LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG021323\
Data File : BG056626.D
Acq On : 13 Feb 2023 19:28
Operator : CG/JU
Sample : 01529-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-06-0-2.0

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-BG012723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056626.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.240	326	332	343	rVB	69265	119264	8.32%	0.916%
2	5.739	410	417	429	rBV	293361	509514	35.54%	3.914%
3	7.372	685	695	707	rBV	302594	532179	37.12%	4.088%
4	8.213	831	838	845	rBV	133985	225501	15.73%	1.732%
5	9.388	1030	1038	1049	rBB	187491	340757	23.77%	2.618%
6	10.980	1303	1309	1312	rBV2	10262	15812	1.10%	0.121%
7	11.045	1312	1320	1326	rVV	170195	310469	21.66%	2.385%
8	12.220	1513	1520	1526	rBV3	9481	15615	1.09%	0.120%
9	12.408	1547	1552	1557	rBV2	17482	27010	1.88%	0.207%
10	12.684	1593	1599	1604	rVB2	14243	24610	1.72%	0.189%
11	12.907	1630	1637	1644	rVB7	12260	29742	2.07%	0.228%
12	13.459	1724	1731	1738	rBV	665936	1041060	72.62%	7.998%
13	13.630	1754	1760	1765	rVB4	21024	33052	2.31%	0.254%
14	13.777	1778	1785	1790	rBV8	9983	17664	1.23%	0.136%
15	14.012	1818	1825	1826	rBV5	11201	20548	1.43%	0.158%
16	14.159	1845	1850	1854	rBV3	17986	32841	2.29%	0.252%
17	14.211	1854	1859	1862	rVB2	13046	19617	1.37%	0.151%
18	14.282	1868	1871	1875	rVB4	14881	20461	1.43%	0.157%
19	14.400	1886	1891	1894	rBV6	12164	18874	1.32%	0.145%
20	14.570	1914	1920	1926	rBV4	14613	31872	2.22%	0.245%
21	14.693	1938	1941	1945	rVB2	17435	20425	1.42%	0.157%
22	14.840	1957	1966	1972	rBV	291609	447694	31.23%	3.439%
23	14.905	1972	1977	1985	rVB2	28308	44988	3.14%	0.346%
24	15.034	1994	1999	2000	rBV4	10618	14751	1.03%	0.113%
25	15.228	2027	2032	2038	rVB2	23540	43165	3.01%	0.332%
26	15.304	2041	2045	2054	rVB4	15761	26602	1.86%	0.204%
27	15.445	2063	2069	2074	rBV5	14893	30128	2.10%	0.231%
28	15.498	2075	2078	2082	rVB3	10212	15055	1.05%	0.116%
29	15.639	2090	2102	2110	rBV6	23455	57988	4.04%	0.445%
30	15.880	2137	2143	2148	rBV3	26425	51273	3.58%	0.394%
31	16.039	2167	2170	2174	rVB4	17737	23848	1.66%	0.183%
32	16.180	2189	2194	2199	rVB	54355	80030	5.58%	0.615%
33	16.327	2212	2219	2226	rBV	411262	655527	45.72%	5.036%
34	16.521	2244	2252	2258	rBV3	25320	61852	4.31%	0.475%
35	16.932	2319	2322	2327	rBV5	11296	17610	1.23%	0.135%
36	17.231	2369	2373	2378	rVB3	18931	33798	2.36%	0.260%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG021323\
Data File : BG056626.D
Acq On : 13 Feb 2023 19:28
Operator : CG/JU
Sample : 01529-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

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-BG012723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.290	2380	2383	2386	rVV5	17361	26538	1.85%	0.204%
38	17.337	2389	2391	2394	rVV4	16332	18970	1.32%	0.146%
39	17.402	2397	2402	2406	rVB	20920	32083	2.24%	0.246%
40	17.578	2426	2432	2436	rBV	348749	547468	38.19%	4.206%
41	17.619	2436	2439	2445	rVB	382458	522678	36.46%	4.015%
42	17.713	2450	2455	2461	rBV	84388	124535	8.69%	0.957%
43	17.978	2497	2500	2505	rVV	34908	50490	3.52%	0.388%
44	18.025	2506	2508	2513	rVB4	19585	22107	1.54%	0.170%
45	18.448	2574	2580	2584	rBV2	62568	126701	8.84%	0.973%
46	18.495	2585	2588	2593	rVB	87031	122248	8.53%	0.939%
47	18.647	2608	2614	2617	rBV2	79082	161161	11.24%	1.238%
48	18.935	2659	2663	2668	rBV	52492	77516	5.41%	0.596%
49	18.988	2669	2672	2680	rVB2	43431	68210	4.76%	0.524%
50	19.617	2774	2779	2784	rBV	875276	1236159	86.22%	9.497%
51	19.946	2830	2835	2837	rBV2	146983	258795	18.05%	1.988%
52	19.981	2837	2841	2847	rVB	815327	1129430	78.78%	8.677%
53	20.040	2848	2851	2855	rBV	49942	76462	5.33%	0.587%
54	20.157	2866	2871	2877	rVB	1131419	1433655	100.00%	11.014%
55	20.563	2937	2940	2943	rBV	61220	70468	4.92%	0.541%
56	21.844	3153	3158	3165	rBV4	500655	1335629	93.16%	10.261%
57	21.908	3166	3169	3175	rVB	370377	564427	39.37%	4.336%

