LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051024\
Data File : BG061168.D
Acq On : 10 May 2024 18:20
Operator : MA/JU
Sample : P2430-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-SS001-1224-01

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-BG043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061168.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.076	9	15	21	rBV4	10649	21550	2.07%	0.202%
2	3.147	22	27	42	rVB	210157	345745	33.16%	3.235%
3	3.670	112	116	123	rBV	19424	30877	2.96%	0.289%
4	5.526	425	432	439	rBV	303302	494638	47.44%	4.628%
5	7.107	693	701	710	rBV	333708	563453	54.04%	5.272%
6	7.929	833	841	848	rBV	119668	192396	18.45%	1.800%
7	9.087	1030	1038	1046	rBV	207658	368413	35.34%	3.447%
8	9.639	1125	1132	1138	rVB3	7678	12642	1.21%	0.118%
9	10.726	1308	1317	1324	rBV	153553	270641	25.96%	2.532%
10	11.461	1436	1442	1451	rBV4	9151	18464	1.77%	0.173%
11	13.182	1728	1735	1741	rBV	500024	749256	71.87%	7.010%
12	14.557	1957	1969	1976	rBV	242439	381193	36.56%	3.566%
13	14.622	1976	1980	1986	rVB	10638	16457	1.58%	0.154%
14	14.763	1999	2004	2005	rBV3	10118	13241	1.27%	0.124%
15	14.780	2005	2007	2012	rVB2	10604	12241	1.17%	0.115%
16	14.962	2033	2038	2042	rVB2	7843	12211	1.17%	0.114%
17	15.609	2142	2148	2153	rBV5	8745	14670	1.41%	0.137%
18	16.049	2217	2223	2233	rBV	445768	701647	67.30%	6.565%
19	16.296	2258	2265	2270	rVB4	8933	20155	1.93%	0.189%
20	16.960	2374	2378	2383	rBV2	11017	15918	1.53%	0.149%
21	17.066	2388	2396	2401	rVV6	4644	11129	1.07%	0.104%
22	17.124	2401	2406	2414	rVB2	9476	15016	1.44%	0.140%
23	17.224	2419	2423	2427	rBV4	8500	11240	1.08%	0.105%
24	17.307	2431	2437	2441	rBV	299022	469352	45.02%	4.391%
25	17.348	2441	2444	2451	rVV	184572	262718	25.20%	2.458%
26	17.442	2451	2460	2466	rVV	19498	35211	3.38%	0.329%
27	17.501	2466	2470	2475	rVB3	8770	12287	1.18%	0.115%
28	17.712	2498	2506	2511	rBV	28310	50053	4.80%	0.468%
29	18.182	2583	2586	2588	rBV	12985	15244	1.46%	0.143%
30	18.229	2588	2594	2599	rVB2	25911	53704	5.15%	0.502%
31	18.382	2614	2620	2623	rBV4	28954	49137	4.71%	0.460%
32	18.417	2624	2626	2631	rVB	12279	13495	1.29%	0.126%
33	18.681	2665	2671	2674	rBV	15797	24907	2.39%	0.233%
34	18.723	2674	2678	2683	rVB2	44111	63352	6.08%	0.593%
35	19.105	2738	2743	2746	rVV3	13247	21628	2.07%	0.202%
36	19.240	2762	2766	2773	rVB3	18570	27324	2.62%	0.256%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051024\
Data File : BG061168.D
Acq On : 10 May 2024 18:20
Operator : MA/JU
Sample : P2430-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-SS001-1224-01

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-BG043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.363	2781	2787	2793	rBV	411980	573239	54.98%	5.363%
38	19.463	2800	2804	2808	rVB4	10506	12652	1.21%	0.118%
39	19.563	2815	2821	2825	rBV7	9399	18958	1.82%	0.177%
40	19.610	2825	2829	2832	rVV	11201	11869	1.14%	0.111%
41	19.727	2838	2849	2857	rBV	318075	547748	52.54%	5.125%
42	19.798	2857	2861	2868	rVB3	15231	25581	2.45%	0.239%
43	19.927	2874	2883	2888	rBV	791545	1042578	100.00%	9.754%
44	20.056	2898	2905	2910	rBV2	20134	51794	4.97%	0.485%
45	20.097	2910	2912	2917	rBV4	7594	13075	1.25%	0.122%
46	20.186	2923	2927	2928	rBV4	11816	15366	1.47%	0.144%
47	20.221	2929	2933	2939	rVB2	34985	58993	5.66%	0.552%
48	20.321	2945	2950	2955	rBV	24004	40481	3.88%	0.379%
49	20.380	2955	2960	2963	rVV2	26690	45052	4.32%	0.422%
50	20.415	2964	2966	2969	rVB4	16094	16048	1.54%	0.150%
51	20.521	2981	2984	2987	rBV	13015	15935	1.53%	0.149%
52	20.568	2988	2992	2995	rBV3	15101	21540	2.07%	0.202%
53	20.732	3018	3020	3023	rVB3	15792	14954	1.43%	0.140%
54	20.973	3057	3061	3068	rVB3	38995	65215	6.26%	0.610%
55	21.155	3087	3092	3096	rBV2	30364	51983	4.99%	0.486%
56	21.196	3096	3099	3102	rVV2	18347	26233	2.52%	0.245%
57	21.237	3102	3106	3112	rVV3	56527	119733	11.48%	1.120%
58	21.302	3113	3117	3125	rVB	48662	79782	7.65%	0.746%
59	21.566	3154	3162	3167	rBV2	367579	820865	78.73%	7.680%
60	21.613	3167	3170	3178	rVB	161191	259341	24.87%	2.426%
61	21.760	3192	3195	3200	rVB3	29428	43073	4.13%	0.403%
62	21.819	3203	3205	3210	rBV5	12460	17502	1.68%	0.164%
63	22.360	3290	3297	3303	rBV7	32519	74191	7.12%	0.694%
64	23.705	3519	3526	3534	rBV2	125598	417451	40.04%	3.906%
65	24.398	3639	3644	3656	rVB2	58012	173634	16.65%	1.625%
66	24.545	3663	3669	3680	rVB	67314	196253	18.82%	1.836%
67	24.692	3687	3694	3711	rVB2	125871	425661	40.83%	3.982%

