

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112922\
 Data File : BG055835.D
 Acq On : 29 Nov 2022 19:27
 Operator : CG/JU
 Sample : N5791-01 5X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WSH-STOCK-1128

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: BG055835.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.274	332	338	347	rBV	82486	127424	11.45%	1.406%
2	5.756	412	420	433	rBV	125463	207255	18.63%	2.287%
3	7.372	688	695	707	rBV	123615	222710	20.02%	2.457%
4	8.224	833	840	847	rVB	193431	325936	29.30%	3.596%
5	9.393	1031	1039	1050	rBV	74645	137268	12.34%	1.515%
6	10.803	1273	1279	1300	rBV4	8687	32914	2.96%	0.363%
7	11.050	1312	1321	1335	rBV	272593	497368	44.71%	5.488%
8	13.471	1726	1733	1745	rBV	233125	349298	31.40%	3.854%
9	14.845	1957	1967	1974	rBV	443625	703404	63.23%	7.761%
10	14.910	1974	1978	1985	rVB2	14495	22455	2.02%	0.248%
11	15.245	2030	2035	2039	rVB3	7335	11941	1.07%	0.132%
12	15.891	2139	2145	2155	rVB	19159	32170	2.89%	0.355%
13	16.185	2190	2195	2202	rVB3	8488	14978	1.35%	0.165%
14	16.332	2214	2220	2231	rBV	159758	252547	22.70%	2.787%
15	16.884	2307	2314	2319	rBV3	8683	17310	1.56%	0.191%
16	17.407	2399	2403	2411	rVB2	9273	14959	1.34%	0.165%
17	17.589	2427	2434	2438	rBV	544735	827269	74.37%	9.128%
18	17.630	2438	2441	2447	rVV	166609	238957	21.48%	2.637%
19	17.724	2451	2457	2462	rVV	38409	60629	5.45%	0.669%
20	17.989	2496	2502	2509	rBV3	9577	23032	2.07%	0.254%
21	18.165	2527	2532	2537	rVV2	8599	13366	1.20%	0.147%
22	18.459	2577	2582	2586	rBV	43545	68398	6.15%	0.755%
23	18.506	2586	2590	2597	rVB	51393	75539	6.79%	0.833%
24	18.588	2597	2604	2609	rBV2	19327	30911	2.78%	0.341%
25	18.659	2609	2616	2619	rBV3	57699	115409	10.37%	1.273%
26	18.688	2619	2621	2627	rVB2	30187	35269	3.17%	0.389%
27	18.853	2645	2649	2653	rBV5	16721	21121	1.90%	0.233%
28	18.947	2661	2665	2669	rBV	25462	32687	2.94%	0.361%
29	18.994	2669	2673	2680	rVB3	18510	28910	2.60%	0.319%
30	19.187	2703	2706	2711	rVB3	11465	15471	1.39%	0.171%
31	19.240	2711	2715	2718	rBV	14100	18637	1.68%	0.206%
32	19.281	2718	2722	2727	rVB3	11720	15353	1.38%	0.169%
33	19.358	2731	2735	2742	rBV	37745	75544	6.79%	0.834%
34	19.417	2742	2745	2746	rBV3	11318	13348	1.20%	0.147%
35	19.511	2754	2761	2773	rBV7	19023	57825	5.20%	0.638%
36	19.628	2775	2781	2786	rBV	337497	459066	41.27%	5.065%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112922\
Data File : BG055835.D
Acq On : 29 Nov 2022 19:27
Operator : CG/JU
Sample : N5791-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WSH-STOCK-1128

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	19.716	2794	2796	2800	rVB4	14040	16007	1.44%	0.177%
38	19.957	2832	2837	2838	rBV2	54592	76934	6.92%	0.849%
39	19.986	2838	2842	2850	rVV	274264	427471	38.43%	4.717%
40	20.057	2850	2854	2857	rVB2	21608	32693	2.94%	0.361%
41	20.169	2868	2873	2878	rBV	390049	513986	46.20%	5.671%
42	20.310	2890	2897	2904	rBV4	31174	84423	7.59%	0.932%
43	20.474	2922	2925	2931	rVB	64839	83547	7.51%	0.922%
44	20.574	2938	2942	2945	rBV2	52773	64310	5.78%	0.710%
45	20.774	2972	2976	2980	rBV2	32108	48216	4.33%	0.532%
46	21.878	3156	3164	3169	rBV2	551624	1112431	100.00%	12.274%
47	21.925	3169	3172	3180	rVB	123569	193765	17.42%	2.138%
48	24.182	3551	3556	3563	rBV	58168	173086	15.56%	1.910%
49	25.104	3708	3713	3723	rVB	75823	198906	17.88%	2.195%
50	25.269	3732	3741	3750	rBV2	292143	840600	75.56%	9.275%

