

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081721\
 Data File : BG049886.D
 Acq On : 17 Aug 2021 20:35
 Operator : CG/JU
 Sample : M3431-02
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 2

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-BG080321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049886.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.133	11	16	33	rVB	63937	136499	9.57%	1.725%
2	5.106	346	352	363	rVB2	18467	34268	2.40%	0.433%
3	5.588	425	434	444	rBV	421918	717914	50.32%	9.073%
4	7.198	699	708	719	rBV	457754	817456	57.30%	10.331%
5	8.026	842	849	856	rBV	123696	215011	15.07%	2.717%
6	9.201	1041	1049	1059	rBV	294335	542338	38.02%	6.854%
7	10.611	1283	1289	1298	rBV3	8746	19693	1.38%	0.249%
8	10.846	1317	1329	1337	rBV	160687	294014	20.61%	3.716%
9	13.295	1738	1746	1754	rBV	789460	1217041	85.31%	15.381%
10	14.682	1974	1982	1988	rVB	241002	382269	26.80%	4.831%
11	16.174	2230	2236	2246	rBV	605903	932514	65.37%	11.785%
12	17.431	2443	2450	2456	rBV	269934	415510	29.13%	5.251%
13	19.487	2796	2800	2805	rVB2	37423	52607	3.69%	0.665%
14	19.851	2858	2862	2868	rVB	31895	48593	3.41%	0.614%
15	20.039	2889	2894	2899	rVB	1102624	1426617	100.00%	18.029%
16	21.713	3173	3179	3185	rBV2	217575	380956	26.70%	4.814%
17	24.991	3731	3737	3745	rVB3	106010	279497	19.59%	3.532%

