

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
 Data File : BF125010.D
 Acq On : 9 Aug 2021 19:55
 Operator : JU/CG
 Sample : M3318-04
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20210595-AMENDED-COM-9

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-BF080421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125010.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	13	15	18	rBB	2659	2344	1.65%	0.246%
2	5.028	497	500	505	rBB	8833	9134	6.43%	0.959%
3	5.434	566	569	573	rBV	129933	112151	78.94%	11.773%
4	6.451	737	742	745	rBV	135753	126812	89.26%	13.312%
5	6.816	801	804	807	rBB	43760	32239	22.69%	3.384%
6	7.380	896	900	903	rBB	94563	83545	58.81%	8.770%
7	7.533	924	926	928	rBB	2804	2054	1.45%	0.216%
8	8.004	1003	1006	1011	rBB	9380	8424	5.93%	0.884%
9	8.098	1019	1022	1026	rBB	52946	43221	30.42%	4.537%
10	9.174	1201	1205	1208	rBV	187607	142064	100.00%	14.913%
11	9.816	1312	1314	1317	rBV	4111	3489	2.46%	0.366%
12	9.851	1317	1320	1323	rVB	57610	48912	34.43%	5.135%
13	10.639	1451	1454	1458	rBB	82572	71548	50.36%	7.511%
14	10.769	1473	1476	1478	rBB	14752	11330	7.98%	1.189%
15	11.210	1548	1551	1553	rBB	3831	2985	2.10%	0.313%
16	11.339	1570	1573	1576	rBV	69742	51557	36.29%	5.412%
17	12.921	1839	1842	1845	rBV	158259	139279	98.04%	14.621%
18	13.974	2018	2021	2025	rBB	40692	35263	24.82%	3.702%
19	15.433	2265	2269	2273	rBB	22741	26259	18.48%	2.757%

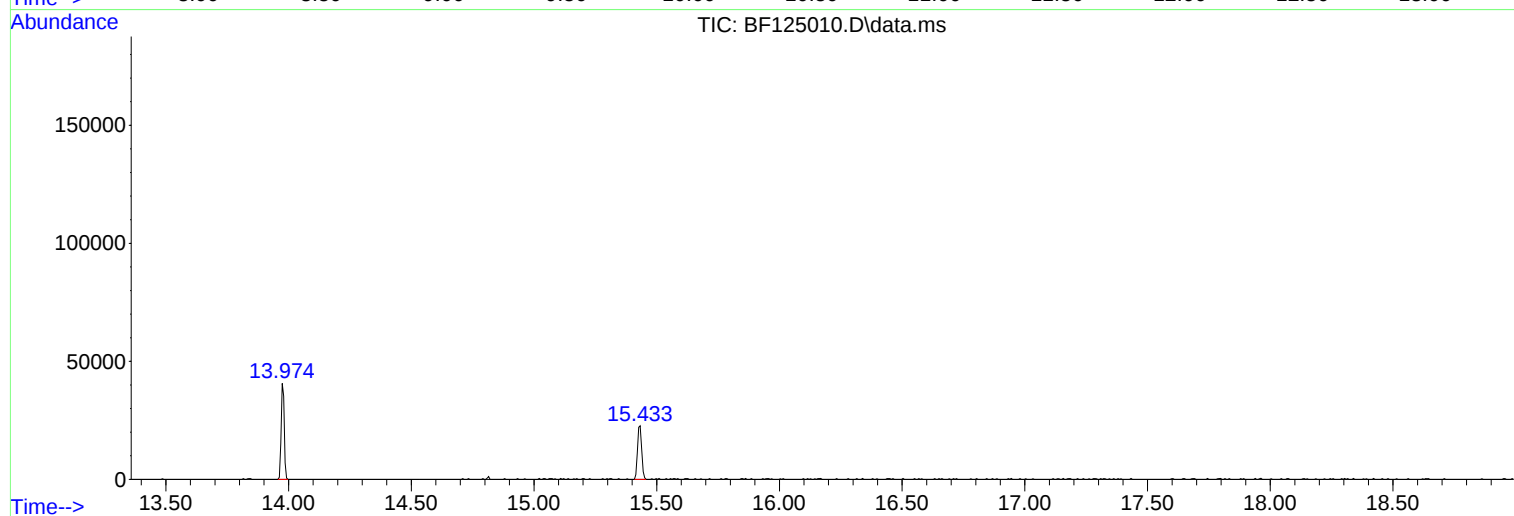
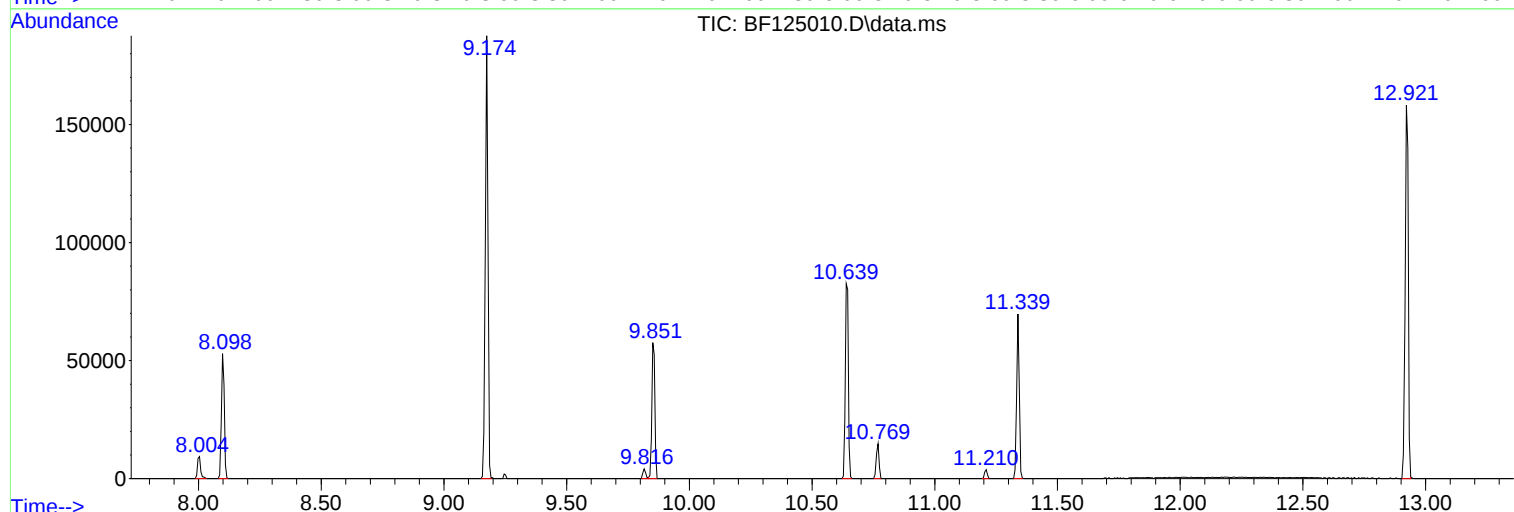
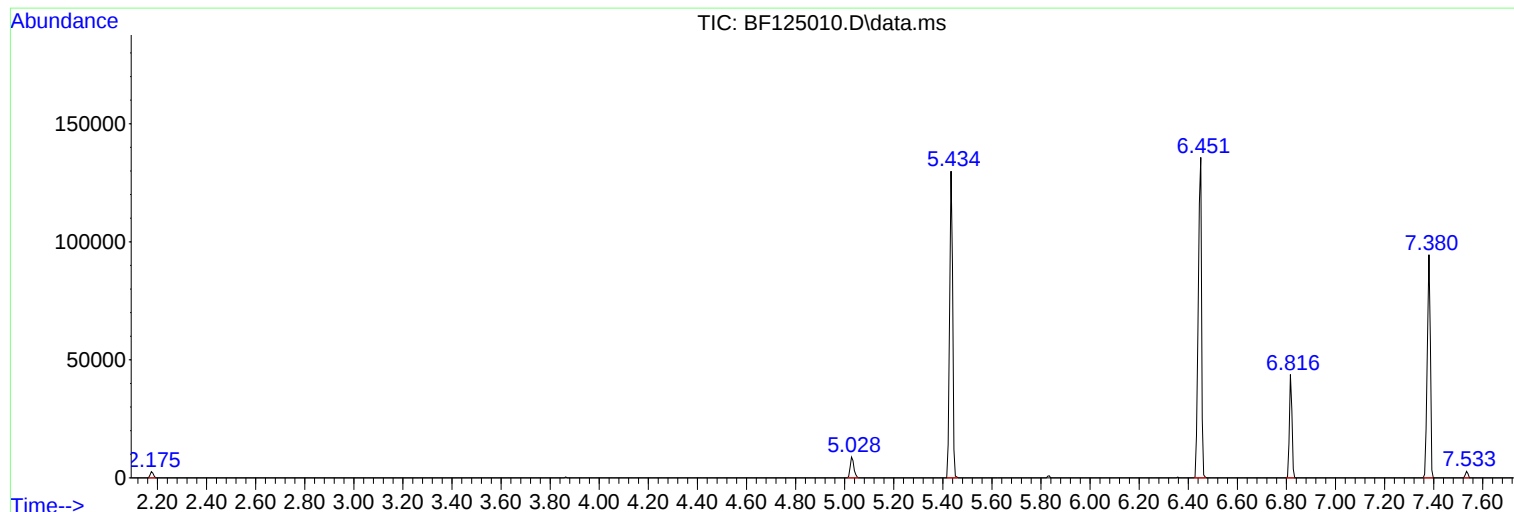
Sum of corrected areas: 952610

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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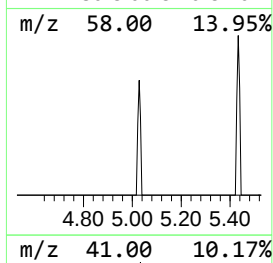
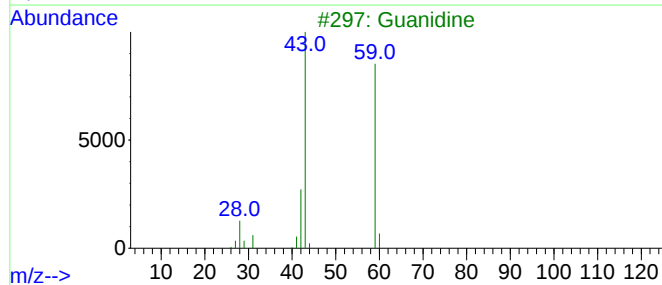