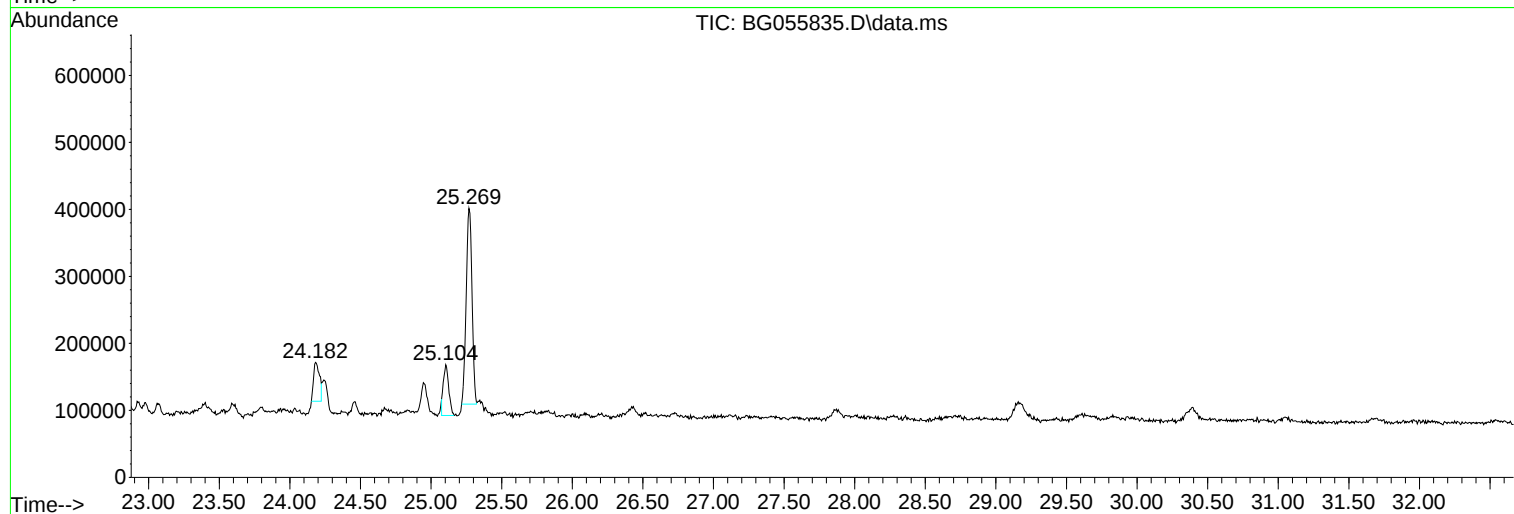
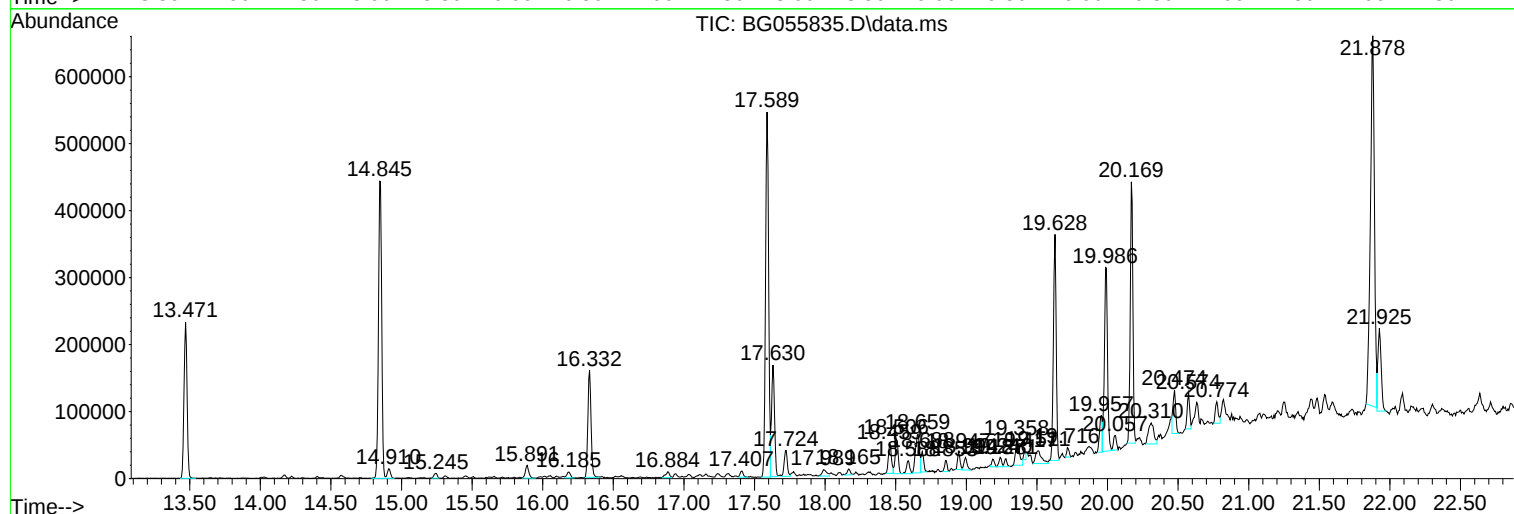
