LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053023\
Data File : BG057617.D
Acq On : 30 May 2023 22:18
Operator : CG/JU
Sample : 02953-03 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PNNL-RH-524-2

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-BG052723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057617.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.371	306	312	320	rBV2	15364	24458	3.82%	0.443%
2	5.864	389	396	408	rBV	146871	256034	39.96%	4.633%
3	7.492	665	673	685	rBV	159515	291993	45.58%	5.283%
4	8.343	810	818	827	rVB	99813	169526	26.46%	3.067%
5	9.524	1012	1019	1031	rBV	97233	181960	28.40%	3.292%
6	11.181	1293	1301	1308	rBV	133047	241890	37.76%	4.377%
7	13.578	1702	1709	1717	rBV	302137	470605	73.45%	8.515%
8	14.958	1937	1944	1951	rBV	233054	352235	54.98%	6.373%
9	15.023	1951	1955	1961	rVB	17283	25024	3.91%	0.453%
10	15.352	2004	2011	2018	rBV2	6692	10820	1.69%	0.196%
11	15.998	2114	2121	2128	rBV2	18309	27371	4.27%	0.495%
12	16.292	2166	2171	2177	rVB2	21588	32663	5.10%	0.591%
13	16.444	2190	2197	2205	rBV	210937	343847	53.67%	6.222%
14	17.361	2347	2353	2356	rBV5	5096	7406	1.16%	0.134%
15	17.519	2376	2380	2384	rVB	7106	10461	1.63%	0.189%
16	17.696	2404	2410	2414	rBV	270498	425782	66.46%	7.704%
17	17.737	2414	2417	2425	rVV	169852	251730	39.29%	4.555%
18	17.831	2425	2433	2441	rVV	44908	65765	10.26%	1.190%
19	18.101	2471	2479	2488	rBV2	15973	41506	6.48%	0.751%
20	18.271	2505	2508	2511	rBV5	4361	6890	1.08%	0.125%
21	18.536	2549	2553	2555	rBV4	16046	21878	3.41%	0.396%
22	18.565	2555	2558	2562	rVV	26229	31112	4.86%	0.563%
23	18.612	2562	2566	2571	rVB2	33422	48969	7.64%	0.886%
24	18.694	2575	2580	2585	rVB	14548	20457	3.19%	0.370%
25	18.765	2585	2592	2596	rBV3	35718	75260	11.75%	1.362%
26	19.047	2636	2640	2645	rBV	19515	26465	4.13%	0.479%
27	19.105	2646	2650	2654	rVB4	10537	16014	2.50%	0.290%
28	19.158	2657	2659	2665	rBV7	4666	7997	1.25%	0.145%
29	19.293	2679	2682	2685	rVB5	6535	6878	1.07%	0.124%
30	19.381	2695	2697	2700	rBV4	7811	7341	1.15%	0.133%
31	19.464	2707	2711	2714	rBV2	13792	17957	2.80%	0.325%
32	19.728	2750	2756	2762	rBV	250237	366970	57.28%	6.640%
33	20.057	2807	2812	2814	rBV2	46042	74657	11.65%	1.351%
34	20.092	2814	2818	2825	rVB	222896	302772	47.26%	5.478%
35	20.263	2842	2847	2852	rBV	502964	640678	100.00%	11.593%
36	20.574	2897	2900	2904	rVB	36054	45388	7.08%	0.821%

LSC Area Percent Report

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Integration Parameters: rteint.p
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Smoothing : ON Filtering: 5
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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-BG052723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.668	2914	2916	2920	rVB	24612	27988	4.37%	0.506%
38	22.001	3135	3143	3148	rBV2	248032	549902	85.83%	9.950%

