LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072722\
Data File : BG054420.D
Acq On : 27 Jul 2022 17:46
Operator : CG/JU
Sample : N3912-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
6601-S

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-BG071522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054420.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.030	3	7	14	rVV2	11230	21335	1.97%	0.300%
2	3.106	16	20	34	rVB	85177	145300	13.40%	2.046%
3	5.562	431	438	452	rBV	214339	369980	34.11%	5.210%
4	7.172	705	712	722	rVB	237382	414116	38.18%	5.832%
5	7.989	844	851	858	rVB	55211	96031	8.85%	1.352%
6	9.152	1041	1049	1057	rBV	143576	263534	24.30%	3.711%
7	10.791	1319	1328	1335	rBV	75354	141116	13.01%	1.987%
8	13.241	1738	1745	1754	rBV	403332	661599	60.99%	9.317%
9	13.946	1859	1865	1870	rBV2	7195	13426	1.24%	0.189%
10	14.622	1970	1980	1986	rBV	138961	226236	20.86%	3.186%
11	14.687	1986	1991	1997	rVB	20490	33228	3.06%	0.468%
12	15.021	2040	2048	2054	rBV	12904	21156	1.95%	0.298%
13	15.668	2152	2158	2169	rBV	29016	48095	4.43%	0.677%
14	15.962	2202	2208	2214	rVB2	10676	19668	1.81%	0.277%
15	16.114	2223	2234	2247	rBV3	449828	720824	66.45%	10.151%
16	16.343	2264	2273	2280	rBV6	10898	25255	2.33%	0.356%
17	16.667	2317	2328	2334	rBV7	8537	20354	1.88%	0.287%
18	16.896	2360	2367	2372	rBV5	7184	15442	1.42%	0.217%
19	16.937	2372	2374	2384	rVV6	7363	16246	1.50%	0.229%
20	17.025	2384	2389	2394	rVV3	7654	12746	1.18%	0.179%
21	17.107	2396	2403	2408	rVV4	11191	22582	2.08%	0.318%
22	17.184	2408	2416	2424	rVB3	10604	24487	2.26%	0.345%
23	17.366	2441	2447	2451	rBV	184762	288645	26.61%	4.065%
24	17.407	2451	2454	2460	rVB	116028	170576	15.73%	2.402%
25	17.501	2464	2470	2476	rBV	136452	216467	19.96%	3.048%
26	17.777	2510	2517	2520	rBV4	6710	13134	1.21%	0.185%
27	17.848	2525	2529	2532	rVV2	8586	11748	1.08%	0.165%
28	18.247	2590	2597	2601	rBV3	23370	43277	3.99%	0.609%
29	18.294	2601	2605	2611	rVB	26549	39667	3.66%	0.559%
30	18.371	2612	2618	2624	rBV	13557	24280	2.24%	0.342%
31	18.441	2624	2630	2634	rBV2	33844	62826	5.79%	0.885%
32	18.547	2644	2648	2653	rVB3	9977	14882	1.37%	0.210%
33	18.735	2677	2680	2686	rVB	17595	22327	2.06%	0.314%
34	18.982	2719	2722	2726	rVB5	8271	13589	1.25%	0.191%
35	19.170	2747	2754	2758	rBV3	20056	44126	4.07%	0.621%
36	19.299	2772	2776	2781	rBV	17151	27959	2.58%	0.394%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072722\
Data File : BG054420.D
Acq On : 27 Jul 2022 17:46
Operator : CG/JU
Sample : N3912-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
6601-S

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-BG071522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.422	2791	2797	2802	rBV	179067	262218	24.17%	3.693%
38	19.475	2802	2806	2809	rVB5	11241	15557	1.43%	0.219%
39	19.745	2848	2852	2854	rBV2	39858	53669	4.95%	0.756%
40	19.781	2854	2858	2864	rVB	157917	244534	22.54%	3.444%
41	19.975	2885	2891	2896	rBV	828367	1084724	100.00%	15.275%
42	20.274	2938	2942	2945	rVB	32724	46011	4.24%	0.648%
43	20.374	2956	2959	2963	rVB2	14561	18618	1.72%	0.262%
44	20.433	2965	2969	2974	rVV2	14391	23631	2.18%	0.333%
45	21.631	3165	3173	3178	rBV2	222672	473689	43.67%	6.670%
46	21.672	3178	3180	3188	rVB	56816	88656	8.17%	1.248%
47	23.071	3413	3418	3433	rVB3	51838	134828	12.43%	1.899%
48	24.834	3710	3718	3730	rBV2	117667	328884	30.32%	4.631%

