

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
 Data File : BF124069.D
 Acq On : 26 May 2021 17:34
 Operator : JU/CG
 Sample : PB136648BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB136648BL

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_F\METHODS\8270-BF051421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124069.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.252	22	28	33	rVB	63013	77399	2.74%	0.506%
2	5.128	511	517	527	rBV	535319	746015	26.41%	4.876%
3	5.528	579	585	588	rBV	1795845	1881380	66.60%	12.297%
4	5.910	647	650	655	rBB	67807	54130	1.92%	0.354%
5	6.522	748	754	757	rBV	1686341	1846428	65.37%	12.069%
6	6.892	813	817	820	rBV	394203	340262	12.05%	2.224%
7	7.457	907	913	916	rBV	1167525	1284182	45.46%	8.394%
8	8.175	1030	1035	1038	rBV	509952	419618	14.85%	2.743%
9	9.251	1212	1218	1221	rBV	2752753	2302751	81.52%	15.051%
10	9.933	1329	1334	1340	rBV	534752	510621	18.08%	3.338%
11	10.722	1463	1468	1471	rBV	1765018	1601344	56.69%	10.467%
12	11.422	1583	1587	1594	rBV	584600	537819	19.04%	3.515%
13	13.010	1852	1857	1860	rBV	2963696	2824783	100.00%	18.463%
14	14.063	2032	2036	2042	rVB	534542	481635	17.05%	3.148%
15	15.557	2285	2290	2300	rBV	247099	391131	13.85%	2.556%

