

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
 Data File : BF128681.D
 Acq On : 03 Jun 2022 16:08
 Operator : CG\JU
 Sample : N3170-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220422-AMENDED-COMPOSITE-B

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-BF060222.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128681.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.087	458	476	479	rBV	3272166	8750733	100.00%	42.203%
2	5.481	540	543	553	rVB	283169	291834	3.33%	1.407%
3	6.463	707	710	712	rBV	108565	89109	1.02%	0.430%
4	6.487	712	714	725	rVB	602141	688070	7.86%	3.318%
5	6.822	767	771	777	rBV	610675	485144	5.54%	2.340%
6	7.386	859	867	870	rBV	1734400	1764093	20.16%	8.508%
7	7.539	889	893	896	rBV	628455	609205	6.96%	2.938%
8	8.104	984	989	992	rBV	717428	581617	6.65%	2.805%
9	9.186	1168	1173	1176	rBV	2493913	2295003	26.23%	11.068%
10	9.863	1284	1288	1291	rVB	699763	580124	6.63%	2.798%
11	10.651	1419	1422	1428	rVB3	101937	113935	1.30%	0.549%
12	10.774	1438	1443	1451	rVB4	81230	114988	1.31%	0.555%
13	11.216	1515	1518	1522	rBV2	79401	106178	1.21%	0.512%
14	11.351	1537	1541	1543	rBV	557232	512286	5.85%	2.471%