Sum of corrected areas: 7101278

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072722\
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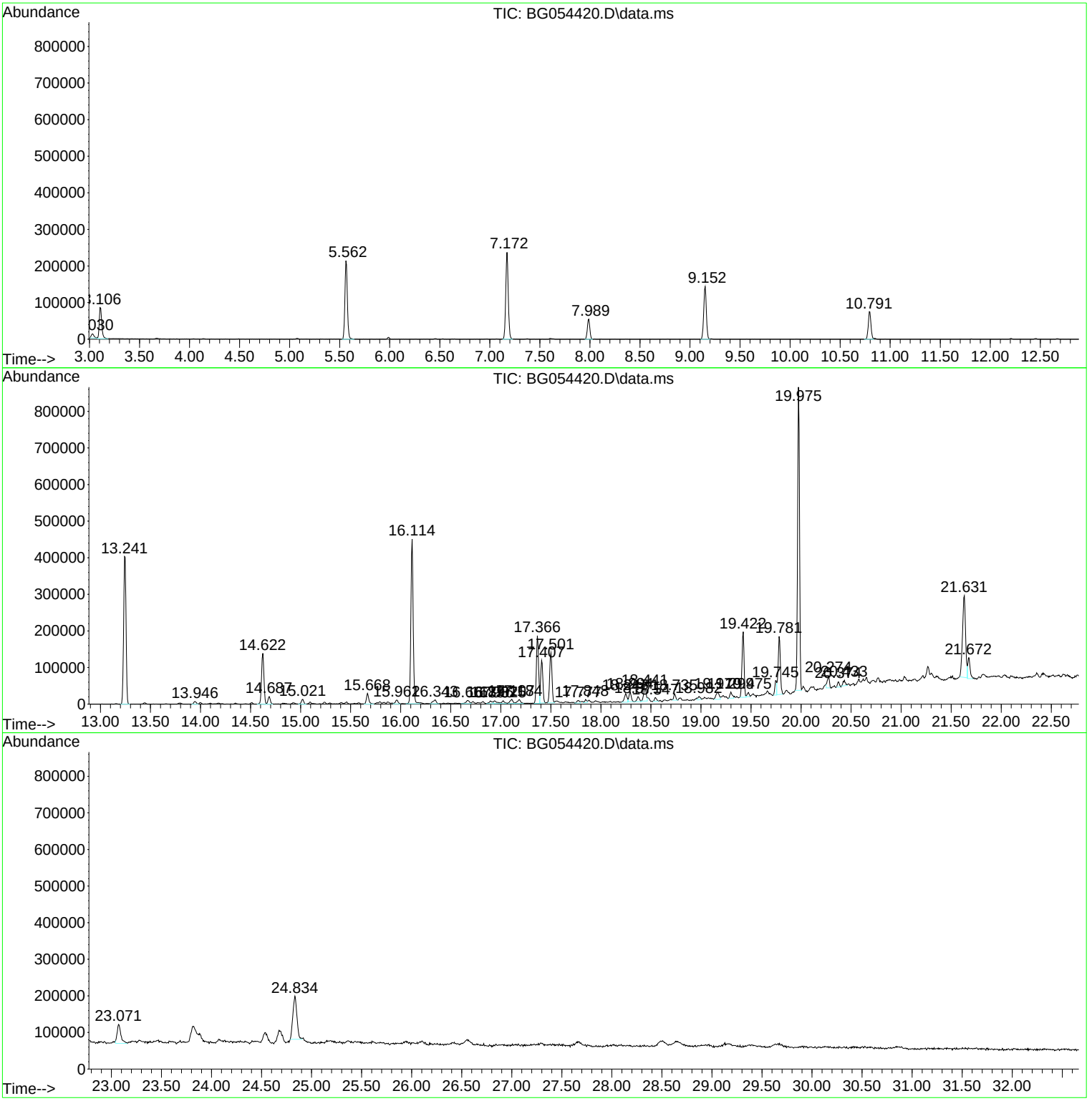
Operator : CG/JU
Sample : N3912-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
6601-S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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\BG072722\
Data File : BG054420.D
Acq On : 27 Jul 2022 17:46
Operator : CG/JU
Sample : N3912-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
6601-S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

