LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072722\
Data File : BG054419.D
Acq On : 27 Jul 2022 17:03
Operator : CG/JU
Sample : N3891-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 4553-E

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: BG054419.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.025	3	6	15	rVB2	12534	25507	2.31%	0.354%
2	3.108	15	20	33	rVB	84444	137143	12.42%	1.901%
3	5.070	349	354	360	rBV2	13984	22933	2.08%	0.318%
4	5.564	431	438	453	rVB	169736	289779	26.23%	4.017%
5	7.168	704	711	722	rBV	177100	325047	29.43%	4.506%
6	7.984	842	850	859	rBB	57167	96797	8.76%	1.342%
7	9.148	1041	1048	1058	rBV	116844	212162	19.21%	2.941%
8	10.793	1321	1328	1338	rBV	77954	142181	12.87%	1.971%
9	13.243	1737	1745	1756	rBB	397233	617693	55.92%	8.563%
10	14.624	1973	1980	1987	rBB	142985	232089	21.01%	3.218%
11	16.110	2227	2233	2248	rBV2	343536	553015	50.06%	7.667%
12	17.367	2439	2447	2451	rBV	196699	313911	28.42%	4.352%
13	17.409	2451	2454	2461	rVB	70338	101374	9.18%	1.405%
14	17.503	2465	2470	2475	rVB	13463	20401	1.85%	0.283%
15	18.243	2591	2596	2601	rBV2	13669	24465	2.21%	0.339%
16	18.290	2601	2604	2612	rVB	17704	28450	2.58%	0.394%
17	18.372	2612	2618	2623	rBV	7062	12345	1.12%	0.171%
18	18.431	2623	2628	2633	rVV2	19223	41038	3.72%	0.569%
19	18.472	2633	2635	2642	rVB	10178	14503	1.31%	0.201%
20	18.736	2675	2680	2684	rBV	13144	19892	1.80%	0.276%
21	18.783	2684	2688	2694	rVB3	9407	14807	1.34%	0.205%
22	18.983	2715	2722	2727	rBV4	6045	12410	1.12%	0.172%
23	19.159	2745	2752	2757	rBV2	14899	31383	2.84%	0.435%
24	19.218	2759	2762	2771	rVB7	7807	18558	1.68%	0.257%
25	19.301	2771	2776	2782	rBV4	11136	22477	2.03%	0.312%
26	19.418	2788	2796	2803	rBV	225942	326710	29.58%	4.529%
27	19.753	2847	2853	2854	rBV2	39930	57575	5.21%	0.798%
28	19.782	2854	2858	2866	rVB	211486	312064	28.25%	4.326%
29	19.847	2866	2869	2877	rBV3	11645	21335	1.93%	0.296%
30	19.976	2879	2891	2896	rBV	817908	1104630	100.00%	15.314%
31	20.111	2904	2914	2919	rBV4	18834	51246	4.64%	0.710%
32	20.270	2931	2941	2946	rBV3	28208	65948	5.97%	0.914%
33	20.376	2955	2959	2963	rBV	13908	19242	1.74%	0.267%
34	20.434	2963	2969	2973	rBV3	20856	39819	3.60%	0.552%
35	20.575	2986	2993	2996	rBV	16757	33032	2.99%	0.458%
36	20.617	2996	3000	3005	rVV	17005	28347	2.57%	0.393%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072722\
Data File : BG054419.D
Acq On : 27 Jul 2022 17:03
Operator : CG/JU
Sample : N3891-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4553-E

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	21.028	3067	3070	3077	rVB	19365	29647	2.68%	0.411%
38	21.263	3106	3110	3114	rBV3	23006	37655	3.41%	0.522%
39	21.510	3145	3152	3158	rBV2	42470	68993	6.25%	0.956%
40	21.627	3164	3172	3177	rBV2	260961	603278	54.61%	8.364%
41	21.674	3177	3180	3192	rVB	96391	167208	15.14%	2.318%
42	21.827	3203	3206	3210	rVB	17897	27790	2.52%	0.385%
43	23.813	3537	3544	3552	rBV2	73385	243938	22.08%	3.382%
44	24.530	3662	3666	3678	rVB	45828	124340	11.26%	1.724%
45	24.677	3684	3691	3699	rBV	62167	162085	14.67%	2.247%
46	24.829	3709	3717	3727	rBV2	125508	357855	32.40%	4.961%