Sum of corrected areas: 13016926

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG021323\
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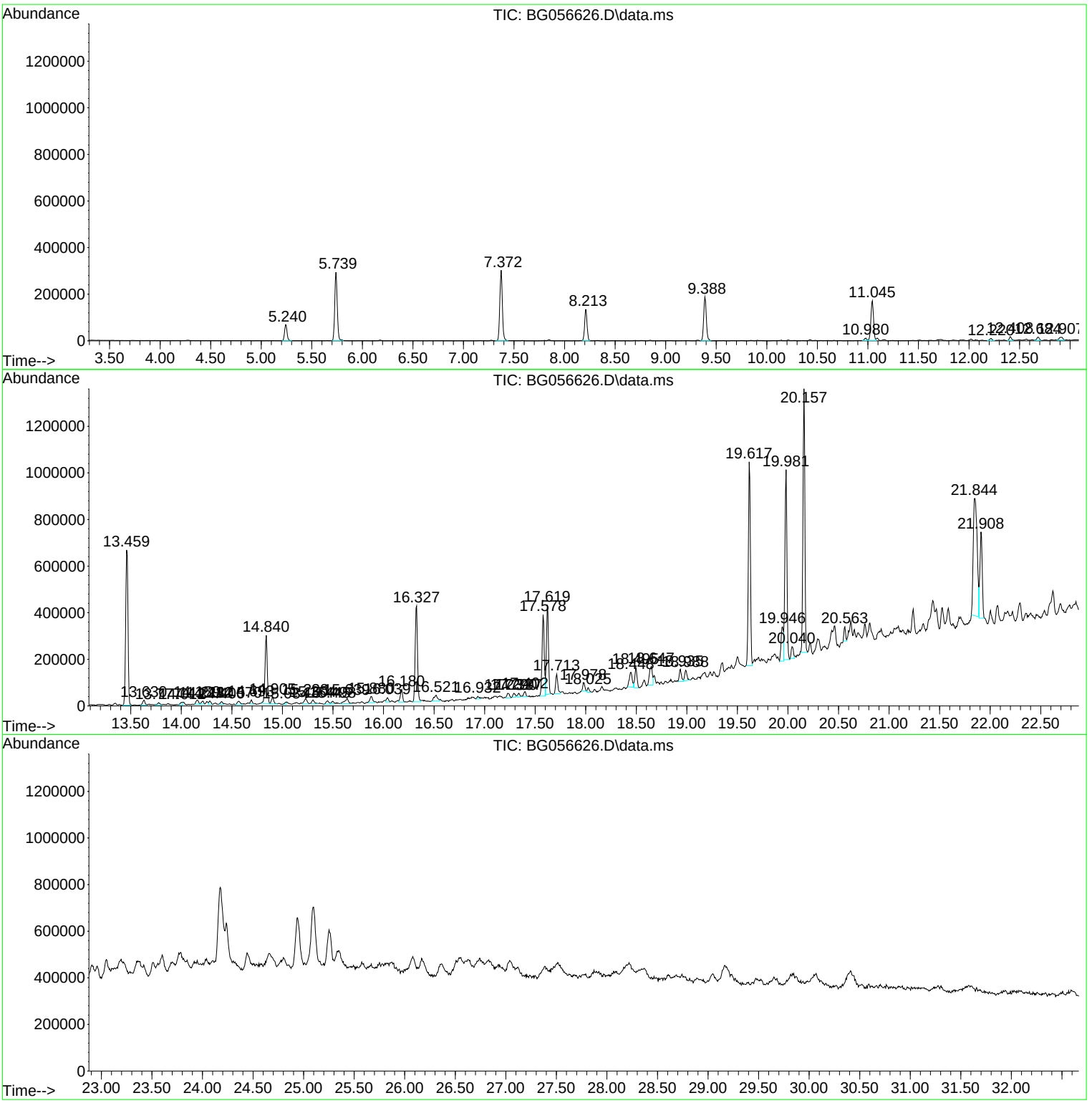
Acq On : 13 Feb 2023 19:28
Operator : CG/JU
Sample : 01529-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.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\BG021323\
Data File : BG056626.D
Acq On : 13 Feb 2023 19:28
Operator : CG/JU
Sample : 01529-01
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Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

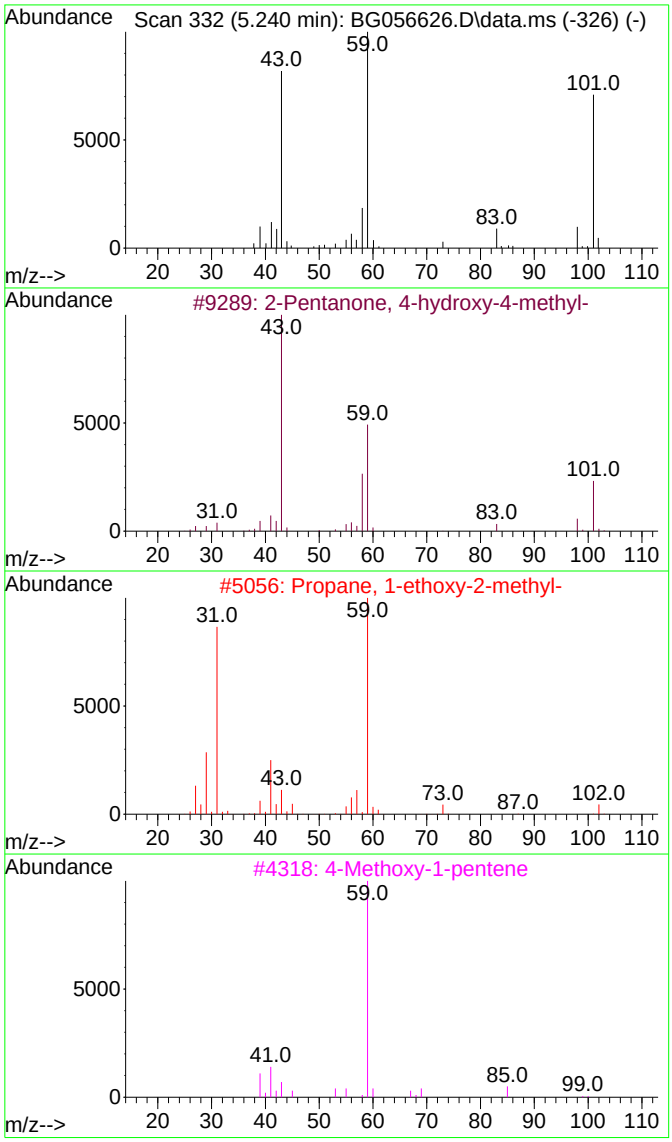
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