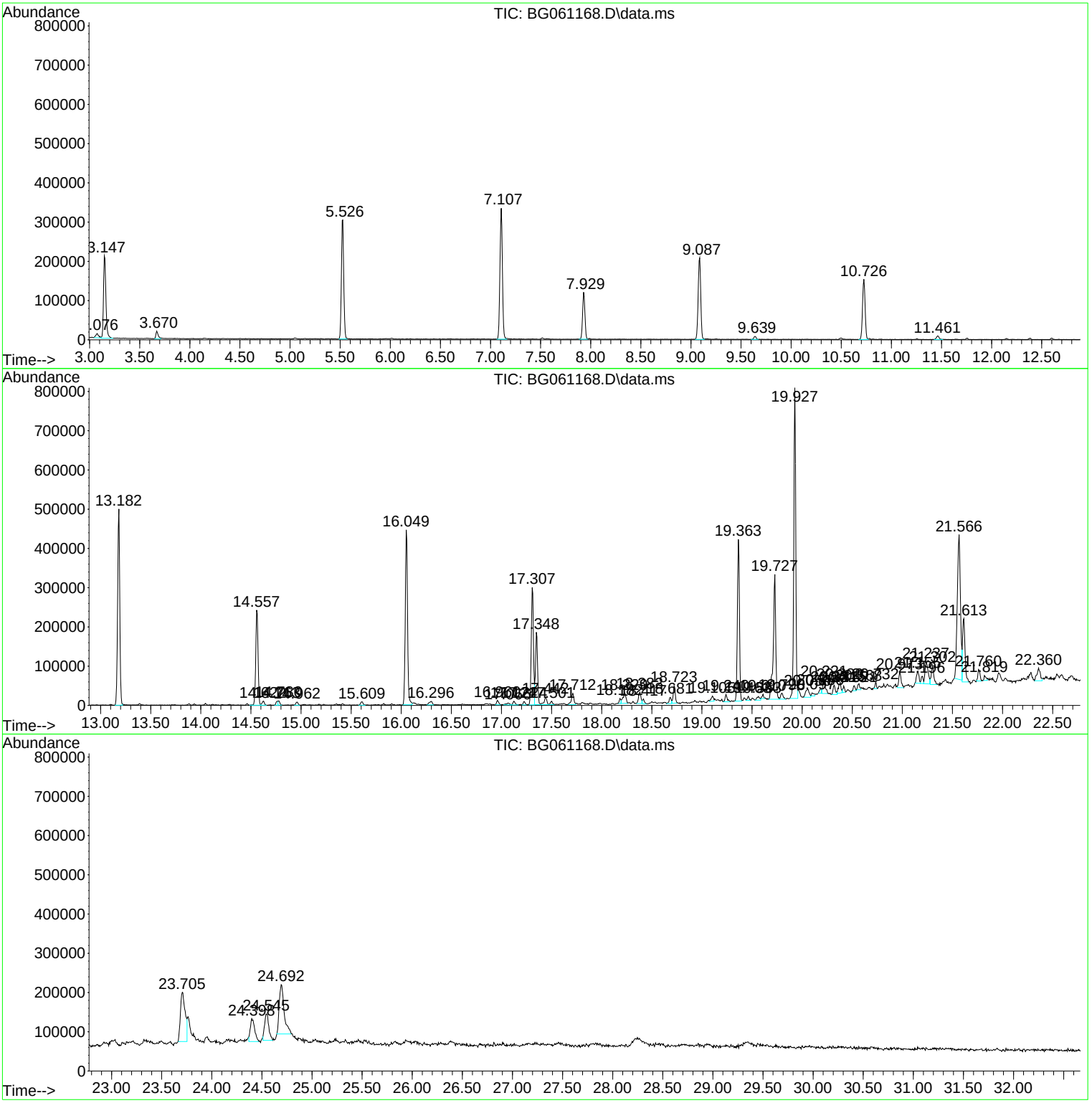
Sum of corrected areas: 10688385

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051024\
Data File : BG061168.D
Acq On : 10 May 2024 18:20
Operator : MA/JU
Sample : P2430-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-SS001-1224-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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\BG051024\
Data File : BG061168.D
Acq On : 10 May 2024 18:20
Operator : MA/JU
Sample : P2430-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-SS001-1224-01

