LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055895.D
Acq On : 5 Dec 2022 21:55
Operator : CG/JU
Sample : N5868-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055895.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.215	321	328	339	rBV	236842	366464	19.59%	2.678%
2	5.703	404	411	422	rBV	597940	960562	51.35%	7.019%
3	6.320	510	516	522	rVB	13426	21066	1.13%	0.154%
4	7.330	680	688	704	rBV	601912	1050084	56.13%	7.673%
5	8.171	824	831	837	rBV	138189	228980	12.24%	1.673%
6	9.346	1023	1031	1040	rBV	353478	630304	33.69%	4.606%
7	10.997	1305	1312	1319	rBV	200088	360061	19.25%	2.631%
8	13.423	1718	1725	1736	rBV	915207	1406832	75.21%	10.280%
9	14.804	1950	1960	1966	rBV	342948	521806	27.89%	3.813%
10	14.863	1966	1970	1978	rVB	12837	19976	1.07%	0.146%
11	15.844	2131	2137	2146	rVB3	12528	22562	1.21%	0.165%
12	16.144	2182	2188	2198	rVB	104901	156170	8.35%	1.141%
13	16.285	2206	2212	2226	rBV	727799	1156904	61.84%	8.454%
14	16.708	2278	2284	2291	rVB2	13264	20006	1.07%	0.146%
15	17.542	2420	2426	2430	rBV	406772	617360	33.00%	4.511%
16	17.583	2430	2433	2440	rVB	151438	216000	11.55%	1.578%
17	17.677	2440	2449	2453	rBV	27675	49773	2.66%	0.364%
18	17.947	2484	2495	2501	rBV3	14810	32197	1.72%	0.235%
19	18.406	2568	2573	2579	rBV2	79390	150794	8.06%	1.102%
20	18.464	2579	2583	2590	rVV	44653	73649	3.94%	0.538%
21	18.547	2593	2597	2602	rVV	12773	21679	1.16%	0.158%
22	18.605	2602	2607	2611	rVV2	36480	76287	4.08%	0.557%
23	18.647	2611	2614	2618	rVB	22905	31078	1.66%	0.227%
24	18.905	2653	2658	2662	rBV	21508	32940	1.76%	0.241%
25	18.958	2662	2667	2676	rVB2	16443	29010	1.55%	0.212%
26	19.316	2723	2728	2733	rBV3	32437	55822	2.98%	0.408%
27	19.463	2748	2753	2758	rBV3	20538	43898	2.35%	0.321%
28	19.587	2767	2774	2779	rBV	237126	343575	18.37%	2.511%
29	19.669	2785	2788	2795	rVB7	16515	29659	1.59%	0.217%
30	19.916	2825	2830	2831	rBV2	40078	56410	3.02%	0.412%
31	19.945	2831	2835	2842	rVV	232657	352902	18.87%	2.579%
32	20.010	2842	2846	2853	rVB3	23146	34412	1.84%	0.251%
33	20.133	2861	2867	2872	rBV	1469141	1870661	100.00%	13.669%
34	20.262	2884	2889	2890	rBV3	26333	37546	2.01%	0.274%
35	20.415	2910	2915	2916	rBV3	25471	39916	2.13%	0.292%
36	20.533	2931	2935	2938	rBV2	19442	26097	1.40%	0.191%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055895.D
Acq On : 5 Dec 2022 21:55
Operator : CG/JU
Sample : N5868-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.591	2943	2945	2949	rVB	31868	37428	2.00%	0.273%
38	20.726	2965	2968	2973	rBV	34265	47848	2.56%	0.350%
39	20.779	2973	2977	2984	rVB	37018	61689	3.30%	0.451%
40	21.202	3046	3049	3056	rVB	28152	48974	2.62%	0.358%
41	21.432	3083	3088	3095	rBV2	74783	148575	7.94%	1.086%
42	21.825	3147	3155	3160	rBV3	412092	856494	45.79%	6.258%
43	21.872	3160	3163	3174	rVB	108505	190533	10.19%	1.392%
44	24.111	3538	3544	3562	rVB2	73463	368958	19.72%	2.696%
45	25.016	3693	3698	3706	rVB	72009	180935	9.67%	1.322%
46	25.180	3718	3726	3735	rVB2	213119	600500	32.10%	4.388%