15	11.945	1639	1642	1654	rVB7	38558	92206	1.05%	0.445%
16	12.792	1780	1786	1788	rBV	82184	105766	1.21%	0.510%
17	12.939	1807	1811	1814	rBV	1991062	1622812	18.54%	7.827%
18	13.074	1831	1834	1837	rBV	115908	94595	1.08%	0.456%
19	13.992	1985	1990	1993	rBV	480116	496780	5.68%	2.396%
20	14.092	2002	2007	2012	rBV	416080	436783	4.99%	2.107%
21	15.109	2177	2180	2187	rVB2	85615	100385	1.15%	0.484%
22	15.457	2234	2239	2242	rBV	356533	438739	5.01%	2.116%
23	16.192	2355	2364	2375	rBV9	55211	229545	2.62%	1.107%
24	16.362	2388	2393	2400	rBV7	68049	134726	1.54%	0.650%

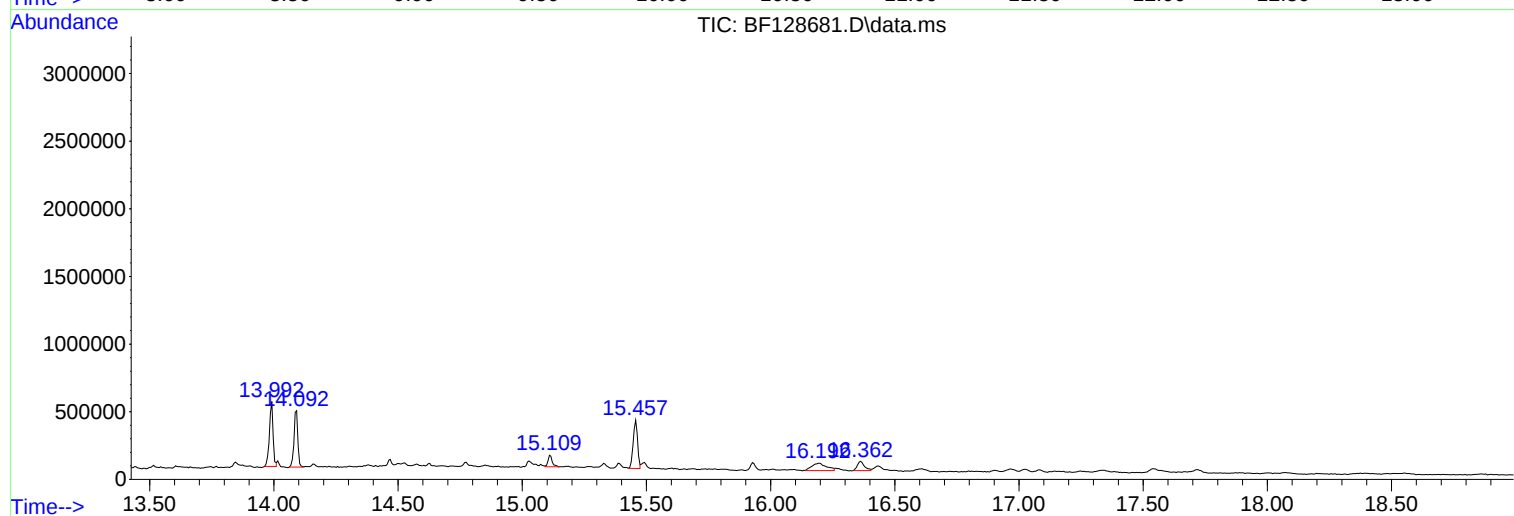
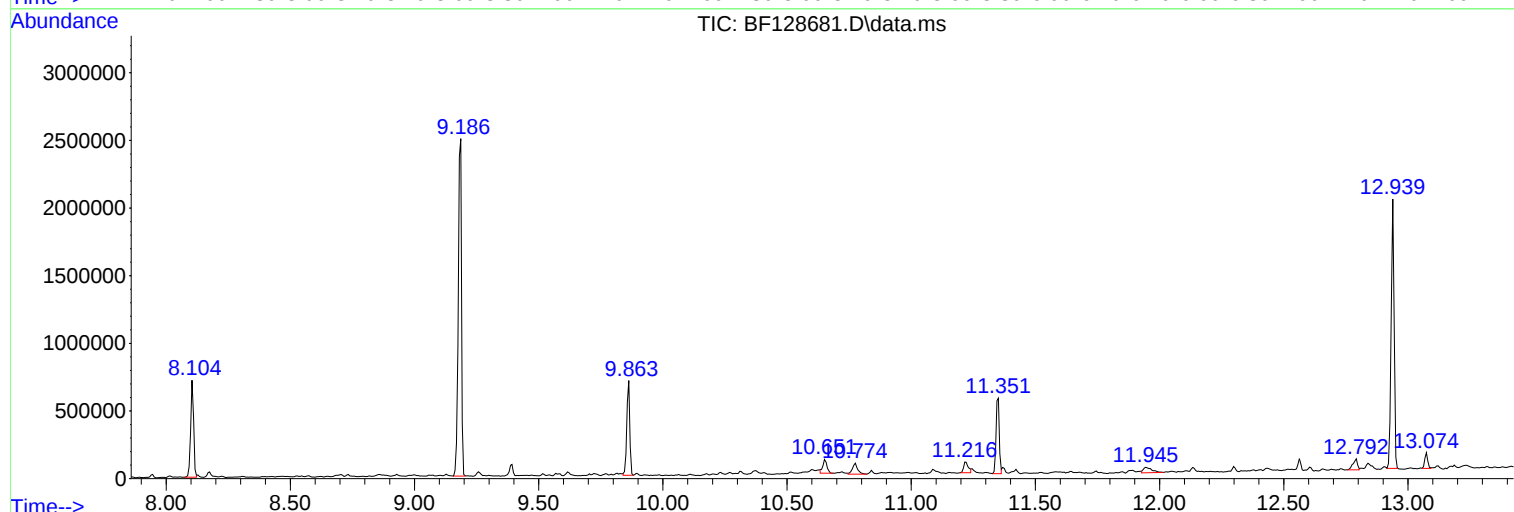
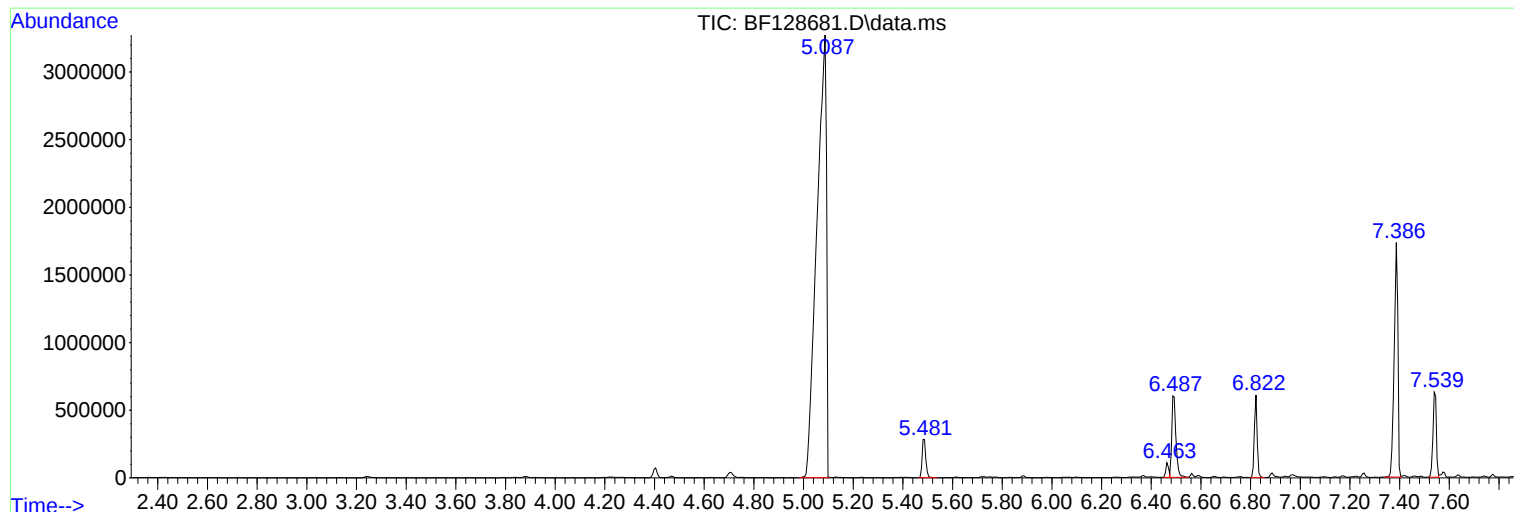
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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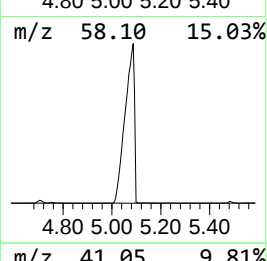
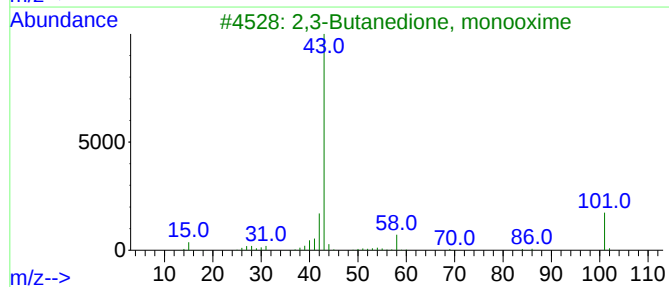
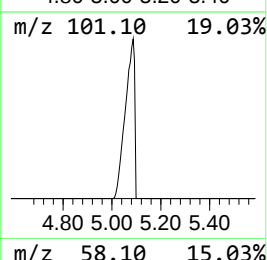
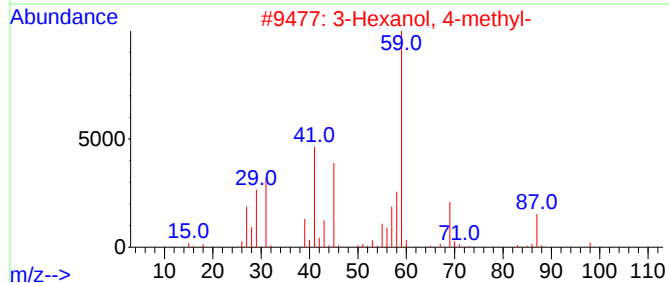
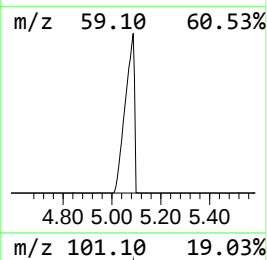
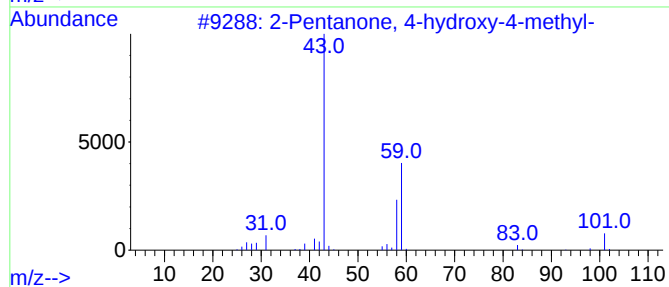
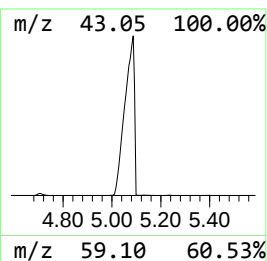
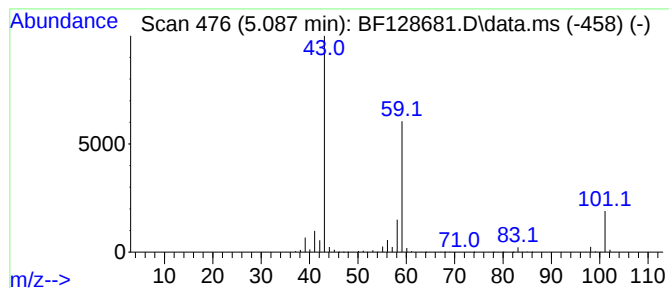
