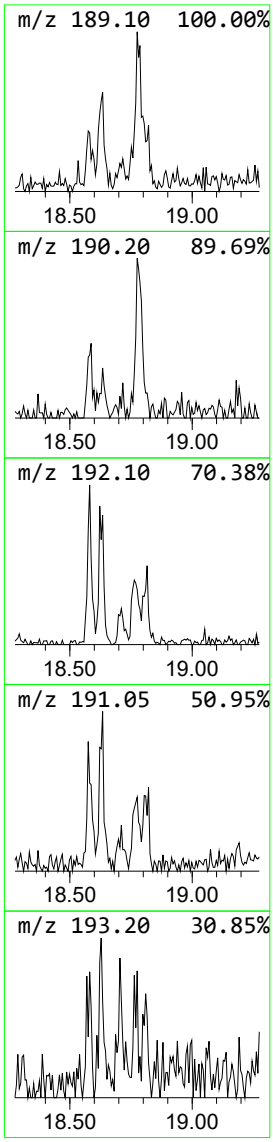
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.775	2.77 ng	95072	Phenanthrene-d10	17.717

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	50
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	47
3	4,6-Dichloro-2-ethylpyrimidin-5-...	191	C6H7Cl2N3	006237-96-3	38
4	2-Amino-4,6-dichloropyrimidine-5...	191	C5H3Cl2N3O	005604-46-6	35
5	2-Bromo-5-fluorophenol	190	C6H4BrFO	147460-41-1	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
Data File : BG059852.D
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Operator : MA/JU
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Misc :
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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
Oxirane, [(1-me...	5.367	5.9	ng	89653	1	8.334	303995	20.0
Benzocyclohepta...	12.811	2.8	ng	58044	2	11.178	420671	20.0
1H-Indene, 1-et...	13.023	2.7	ng	57266	2	11.178	420671	20.0
Benzene, 2,5-cy...	14.274	2.7	ng	77496	3	14.962	568386	20.0
unknown18.528	18.528	4.4	ng	150905	4	17.717	687206	20.0
Anthracene, 2-m...	18.581	2.7	ng	91815	4	17.717	687206	20.0
Anthracene, 1-m...	18.628	2.5	ng	87738	4	17.717	687206	20.0
4H-Cyclopenta[d...	18.775	2.8	ng	95072	4	17.717	687206	20.0