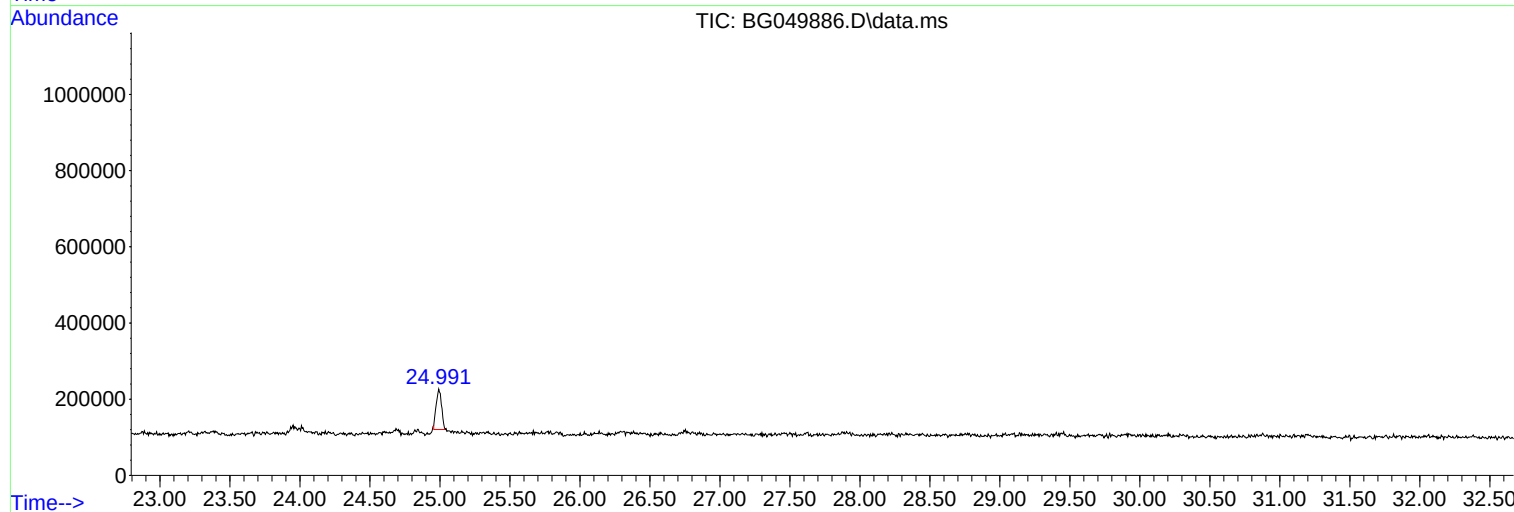
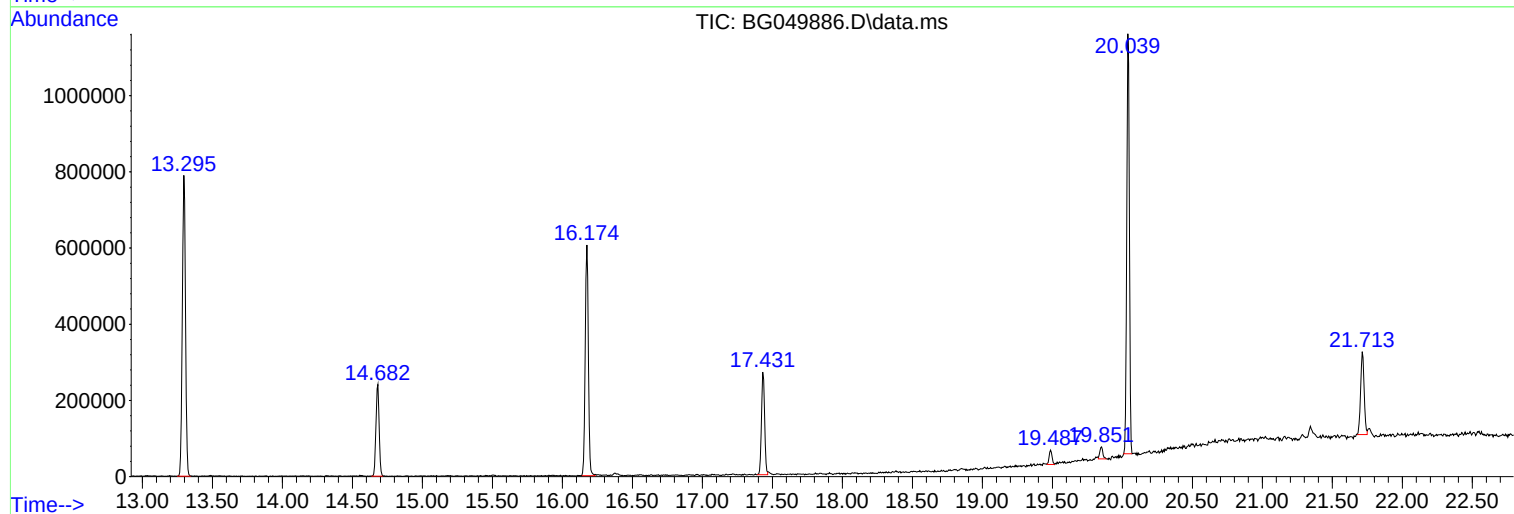
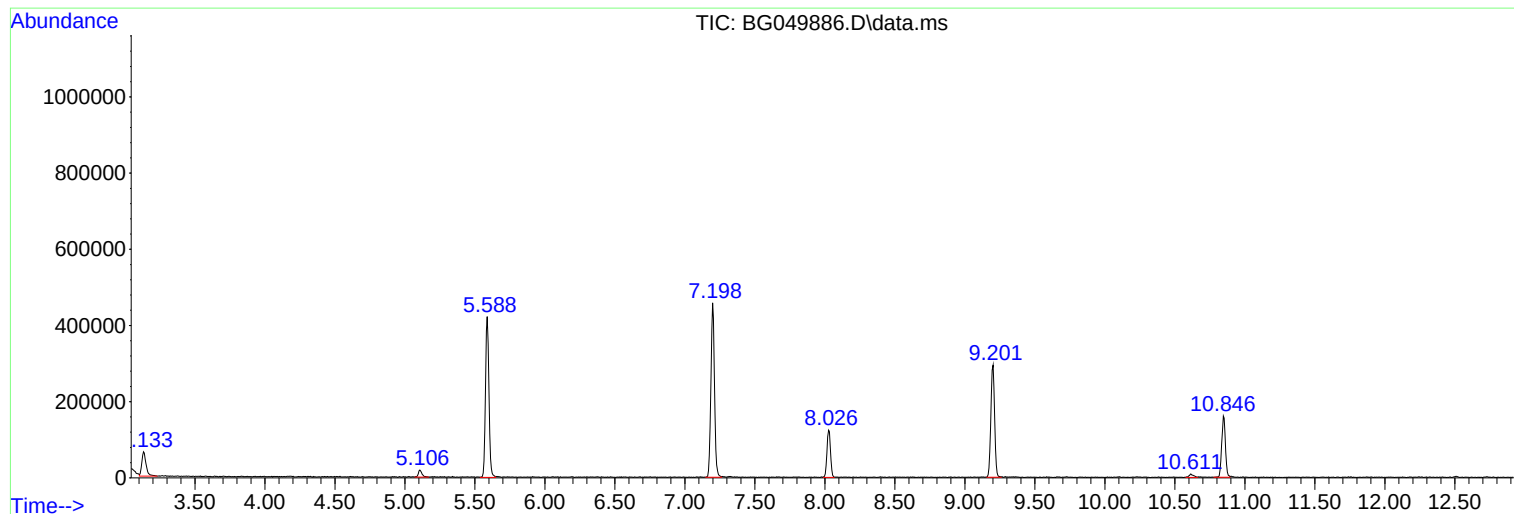
Sum of corrected areas: 7912797

