

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
 Data File : BP019903.D
 Acq On : 27 Feb 2024 18:50
 Operator : MA/JU
 Sample : P1538-12
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 20241105-AMENDED-COMPOSITE-35N-N-4-04

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_P\Methods\8270E-BP022624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019903.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	321	332	337	rBV	6452852	12470280	100.00%	38.319%
2	5.469	399	405	413	rBV	292585	448949	3.60%	1.380%
3	7.069	669	677	692	rVB	531843	922201	7.40%	2.834%
4	7.199	692	699	709	rBV	85048	150642	1.21%	0.463%
5	7.893	807	817	824	rBV	359786	601284	4.82%	1.848%
6	9.069	1008	1017	1033	rBV	765293	1336652	10.72%	4.107%
7	9.428	1070	1078	1089	rVB	215163	406824	3.26%	1.250%
8	10.693	1284	1293	1309	rBV	462436	848868	6.81%	2.608%
9	13.163	1705	1713	1722	rBV	2055211	3028679	24.29%	9.307%
10	14.463	1924	1934	1940	rBV	91933	208818	1.67%	0.642%
11	14.540	1940	1947	1954	rVB	805234	1253096	10.05%	3.851%
12	15.157	2040	2052	2053	rBV4	46250	130974	1.05%	0.402%
13	16.040	2196	2202	2210	rVB	178583	285697	2.29%	0.878%
14	17.075	2372	2378	2388	rBV	335993	572531	4.59%	1.759%
15	17.298	2410	2416	2421	rBV	1031235	1538343	12.34%	4.727%
16	18.198	2565	2569	2575	rBV2	101676	153459	1.23%	0.472%
17	19.869	2848	2853	2859	rBV	4128240	5080870	40.74%	15.613%
18	21.122	3062	3066	3072	rBV	315615	408070	3.27%	1.254%
19	21.398	3107	3113	3118	rBV	1147790	1562477	12.53%	4.801%
20	23.816	3518	3524	3532	rVB	549491	1134790	9.10%	3.487%