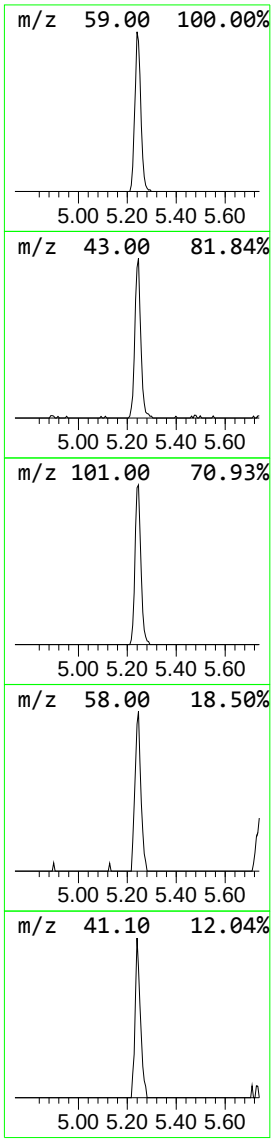
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.240	10.58 ng	119264	1,4-Dichlorobenzene-d4	8.207

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	38
3	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	38
4	Guanidine	59	CH5N3	000113-00-8	28
5	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG021323\
Data File : BG056626.D
Acq On : 13 Feb 2023 19:28
Operator : CG/JU
Sample : 01529-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

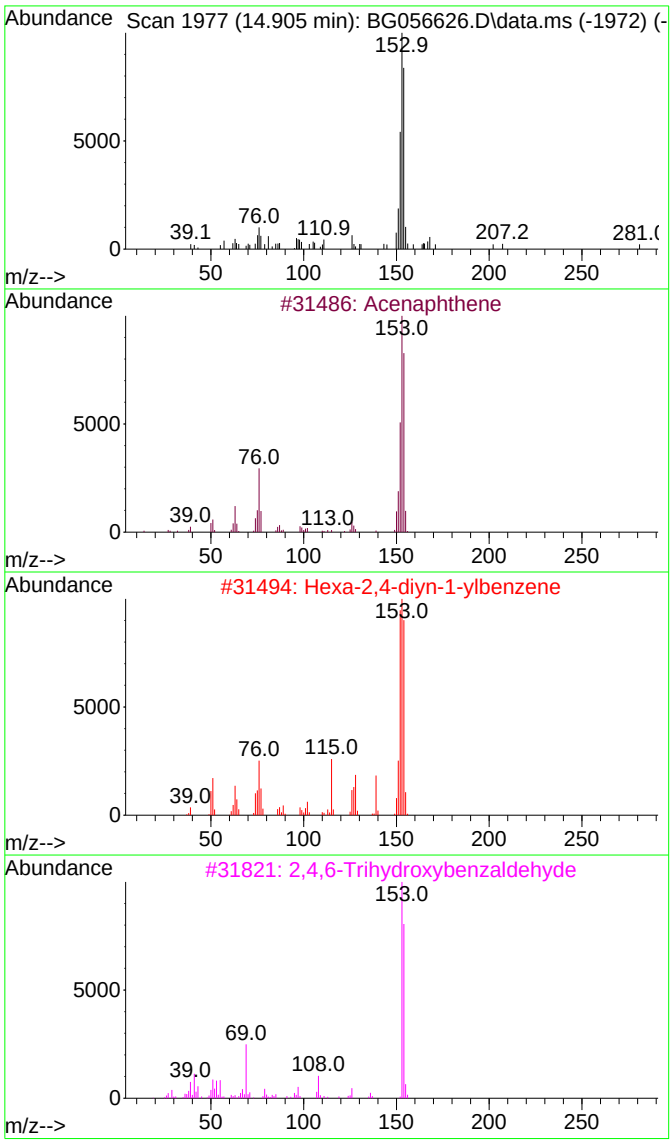
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

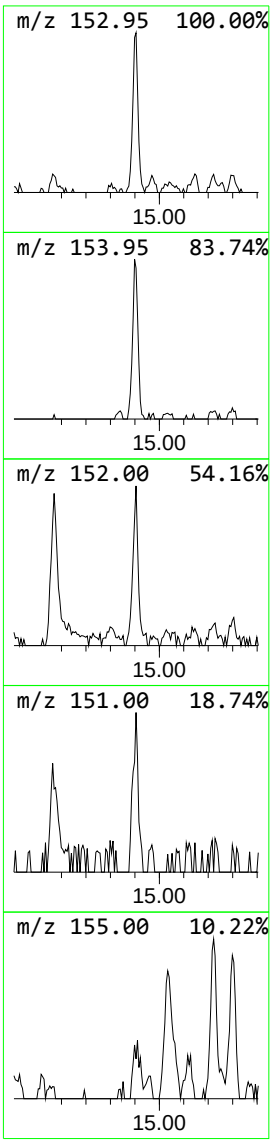
****

Peak Number 2 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.905	2.01 ng	44988	Acenaphthene-d10	14.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene	154	C12H10	000083-32-9	62
2	Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	53
3	2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	52
4	3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50
5	5,10-Methanobenzocycloocten-11-o...	216	C13H9ClO	033655-73-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG021323\
Data File : BG056626.D
Acq On : 13 Feb 2023 19:28
Operator : CG/JU
Sample : 01529-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

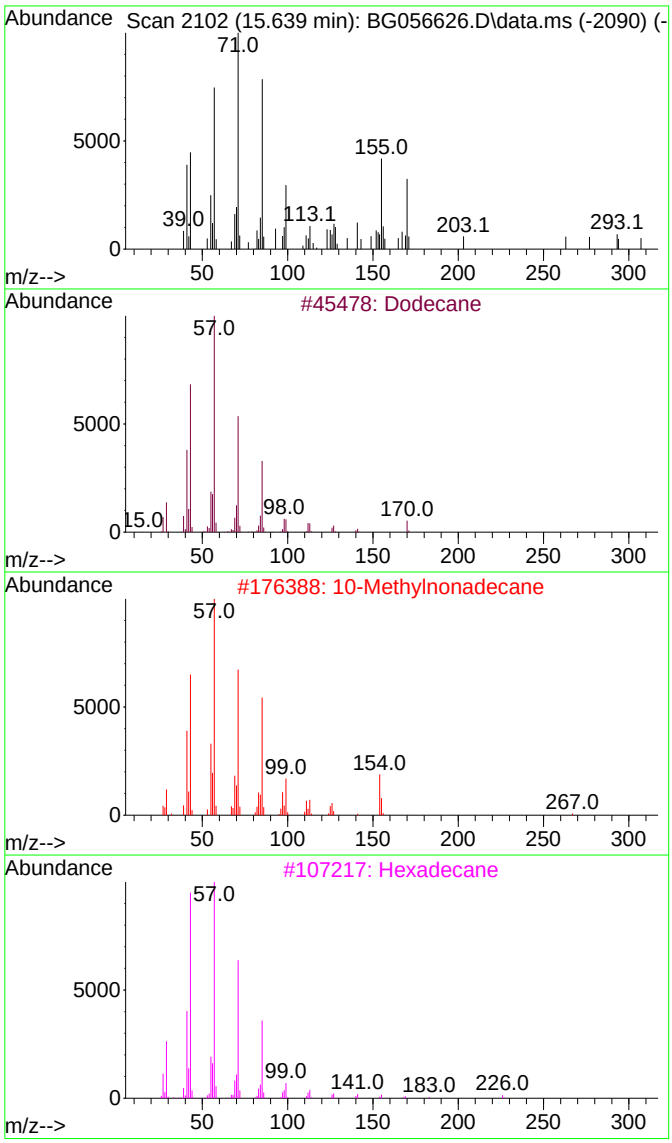
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