Sum of corrected areas: 7213097

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072722\
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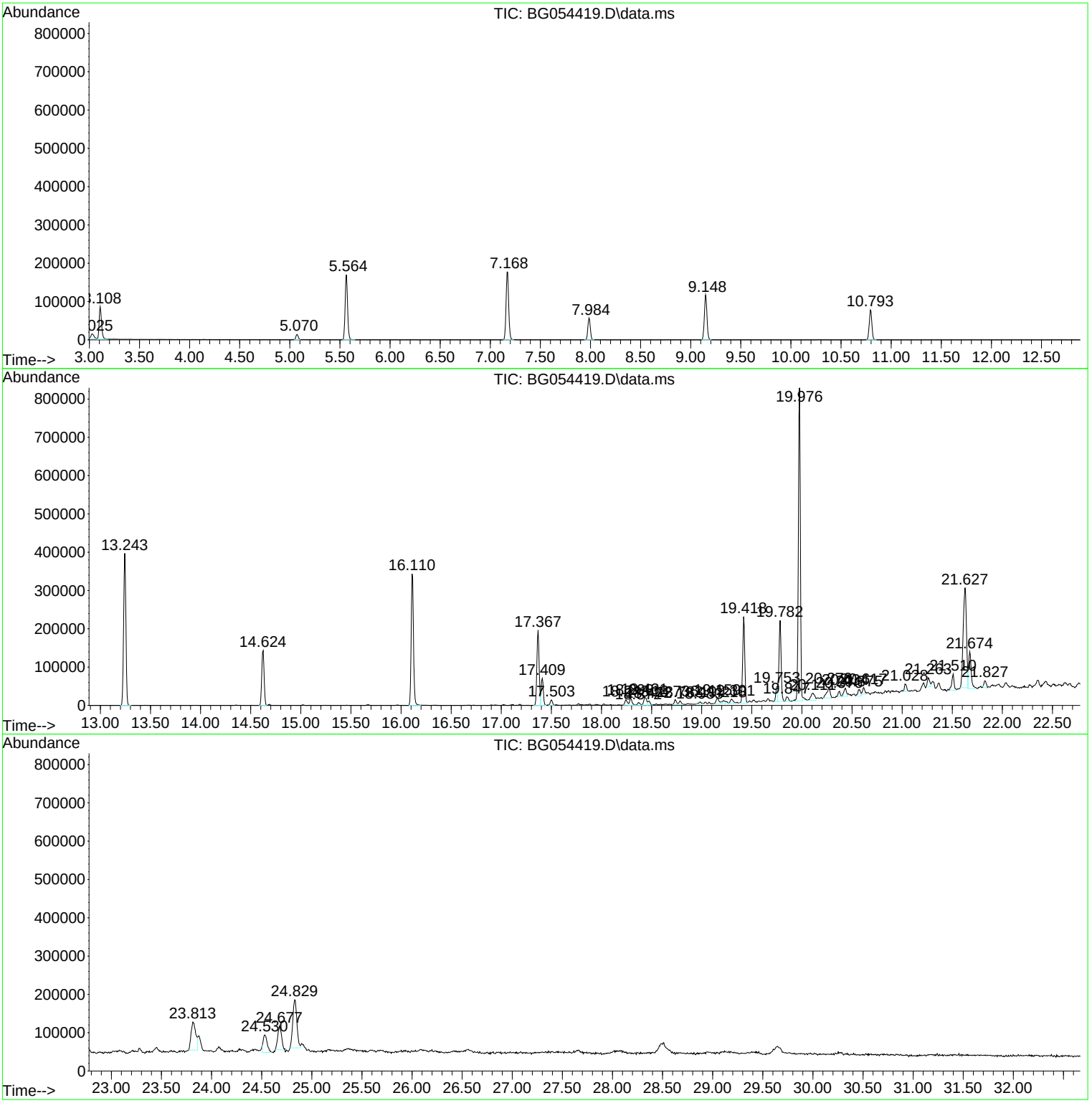
Sample : N3891-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4553-E