Sum of corrected areas: 32543504

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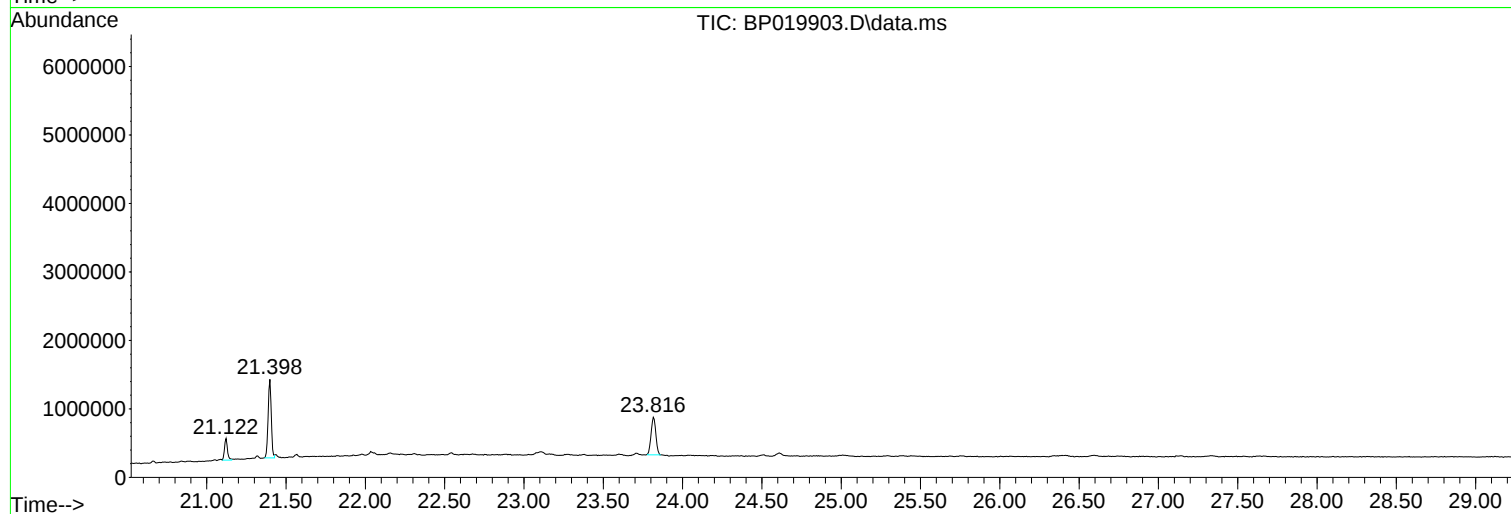
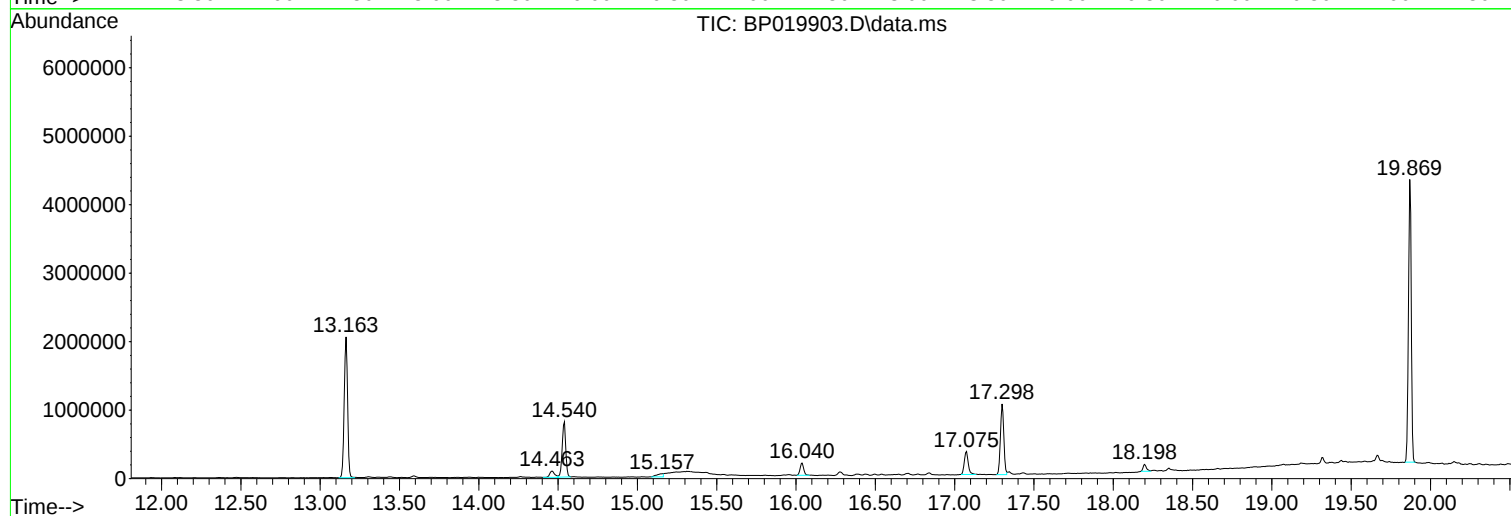
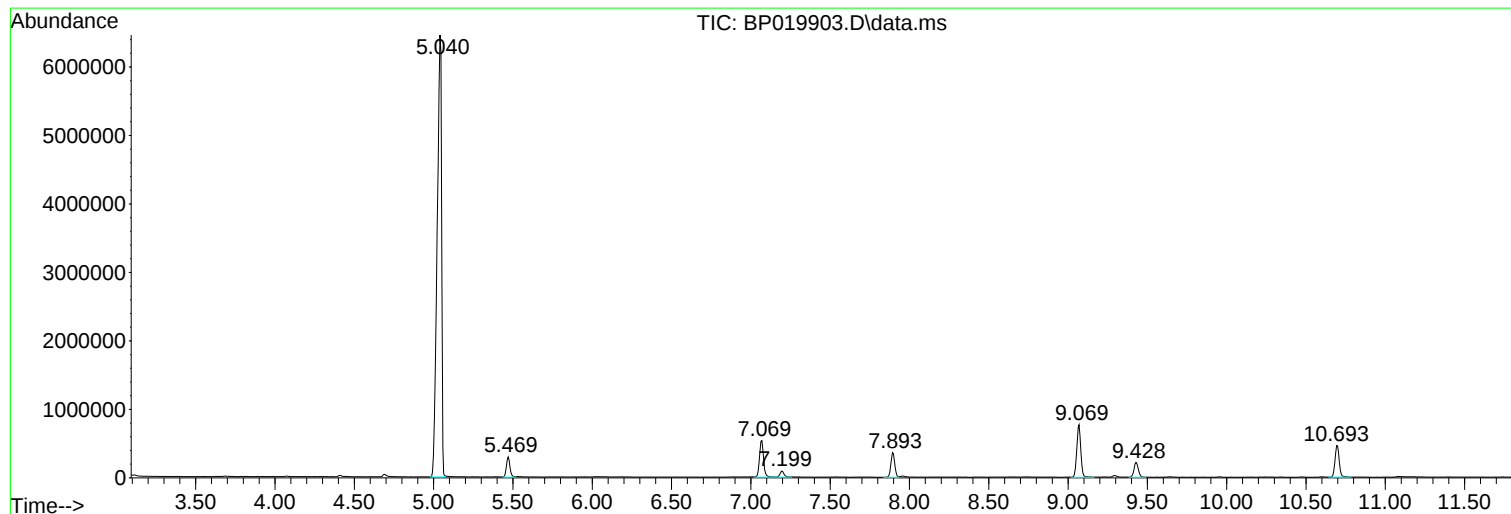
ClientSampleId :

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.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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ClientSampleId :