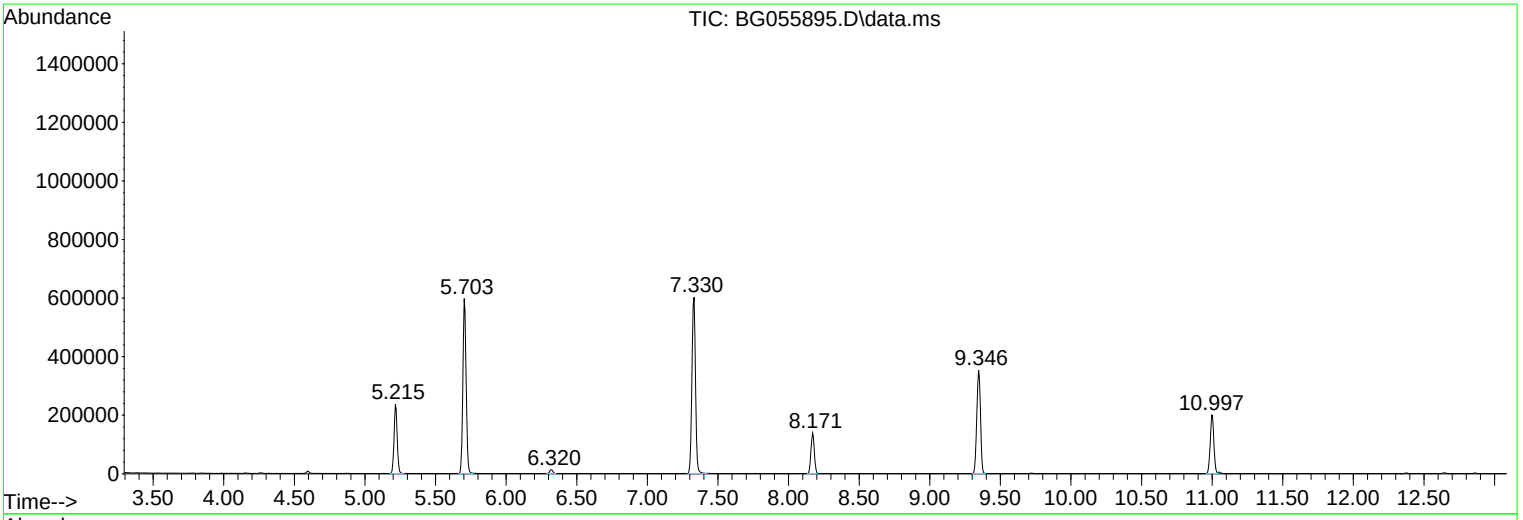
Sum of corrected areas: 13685376

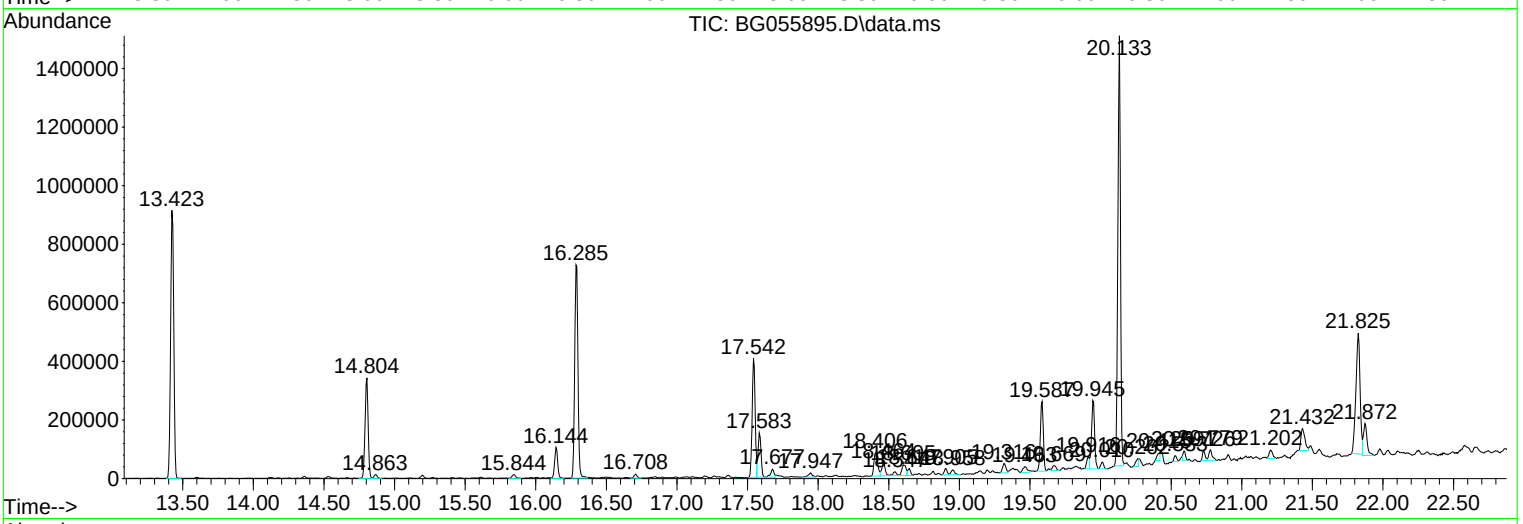
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055895.D
Acq On : 5 Dec 2022 21:55
Operator : CG/JU
Sample : N5868-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