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 : BG054419.D
Acq On : 27 Jul 2022 17:03
Operator : CG/JU
Sample : N3891-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4553-E

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

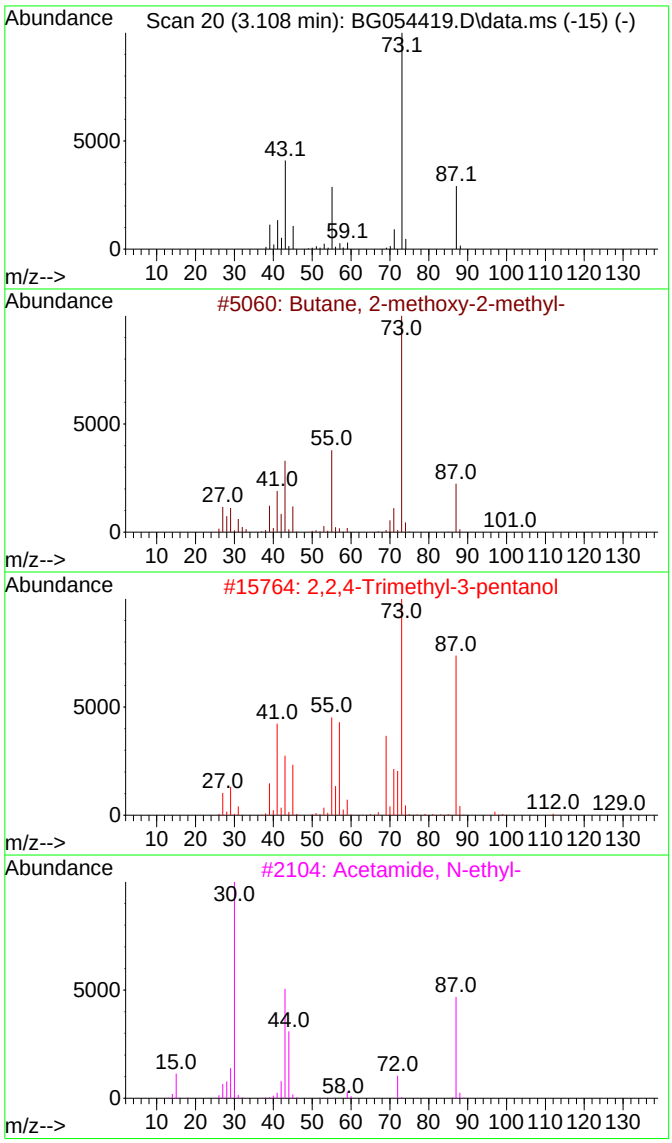
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

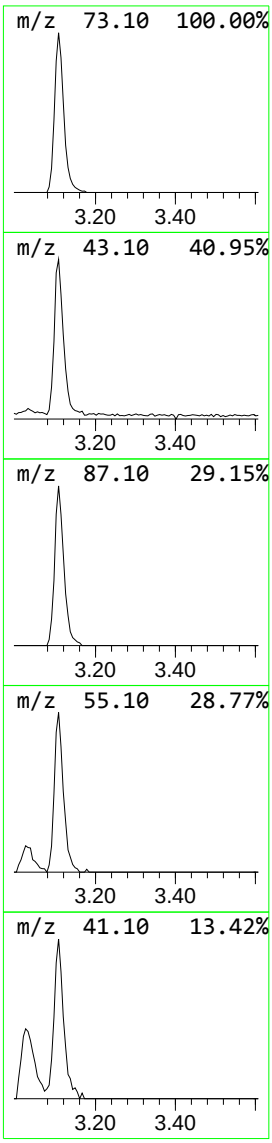
****

Peak Number 2 unknown3.108 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.108	28.34 ng	137143	1,4-Dichlorobenzene-d4	7.984