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

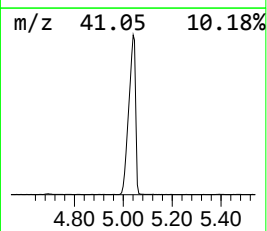
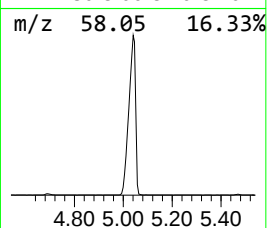
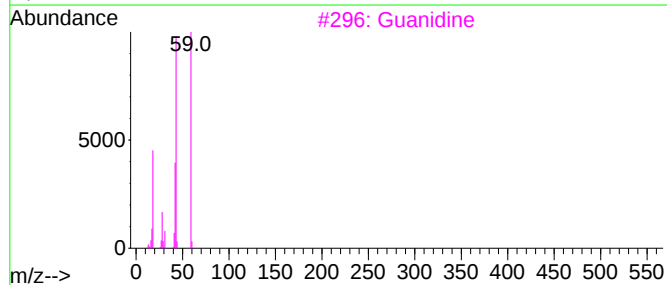
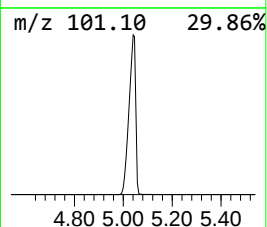
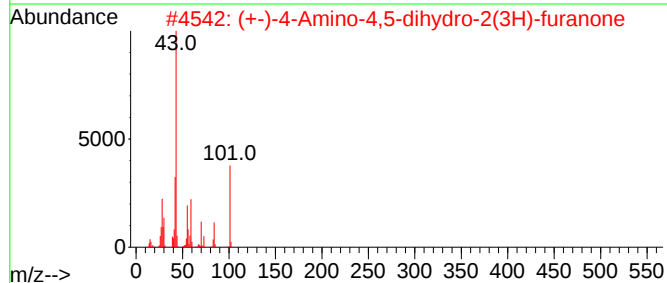
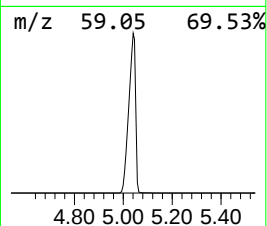
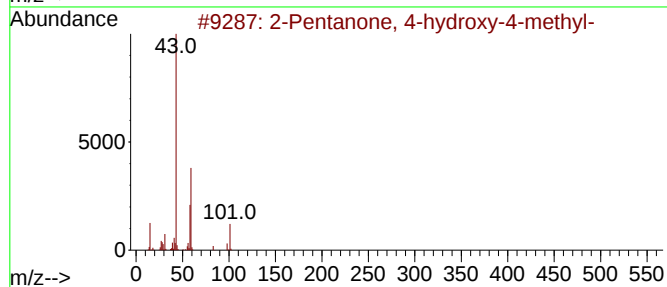
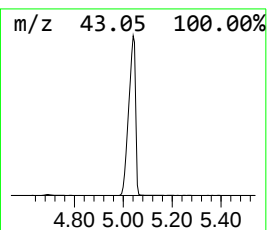
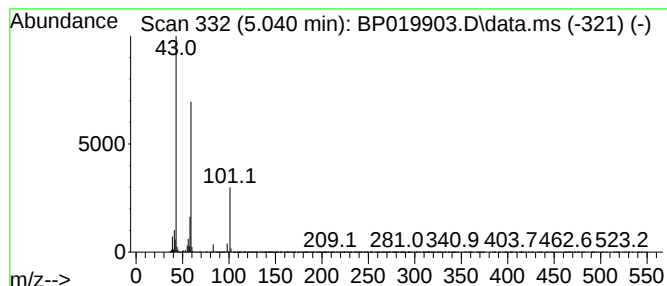
TIC Library : C:\Database\NIST0.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	414.79 ng	12470300	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3			Guanidine	59	CH5N3	000113-00-8	43
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