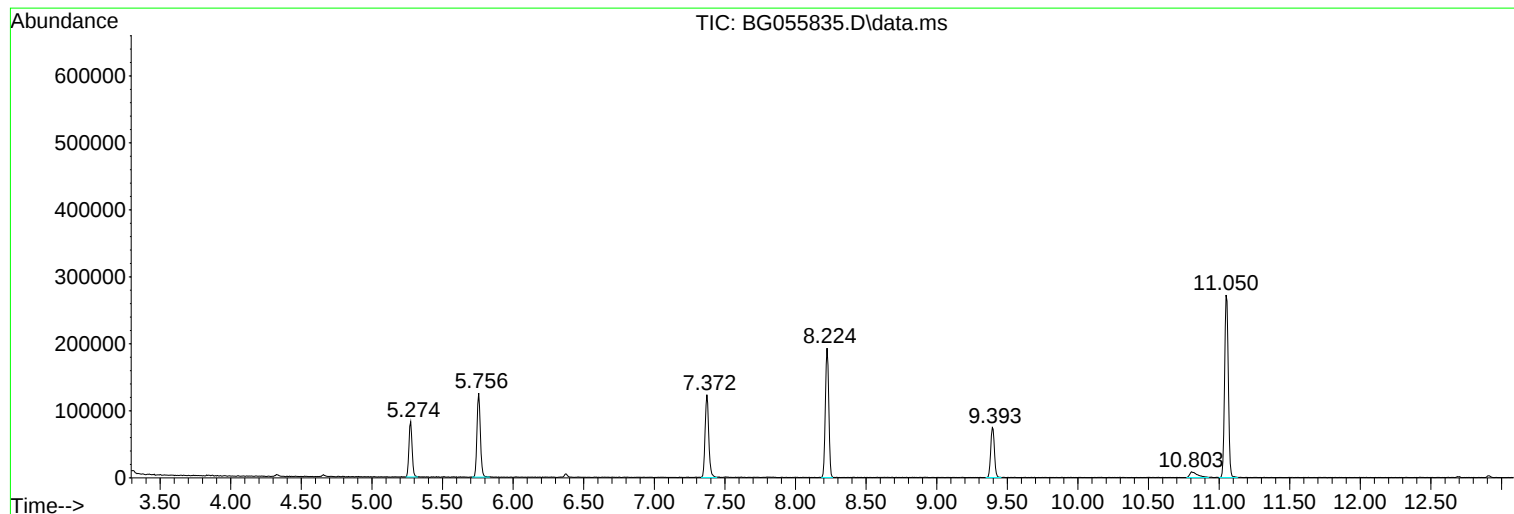
Sum of corrected areas: 9063053

