

Data Path : Z:\HPCHEM1\BNA G\DATA\BG022318\
 Data File : BG032798.D
 Acq On : 23 Feb 2018 20:11
 Operator : SJ/JU
 Sample : J1632-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EFF-180220-01

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:\HPCHEM1\BNA_G\METHODS\8270-BG022118.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.520	31	39	49	rBV	130920	287422	5.24%	1.188%
2	3.614	49	55	73	rVB	889130	1493348	27.21%	6.175%
3	5.828	427	432	442	rVB	49242	88217	1.61%	0.365%
4	6.333	509	518	527	rBV	386247	663934	12.10%	2.745%
5	8.013	794	804	814	rBV	235086	423640	7.72%	1.752%
6	8.319	849	856	863	rVB	57478	100247	1.83%	0.415%
7	8.431	867	875	887	rVV	738595	1341317	24.44%	5.546%
8	8.924	952	959	970	rBV	226792	407701	7.43%	1.686%
9	9.265	1008	1017	1026	rVB	1032757	1917172	34.93%	7.927%
10	10.122	1155	1163	1177	rVB	785774	1480170	26.97%	6.120%
11	11.814	1443	1451	1462	rVB	315794	590397	10.76%	2.441%
12	14.170	1843	1852	1860	rBV	2125400	3512514	63.99%	14.524%
13	15.539	2078	2085	2094	rVB2	476140	778506	14.18%	3.219%
14	16.302	2208	2215	2222	rBV	137367	213312	3.89%	0.882%
15	17.007	2328	2335	2349	rBV	1171276	1810286	32.98%	7.485%
16	18.264	2541	2549	2560	rVB2	632165	1015946	18.51%	4.201%
17	20.790	2972	2979	2988	rBV	4107126	5488962	100.00%	22.697%
18	22.623	3284	3291	3304	rVB	616308	1197331	21.81%	4.951%
19	23.974	3514	3521	3529	rVB	72801	148341	2.70%	0.613%
20	26.441	3928	3941	3960	rBV2	354906	1225372	22.32%	5.067%