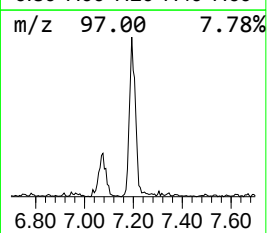
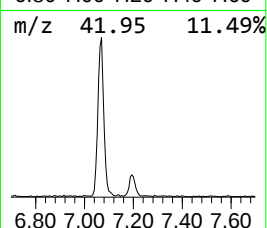
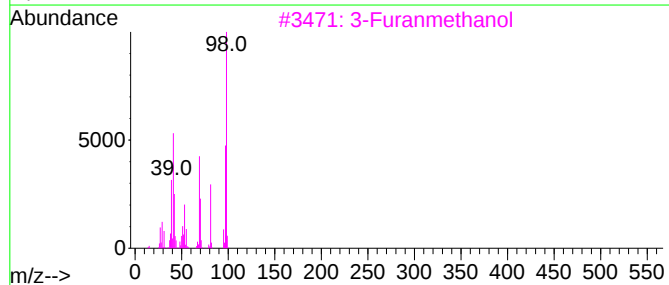
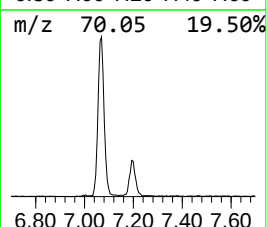
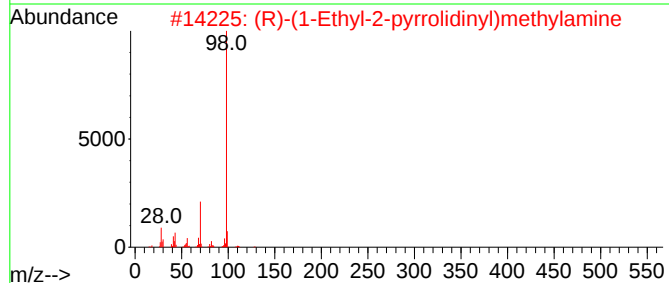
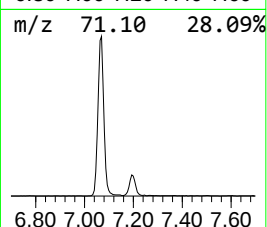
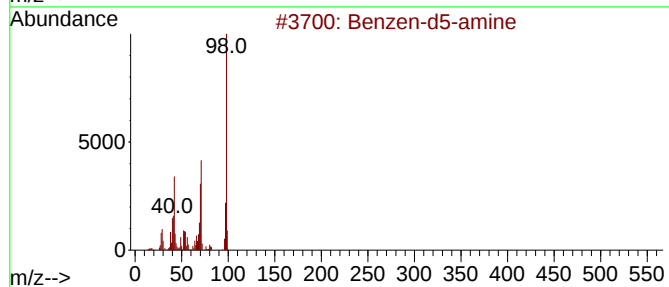
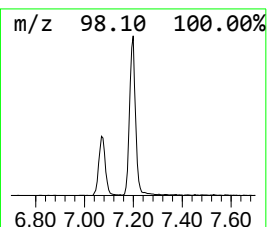
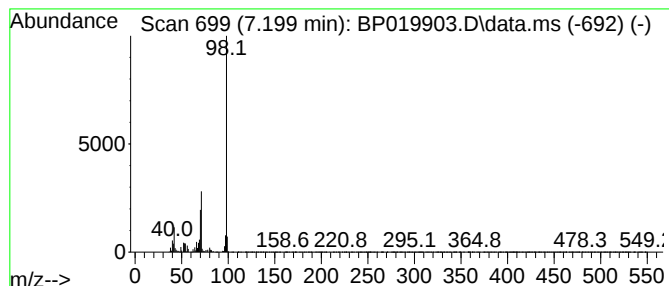
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzen-d5-amine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.199	5.01 ng	150642	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzen-d5-amine	98	C6H2D5N	004165-61-1	87
2			(R)-(1-Ethyl-2-pyrrolidinyl)meth...	128	C7H16N2	022795-97-7	59
3			3-Furanmethanol	98	C5H6O2	004412-91-3	53
4			(R)-1-Ethyl-2-pyrrolidinecarboxa...	142	C7H14N2O	1000237-69-9	53
5			3H-Pyrazole, 3,4-diamino-	98	C3H6N4	1000288-40-0	52



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M

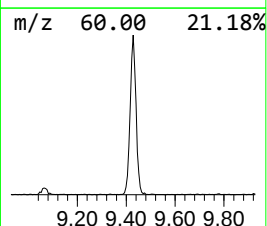
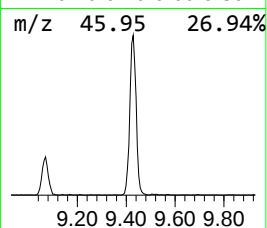
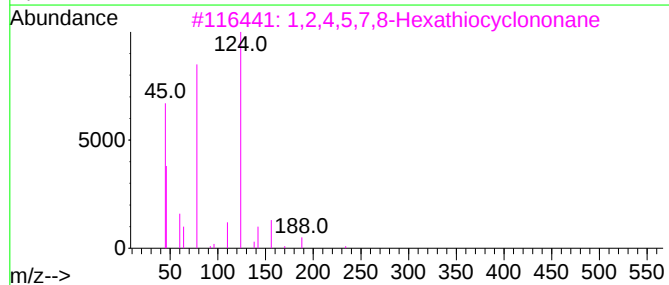
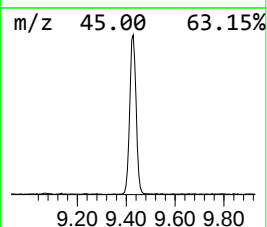
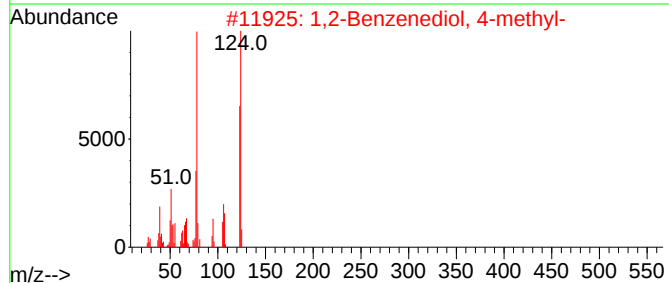
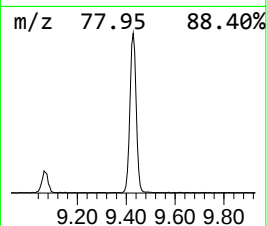
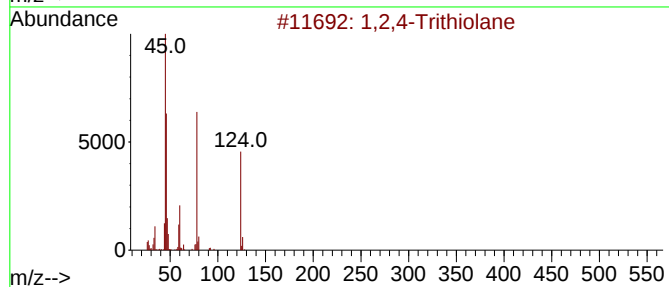
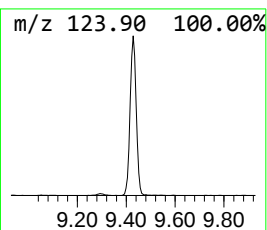
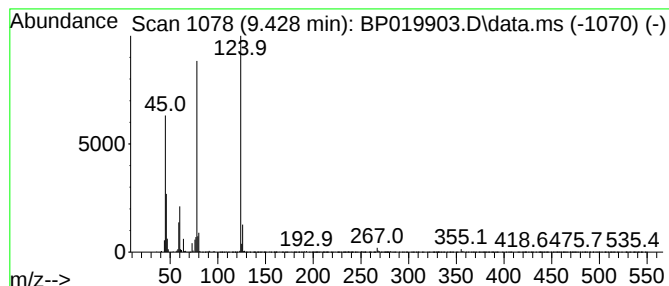
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.428	9.59 ng	406824	Naphthalene-d8	10.699	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Trithiolane	124	C2H4S3	000289-16-7	87
2	1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	45
3	1,2,4,5,7,8-Hexathiocyclononane	234	C3H6S6	081531-38-6	43
4	Fumaronitrile	78	C4H2N2	000764-42-1	28
5	Benzene	78	C6H6	000071-43-2	28