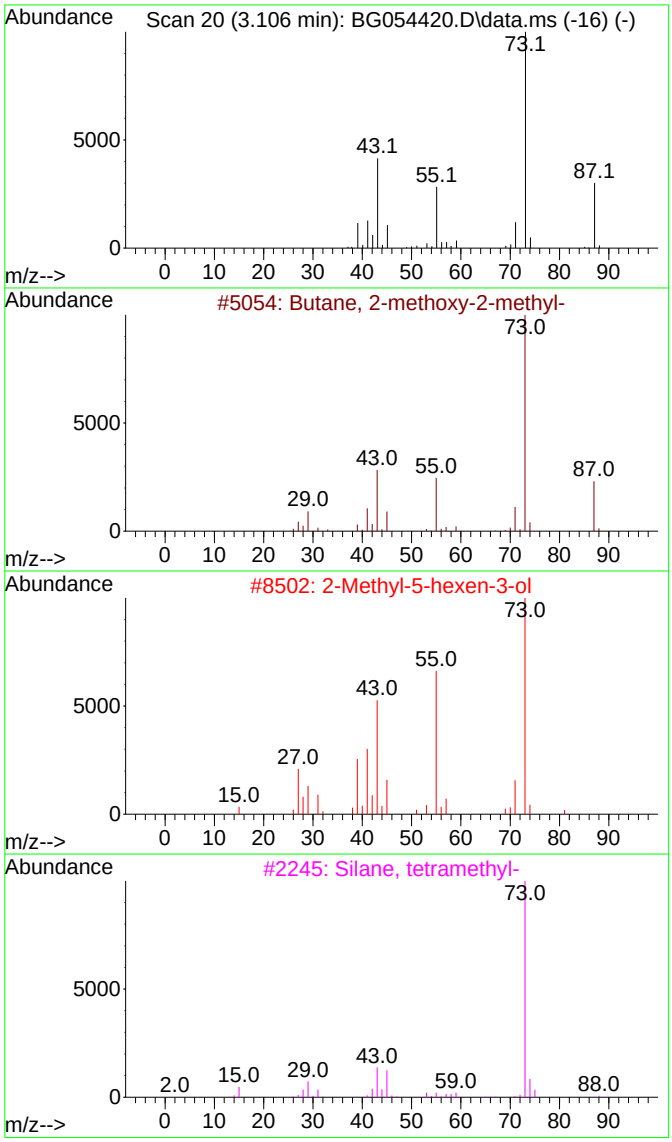
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

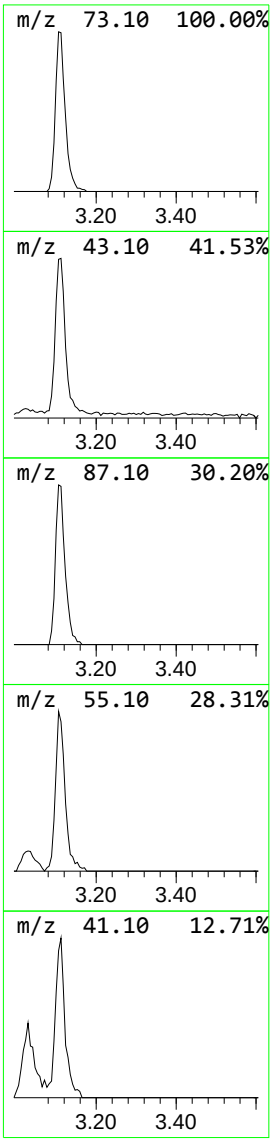
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.106	30.26 ng	145300	1,4-Dichlorobenzene-d4	7.989