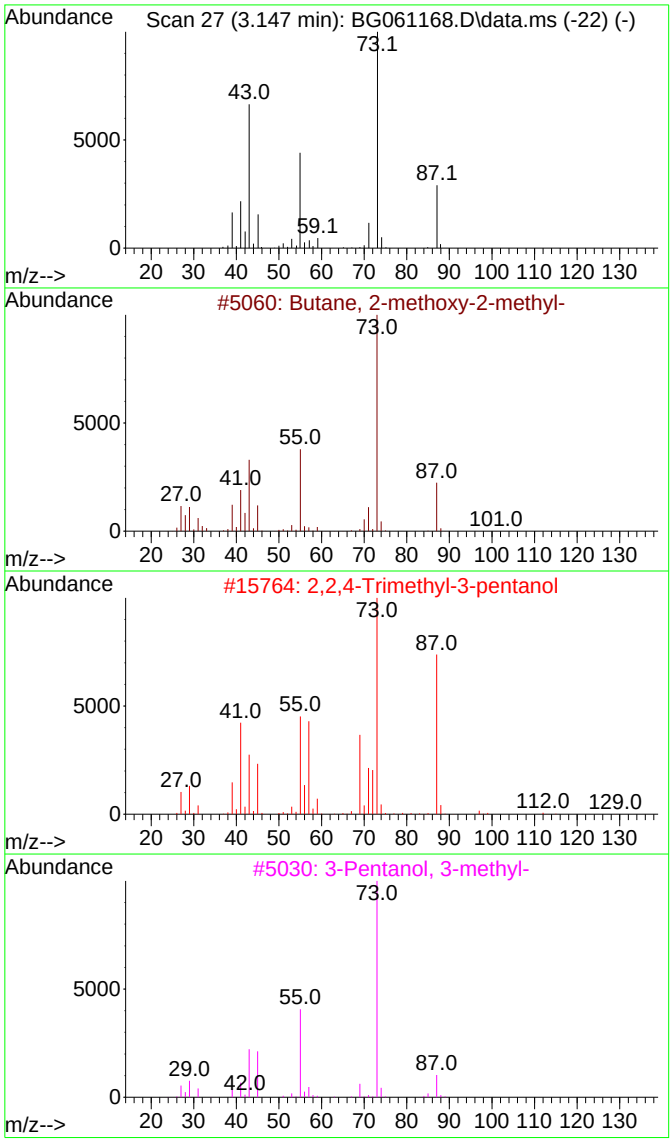
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

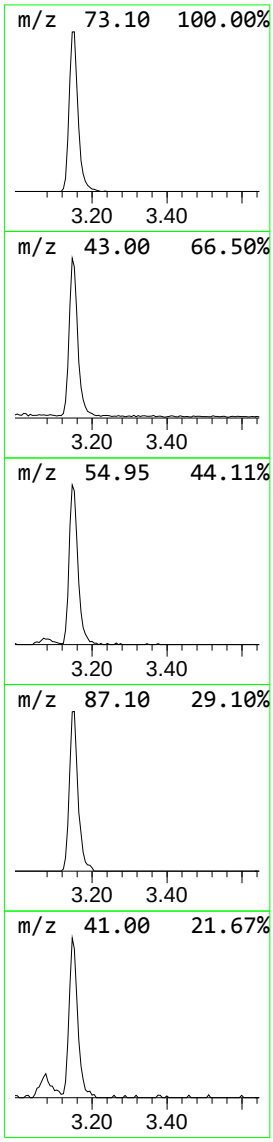
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.147	35.94 ng	345745	1,4-Dichlorobenzene-d4	7.929

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	28
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051024\
Data File : BG061168.D
Acq On : 10 May 2024 18:20
Operator : MA/JU
Sample : P2430-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-SS001-1224-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