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M

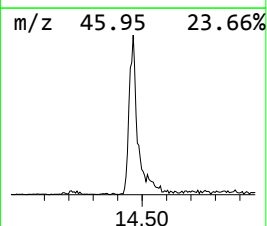
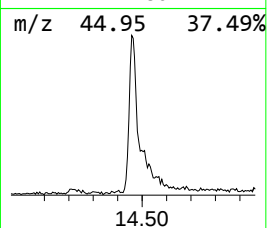
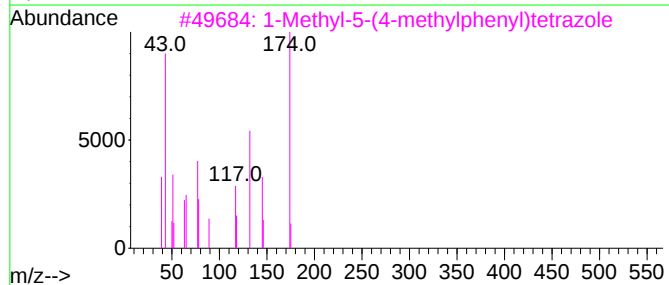
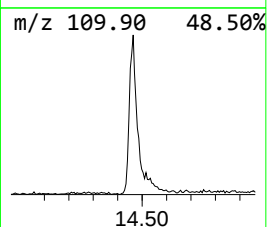
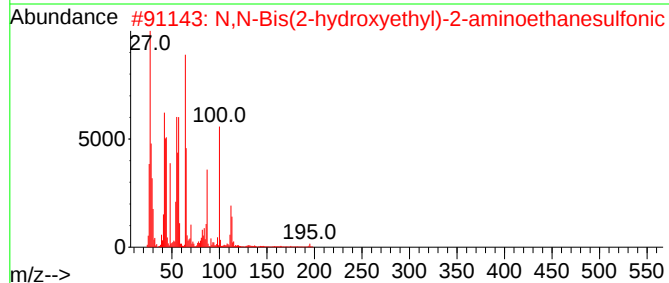
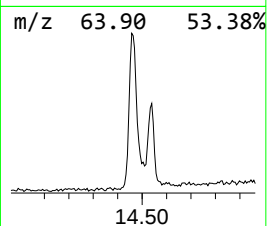
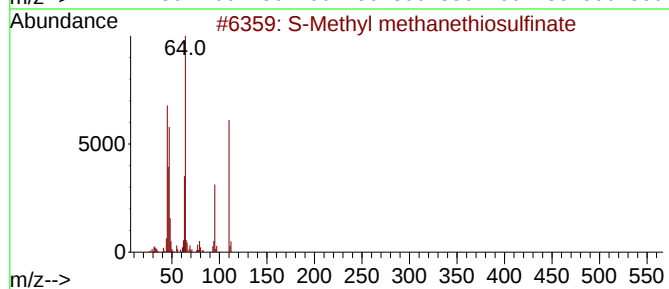
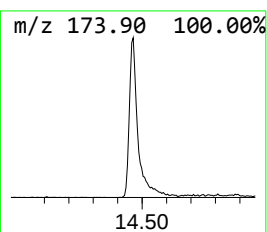
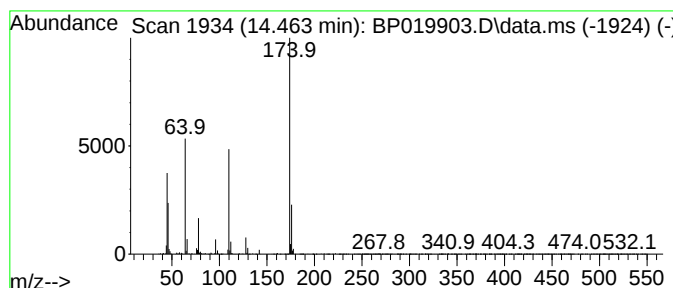
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TIC Integration Parameters: LSCINT.P