Sum of corrected areas: 5526649

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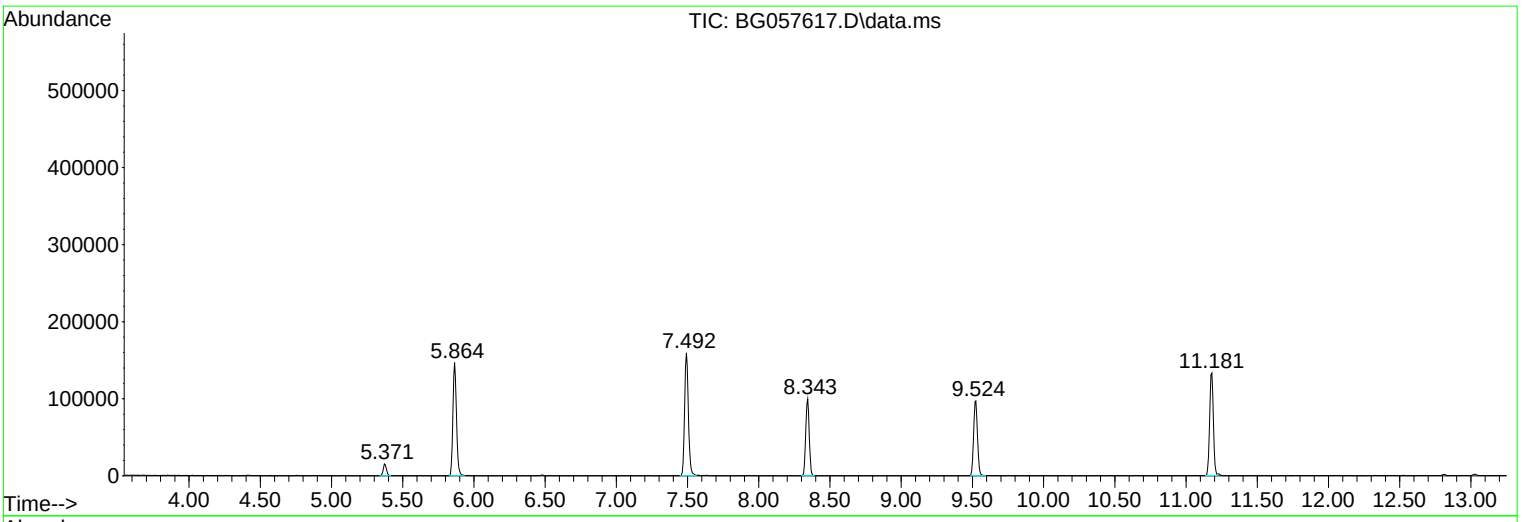
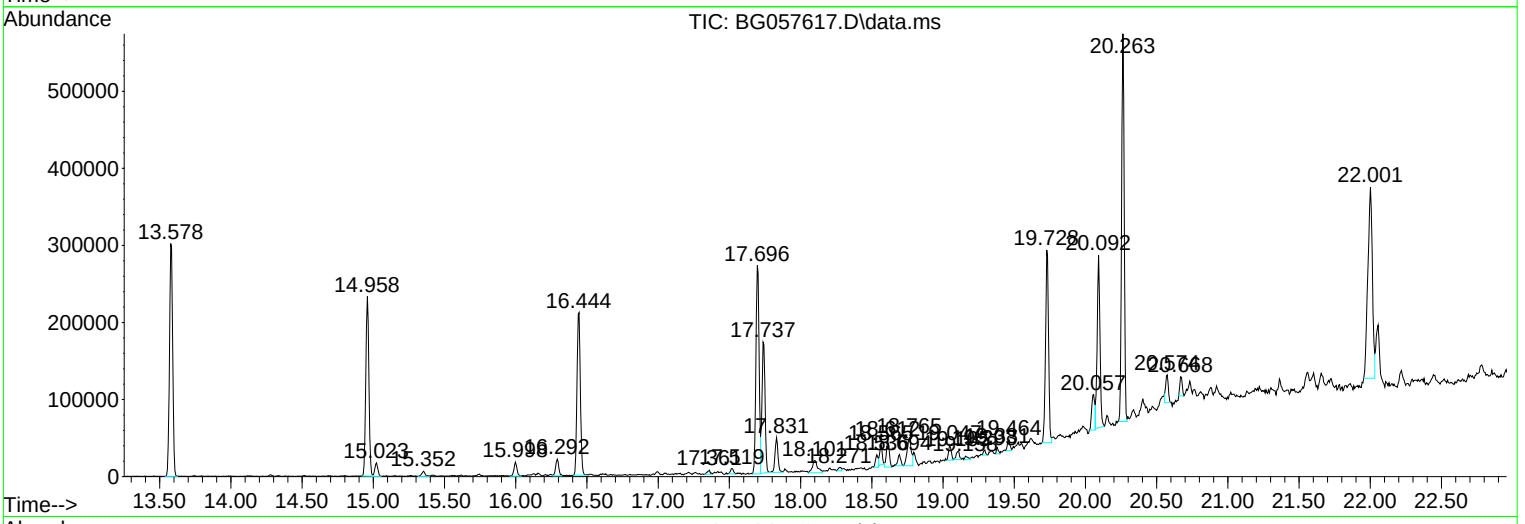
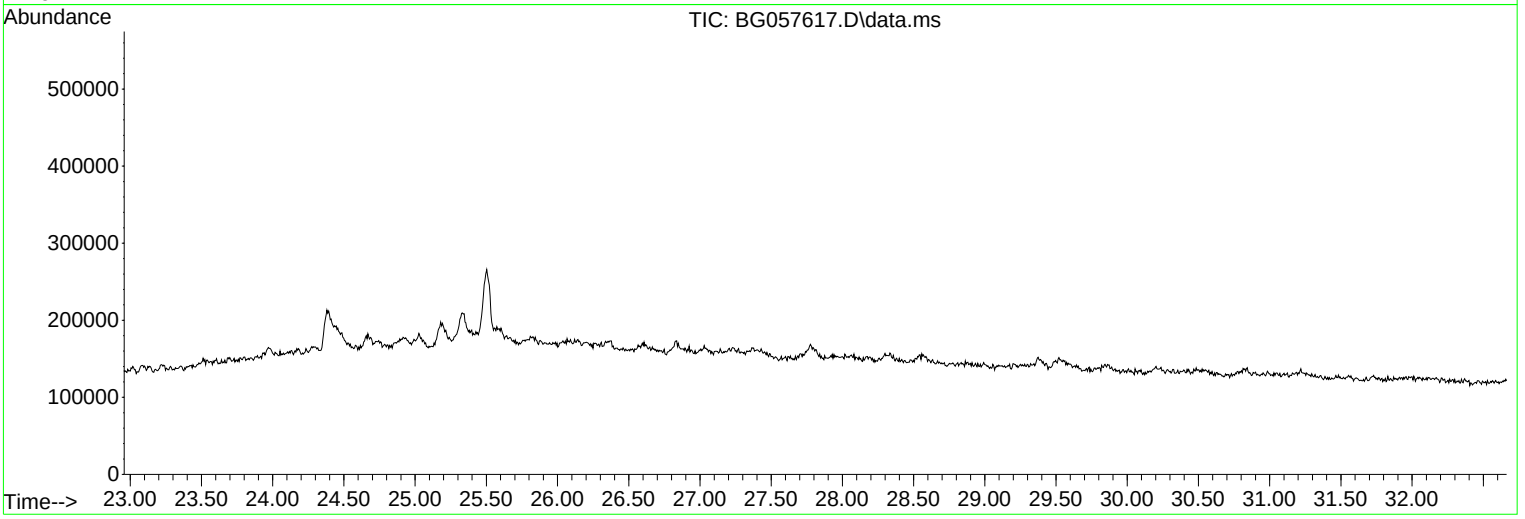