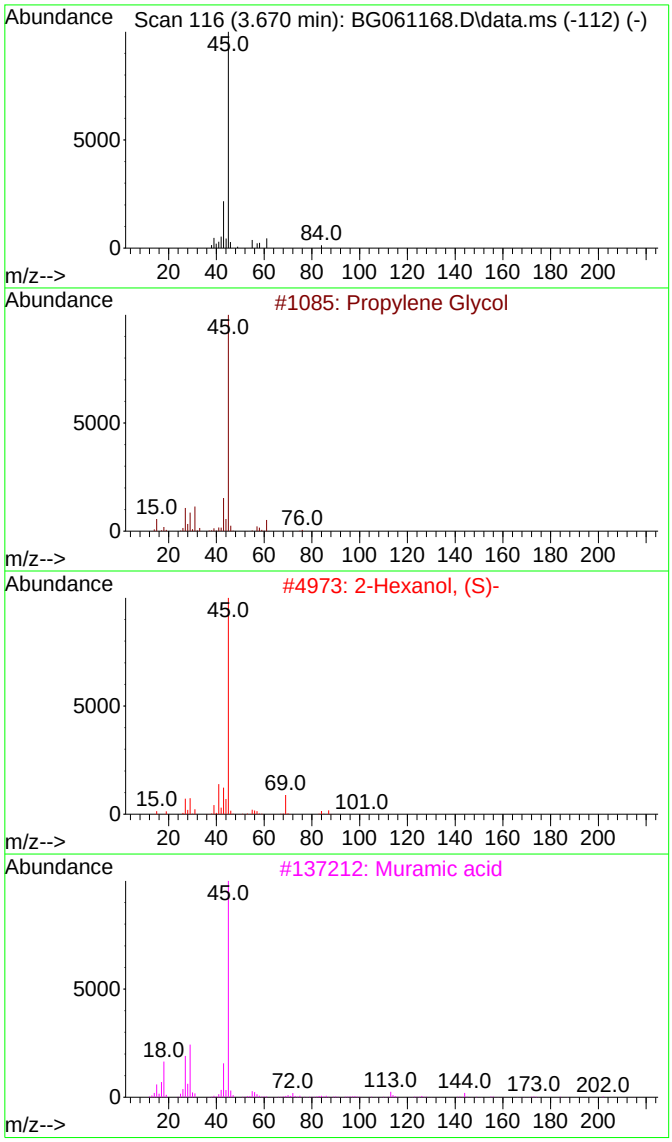
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

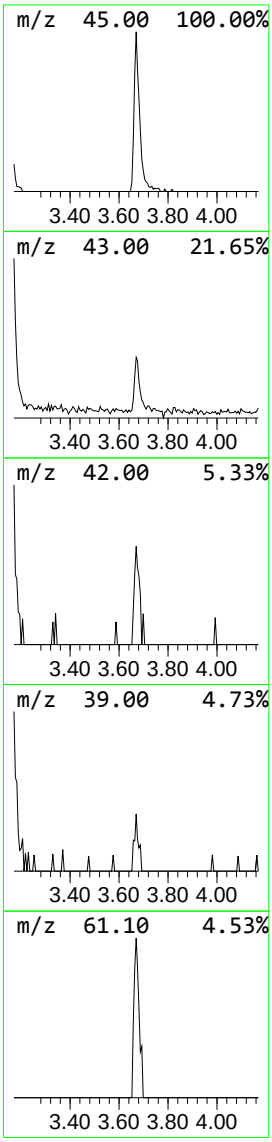
****

Peak Number 3 unknown3.670 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.670	3.21 ng	30877	1,4-Dichlorobenzene-d4	7.929

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	9
2	2-Hexanol, (S)-	102	C6H14O	052019-78-0	9
3	Muramic acid	251	C9H17NO7	001114-41-6	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051024\
Data File : BG061168.D
Acq On : 10 May 2024 18:20
Operator : MA/JU
Sample : P2430-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-SS001-1224-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

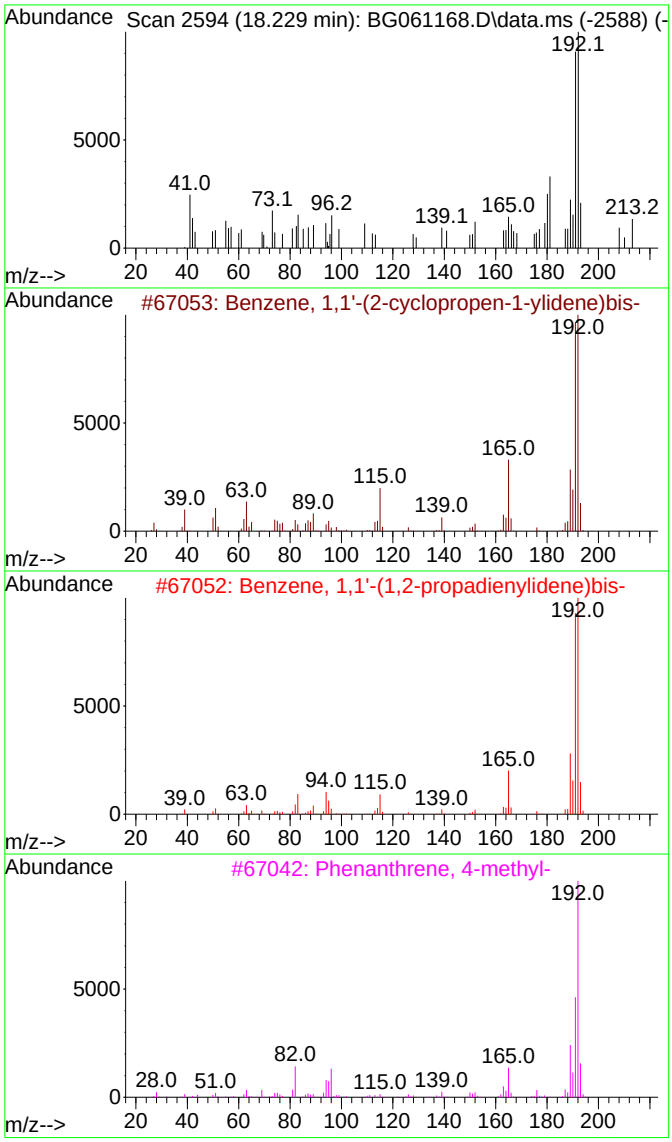
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

