

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080321\
 Data File : BF124917.D
 Acq On : 3 Aug 2021 16:07
 Operator : JU/CG
 Sample : PB138162BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB138162BL

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-BF072221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124917.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	504	508	516	rBB	26764	36137	12.40%	2.300%
2	5.475	571	576	579	rBB	199603	197822	67.89%	12.589%
3	5.863	639	642	644	rBB	6366	4726	1.62%	0.301%
4	6.475	741	746	749	rBV	179479	204195	70.08%	12.994%
5	6.845	806	809	812	rBB	47643	35710	12.26%	2.272%
6	7.410	900	905	908	rBB	136451	132857	45.59%	8.455%
7	8.128	1023	1027	1030	rBB	58721	47153	16.18%	3.001%
8	9.204	1205	1210	1213	rBB	297039	254645	87.39%	16.205%
9	9.880	1321	1325	1328	rBB	73038	56586	19.42%	3.601%
10	10.675	1455	1460	1463	rBV	180933	158749	54.48%	10.102%
11	11.369	1574	1578	1581	rBB	79149	60352	20.71%	3.841%
12	12.957	1843	1848	1851	rBV	339704	291388	100.00%	18.543%
13	13.868	2000	2003	2006	rBB	6133	6658	2.28%	0.424%
14	14.004	2023	2026	2030	rBB	55424	47645	16.35%	3.032%
15	15.468	2271	2275	2279	rBB2	31476	36792	12.63%	2.341%

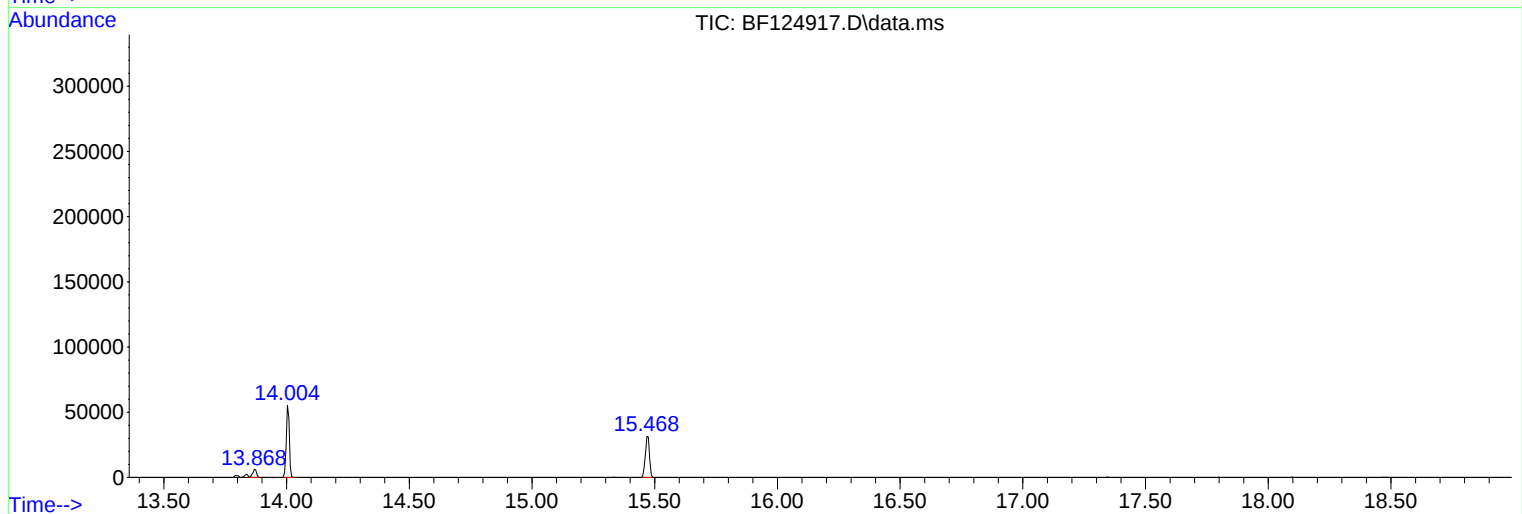
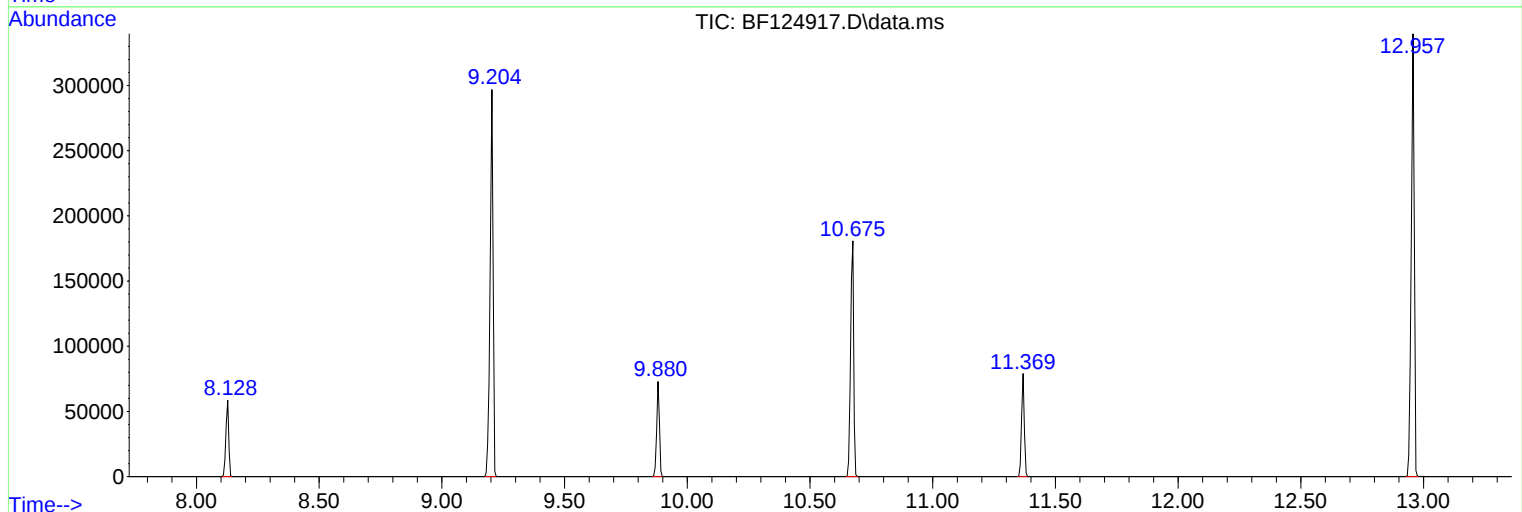
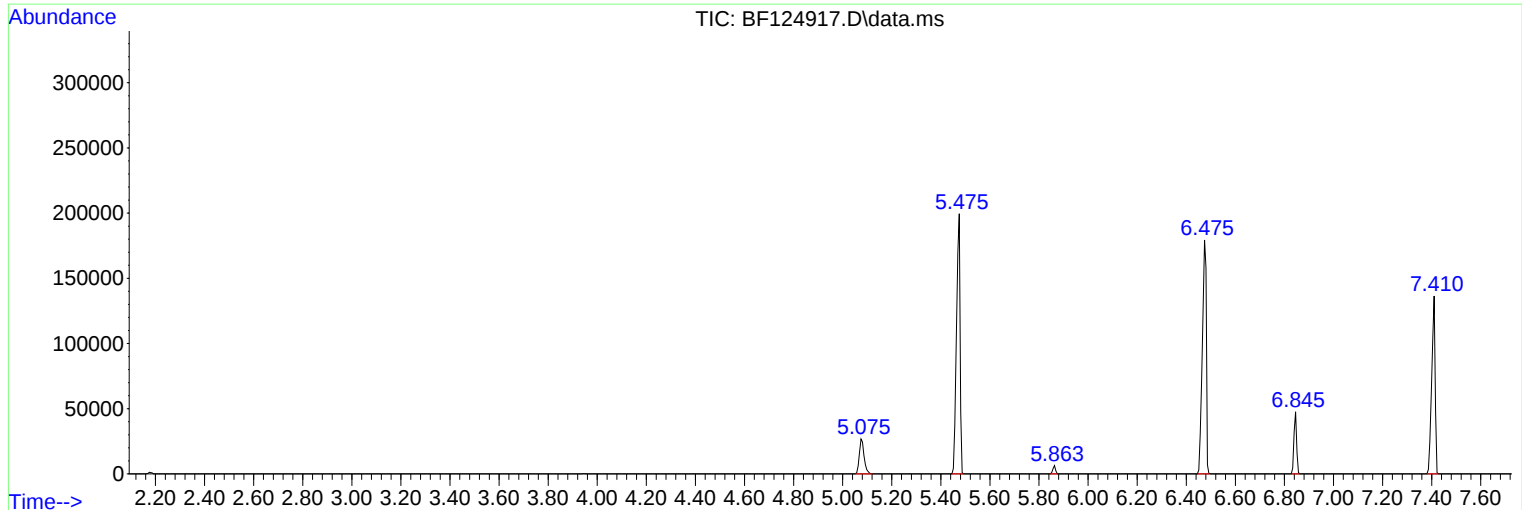
Sum of corrected areas: 1571415

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.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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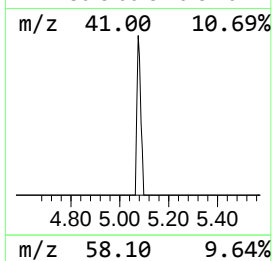
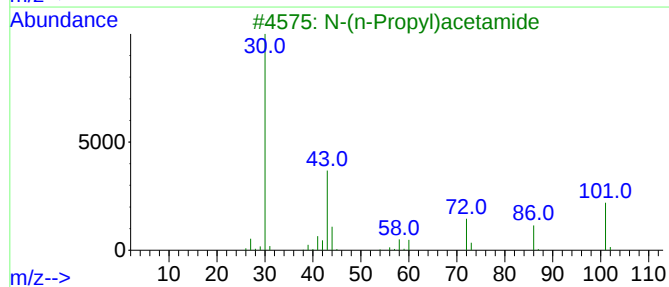
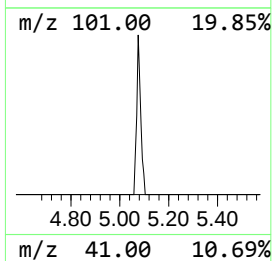