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Instrument :
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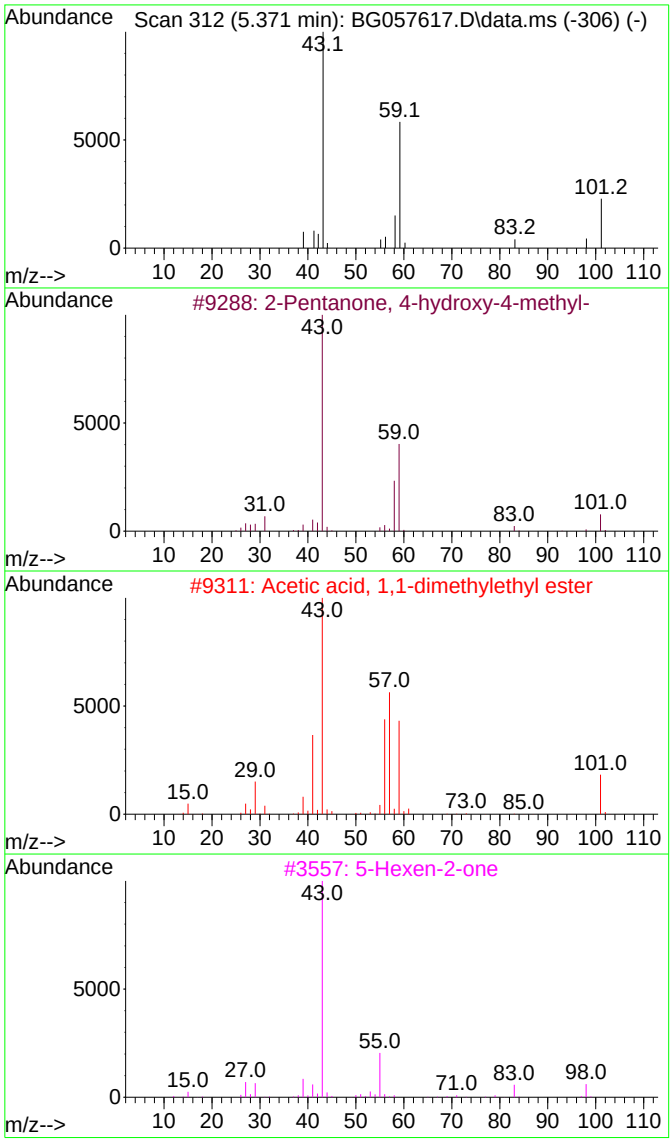
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