Peak Number 4 S-Methyl methanethiosulfinate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.463	3.33 ng	208818	Acenaphthene-d10	14.540	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	S-Methyl methanethiosulfinate	110	C2H6OS2	013882-12-7	52
2	N,N-Bis(2-hydroxyethyl)-2-aminoe...	213	C6H15NO5S	010191-18-1	17
3	1-Methyl-5-(4-methylphenyl)tetra...	174	C9H10N4	068826-33-5	9
4	3-Chloro-5-nitro-2(1H)-pyridinone	174	C5H3ClN2O3	022353-38-4	9
5	3-Chloro-6-hydroxy-4-pyridazinec...	174	C5H3ClN2O3	061404-48-6	9



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M

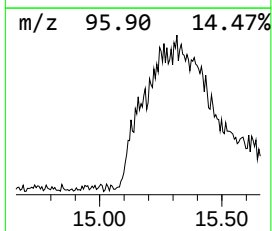
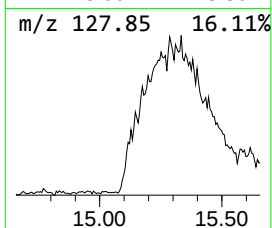
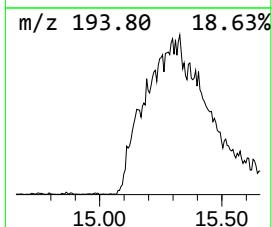
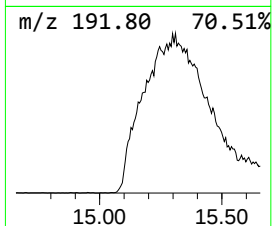
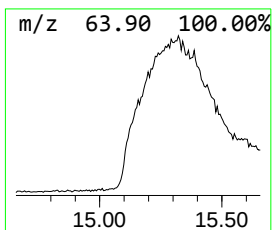
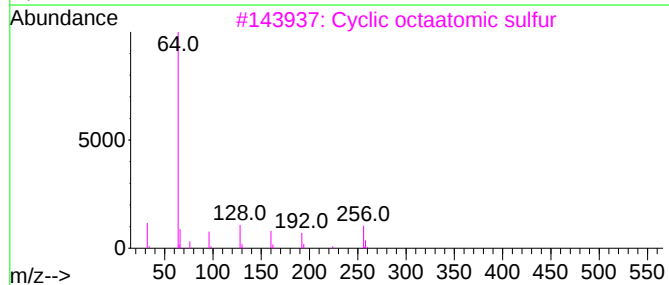
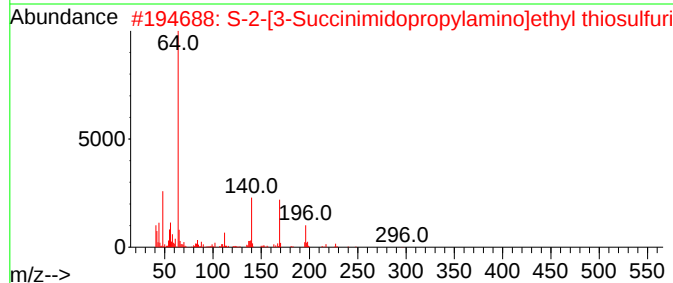
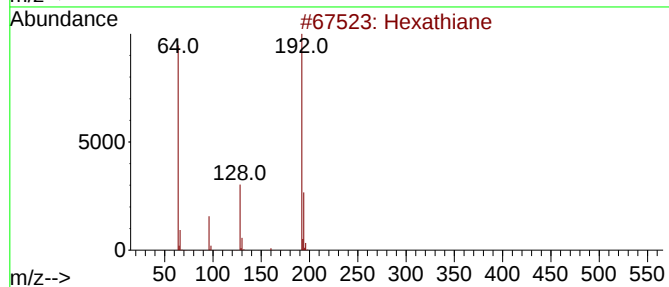
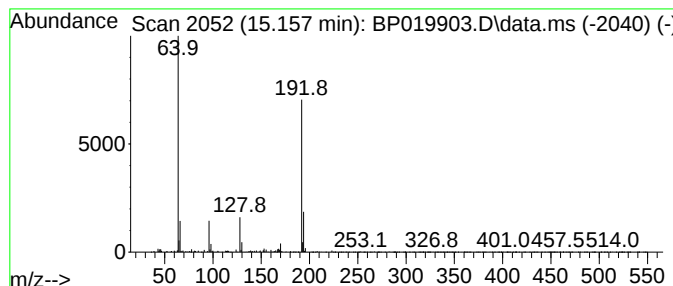
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TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexathiane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.157	2.09 ng	130974	Acenaphthene-d10	14.540	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiane	192	S6	013798-23-7	91
2	S-2-[3-Succinimidopropylamino]et...	296	C9H16N2O5S2	031701-75-4	9
3	Cyclic octaatomic sulfur	256	S8	010544-50-0	9
4	2-Chloro-7-methoxynaphthalene	192	C11H9ClO	067061-67-0	5
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5