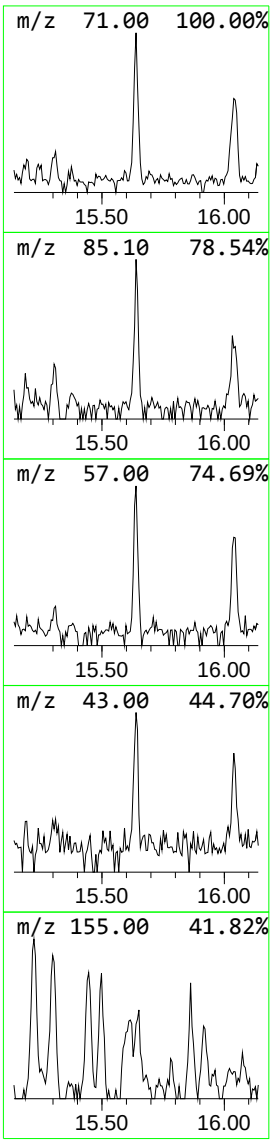
****

Peak Number 3 Dodecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.639	2.59 ng	57988	Acenaphthene-d10	14.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	58
2	10-Methylnonadecane	282	C20H42	056862-62-5	53
3	Hexadecane	226	C16H34	000544-76-3	50
4	Heptadecane	240	C17H36	000629-78-7	50
5	Octacosane	394	C28H58	000630-02-4	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG021323\
Data File : BG056626.D
Acq On : 13 Feb 2023 19:28
Operator : CG/JU
Sample : 01529-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

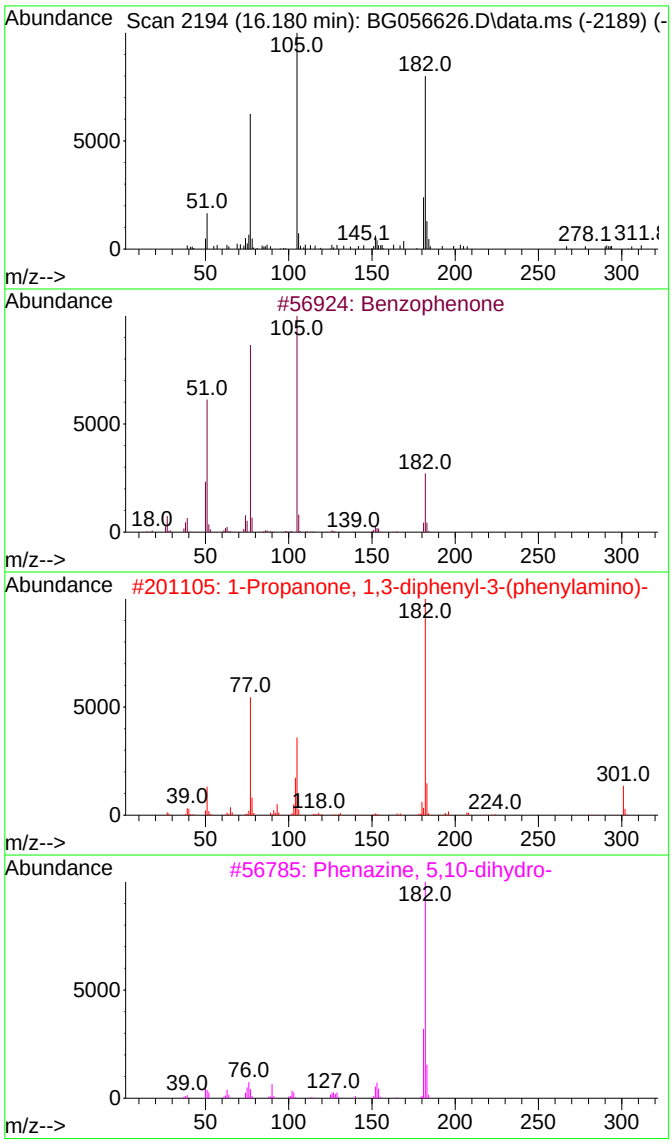
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

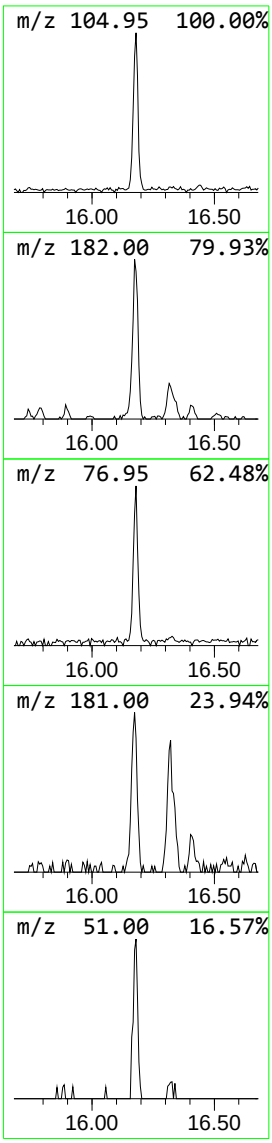
****

Peak Number 5 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.180	3.58 ng	80030	Acenaphthene-d10	14.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	87
2	1-Propanone, 1,3-diphenyl-3-(phe...	301	C21H19NO	000742-43-8	59
3	Phenazine, 5,10-dihydro-	182	C12H10N2	000613-32-1	49
4	Methanimidamide, N'-(4-chlorophe...	182	C9H11ClN2	002103-46-0	47
5	9H-Pyrido[3,4-b]indole, 1-methyl-	182	C12H10N2	000486-84-0	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG021323\
Data File : BG056626.D
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Operator : CG/JU
Sample : 01529-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