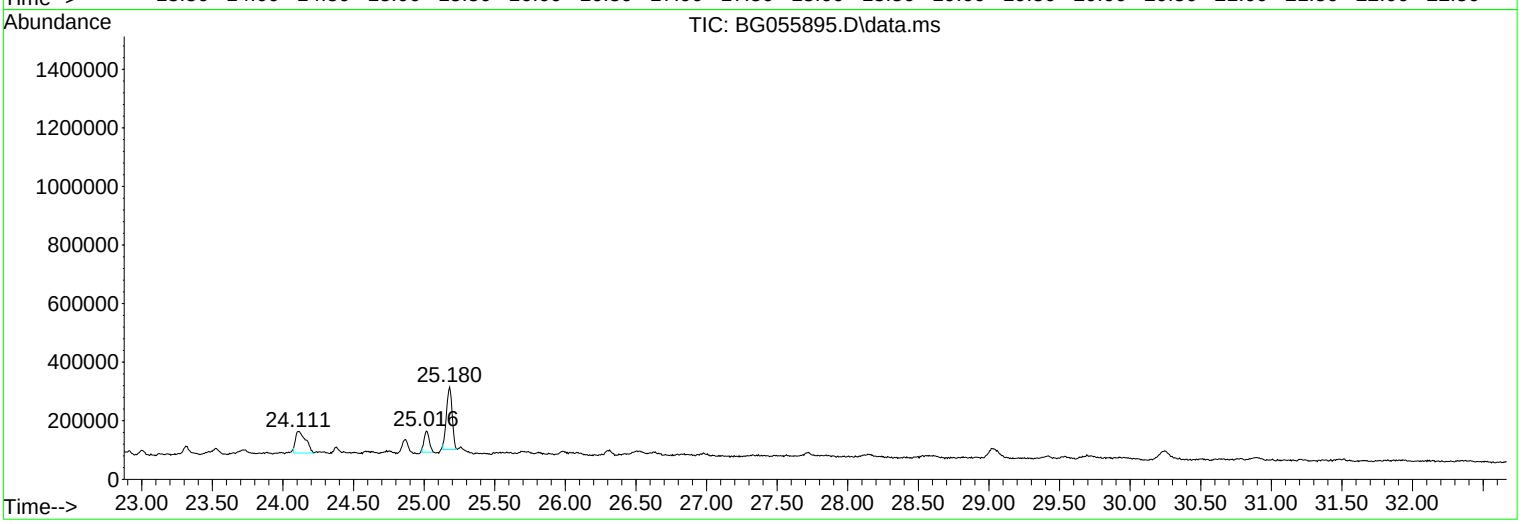
Instrument :
BNA_G
ClientSampleId :
TP-0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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\BG120522\
Data File : BG055895.D
Acq On : 5 Dec 2022 21:55
Operator : CG/JU
Sample : N5868-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-0