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072722\
Data File : BG054420.D
Acq On : 27 Jul 2022 17:46
Operator : CG/JU
Sample : N3912-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
6601-S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

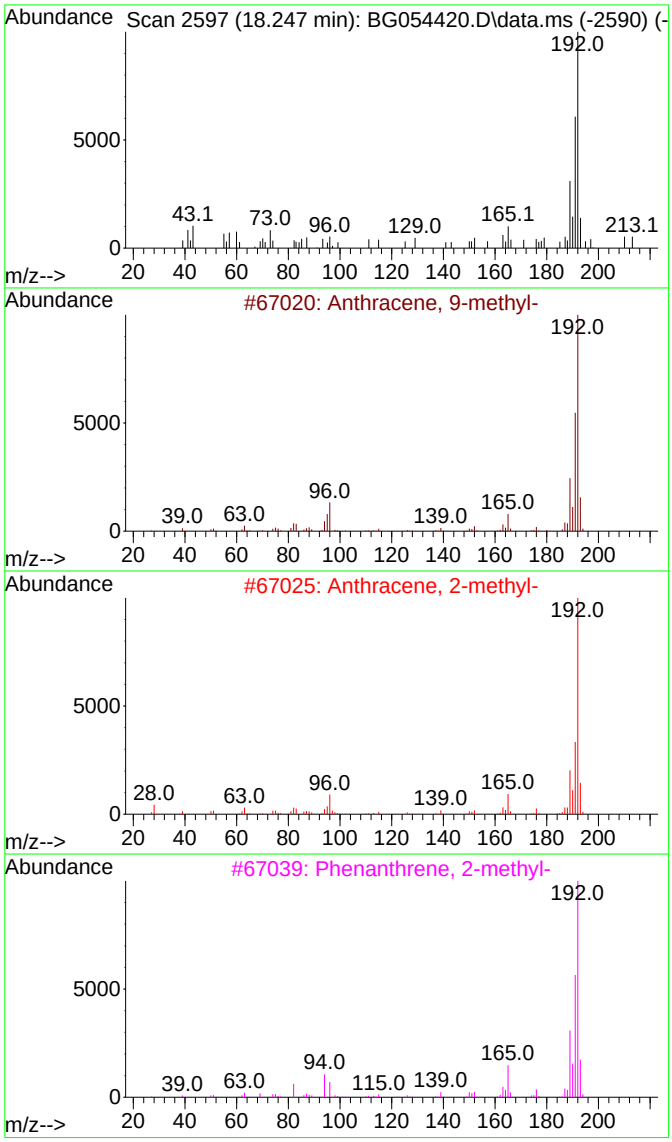
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

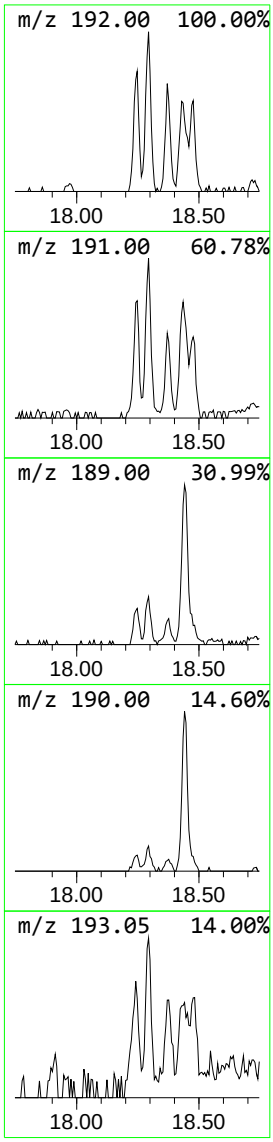
****

Peak Number 3 Anthracene, 9-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.247	3.00 ng	43277	Phenanthrene-d10	17.366

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	83
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	81
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	81
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072722\
Data File : BG054420.D
Acq On : 27 Jul 2022 17:46
Operator : CG/JU
Sample : N3912-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
6601-S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