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TIC Library : C:\Database\NIST20.L

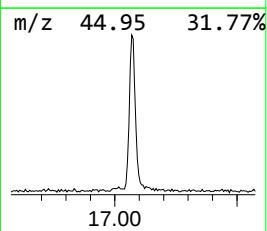
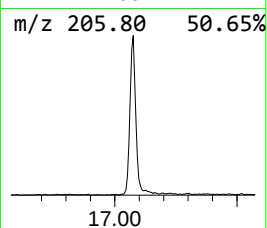
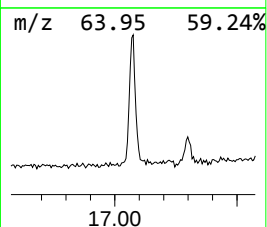
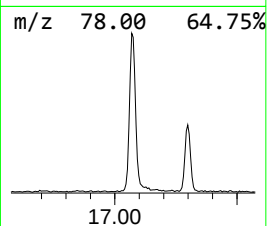
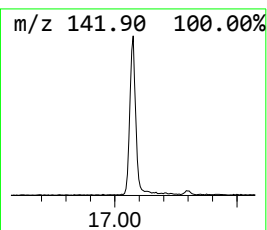
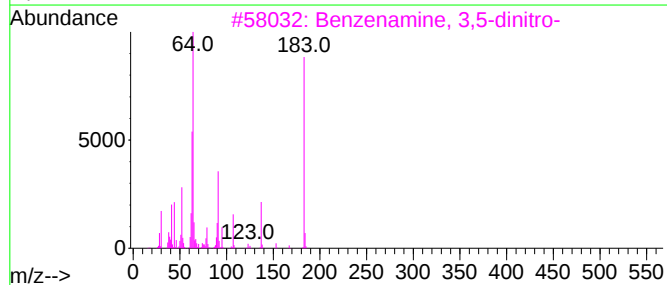
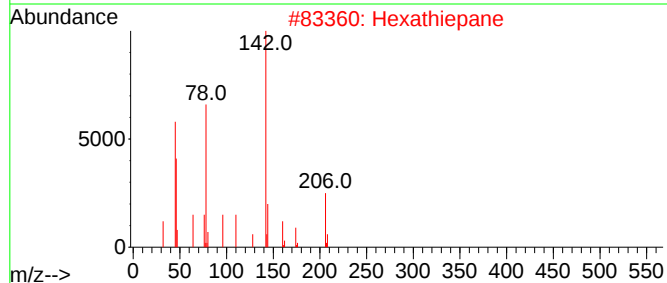
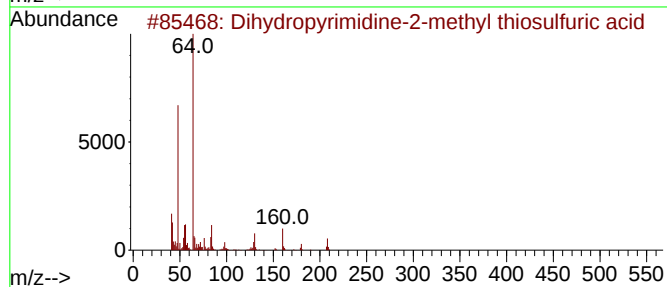
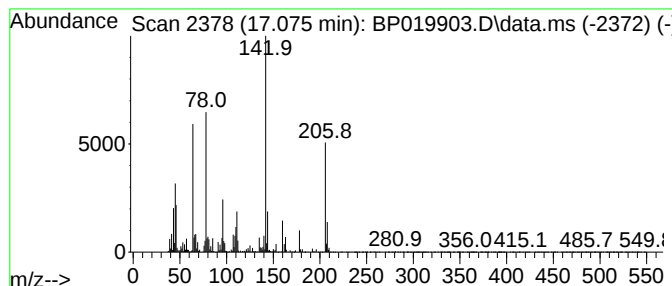
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown17.075

Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.075	7.44 ng	572531	Phenanthrene-d10	17.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	12
2			Hexathiepane	206	CH2S6	017233-71-5	12
3			Benzenamine, 3,5-dinitro-	183	C6H5N3O4	000618-87-1	12
4			Propanoic acid, 2-chloro-	108	C3H5ClO2	000598-78-7	12
5			3,3,4,5,6,6-Hexafluoro-3,6-dihyd...	226	C4F6S2	1000461-21-0	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019903.D
Acq On : 27 Feb 2024 18:50
Operator : MA/JU
Sample : P1538-12
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :