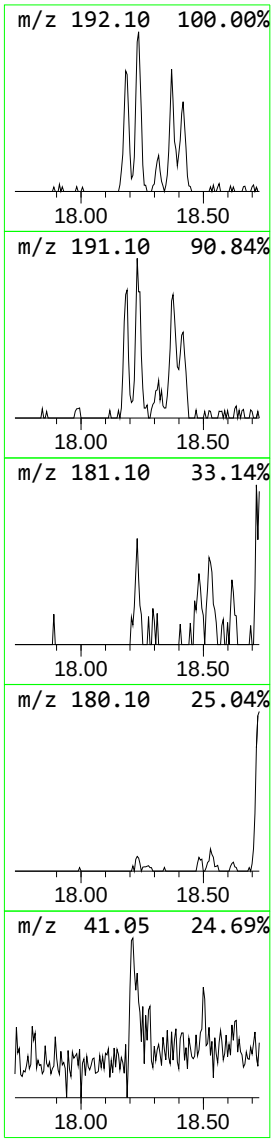
****

Peak Number 4 Benzene, 1,1'-(2-cycloprope... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.229	2.29 ng	53704	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(2-cyclopropen-1-y...	192	C15H12	022825-21-4	64
2	Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	62
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	55
4	2-(4-Fluorobenzyl)thiophene	192	C11H9FS	063877-96-3	52
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051024\
Data File : BG061168.D
Acq On : 10 May 2024 18:20
Operator : MA/JU
Sample : P2430-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-SS001-1224-01

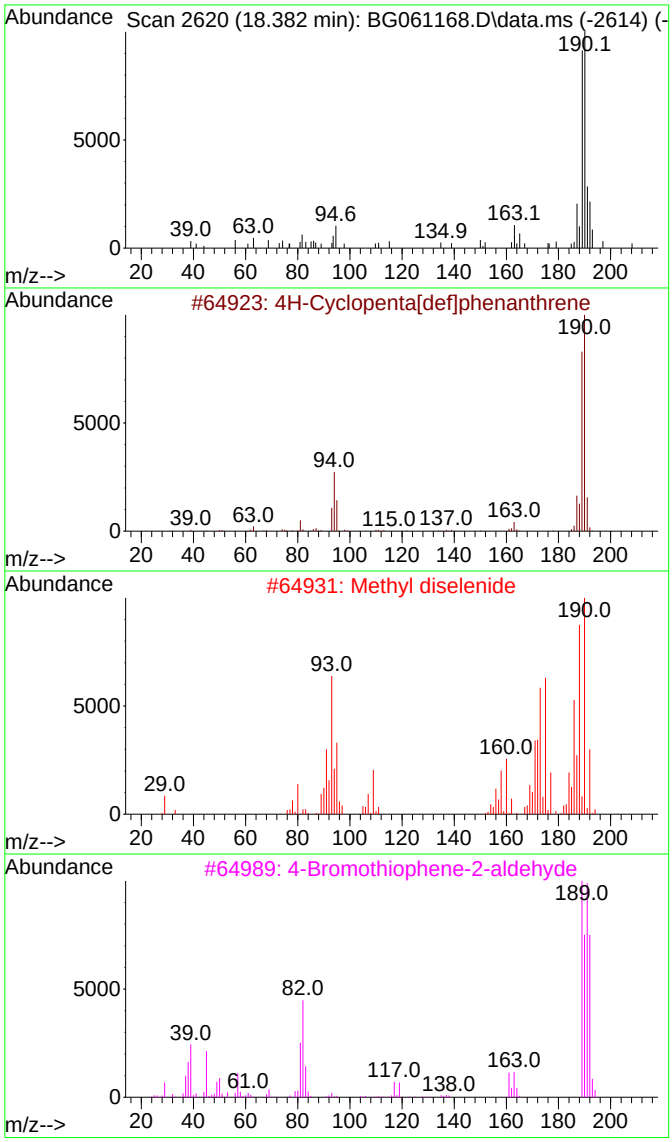
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