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
BNA_G
ClientSampleId :
2

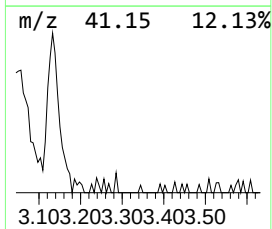
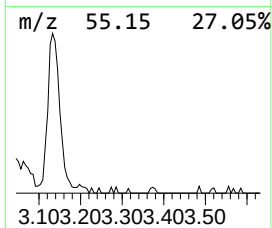
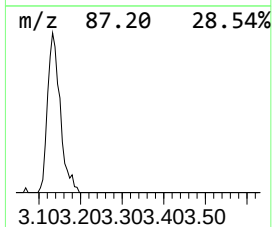
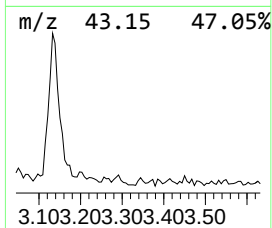
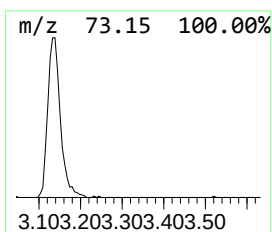
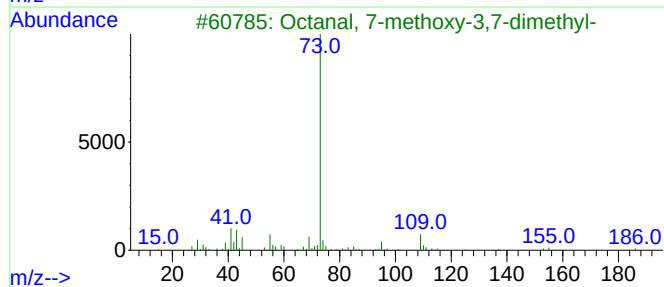
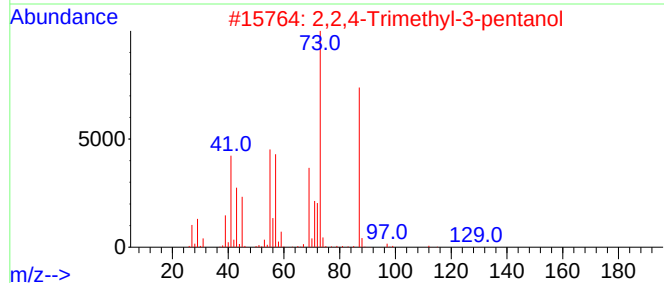
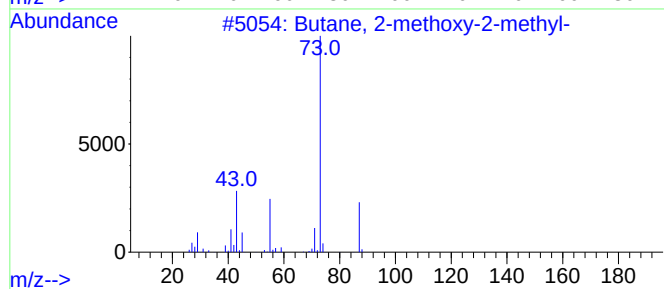
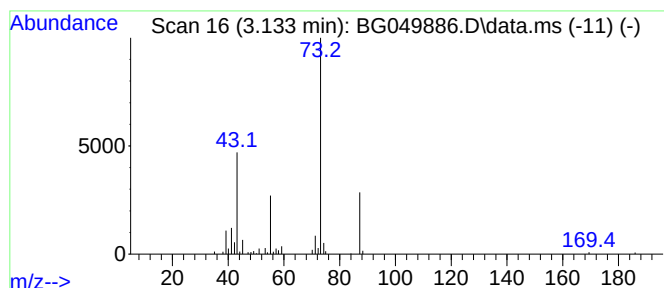
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.133	12.70 ng	136499	1,4-Dichlorobenzene-d4	8.032