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	360.75 ng	8750730	1,4-Dichlorobenzene-d4	6.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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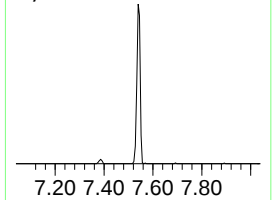
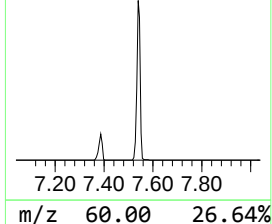
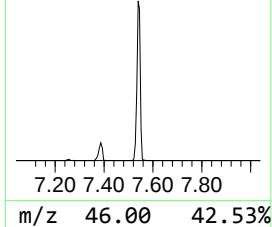
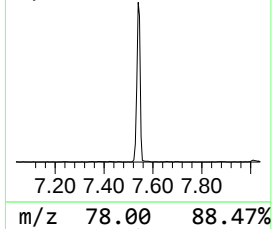
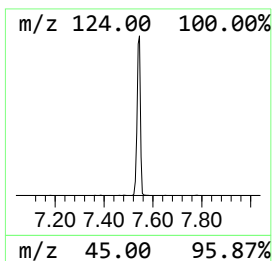
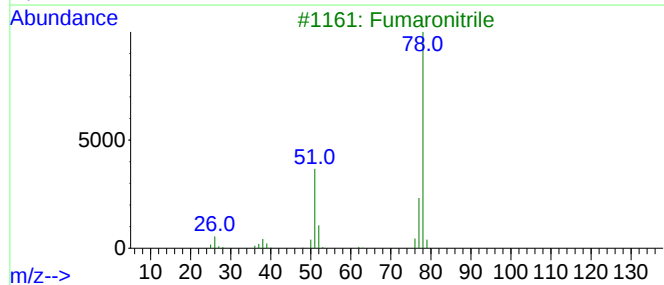
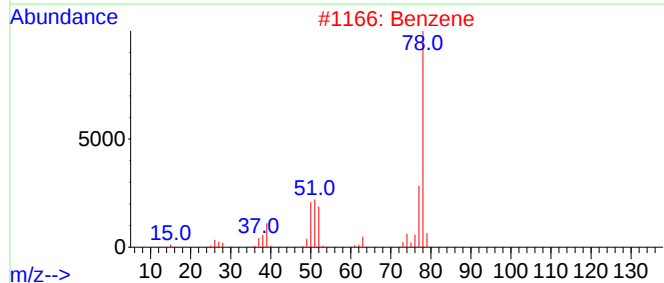
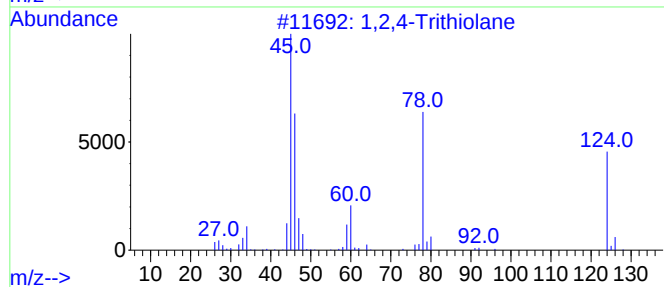
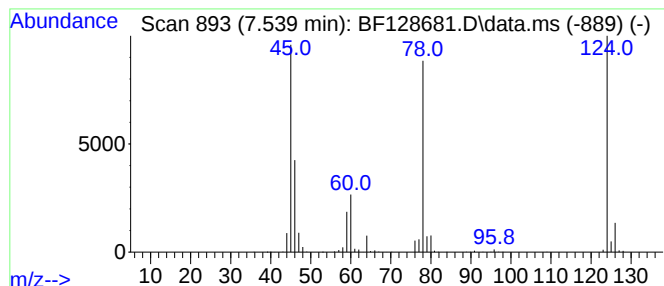
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Peak Number 2 1,2,4-Trithiolane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.539	20.95 ng	609205	Naphthalene-d8	8.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	90
2			Benzene	78	C6H6	000071-43-2	9
3			Fumaronitrile	78	C4H2N2	000764-42-1	9
4			Propane, 1-chloro-3-(2-methoxyet...	152	C6H13ClO2	024255-59-2	9
5			Carbonochloridothioic acid, S-et...	124	C3H5ClOS	002941-64-2	7



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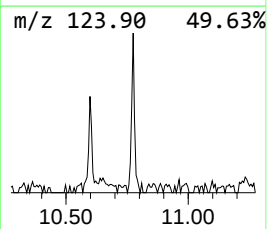
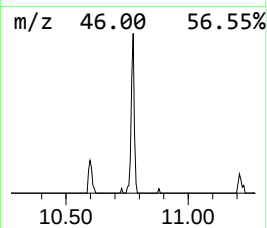