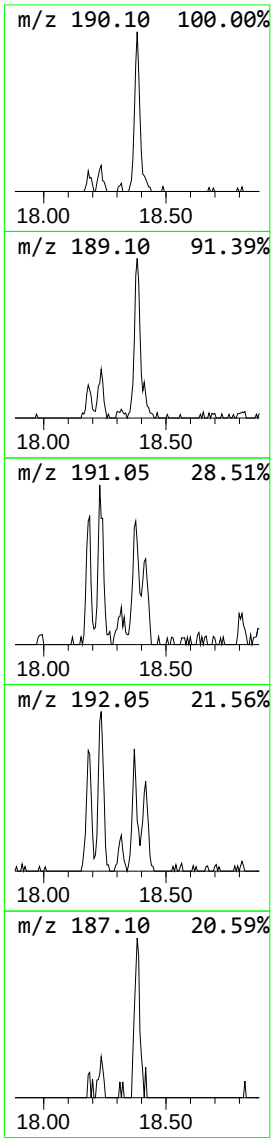
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.382	2.09 ng	49137	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	Methyl diselenide	190	C2H6Se2	007101-31-7	43
3	4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	40
4	8H-Imidazo[4,5-E]-2,1,3-benzothi...	190	C8H6N4S	129485-68-3	25
5	Carbonic acid, 2-formyl-4,6-dich...	276	C11H10Cl2O4	1000331-39-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051024\
Data File : BG061168.D
Acq On : 10 May 2024 18:20
Operator : MA/JU
Sample : P2430-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-SS001-1224-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

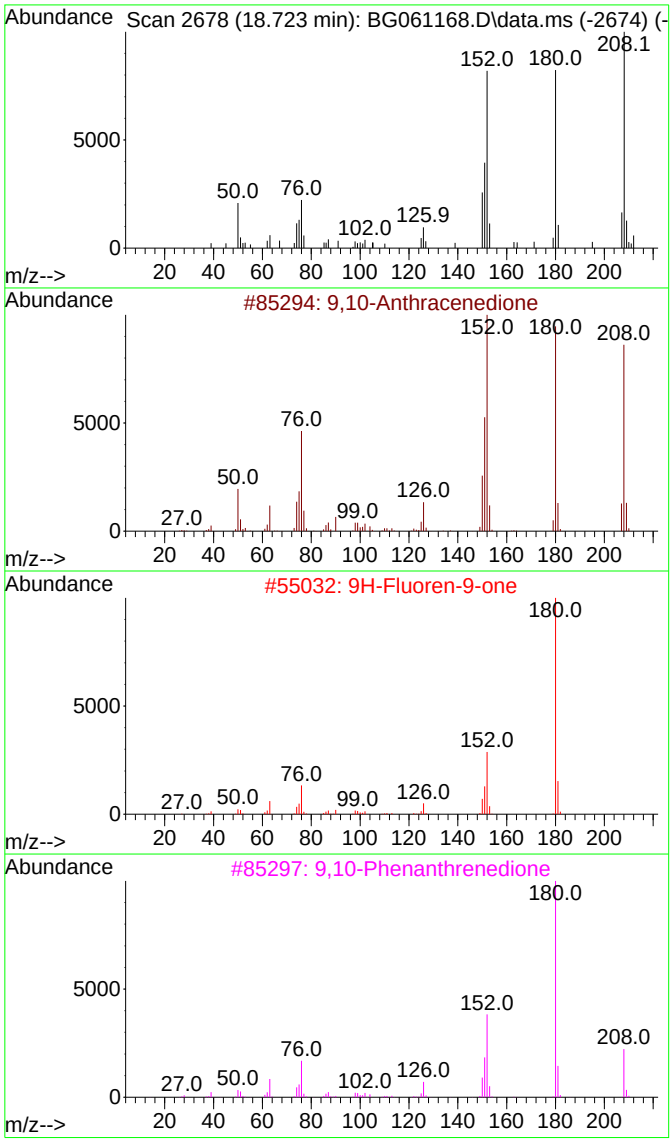
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