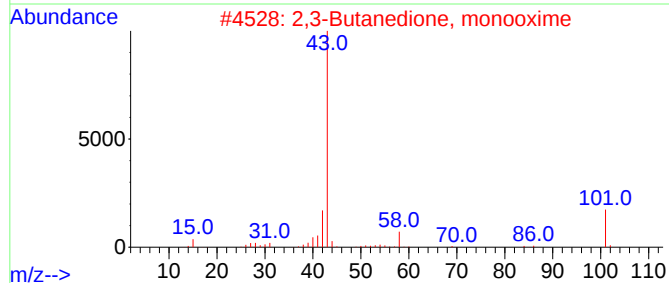
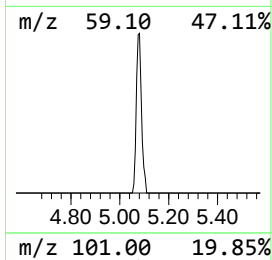
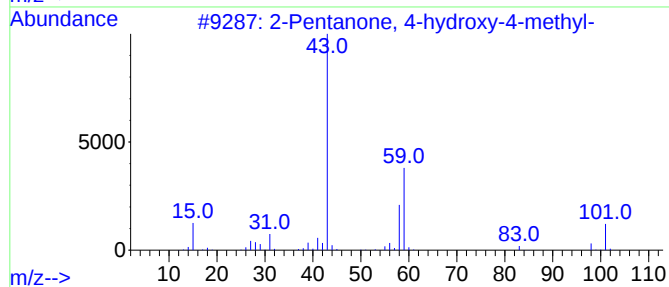
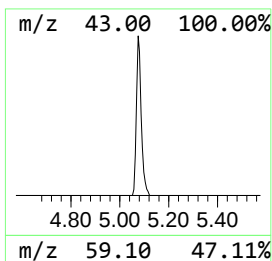
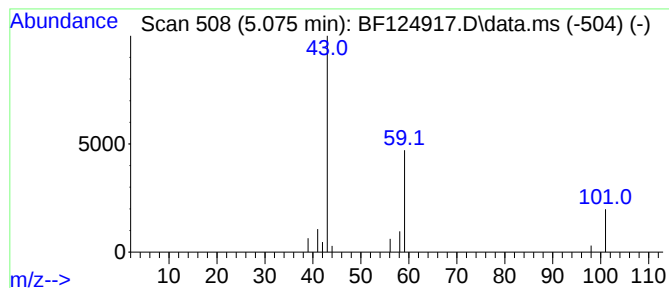
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.075	20.24 ng	36137	1,4-Dichlorobenzene-d4			6.845
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	9
3	N-(n-Propyl)acetamide		101	C5H11NO	005331-48-6	7
4	5-Hexen-2-one		98	C6H10O	000109-49-9	7
5	2-Propyn-1-ol, acetate		98	C5H6O2	000627-09-8	5



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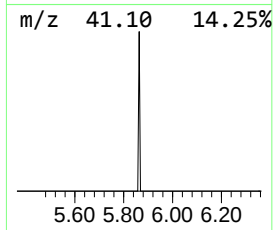
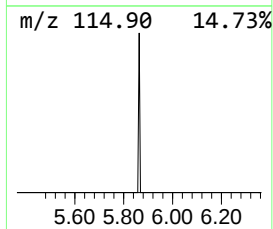
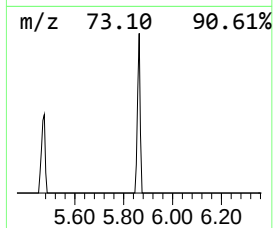
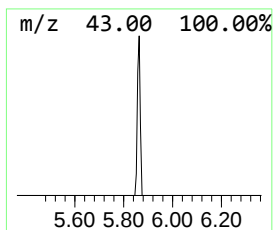
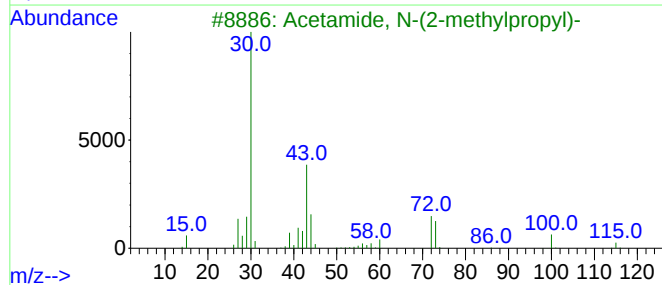
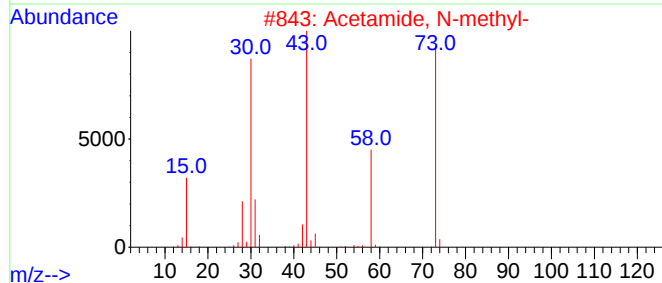
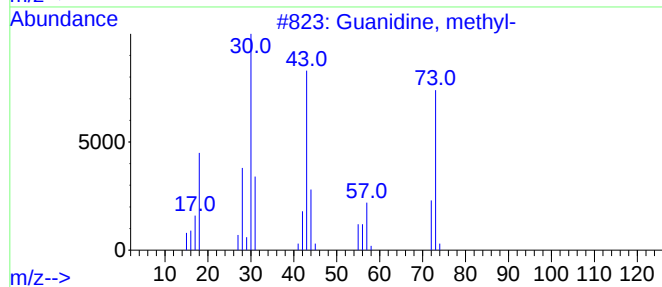