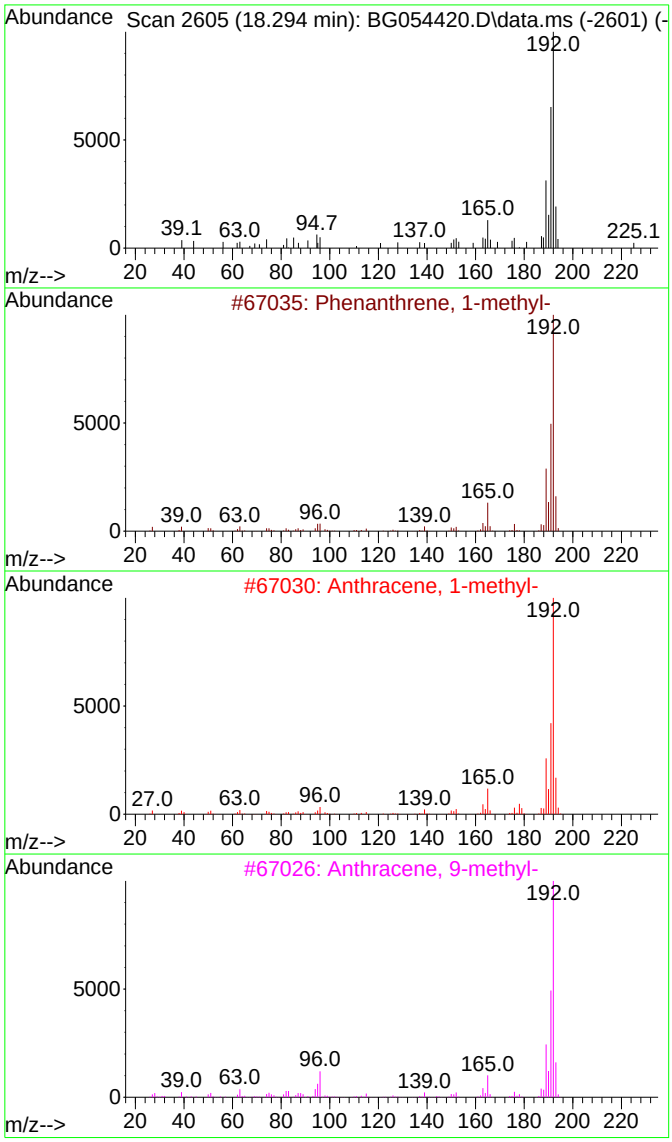
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

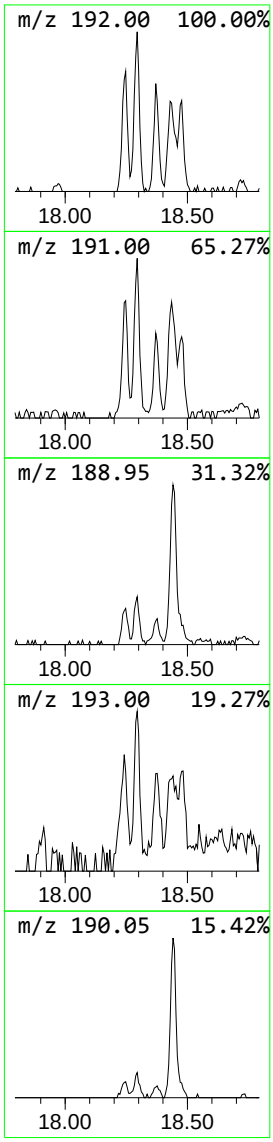
****

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.294	2.75 ng	39667	Phenanthrene-d10	17.366

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	94
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072722\
Data File : BG054420.D
Acq On : 27 Jul 2022 17:46
Operator : CG/JU
Sample : N3912-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
6601-S