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	45
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072722\
Data File : BG054419.D
Acq On : 27 Jul 2022 17:03
Operator : CG/JU
Sample : N3891-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4553-E

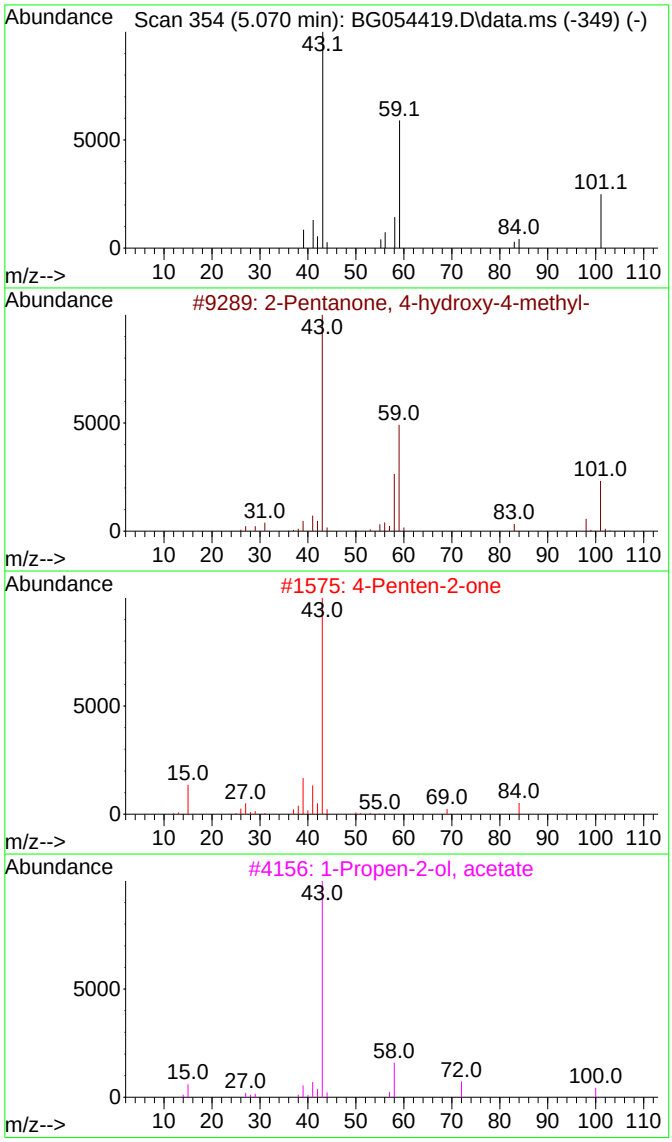
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

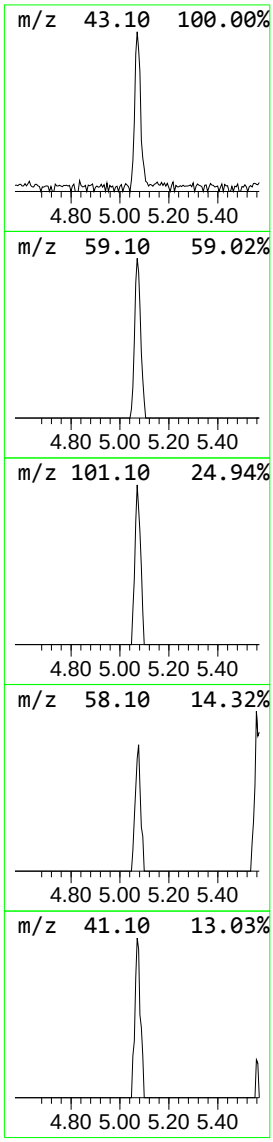
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.070	4.74 ng	22933	1,4-Dichlorobenzene-d4	7.984

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	4-Penten-2-one	84	C5H8O	013891-87-7	9
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5	3-Octanol	130	C8H18O	000589-98-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072722\
Data File : BG054419.D
Acq On : 27 Jul 2022 17:03
Operator : CG/JU
Sample : N3891-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4553-E