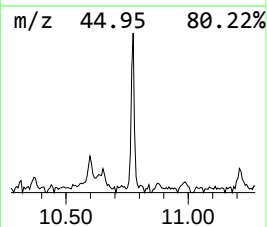
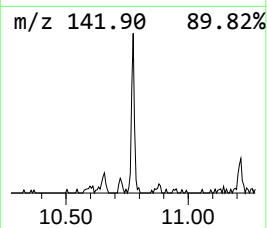
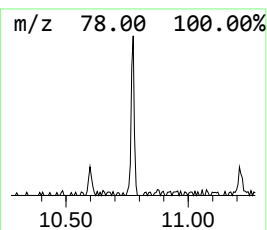
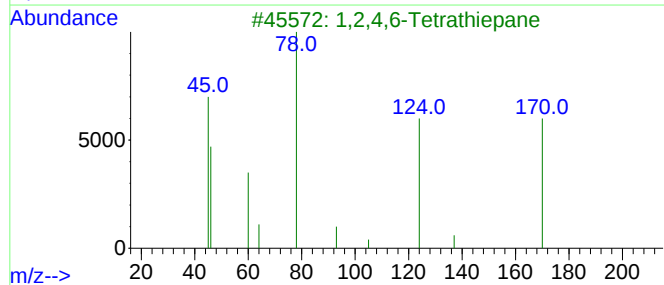
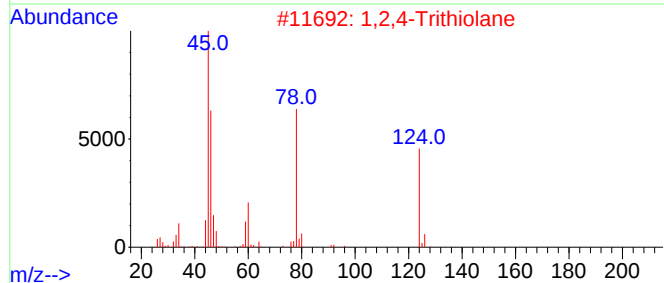
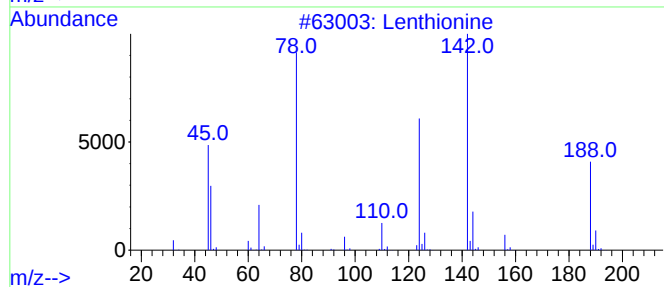
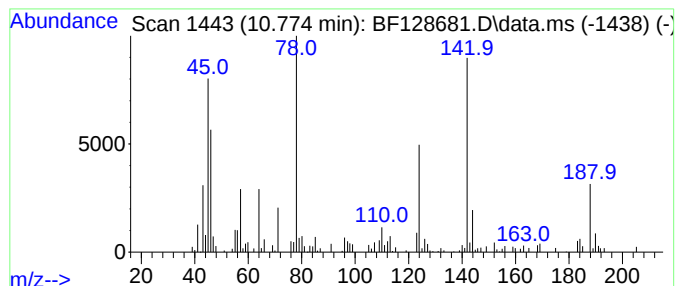
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Peak Number 3 Lenthionine Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.775	4.49 ng	114988	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lenthionine	188	C2H4S5	000292-46-6	93
2			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	59
3			1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	45
4			Ehylthiophosphonamide, o-methyl ...	139	C3H10NOPS	1000306-03-7	33
5			Glyoxal bis(nicotinoylhydrazone)	296	C14H12N6O2	042273-42-7	32



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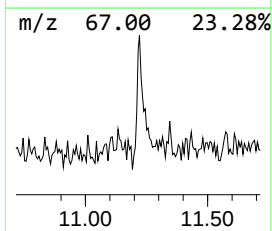
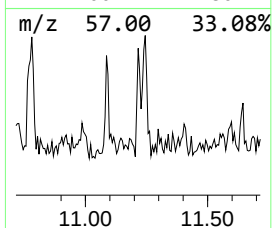
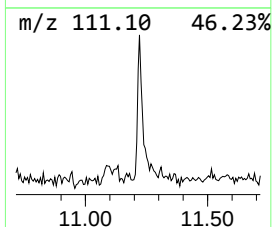
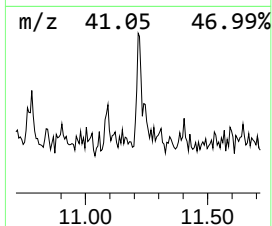
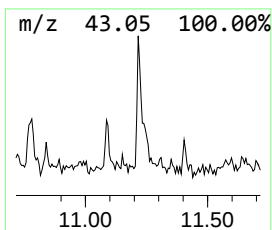
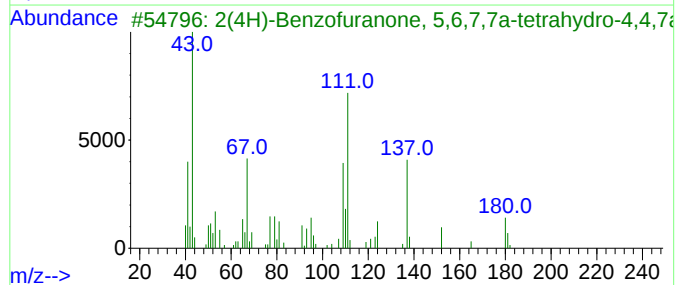
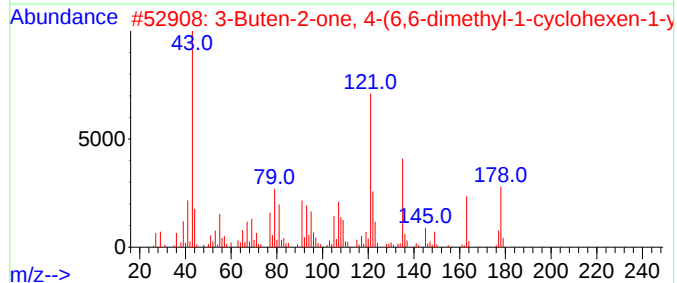
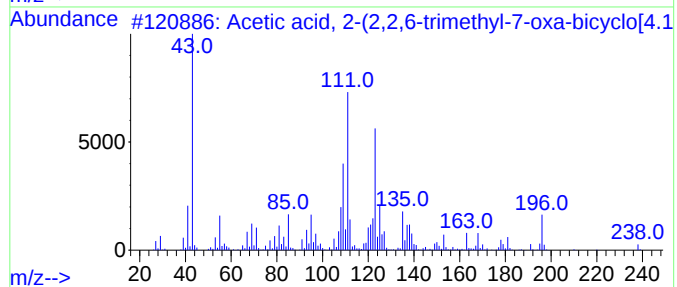