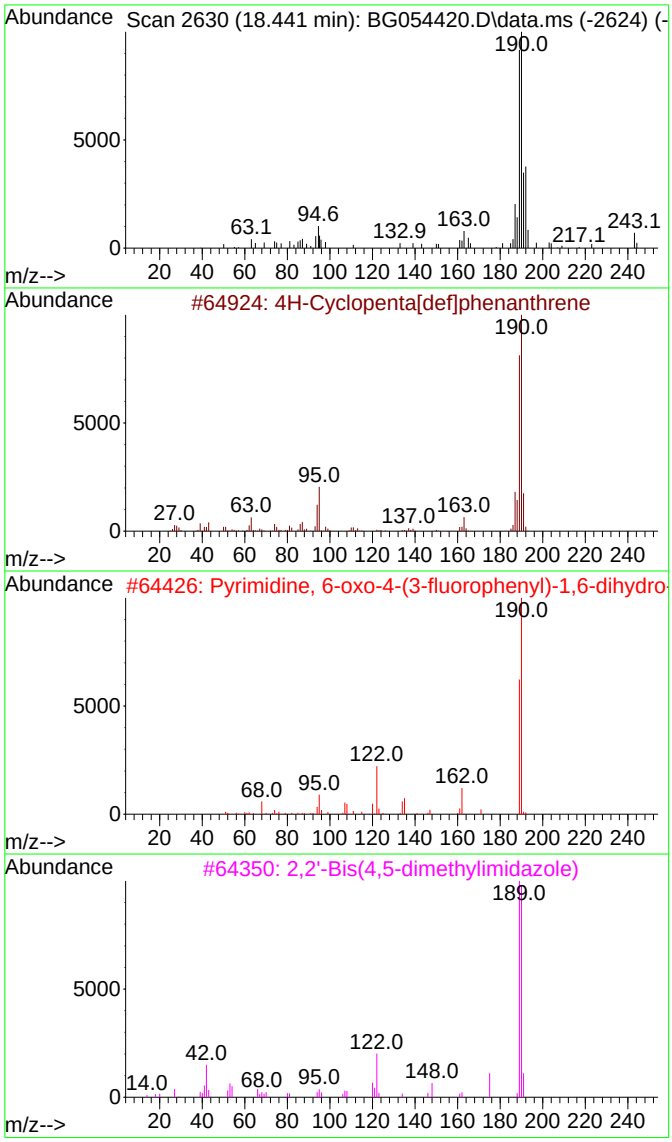
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

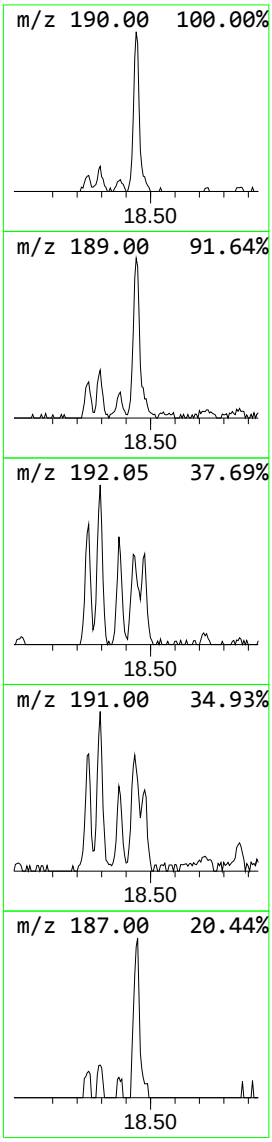
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.441	4.35 ng	62826	Phenanthrene-d10	17.366

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2	Pyrimidine, 6-oxo-4-(3-fluorophe...	190	C10H7FN2O	085979-55-1	50
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
4	1,1'-Biphenyl, 4,4'-difluoro-	190	C12H8F2	000398-23-2	35
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072722\
Data File : BG054420.D
Acq On : 27 Jul 2022 17:46
Operator : CG/JU
Sample : N3912-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
6601-S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