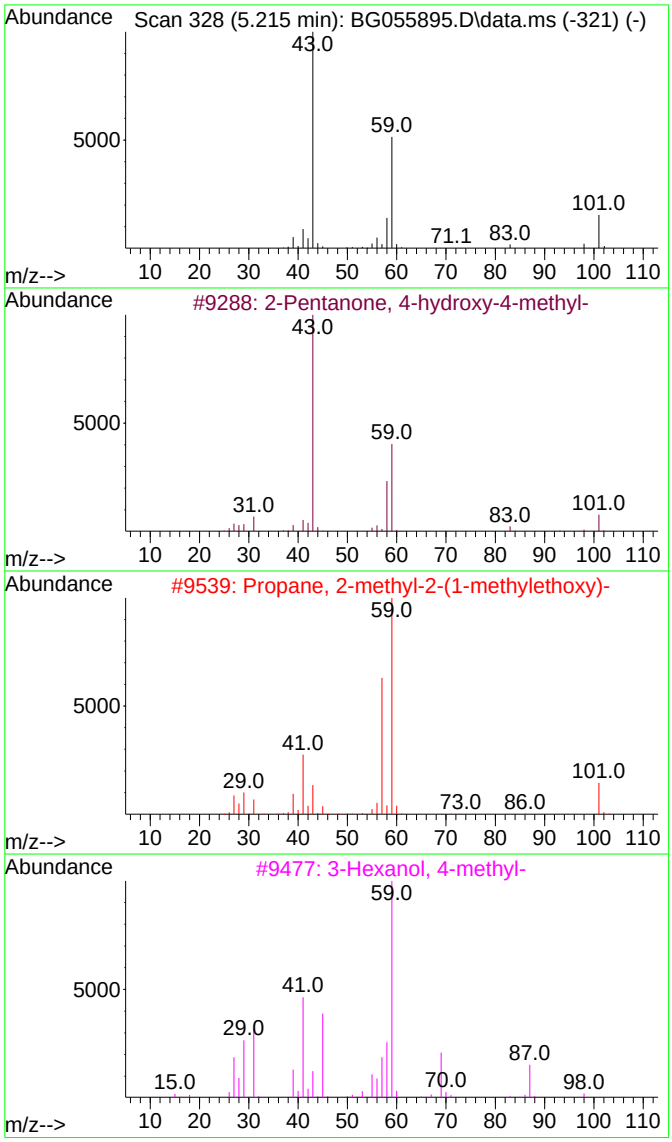
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

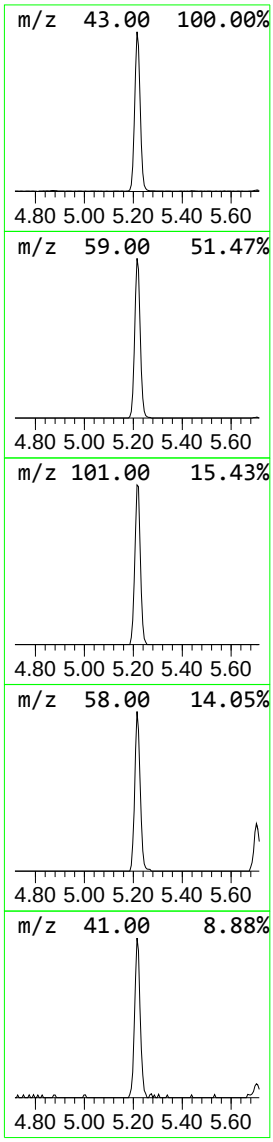
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.215	32.01 ng	366464	1,4-Dichlorobenzene-d4	8.171

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055895.D
Acq On : 5 Dec 2022 21:55
Operator : CG/JU
Sample : N5868-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

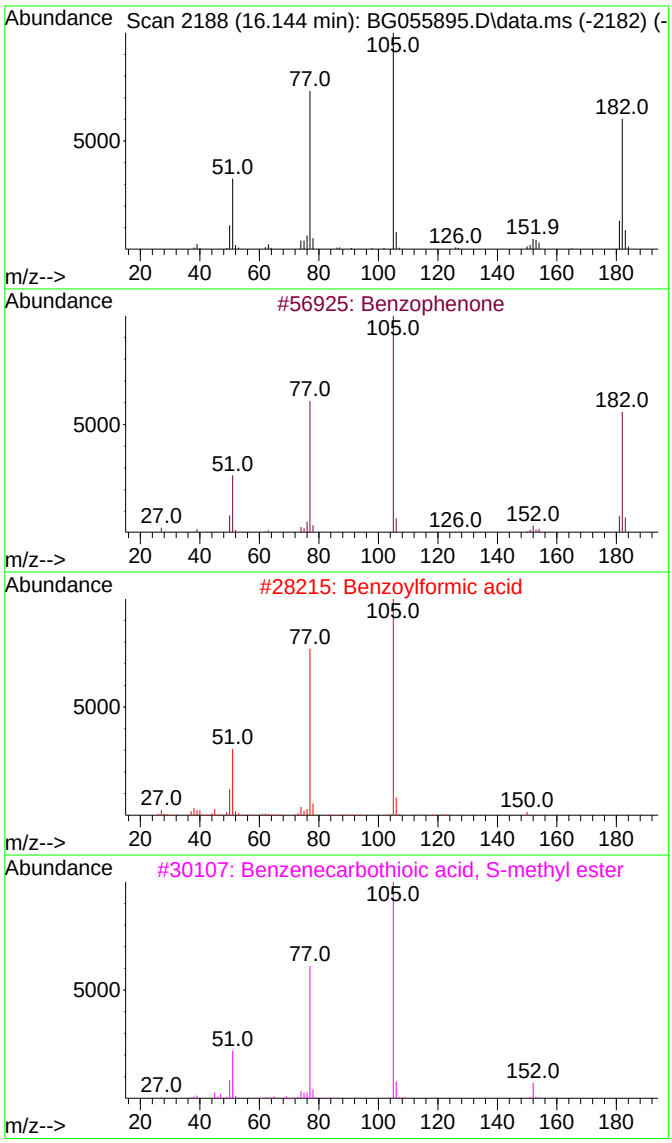
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