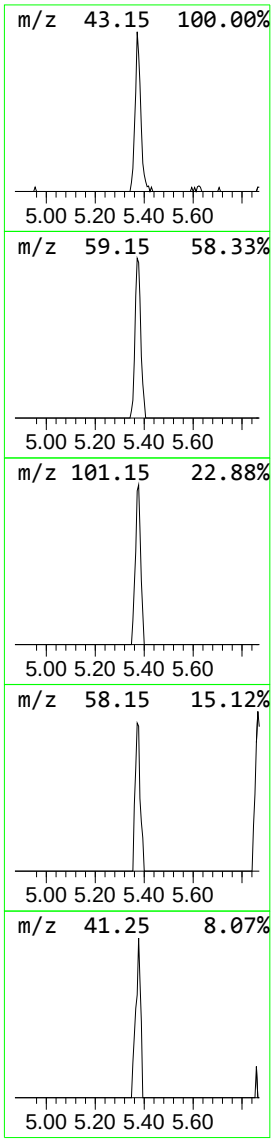
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.371	2.89 ng	24458	1,4-Dichlorobenzene-d4	8.343

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	9
5	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9





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Instrument :
BNA_G
ClientSampleId :
PNNL-RH-524-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

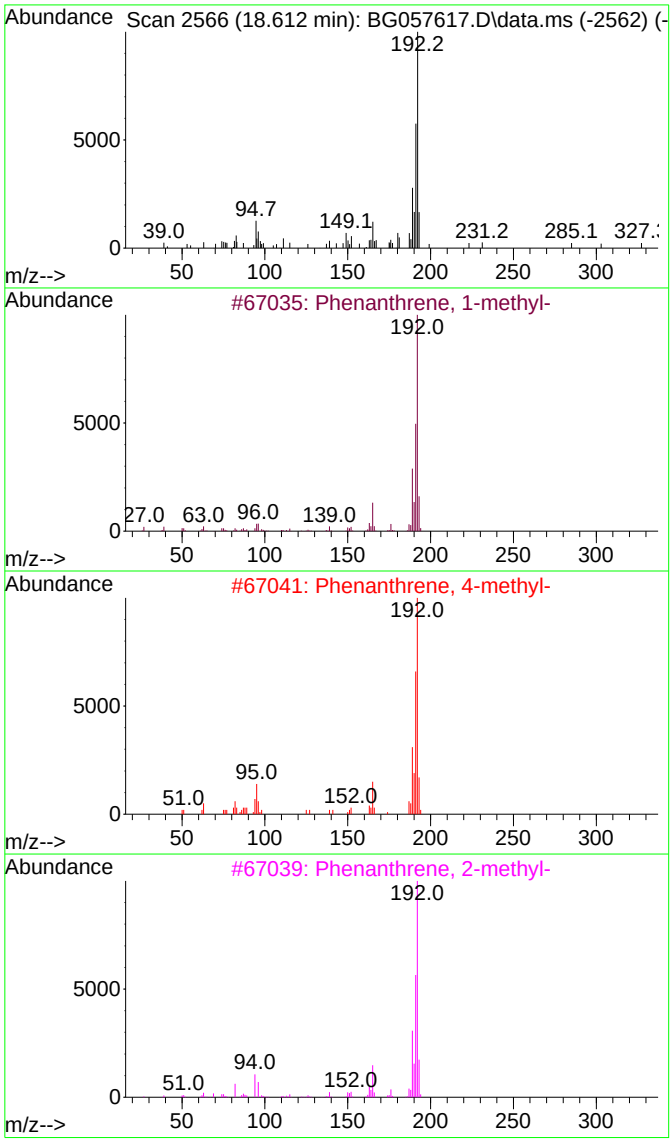
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

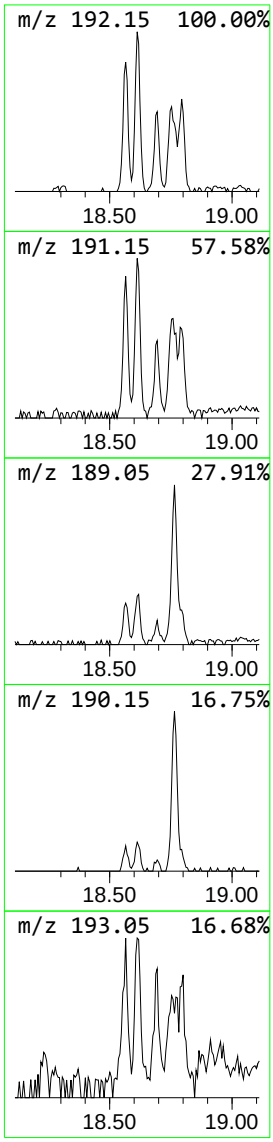
****

Peak Number 2 Phenanthrene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.612	2.30 ng	48969	Phenanthrene-d10	17.695