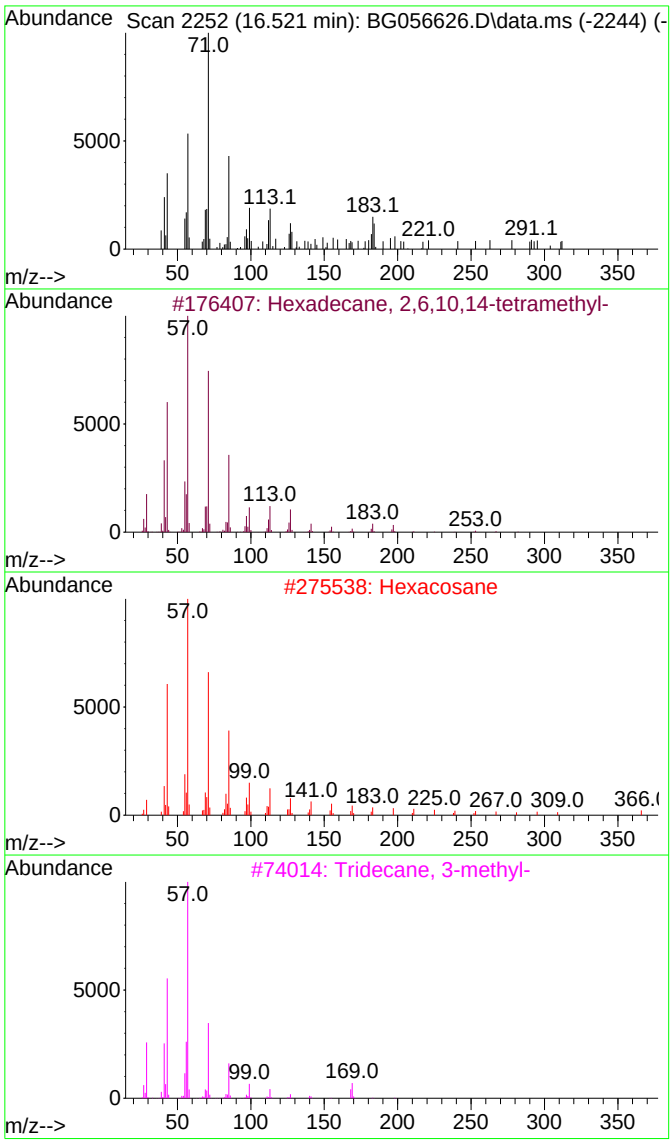
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

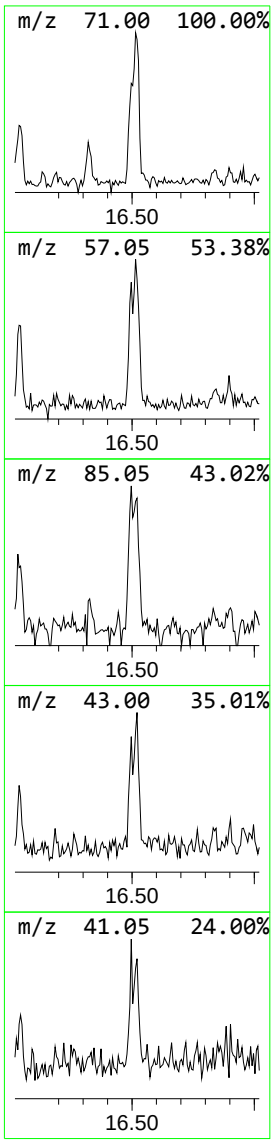
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Hexadecane, 2,6,10,14-tetra... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.521	2.26 ng	61852	Phenanthrene-d10	17.578

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	64
2	Hexacosane	366	C26H54	000630-01-3	64
3	Tridecane, 3-methyl-	198	C14H30	006418-41-3	59
4	Dodecane, 3-methyl-	184	C13H28	017312-57-1	46
5	Bicyclo[3.1.1]heptan-3-one, 2-hy...	168	C10H16O2	010136-65-9	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG021323\
Data File : BG056626.D
Acq On : 13 Feb 2023 19:28
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Sample : 01529-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

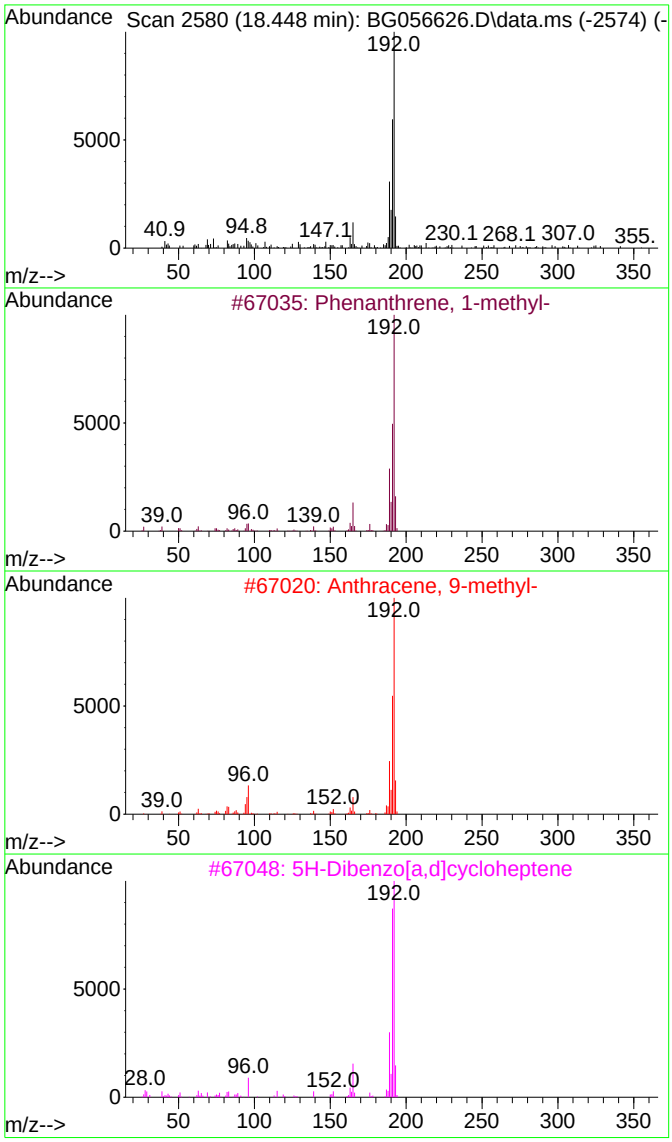
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