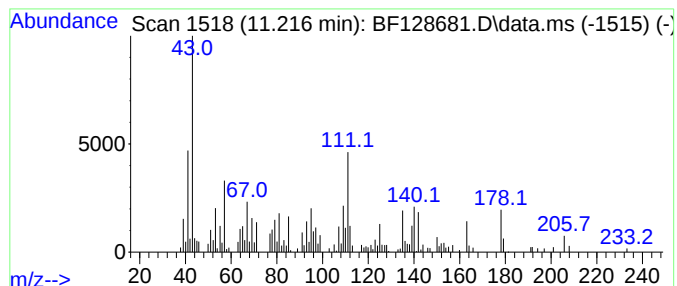
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Peak Number 4 unknown11.216 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.216	4.15 ng	106178	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 2-(2,2,6-trimethyl-...	238	C14H22O3	090165-14-3	27
2			3-Buten-2-one, 4-(6,6-dimethyl-1...	178	C12H18O	065133-79-1	22
3			2(4H)-Benzofuranone, 5,6,7,7a-te...	180	C11H16O2	017092-92-1	16
4			3-Carene, 4-acetyl-	178	C12H18O	1000156-14-1	14
5			Bicyclo[3.1.0]hexane-6-methanol,...	170	C10H18O2	058795-41-8	12



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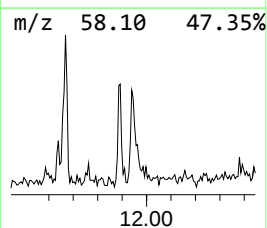
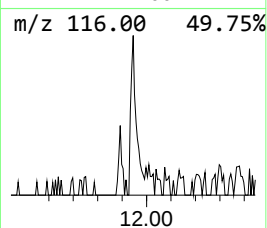
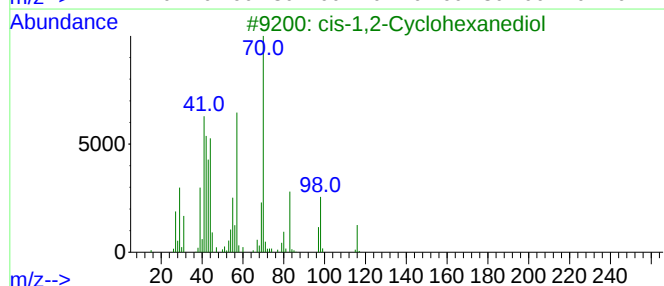
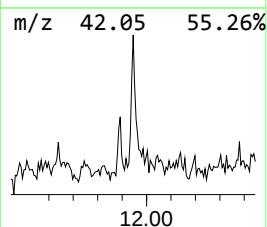
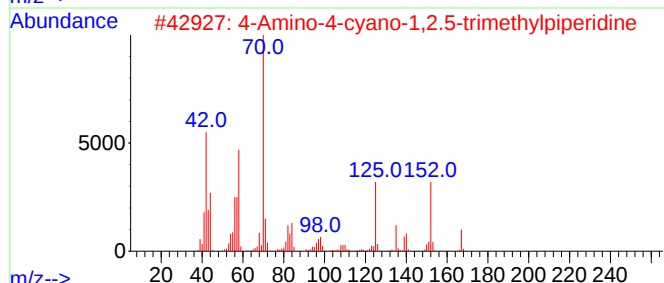
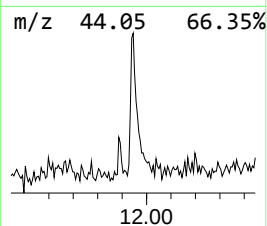
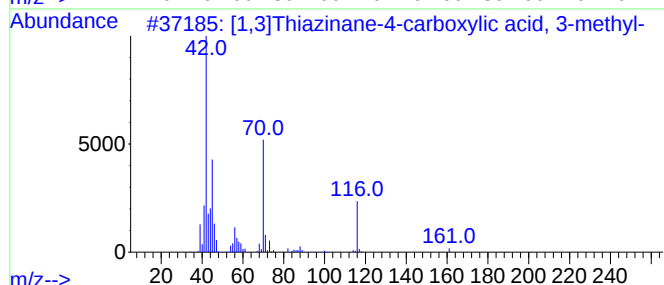
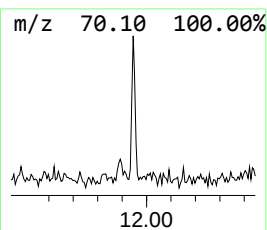
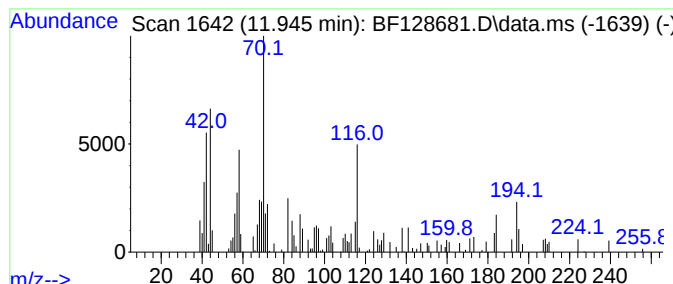
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Peak Number 5 unknown11.945 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	3.60 ng	92206	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			[1,3]Thiazinane-4-carboxylic aci...	161	C6H11N02S	1000305-15-2	43