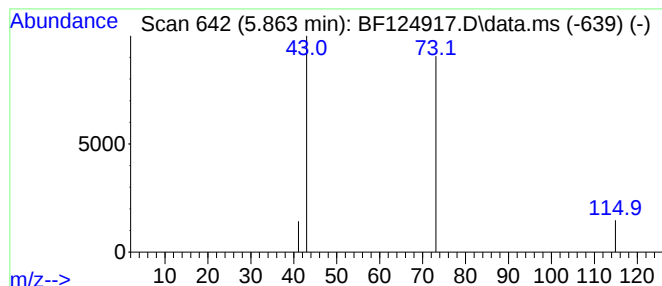
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Peak Number 2 unknown5.863 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.863	2.65 ng	4726	1,4-Dichlorobenzene-d4	6.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Guanidine, methyl-	73	C2H7N3	000471-29-4	4
2			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	4
3			Acetamide, N-(2-methylpropyl)-	115	C6H13NO	001540-94-9	3
4			N-Ethylformamide	73	C3H7NO	000627-45-2	3
5			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	2



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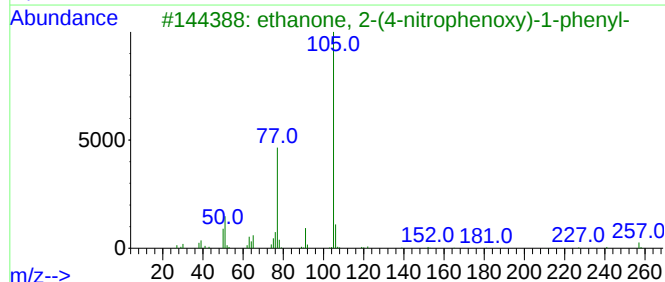
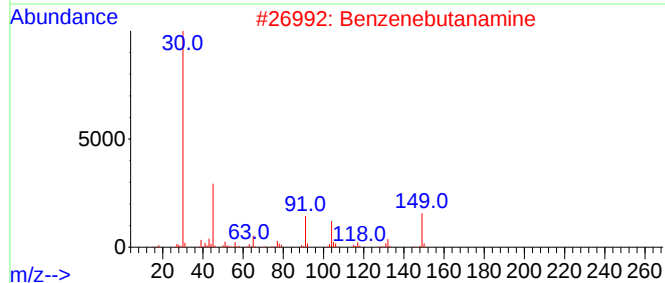
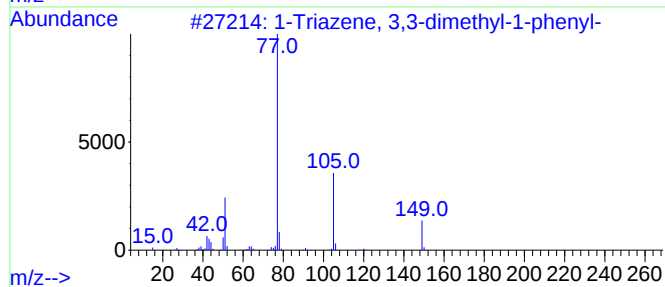
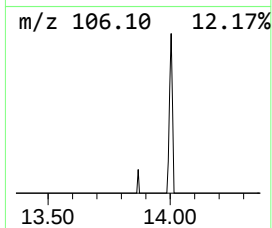
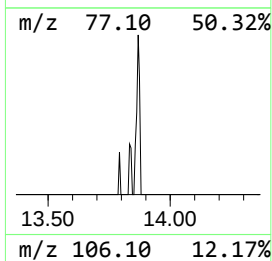