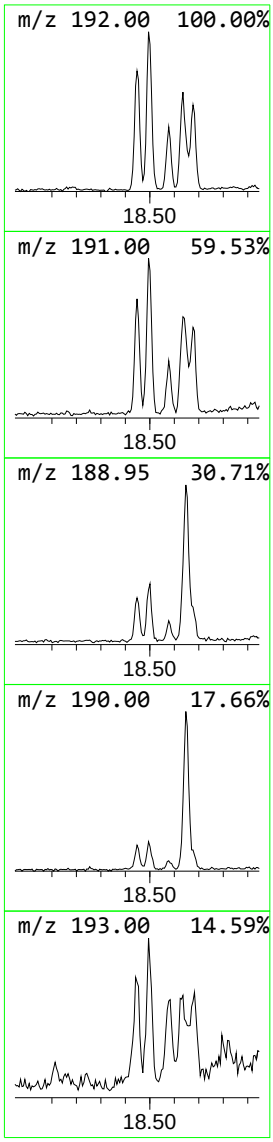
****

Peak Number 7 Phenanthrene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.448	4.63 ng	126701	Phenanthrene-d10	17.578

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	92
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
3	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	90
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	86
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG021323\
Data File : BG056626.D
Acq On : 13 Feb 2023 19:28
Operator : CG/JU
Sample : 01529-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

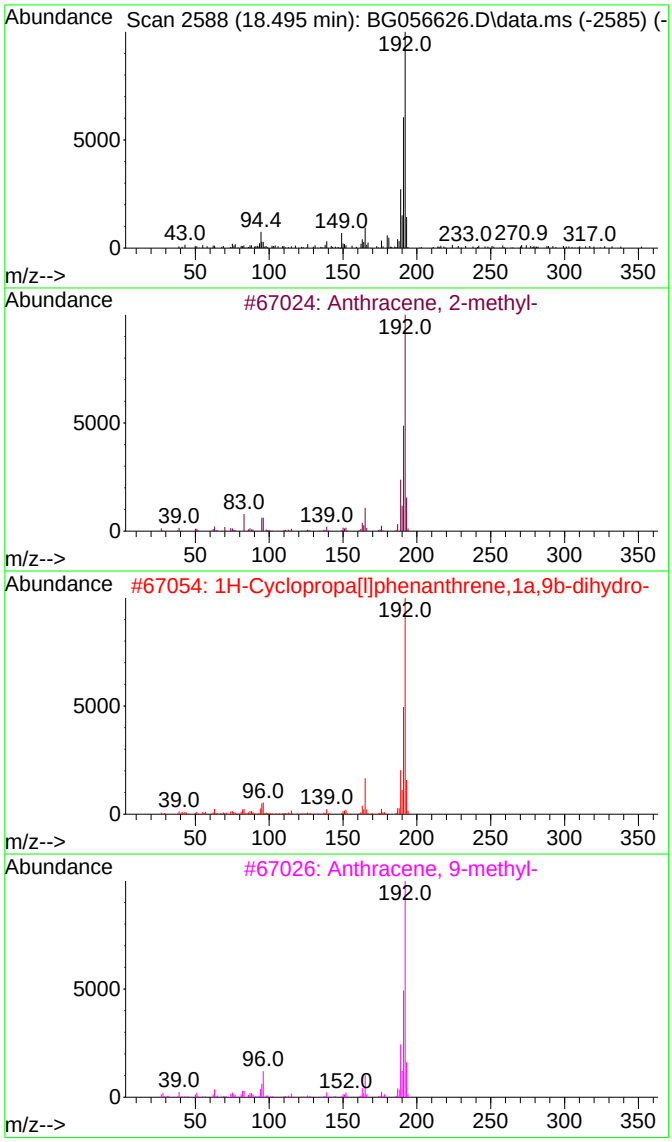
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

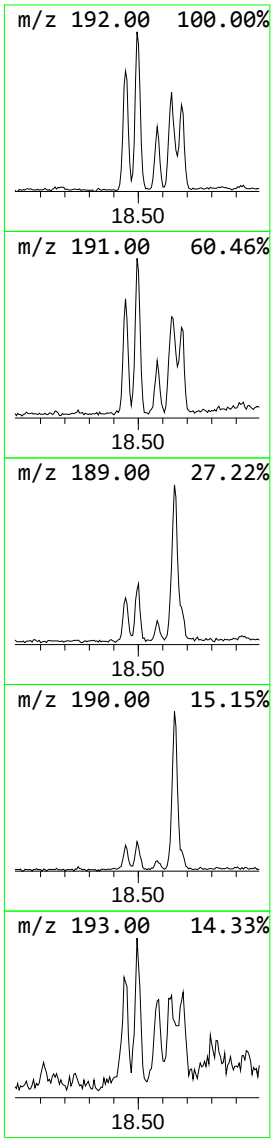
****

Peak Number 8 Anthracene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.495	4.47 ng	122248	Phenanthrene-d10	17.578

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	90
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	81
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	81
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	81
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG021323\
Data File : BG056626.D
Acq On : 13 Feb 2023 19:28
Operator : CG/JU
Sample : 01529-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