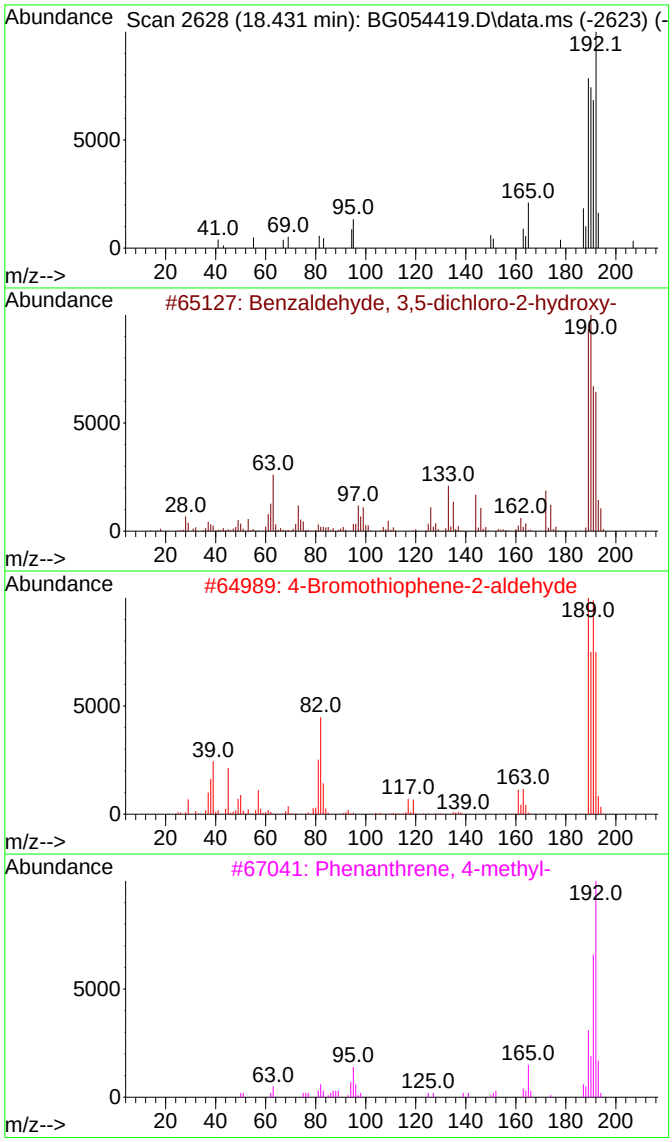
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

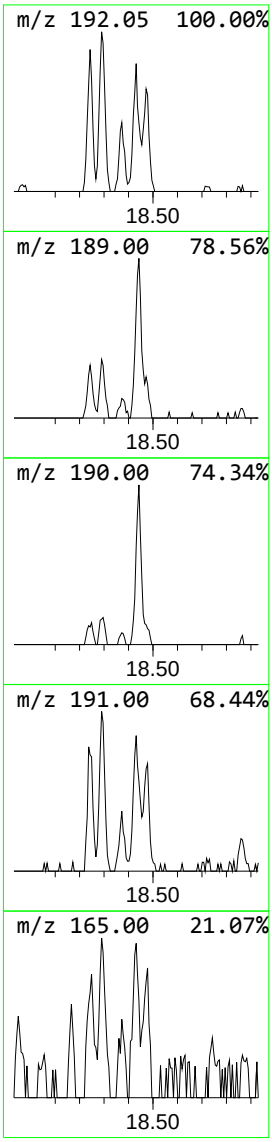
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzaldehyde, 3,5-dichloro-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.431	2.61 ng	41038	Phenanthrene-d10	17.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	58
2	4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	58
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	50
4	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	46
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072722\
Data File : BG054419.D
Acq On : 27 Jul 2022 17:03
Operator : CG/JU
Sample : N3891-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4553-E