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112922\
Data File : BG055835.D
Acq On : 29 Nov 2022 19:27
Operator : CG/JU
Sample : N5791-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WSH-STOCK-1128

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.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\BG112922\
Data File : BG055835.D
Acq On : 29 Nov 2022 19:27
Operator : CG/JU
Sample : N5791-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WSH-STOCK-1128

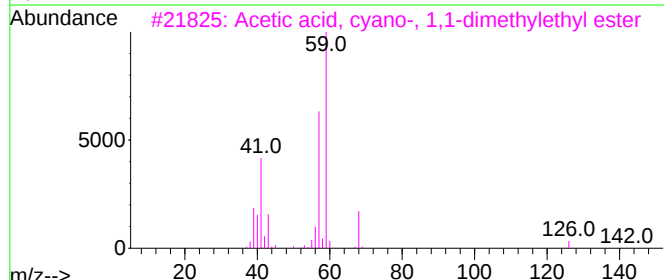
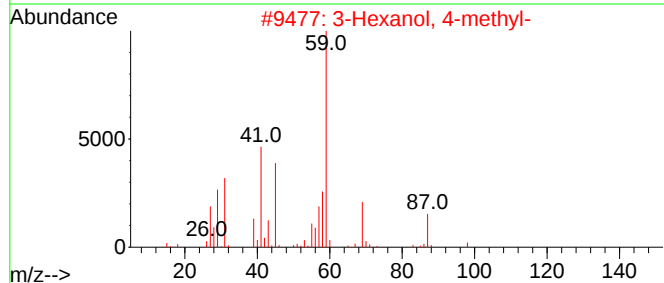
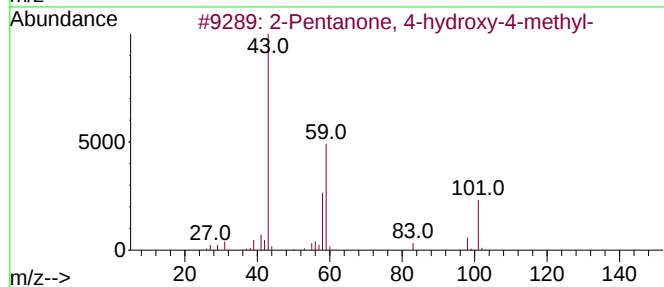
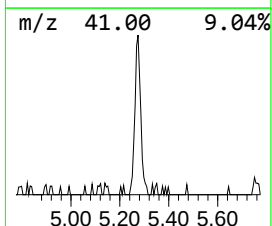
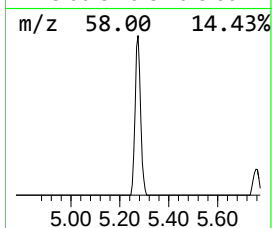
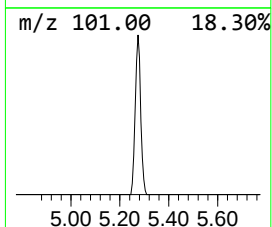
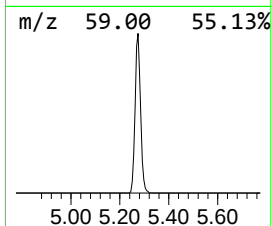
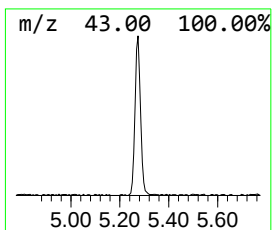
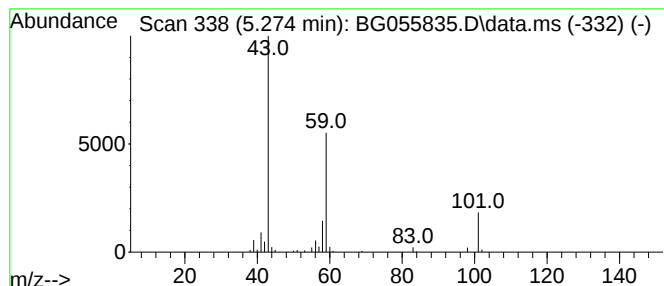
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.274	7.82 ng	127424	1,4-Dichlorobenzene-d4	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112922\
Data File : BG055835.D
Acq On : 29 Nov 2022 19:27
Operator : CG/JU
Sample : N5791-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