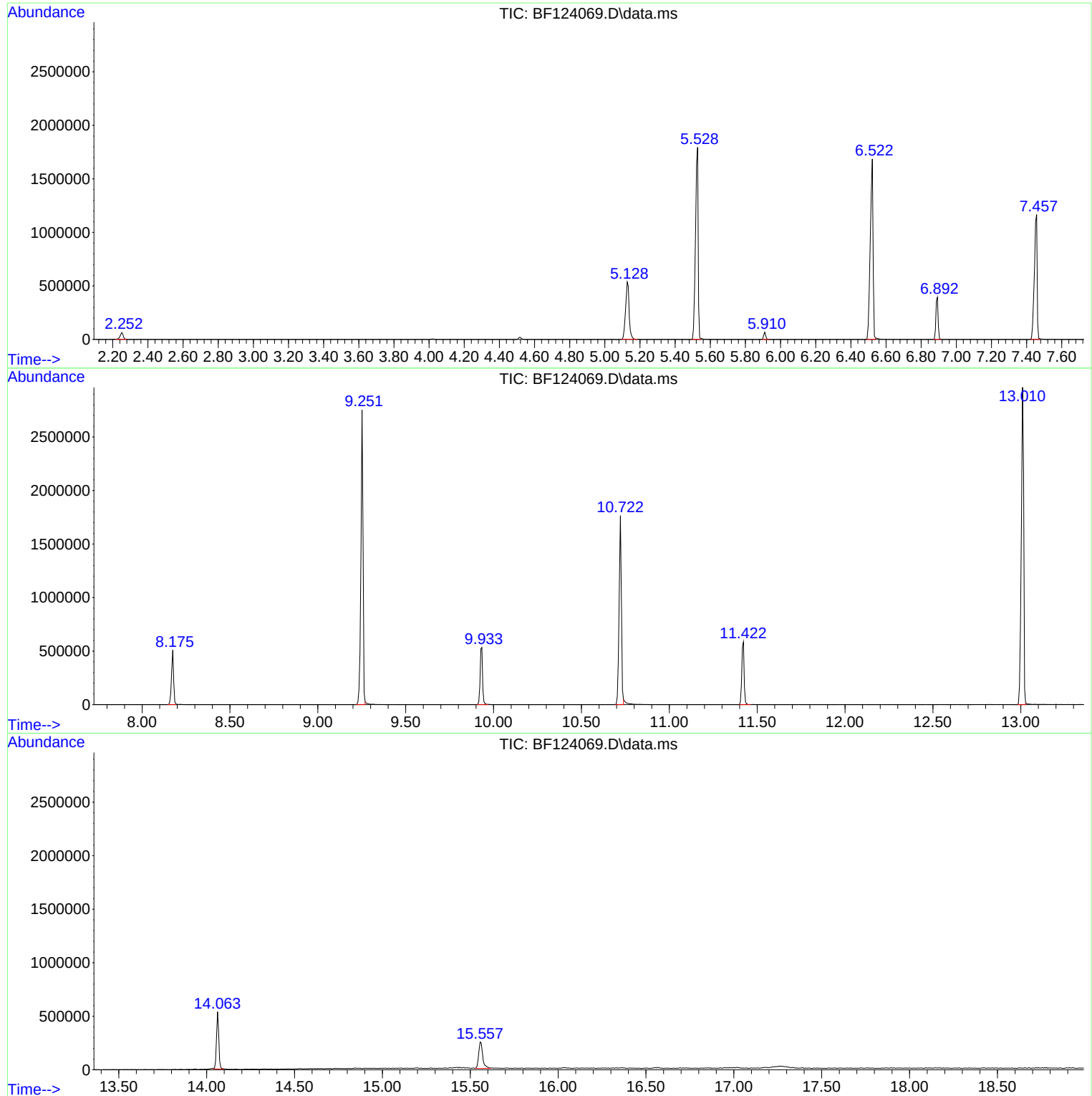
Sum of corrected areas: 15299498

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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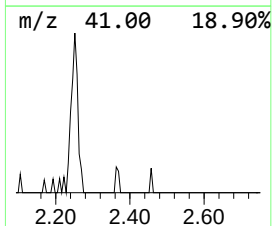
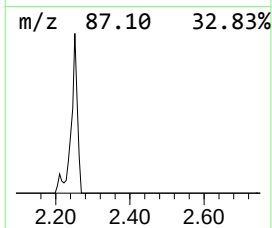
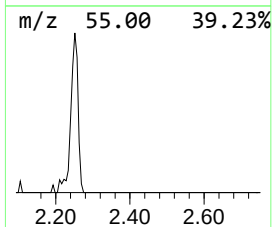
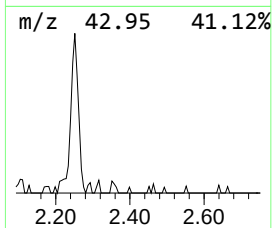
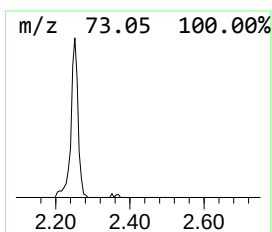
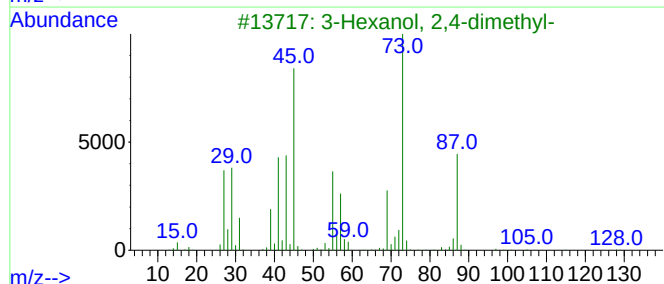
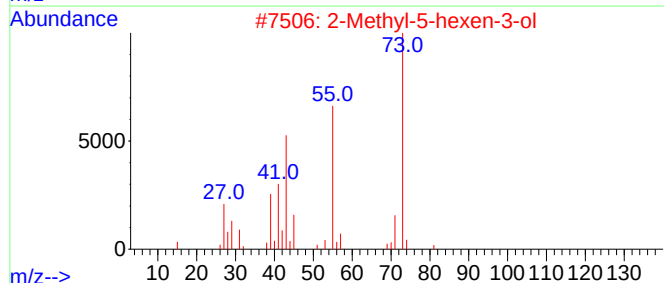
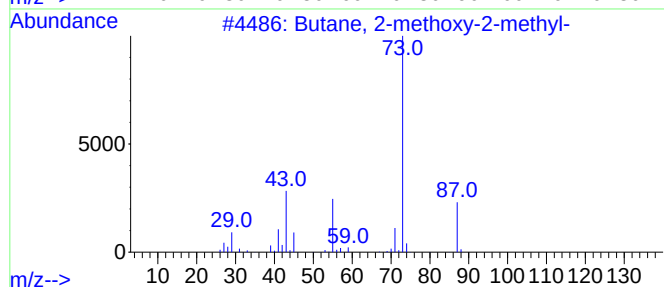
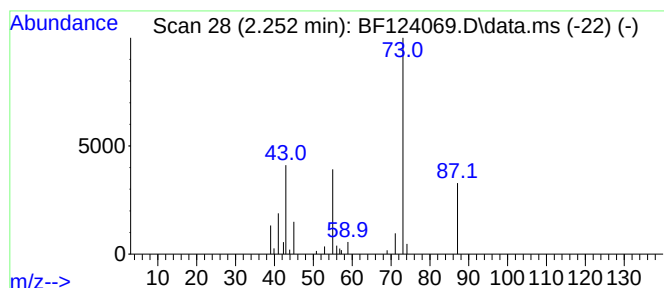
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.252	4.55 ng	77399	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
3			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	9
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	9
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9