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

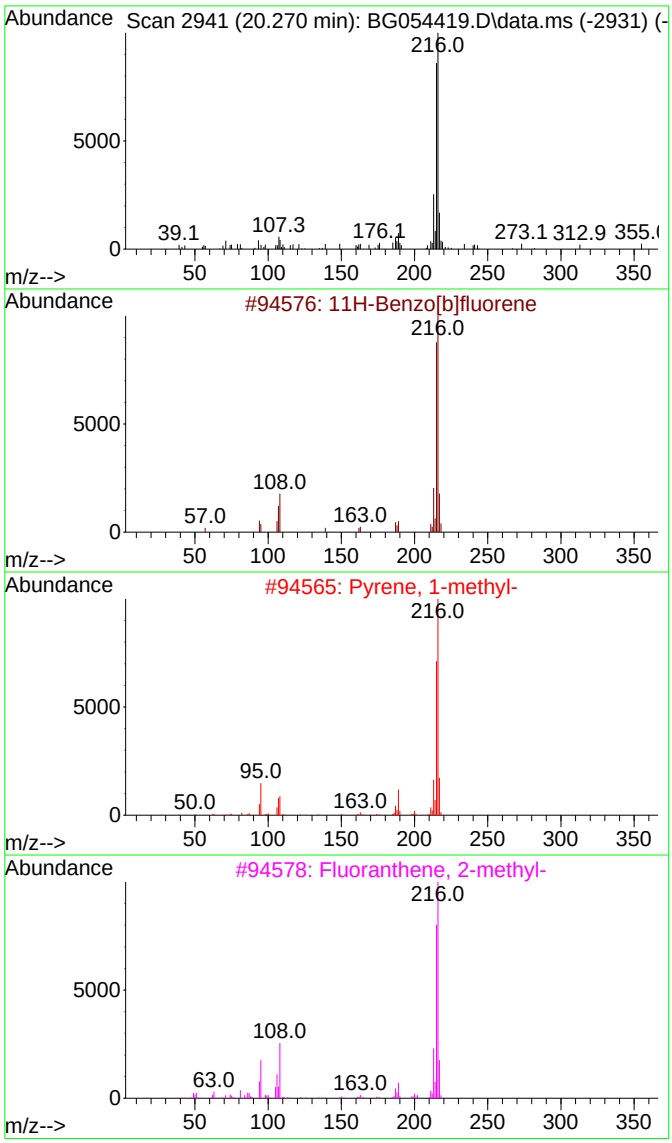
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

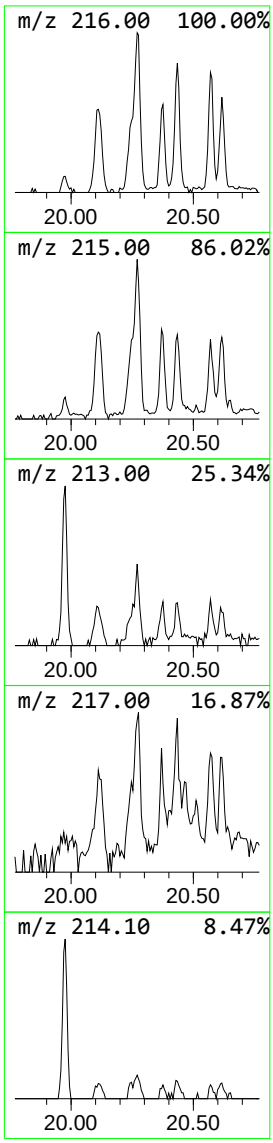
****

Peak Number 5 11H-Benzo[b]fluorene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.270	2.19 ng	65948	Chrysene-d12	21.627

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81
5	Benzoic acid, 3-(3,5-dimethyl-1-...	216	C12H12N2O2	312531-88-7	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072722\
Data File : BG054419.D
Acq On : 27 Jul 2022 17:03
Operator : CG/JU
Sample : N3891-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4553-E