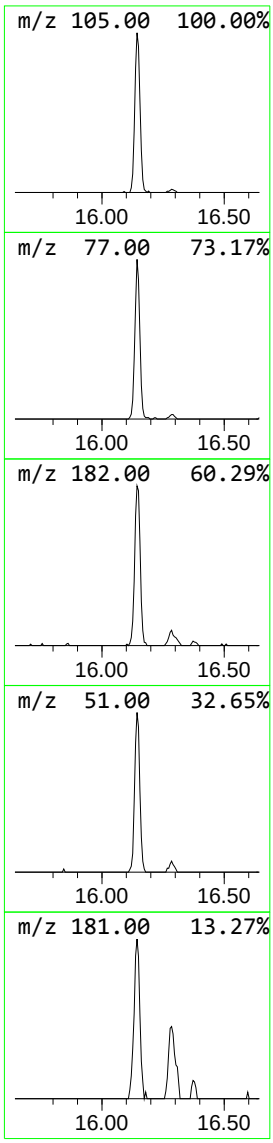
****

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.144	5.99 ng	156170	Acenaphthene-d10	14.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzoylformic acid	150	C8H6O3	000611-73-4	52
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
4	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	52
5	Ethanedione, diphenyl-	210	C14H10O2	000134-81-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055895.D
Acq On : 5 Dec 2022 21:55
Operator : CG/JU
Sample : N5868-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

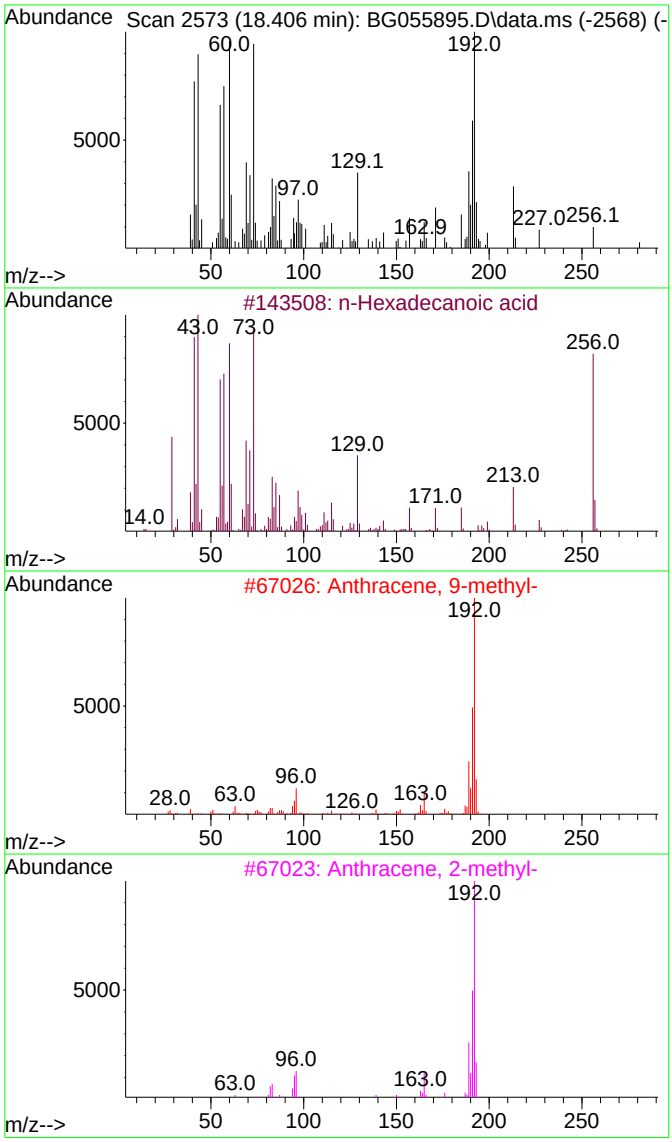
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