2			4-Amino-4-cyano-1,2,5-trimethylp...	167	C9H17N3	037059-45-3	37
3			cis-1,2-Cyclohexanediol	116	C6H12O2	001792-81-0	37
4			Oxazolidine, 2,2-dimethyl-	101	C5H11NO	020515-62-2	35
5			2-[2-(4-Methyl-furazan-3-yloxy)-...	211	C6H9N7O2	1000300-54-6	32



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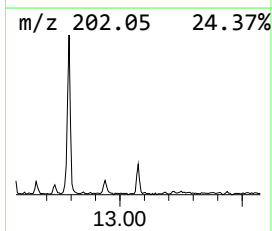
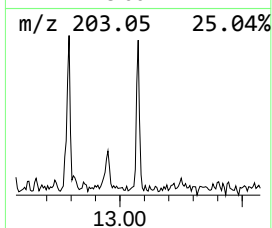
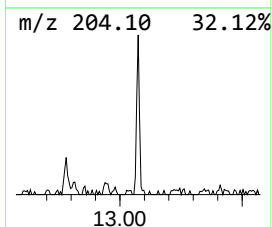
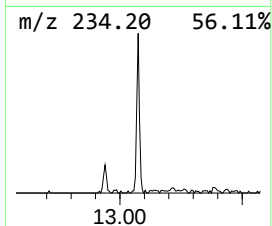
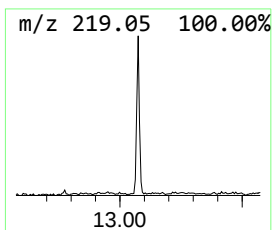
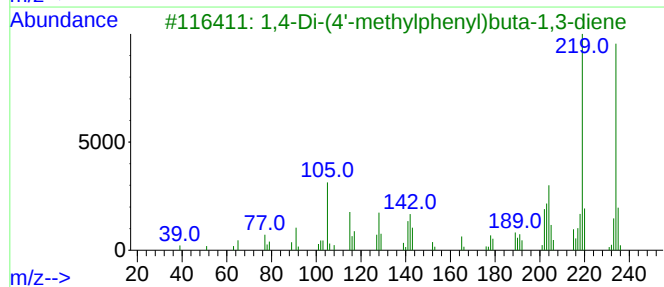
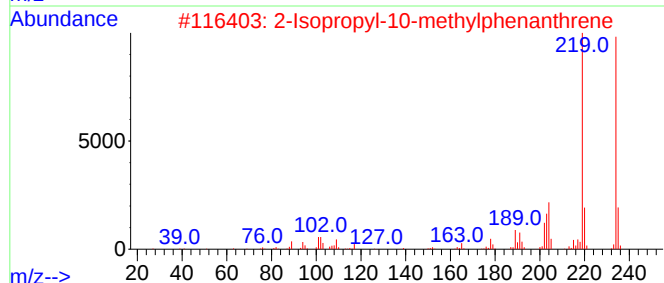
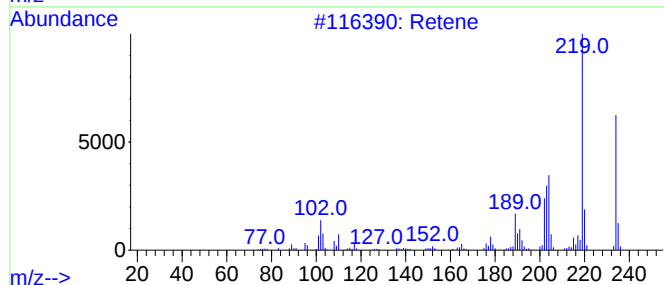
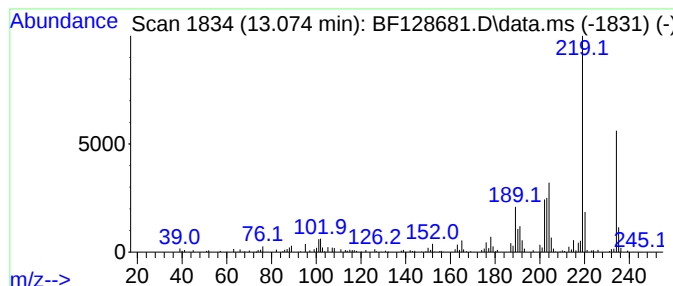
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Retene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.074	3.81 ng	94595	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Retene	234	C18H18	000483-65-8	95
2			2-Isopropyl-10-methylphenanthrene	234	C18H18	066552-97-4	93
3			1,4-Di-(4'-methylphenyl)buta-1,3...	234	C18H18	1000202-17-5	83