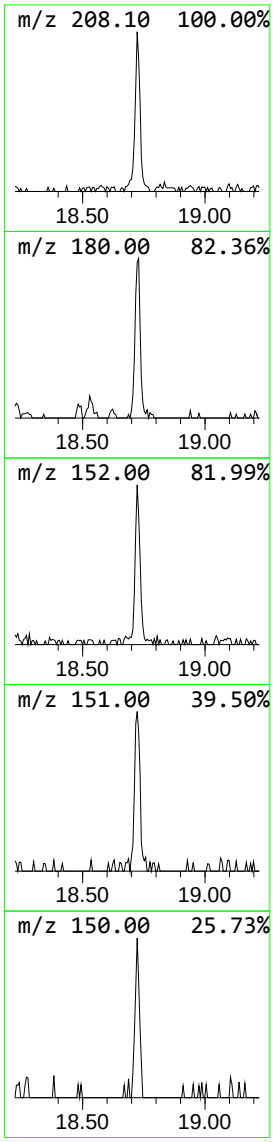
****

Peak Number 6 9,10-Anthracenedione Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.723	2.70 ng	63352	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	97
2	9H-Fluoren-9-one	180	C13H8O	000486-25-9	86
3	9,10-Phenanthrenedione	208	C14H8O2	000084-11-7	64
4	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	64
5	1,4-Anthracenedione	208	C14H8O2	000635-12-1	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051024\
Data File : BG061168.D
Acq On : 10 May 2024 18:20
Operator : MA/JU
Sample : P2430-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-SS001-1224-01

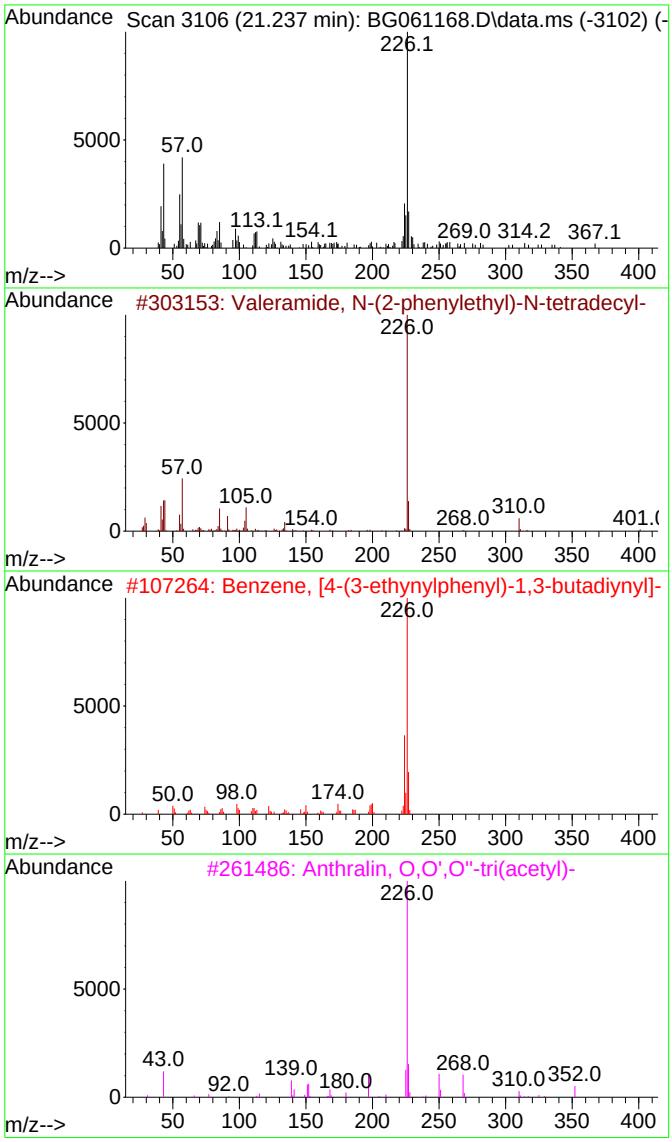
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

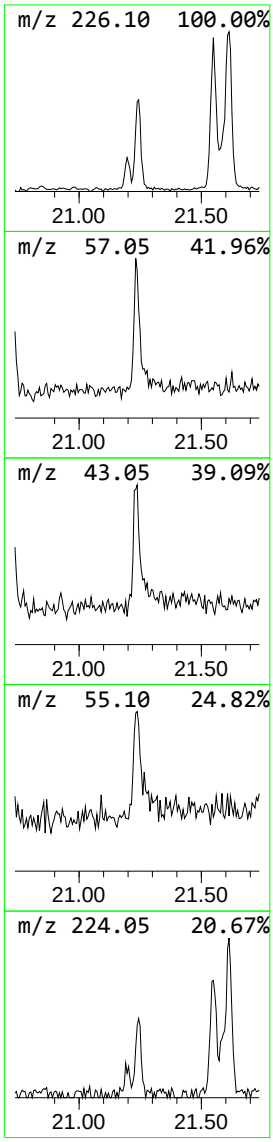
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Valeramide, N-(2-phenylethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.237	2.92 ng	119733	Chrysene-d12	21.566