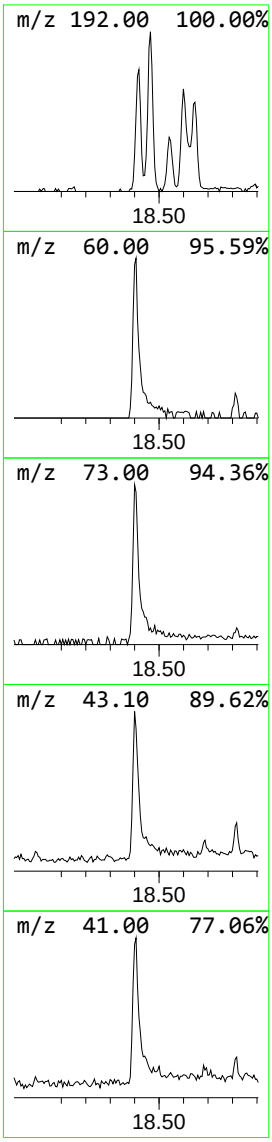
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.406	4.89 ng	150794	Phenanthrene-d10	17.542

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	84
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	83
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	49
4	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	46
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055895.D
Acq On : 5 Dec 2022 21:55
Operator : CG/JU
Sample : N5868-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

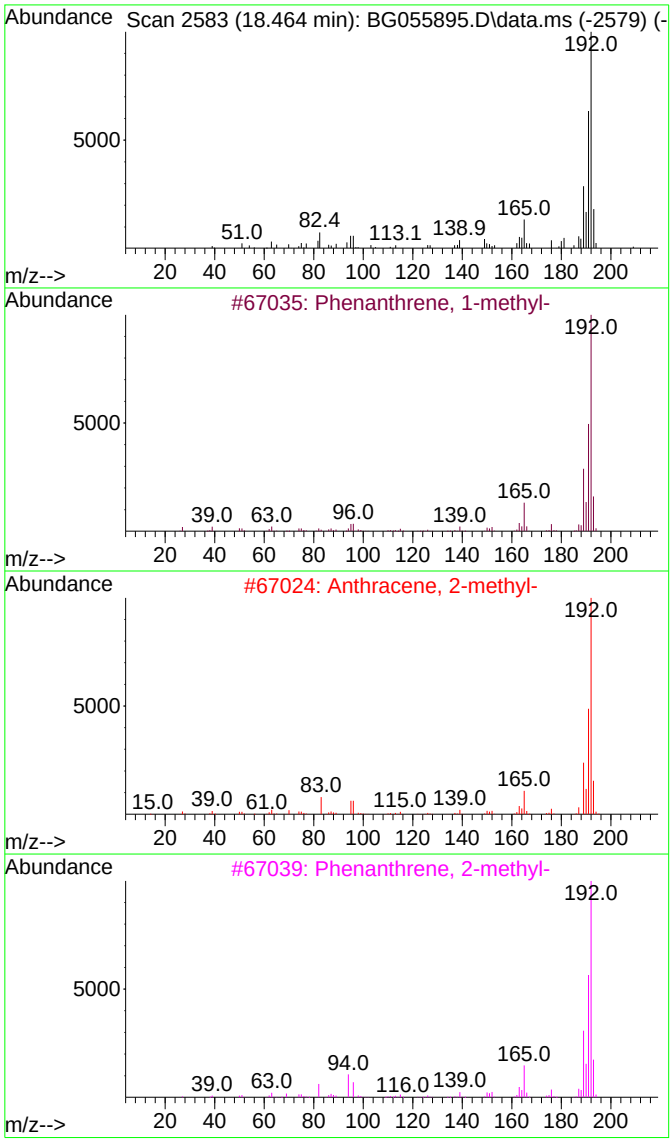
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