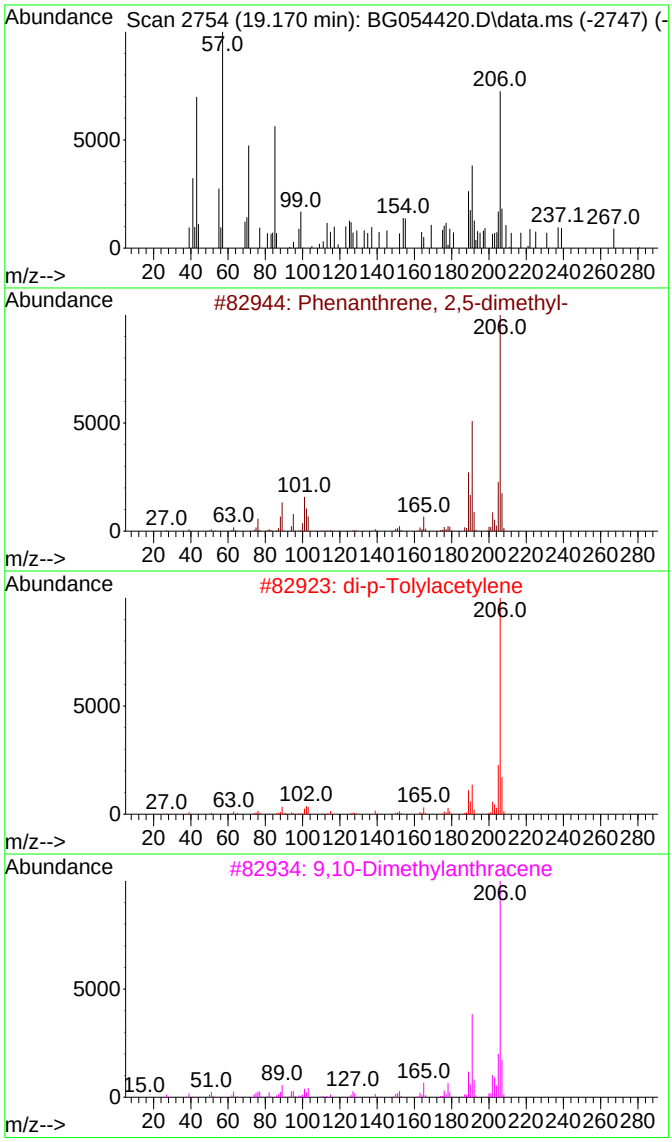
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

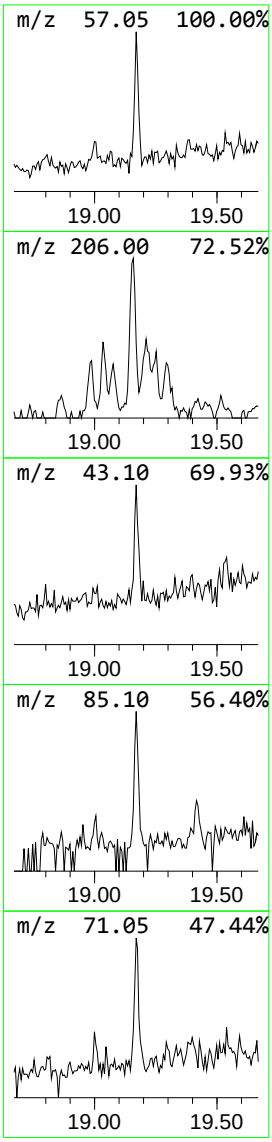
****

Peak Number 6 unknown19.170 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.170	3.06 ng	44126	Phenanthrene-d10	17.366

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	46
2	di-p-Tolylacetylene	206	C16H14	002789-88-0	41
3	9,10-Dimethylanthracene	206	C16H14	000781-43-1	38
4	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	35
5	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	35





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BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