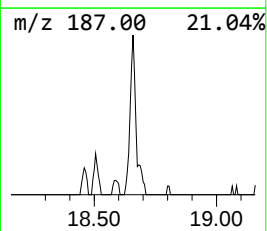
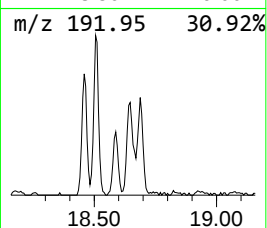
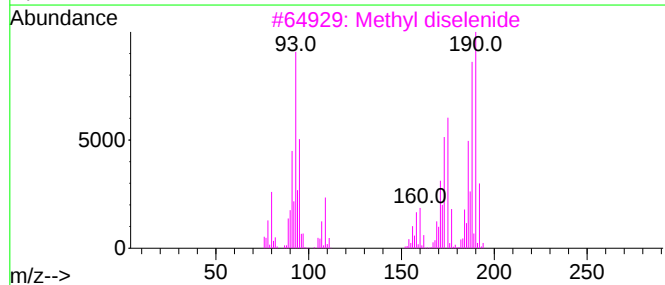
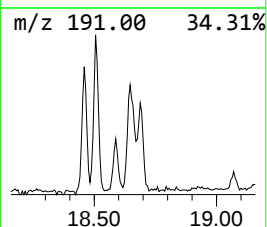
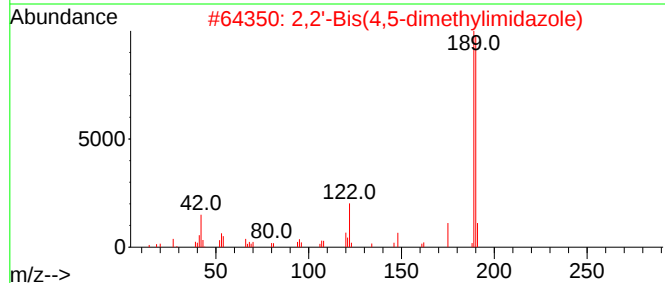
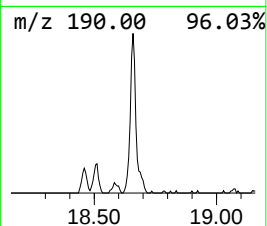
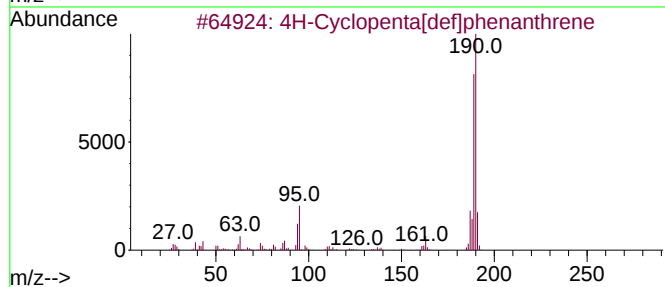
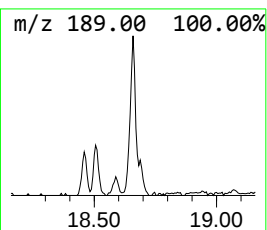
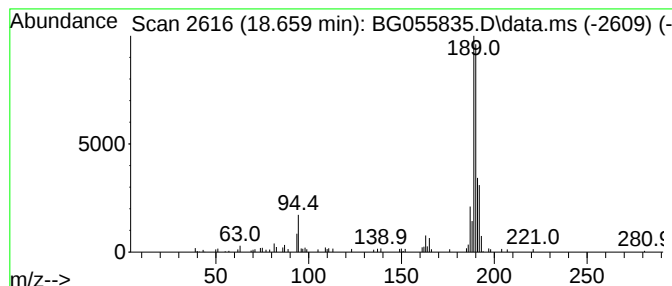
Instrument :
BNA_G
ClientSampleId :
WSH-STOCK-1128

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.659	2.79 ng	115409	Phenanthrene-d10	17.589	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	89
2	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	50
3	Methyl diselenide	190	C2H6Se2	007101-31-7	46
4	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	27
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112922\
Data File : BG055835.D
Acq On : 29 Nov 2022 19:27
Operator : CG/JU
Sample : N5791-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WSH-STOCK-1128

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.274	7.8	ng	127424	1	8.224	325936	20.0
4H-Cyclopenta[d...	18.659	2.8	ng	115409	4	17.589	827269	20.0