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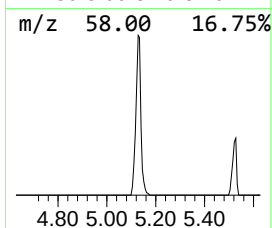
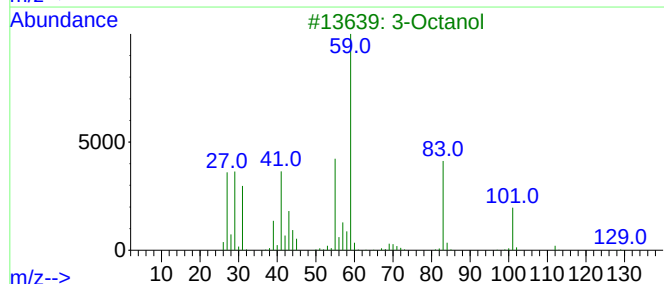
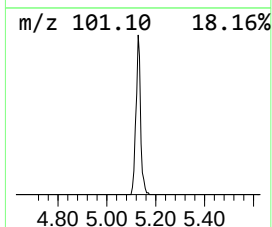
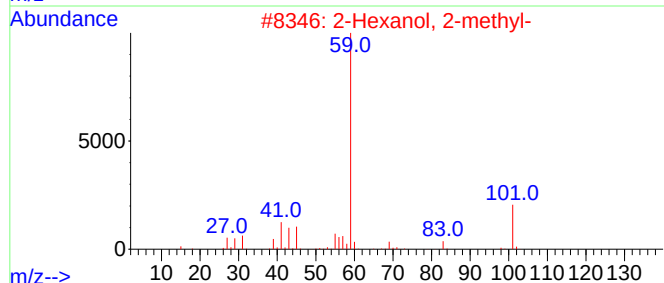
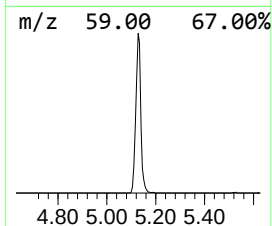
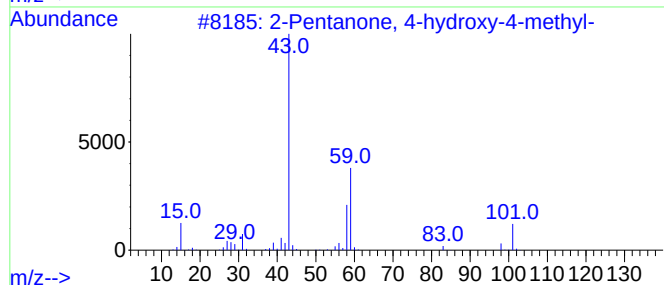
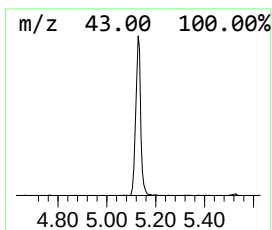
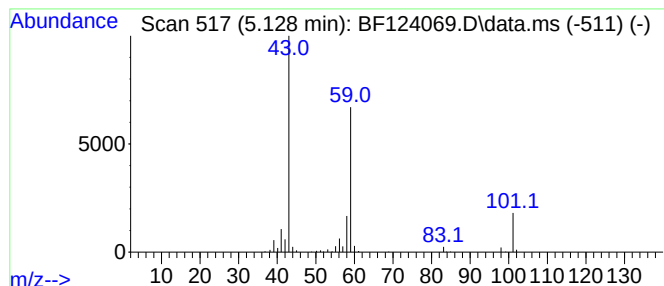
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	43.85 ng	746015	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			3-Octanol	130	C8H18O	000589-98-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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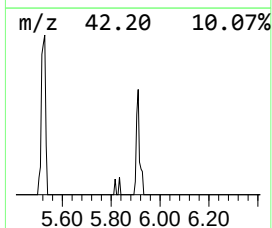
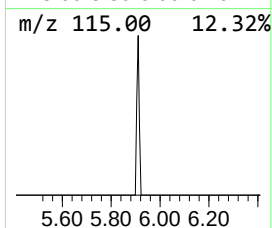
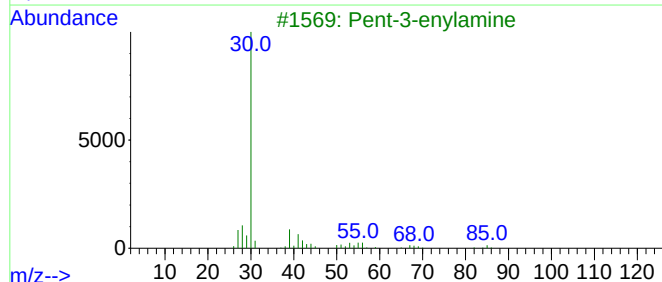
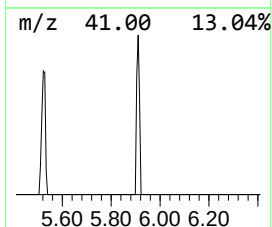