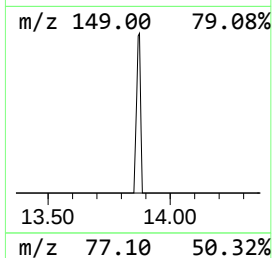
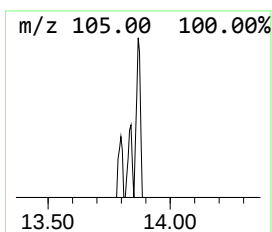
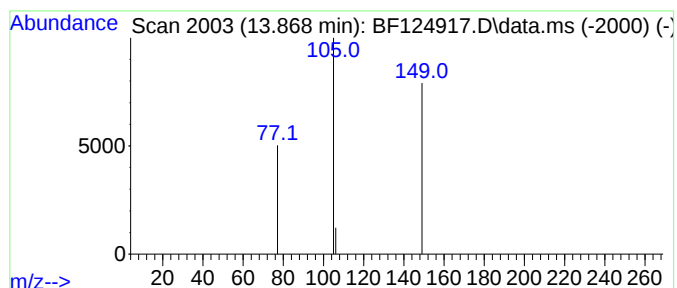
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Peak Number 3 unknown13.868 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	2.79 ng	6658	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Triazene, 3,3-dimethyl-1-phenyl-	149	C8H11N3	007227-91-0	3		
2	Benzenebutanamine	149	C10H15N	013214-66-9	3		
3	ethanone, 2-(4-nitrophenoxy)-1-p...	257	C14H11NO4	1000401-50-9	2		
4	2,6-Piperazinedione, 4-benzoyl-,...	233	C11H11N3O3	035975-25-8	2		
5	Quinoline, N-benzoyl-1,2,3,4-tet...	237	C16H15NO	028748-92-7	2		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.075	20.2	ng	36137	1	6.845	35710	20.0
unknown5.863	5.863	2.6	ng	4726	1	6.845	35710	20.0
unknown13.868	13.868	2.8	ng	6658	5	14.004	47645	20.0