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	93
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	87





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Instrument :
BNA_G
ClientSampleId :
PNNL-RH-524-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

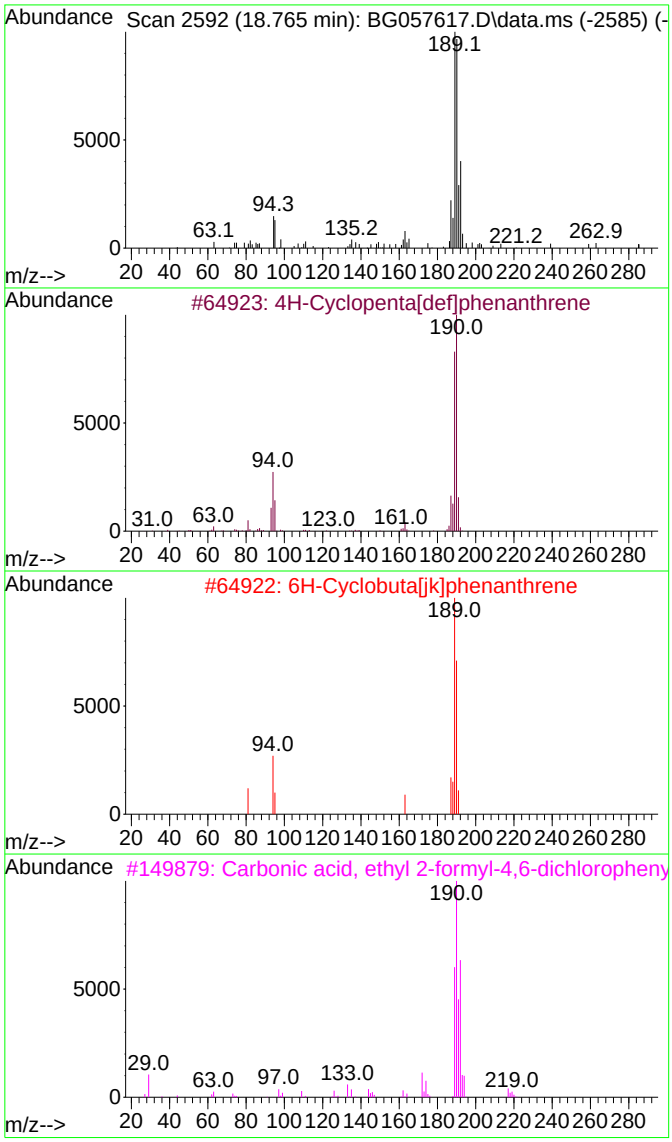
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

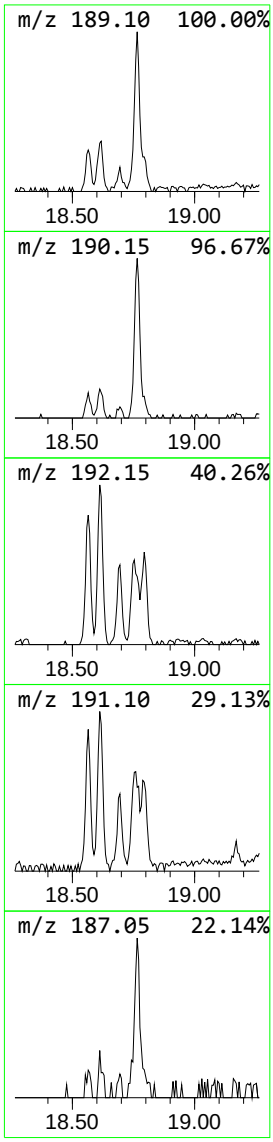
****

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.765	3.54 ng	75260	Phenanthrene-d10	17.695

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
5	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053023\
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Instrument :
BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
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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-...	5.371	2.9	ng	24458	1	8.343	169526	20.0
Phenanthrene, 1...	18.612	2.3	ng	48969	4	17.695	425782	20.0
4H-Cyclopenta[d...	18.765	3.5	ng	75260	4	17.695	425782	20.0