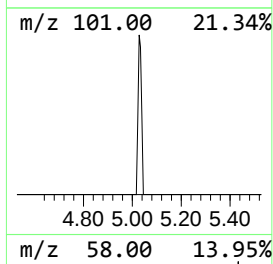
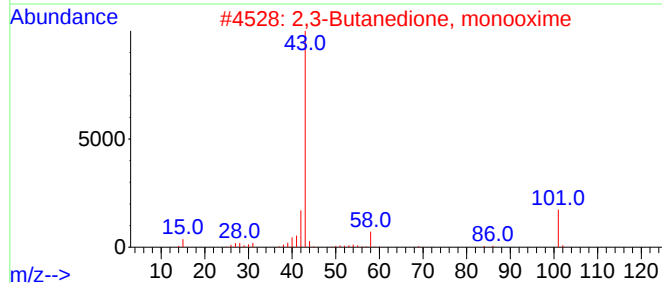
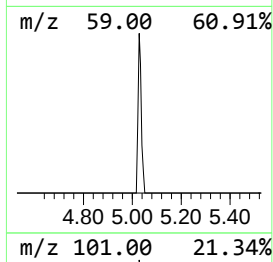
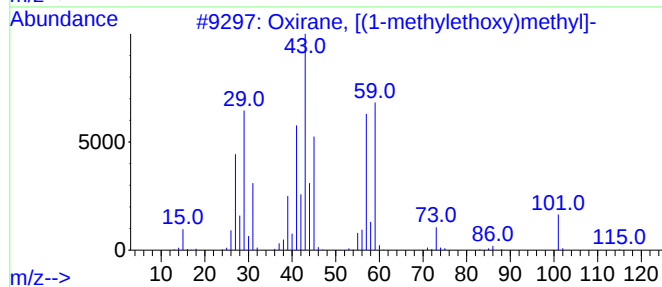
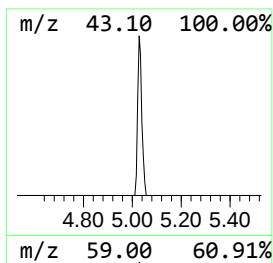
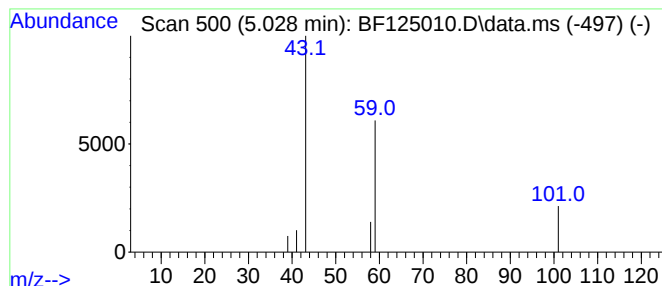
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Peak Number 1 unknown5.028 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	5.67 ng	9134	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	9		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7		
3	Guanidine	59	CH5N3	000113-00-8	4		
4	Diacetamide	101	C4H7NO2	000625-77-4	4		
5	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	4		



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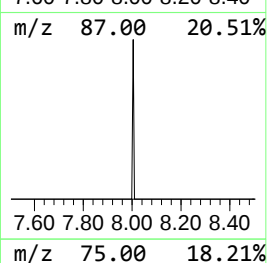
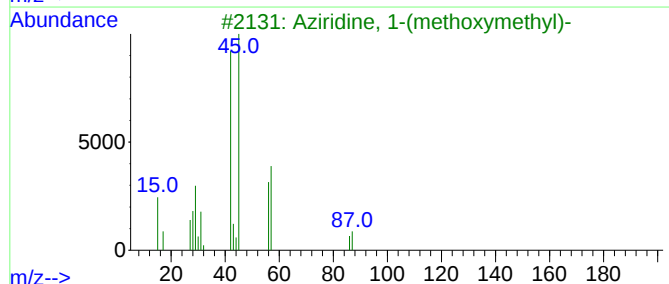
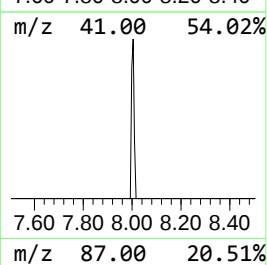