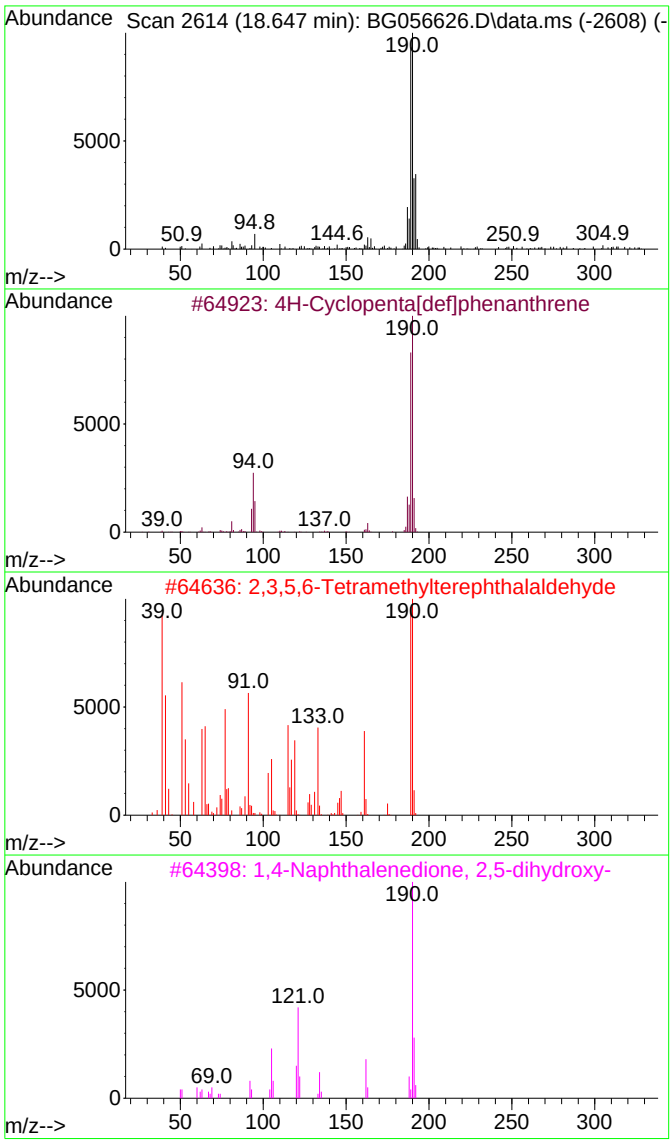
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

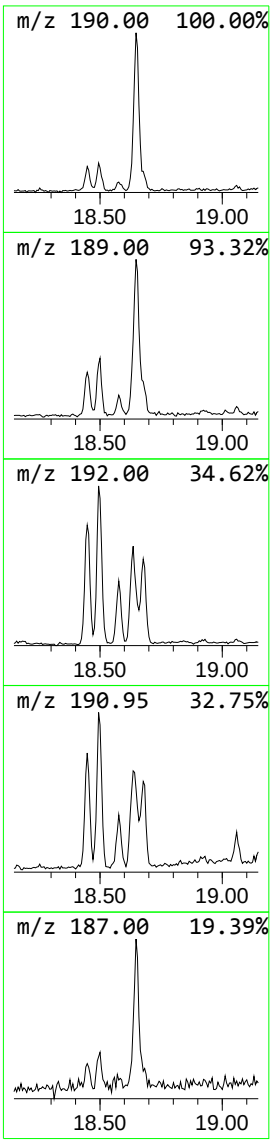
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 4H-Cyclopenta[def]phenanthrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.647	5.89 ng	161161	Phenanthrene-d10	17.578

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	38
3	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	32
4	Pyrimidine, 2-chloro-5-phenyl-	190	C10H7ClN2	022536-62-5	25
5	1-(Phenylethynyl)-1H-1,2,3-benzo...	219	C14H9N3	209912-23-2	25





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Data File : BG056626.D
Acq On : 13 Feb 2023 19:28
Operator : CG/JU
Sample : 01529-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.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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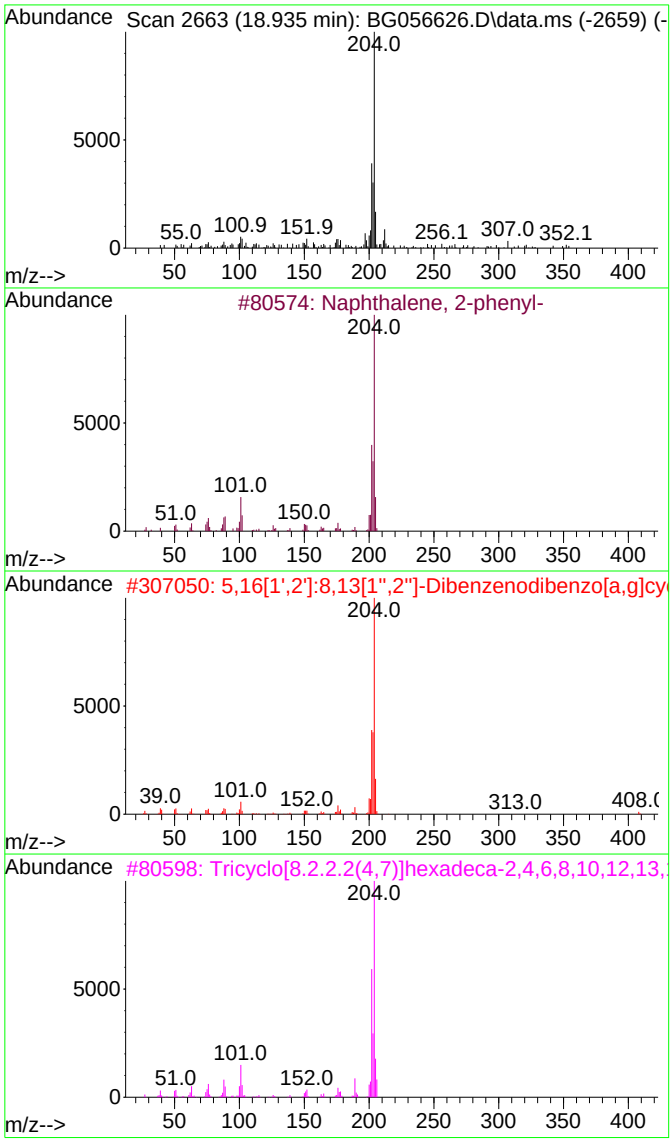
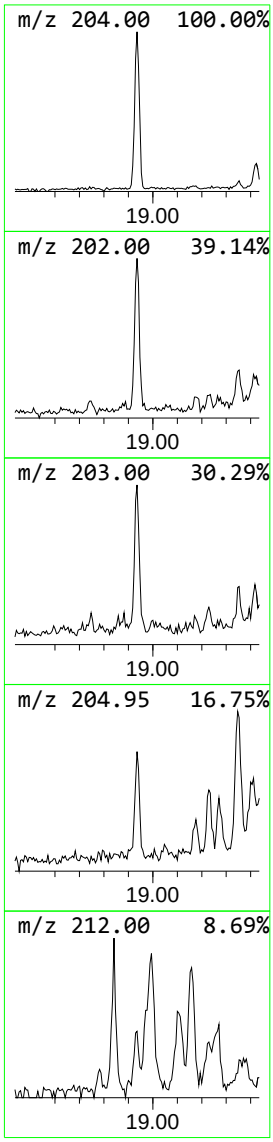
Peak Number 10 Naphthalene, 2-phenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.935	2.83 ng	77516	Phenanthrene-d10	17.578