BNA_P

ClientSampleId :

20241105-AMENDED-COMPOSITE-35N-N-4-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M

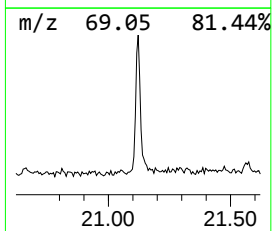
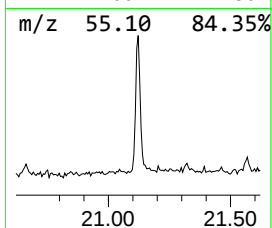
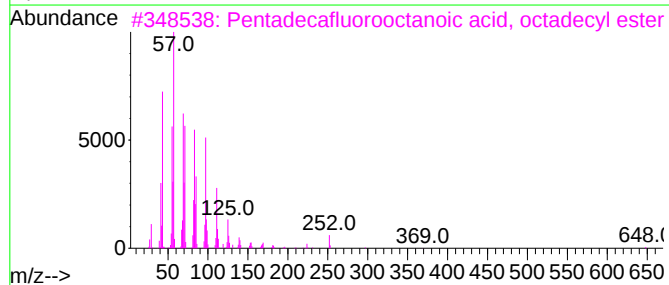
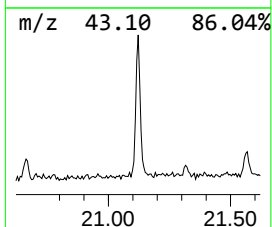
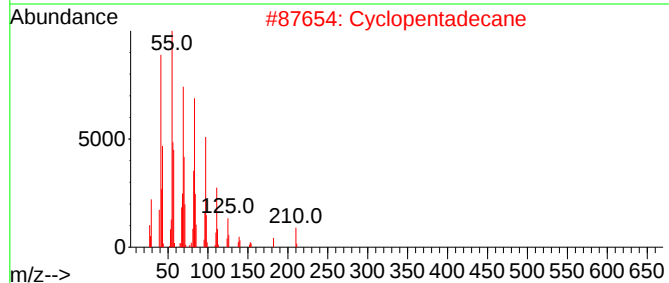
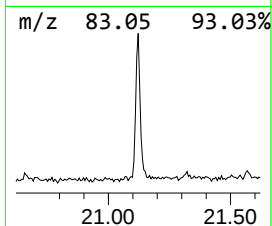
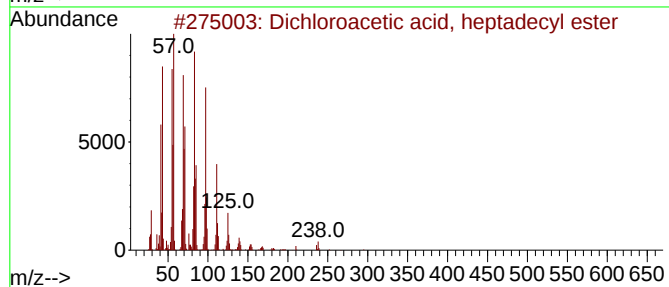
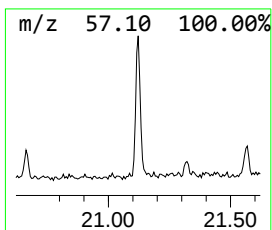
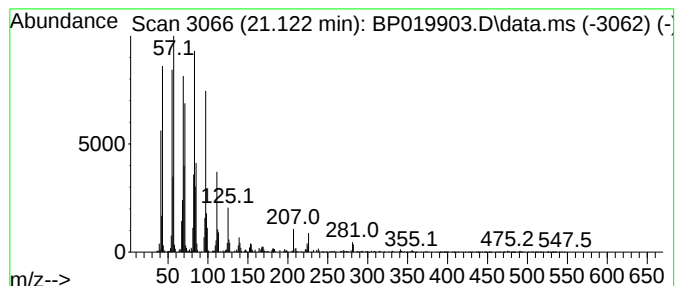
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.122	5.22 ng	408070	Chrysene-d12	21.398	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2	Cyclopentadecane	210	C15H30	000295-48-7	93
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Behenic alcohol	326	C22H46O	000661-19-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019903.D
Acq On : 27 Feb 2024 18:50
Operator : MA/JU
Sample : P1538-12
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :

BNA_P

ClientSampleId :

20241105-AMENDED-COMPOSITE-35N-N-4-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.040	414.8	ng	12470300	1	7.893	601284	20.0
Benzen-d5-amine	7.199	5.0	ng	150642	1	7.893	601284	20.0
1,2,4-Trithiolane	9.428	9.6	ng	406824	2	10.699	848868	20.0
S-Methyl methan...	14.463	3.3	ng	208818	3	14.540	1253100	20.0
Hexathiane	15.157	2.1	ng	130974	3	14.540	1253100	20.0
unknown17.075	17.075	7.4	ng	572531	4	17.298	1538340	20.0
Dichloroacetic ...	21.122	5.2	ng	408070	5	21.398	1562480	20.0