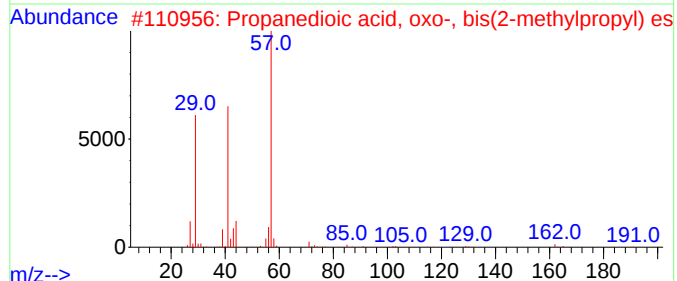
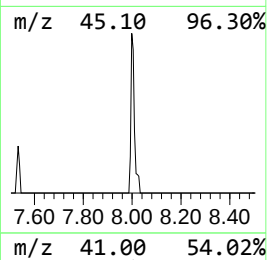
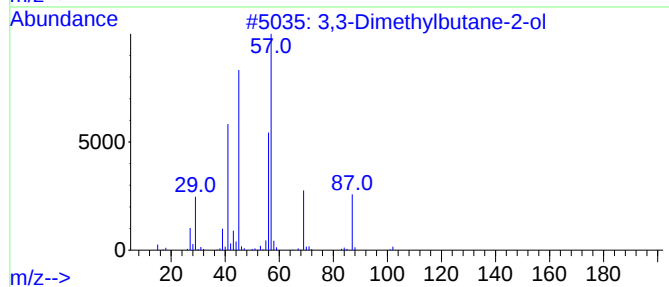
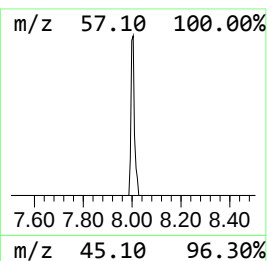
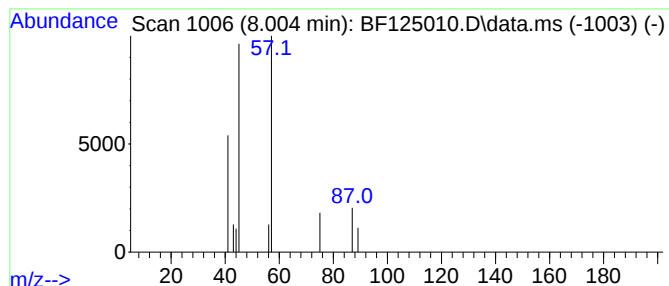
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Peak Number 2 unknown8.004 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.004	3.90 ng	8424	Naphthalene-d8	8.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	9
2			Propanedioic acid, oxo-, bis(2-m...	230	C11H18O5	092778-43-3	9
3			Aziridine, 1-(methoxymethyl)-	87	C4H9NO	001497-83-2	5
4			1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	4
5			Methane, nitroso-	45	CH3NO	000865-40-7	4



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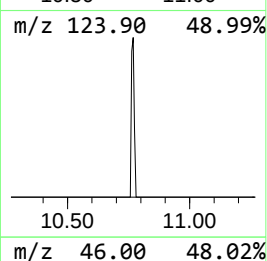
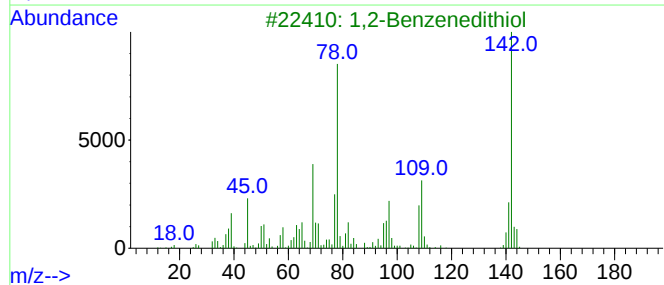
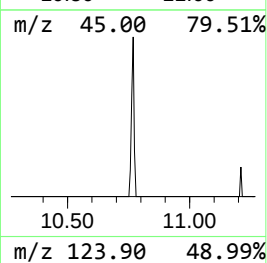
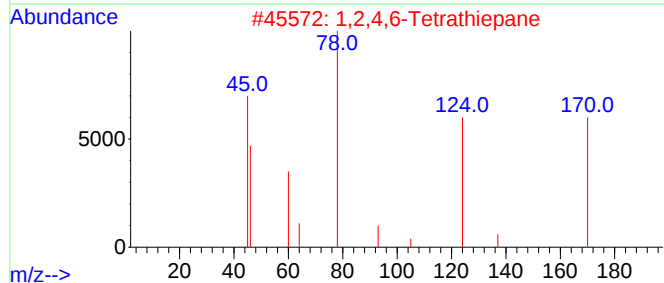