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	32
4			Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	16
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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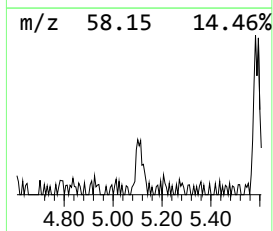
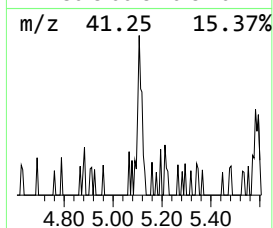
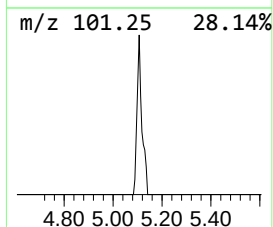
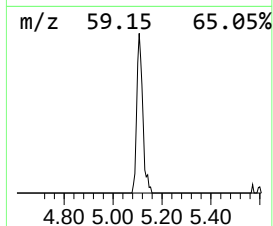
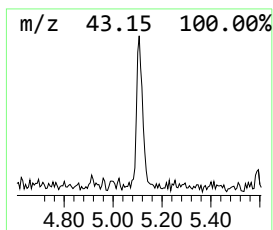
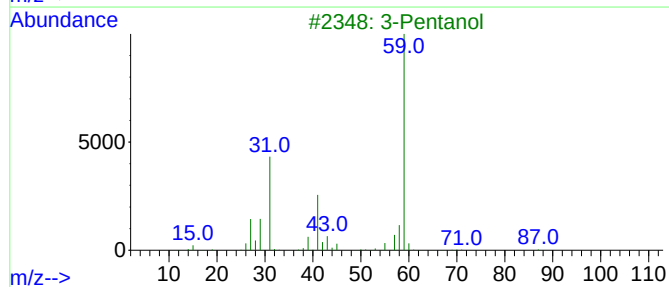
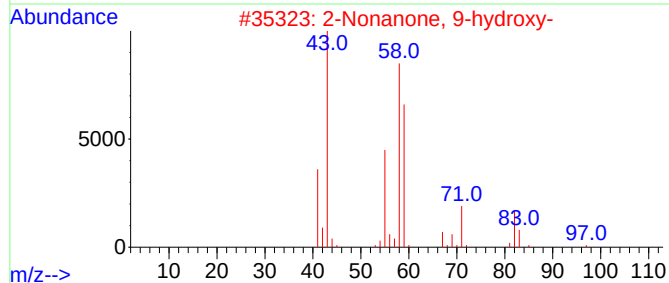
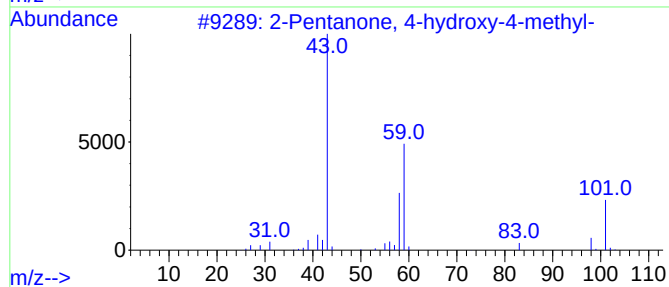
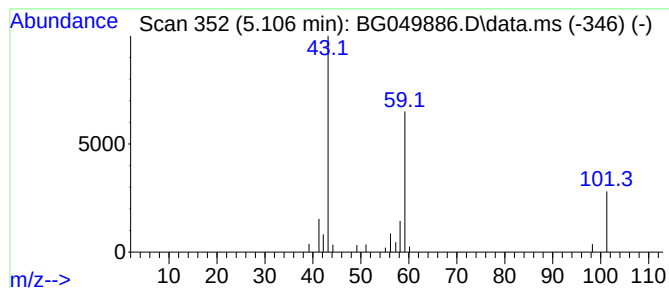
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.106	3.19 ng	34268	1,4-Dichlorobenzene-d4	8.032

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2		2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
3		3-Pentanol	88	C5H12O	000584-02-1	25
4		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17
5		Butane	58	C4H10	000106-97-8	9



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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
Butane, 2-metho...	3.133	12.7	ng	136499	1	8.032	215011	20.0
2-Pentanone, 4-...	5.106	3.2	ng	34268	1	8.032	215011	20.0