4			Phenanthrene, 3,4,5,6-tetramethyl-	234	C18H18	007343-06-8	76
5			Phenanthrene, 2,4,5,7-tetramethyl-	234	C18H18	007396-38-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128681.D
Acq On : 03 Jun 2022 16:08
Operator : CG\JU
Sample : N3170-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220422-AMENDED-COMPOSITE-B

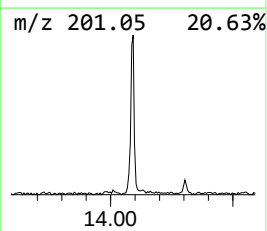
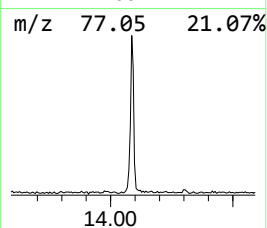
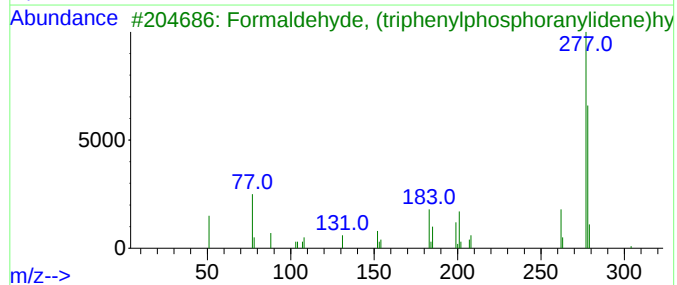
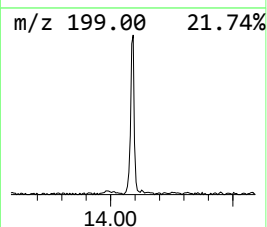
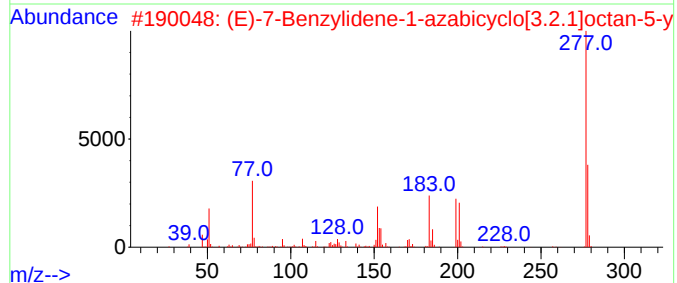
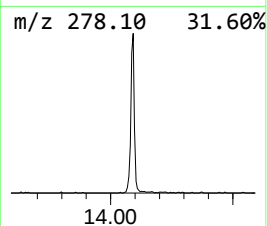
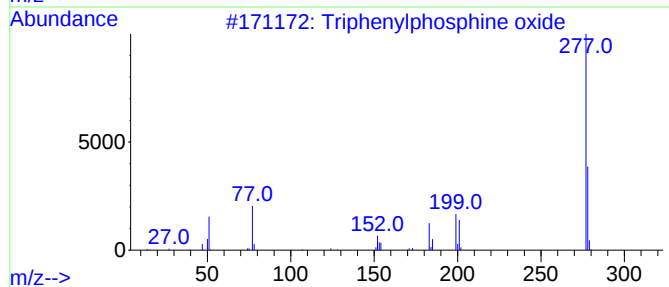
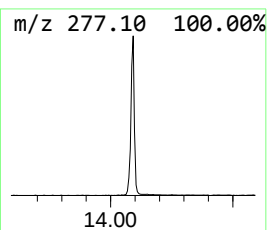
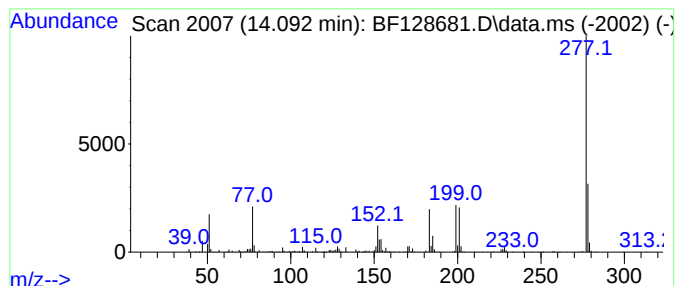
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.092	17.58 ng	436783	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	37
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128681.D
Acq On : 03 Jun 2022 16:08
Operator : CG\JU
Sample : N3170-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220422-AMENDED-COMPOSITE-B

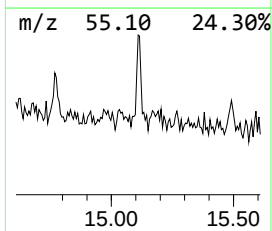
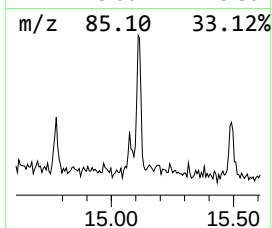
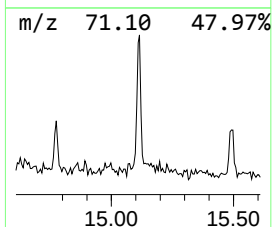