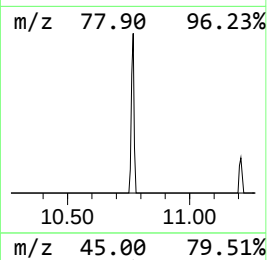
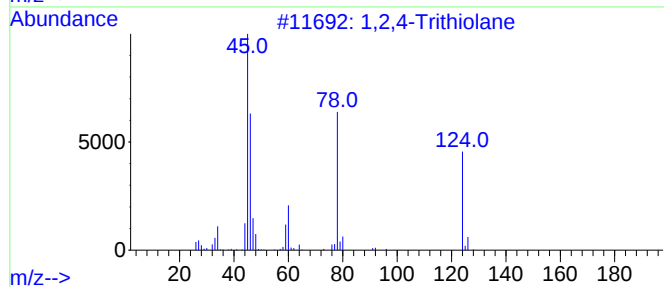
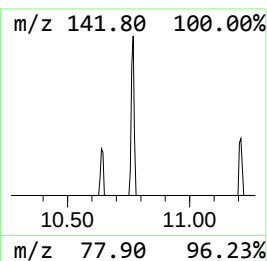
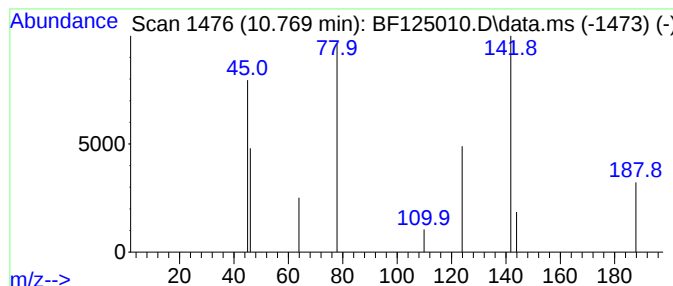
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Peak Number 3 1,2,4-Trithiolane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.769	4.40 ng	11330	Phenanthrene-d10	11.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	64
2			1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	50
3			1,2-Benzenedithiol	142	C6H6S2	017534-15-5	9
4			O-Methyl isopropylphosphonamidot...	153	C4H12NOPS	1000306-04-3	9
5			2,2-Difluorobut-3-en-1-yl 2-fluo...	154	C6H9F3O	1000394-29-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown5.028	5.028	5.7	ng	9134	1	6.816	32239	20.0
unknown8.004	8.004	3.9	ng	8424	2	8.098	43221	20.0
1,2,4-Trithiolane	10.769	4.4	ng	11330	4	11.339	51557	20.0