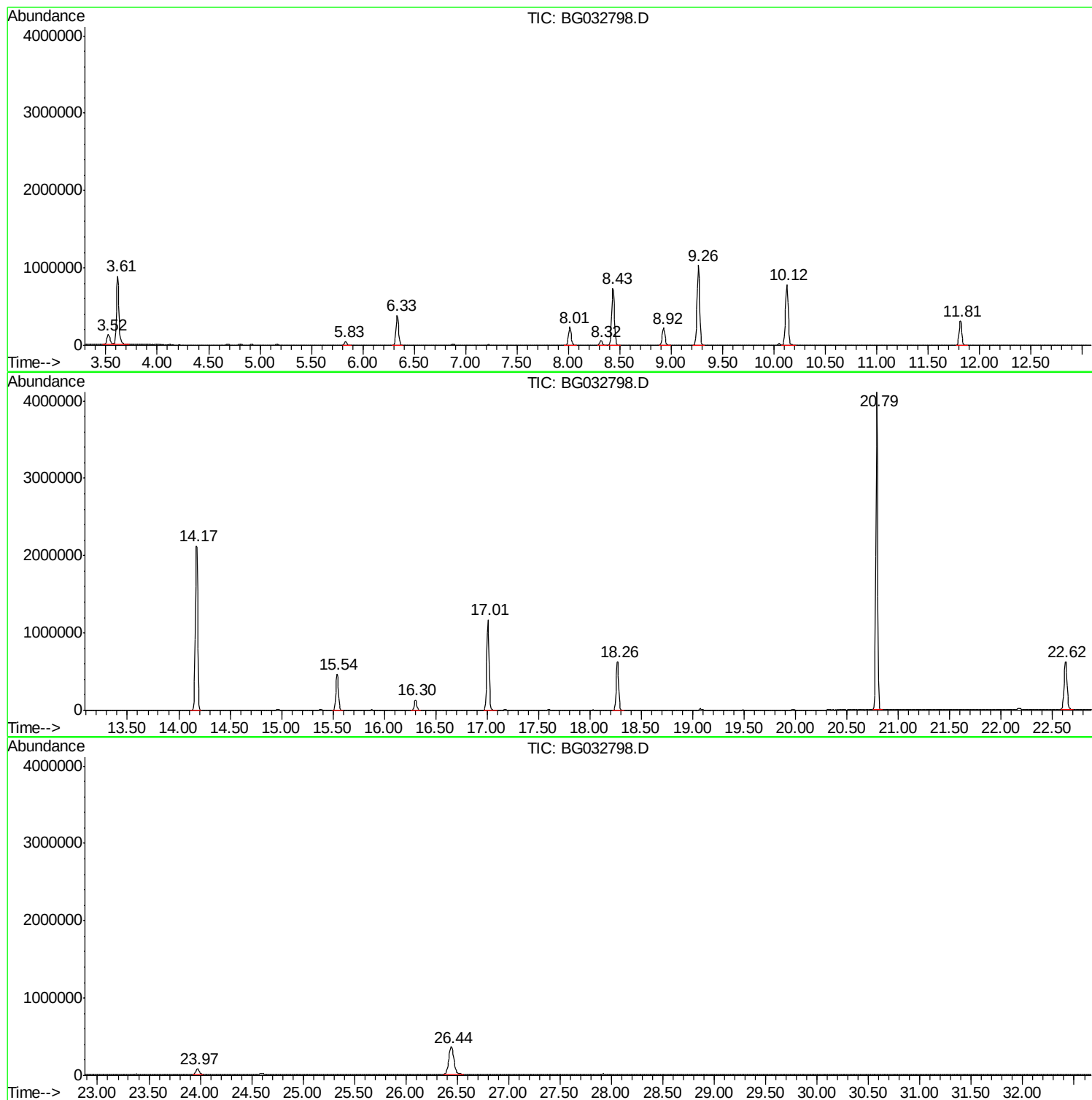
Sum of corrected areas: 24184135

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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG022118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.61	73.26 ng	1493350	1,4-Dichlorobenzene-d4	8.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.83	4.33 ng	88217	1,4-Dichlorobenzene-d4	8.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			(2,3,3-Trimethyloxiranyl)methanol	116	C6H12O2	1000306-64-7	38
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17

Peak Number 3 .alpha.-Methylstyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.32	4.92 ng	100247	1,4-Dichlorobenzene-d4	8.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Methylstyrene	118	C9H10	000098-83-9	94
2			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	64
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	53
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	022250-74-4	52
5			Benzeneethanol, .beta.-ethenyl-....	162	C11H14O	040596-14-3	50

Peak Number 4 unknown8.43 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
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8.43	65.80 ng	1341320	1,4-Dichlorobenzene-d4	8.92
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		3-Chloro-6-fluoro-pyrazine	132 C4H2ClFN2	1000146-10-7 27
2		5-Aminoindole	132 C8H8N2	005192-03-0 12
3		Tranylcypromine-propionyl	189 C12H15NO	1000123-86-3 10
4		(E)-3-Chloro-2-methyl-2-pentenal	132 C6H9ClO	031357-76-3 9
5		4-Chloro-2-fluoro-pyrimidine	132 C4H2ClFN2	051422-00-5 9

Peak Number 5 1,4-Benzenedicarboxylic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.97	2.48 ng	148341	Chrysene-d12	22.63
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		1,4-Benzenedicarboxylic acid, bi...	390 C24H38O4	006422-86-2 72
2		Terephthalic acid, 3-methylbut-2...	348 C21H32O4	1000356-27-6 59
3		1,3-Benzenedicarboxylic acid, bi...	390 C24H38O4	000137-89-3 58
4		Isophthalic acid, 3-methylbut-2...	348 C21H32O4	1000344-72-4 50
5		Terephthalic acid, monochloride,...	296 C16H21ClO3	1000324-22-9 43

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.61	73.3	ng	1493350	1	8.92	407701	20.0
2-Pentanone, 4-hy...	5.83	4.3	ng	88217	1	8.92	407701	20.0
.alpha.-Methylsty...	8.32	4.9	ng	100247	1	8.92	407701	20.0
unknown8.43	8.43	65.8	ng	1341320	1	8.92	407701	20.0
1,4-Benzenedicarb...	23.97	2.5	ng	148341	5	22.63	1197330	20.0