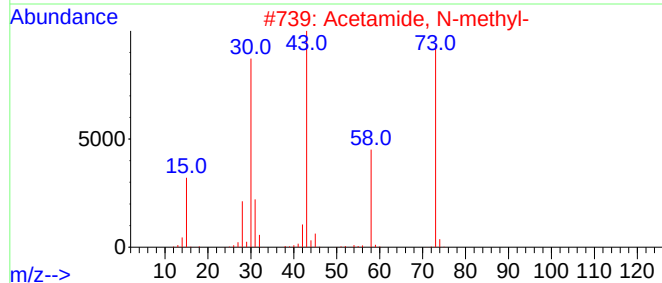
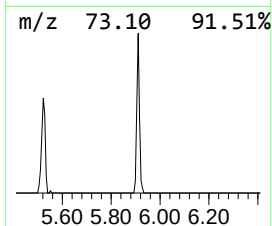
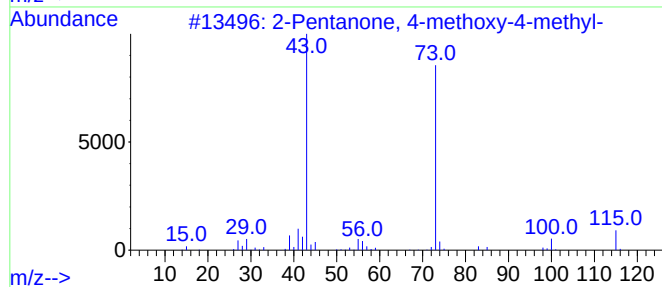
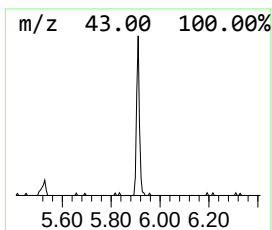
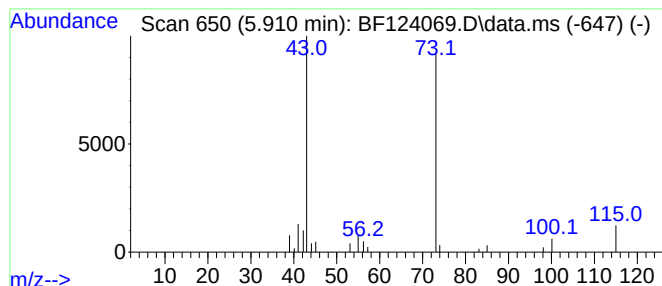
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.910	3.18 ng	54130	1,4-Dichlorobenzene-d4	6.892

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83	
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	43	
3	Pent-3-enylamine	85	C5H11N	087156-70-5	10	
4	Guanidine, methyl-	73	C2H7N3	000471-29-4	9	
5	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9	



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.252	4.5	ng	77399	1	6.892	340262	20.0
2-Pentanone, 4-...	5.128	43.9	ng	746015	1	6.892	340262	20.0
2-Pentanone, 4-...	5.910	3.2	ng	54130	1	6.892	340262	20.0