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	64
2	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	59
3	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	52
4	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	47
5	[1,1'-Biphenyl]-2,2'-dicarbonitrile	204	C14H8N2	004341-02-0	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG021323\
Data File : BG056626.D
Acq On : 13 Feb 2023 19:28
Operator : CG/JU
Sample : 01529-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.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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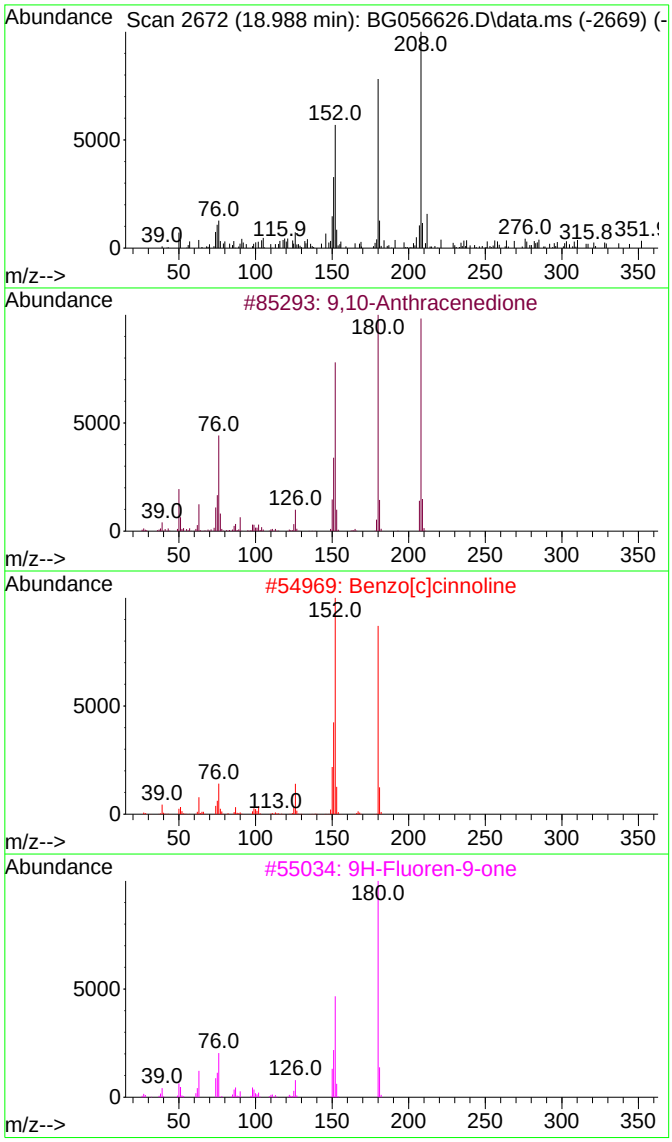
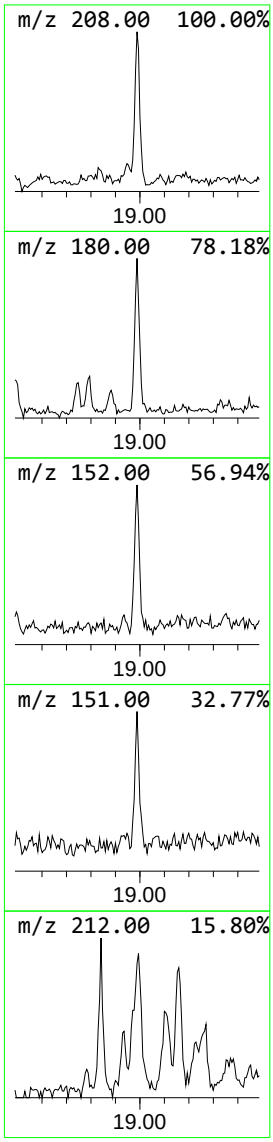
Peak Number 11 9,10-Anthracenedione Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.988	2.49 ng	68210	Phenanthrene-d10	17.578

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	94
2	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	70
3	9H-Fluoren-9-one	180	C13H8O	000486-25-9	49
4	1H-Phenalen-1-one	180	C13H8O	000548-39-0	45
5	1,1'-Biphenyl, 4-ethenyl-	180	C14H12	002350-89-2	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG021323\
Data File : BG056626.D
Acq On : 13 Feb 2023 19:28
Operator : CG/JU
Sample : 01529-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.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
2-Pentanone, 4-...	5.240	10.6	ng	119264	1	8.207	225501	20.0
Hexa-2,4-diyn-1...	14.905	2.0	ng	44988	3	14.840	447694	20.0
Dodecane	15.639	2.6	ng	57988	3	14.840	447694	20.0
Benzophenone	16.180	3.6	ng	80030	3	14.840	447694	20.0
Hexadecane, 2,6...	16.521	2.3	ng	61852	4	17.578	547468	20.0
Phenanthrene, 1...	18.448	4.6	ng	126701	4	17.578	547468	20.0
Anthracene, 2-m...	18.495	4.5	ng	122248	4	17.578	547468	20.0
4H-Cyclopenta[d...	18.647	5.9	ng	161161	4	17.578	547468	20.0
Naphthalene, 2-...	18.935	2.8	ng	77516	4	17.578	547468	20.0
9,10-Anthracene...	18.988	2.5	ng	68210	4	17.578	547468	20.0