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

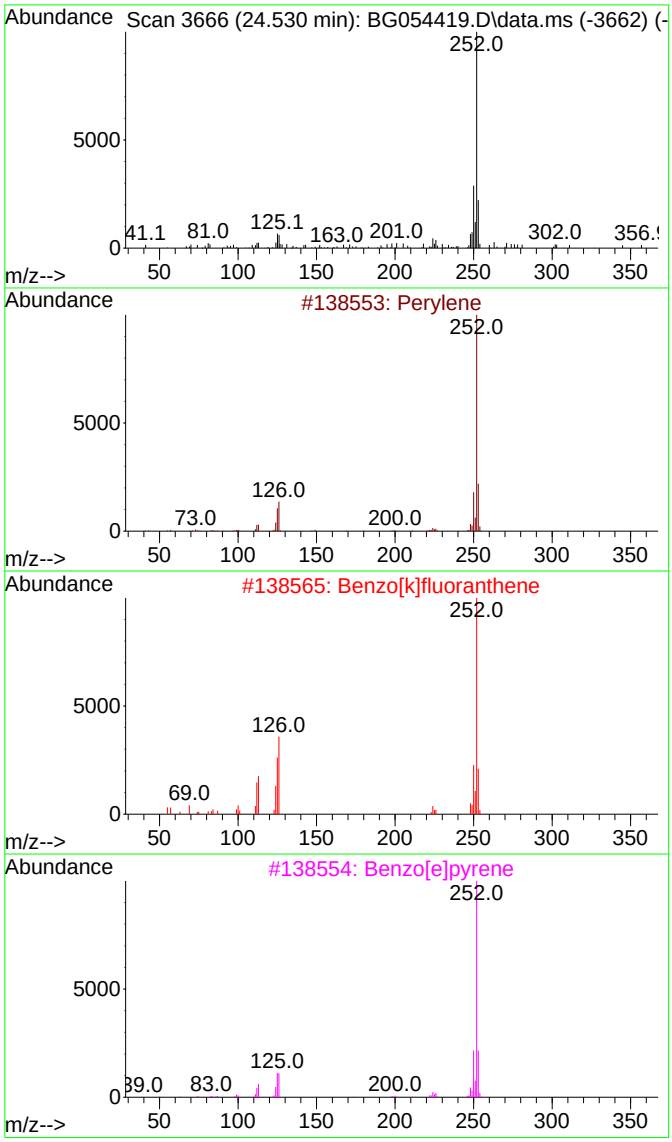
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

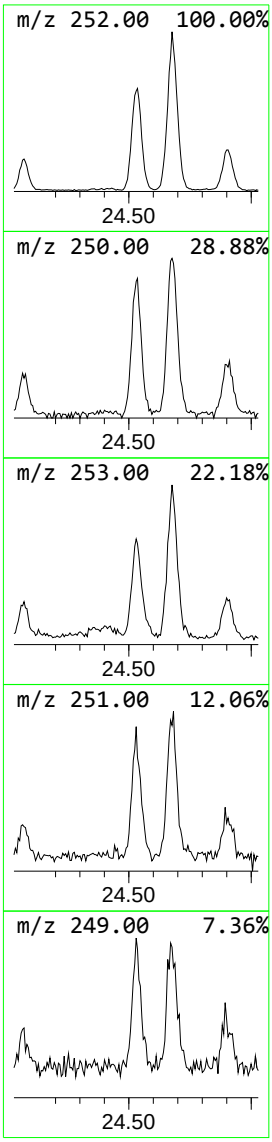
****

Peak Number 6 Perylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.530	6.95 ng	124340	Perylene-d12	24.829

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	81
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	81
3	Benzo[e]pyrene	252	C20H12	000192-97-2	81
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	81
5	(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072722\
Data File : BG054419.D
Acq On : 27 Jul 2022 17:03
Operator : CG/JU
Sample : N3891-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4553-E

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
unknown3.108	3.108	28.3	ng	137143	1	7.984	96797	20.0
2-Pentanone, 4-...	5.070	4.7	ng	22933	1	7.984	96797	20.0
Benzaldehyde, 3...	18.431	2.6	ng	41038	4	17.368	313911	20.0
11H-Benzo[b]flu...	20.270	2.2	ng	65948	5	21.627	603278	20.0
Perylene	24.530	7.0	ng	124340	6	24.829	357855	20.0