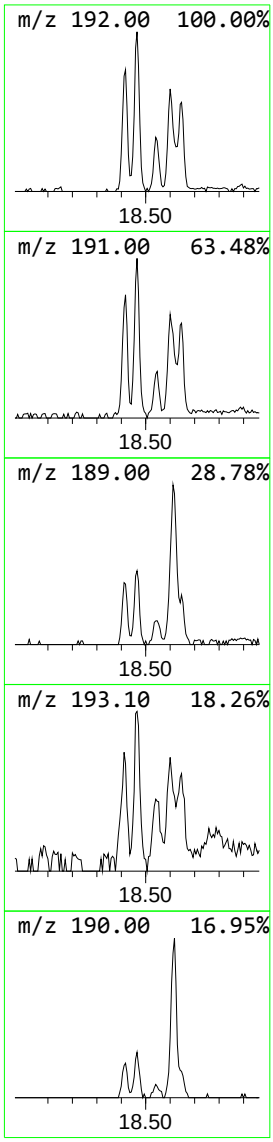
****

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.464	2.39 ng	73649	Phenanthrene-d10	17.542

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	94
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055895.D
Acq On : 5 Dec 2022 21:55
Operator : CG/JU
Sample : N5868-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

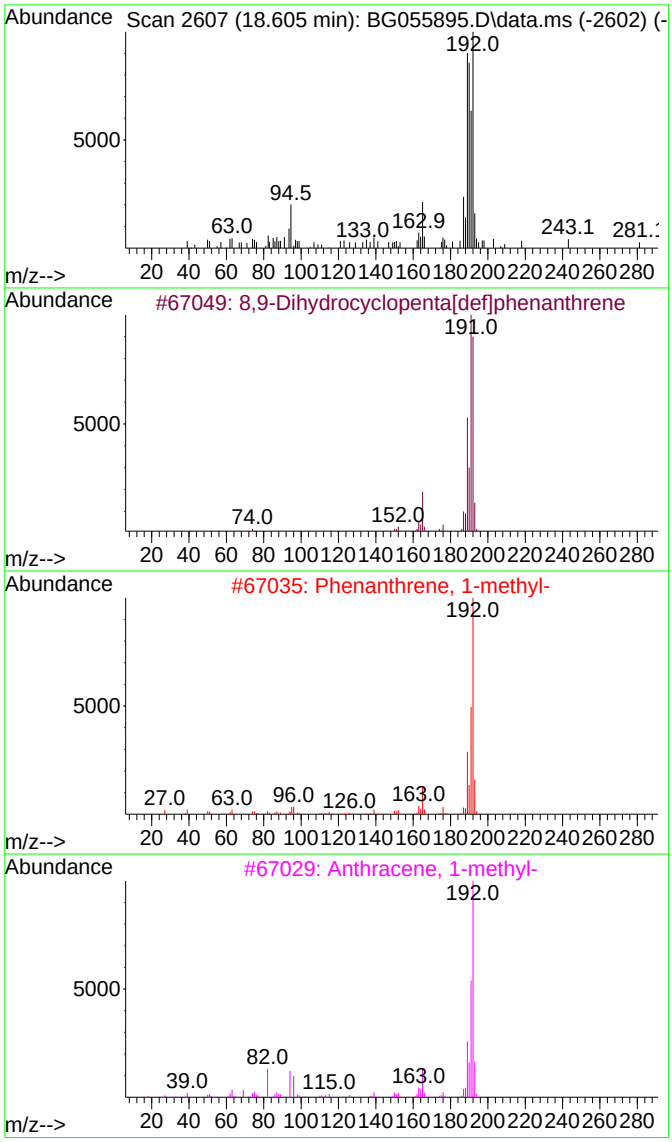
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

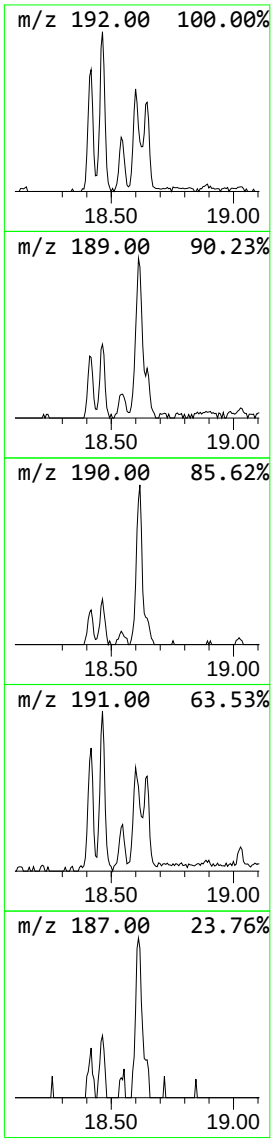
****

Peak Number 5 unknown18.605 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.605	2.47 ng	76287	Phenanthrene-d10	17.542

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	47
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	46
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	46
4	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	43
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	42