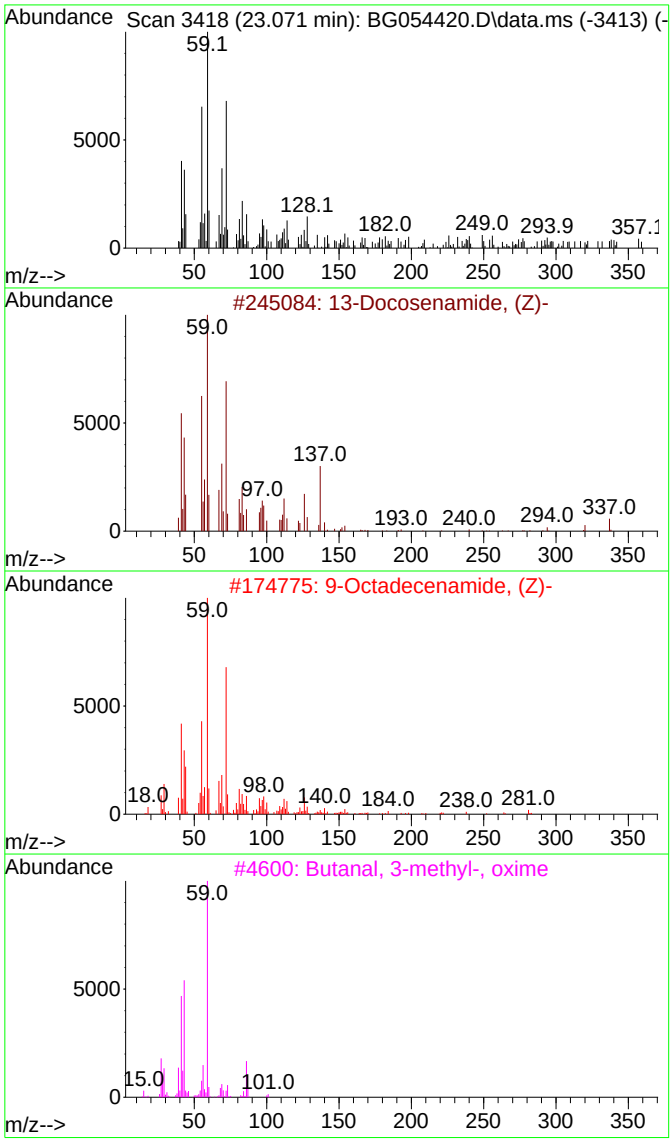
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

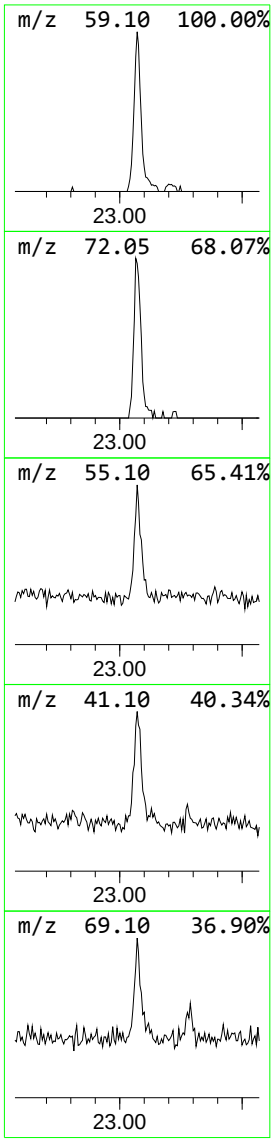
****

Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.071	5.69 ng	134828	Chrysene-d12	21.631

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	76
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	68
3	Butanal, 3-methyl-, oxime	101	C5H11NO	000626-90-4	38
4	14-Hydroxy-14-methylpentadecanoi...	272	C16H32O3	091544-39-7	38
5	1H-Indole-1-acetic acid, 2-cyano...	290	C18H14N2O2	1010327-43-4	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072722\
Data File : BG054420.D
Acq On : 27 Jul 2022 17:46
Operator : CG/JU
Sample : N3912-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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
Butane, 2-metho...	3.106	30.3	ng	145300	1	7.989	96031	20.0
Anthracene, 9-m...	18.247	3.0	ng	43277	4	17.366	288645	20.0
Phenanthrene, 1...	18.294	2.8	ng	39667	4	17.366	288645	20.0
4H-Cyclopenta[d...	18.441	4.3	ng	62826	4	17.366	288645	20.0
unknown19.170	19.170	3.1	ng	44126	4	17.366	288645	20.0
13-Docosenamide...	23.071	5.7	ng	134828	5	21.631	473689	20.0