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Valeramide, N-(2-phenylethyl)-N-...	401	C27H47NO	1000451-53-7	53
2	Benzene, [4-(3-ethynylphenyl)-1,...	226	C18H10	1000115-87-3	52
3	Anthralin, O,O',O''-tri(acetyl)-	352	C20H16O6	1010374-77-5	50
4	p-Anisaldehyde phenylhydrazone	226	C14H14N2O	000622-73-1	50
5	9H-Xanthen-9-one, 3-methoxy-	226	C14H10O3	003722-52-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051024\
Data File : BG061168.D
Acq On : 10 May 2024 18:20
Operator : MA/JU
Sample : P2430-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-SS001-1224-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

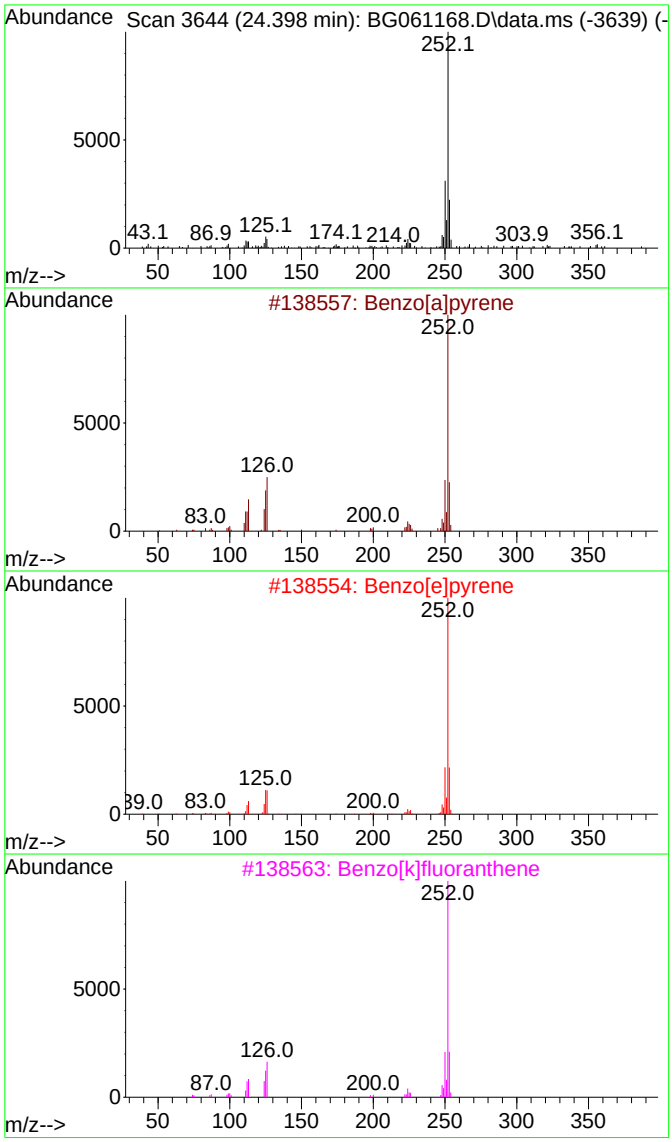
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

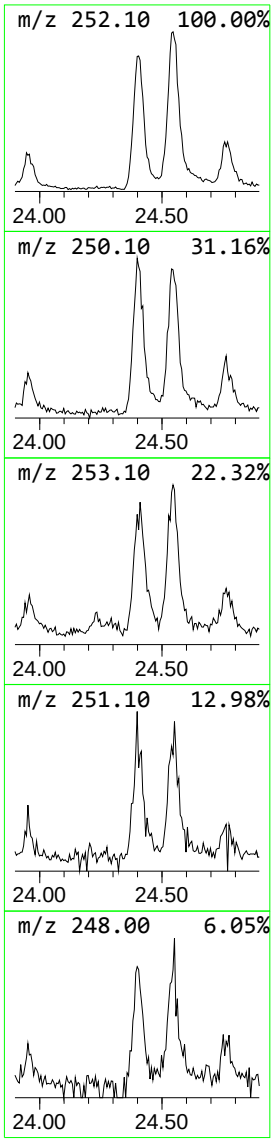
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.398	8.16 ng	173634	Perylene-d12	24.692

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	93
2	Benzo[e]pyrene	252	C20H12	000192-97-2	90
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
5	Perylene	252	C20H12	000198-55-0	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051024\
Data File : BG061168.D
Acq On : 10 May 2024 18:20
Operator : MA/JU
Sample : P2430-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-SS001-1224-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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...	3.147	35.9	ng	345745	1	7.929	192396	20.0
unknown3.670	3.670	3.2	ng	30877	1	7.929	192396	20.0
Benzene, 1,1'-(...	18.229	2.3	ng	53704	4	17.307	469352	20.0
4H-Cyclopenta[d...	18.382	2.1	ng	49137	4	17.307	469352	20.0
9,10-Anthracene...	18.723	2.7	ng	63352	4	17.307	469352	20.0
Valeramide, N-(...	21.237	2.9	ng	119733	5	21.566	820865	20.0
Benzo[e]pyrene	24.398	8.2	ng	173634	6	24.692	425661	20.0