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Data File : BG055895.D
Acq On : 5 Dec 2022 21:55
Operator : CG/JU
Sample : N5868-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

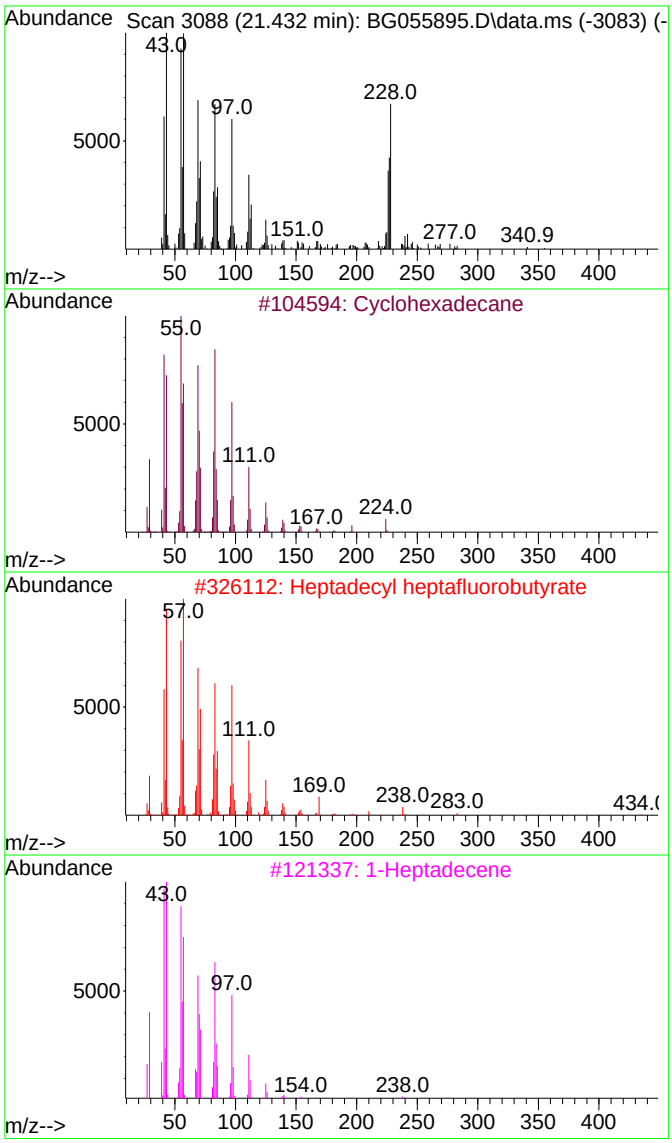
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

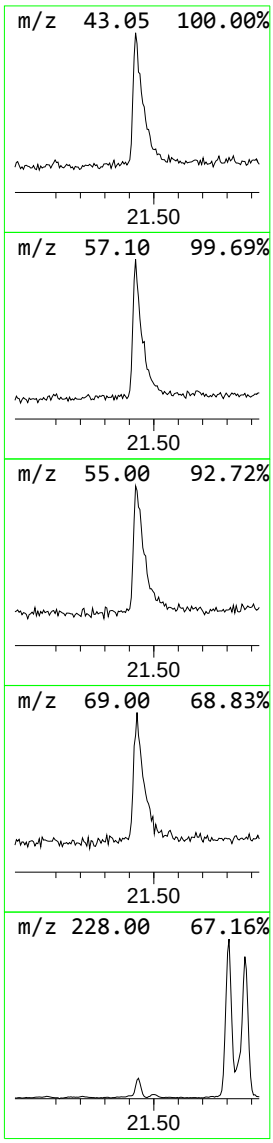
****

Peak Number 6 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.432	3.47 ng	148575	Chrysene-d12	21.825

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	78
3	1-Heptadecene	238	C17H34	006765-39-5	66
4	Cetene	224	C16H32	000629-73-2	64
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	60





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055895.D
Acq On : 5 Dec 2022 21:55
Operator : CG/JU
Sample : N5868-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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-...	5.215	32.0	ng	366464	1	8.171	228980	20.0
Benzophenone	16.144	6.0	ng	156170	3	14.804	521806	20.0
n-Hexadecanoic ...	18.406	4.9	ng	150794	4	17.542	617360	20.0
Phenanthrene, 1...	18.464	2.4	ng	73649	4	17.542	617360	20.0
unknown18.605	18.605	2.5	ng	76287	4	17.542	617360	20.0
Cyclohexadecane	21.432	3.5	ng	148575	5	21.825	856494	20.0