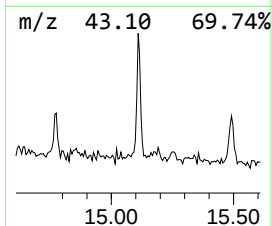
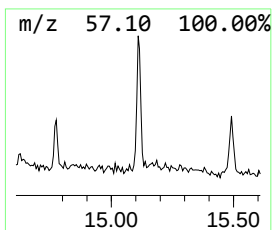
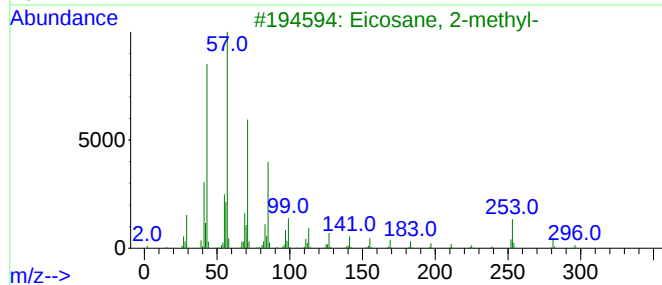
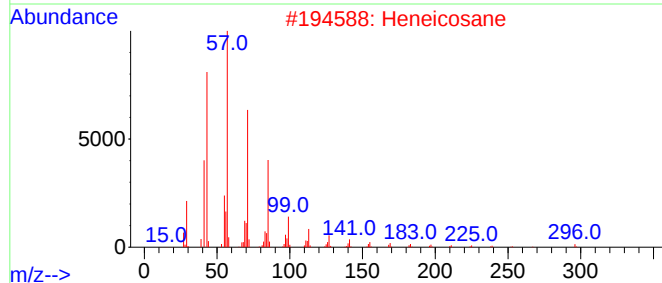
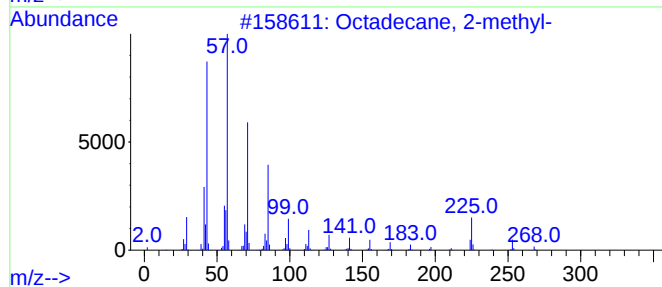
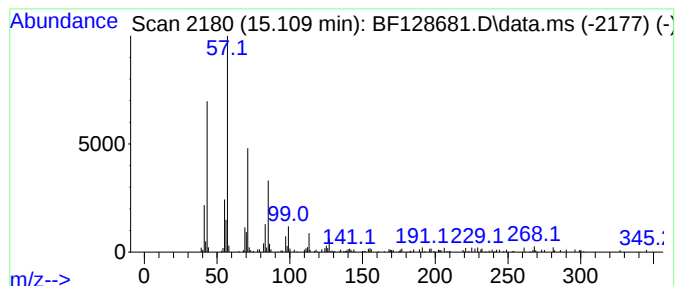
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.110	4.58 ng	100385	Perylene-d12	15.457

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane, 2-methyl-	268	C19H40	001560-88-9	91
2		Heneicosane	296	C21H44	000629-94-7	89
3		Eicosane, 2-methyl-	296	C21H44	001560-84-5	87
4		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	87
5		Eicosane	282	C20H42	000112-95-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128681.D
Acq On : 03 Jun 2022 16:08
Operator : CG\JU
Sample : N3170-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220422-AMENDED-COMPOSITE-B

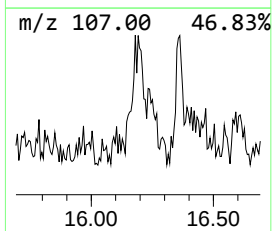
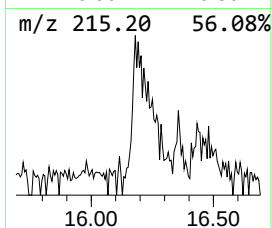
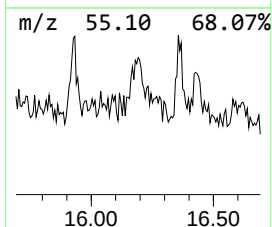
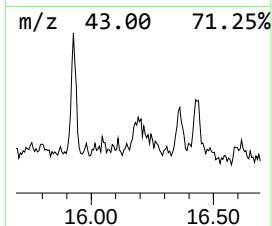
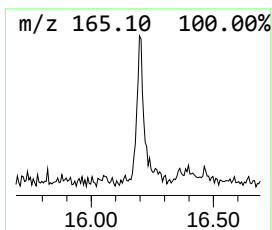
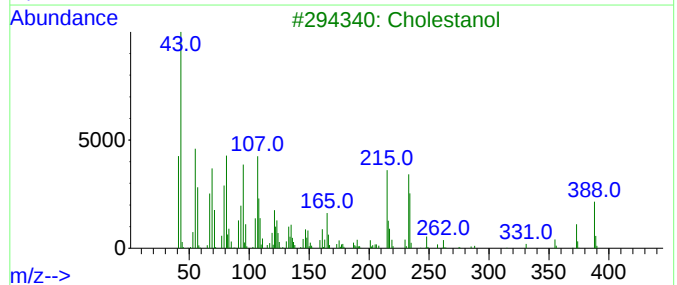
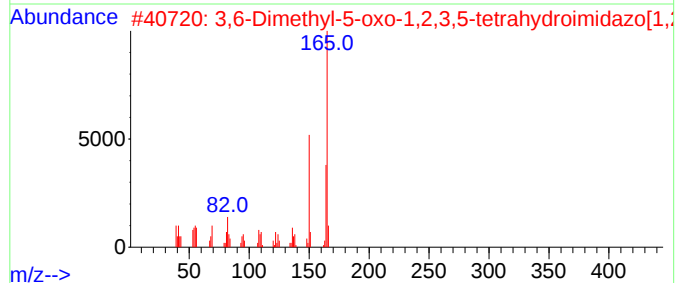
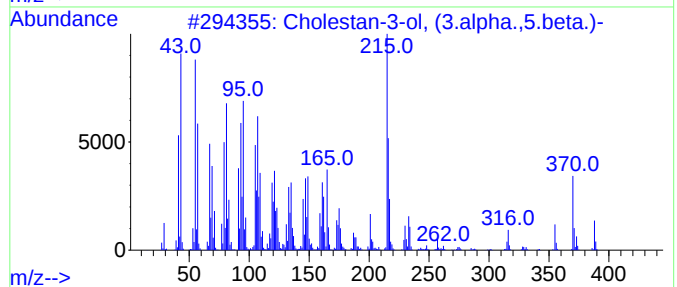
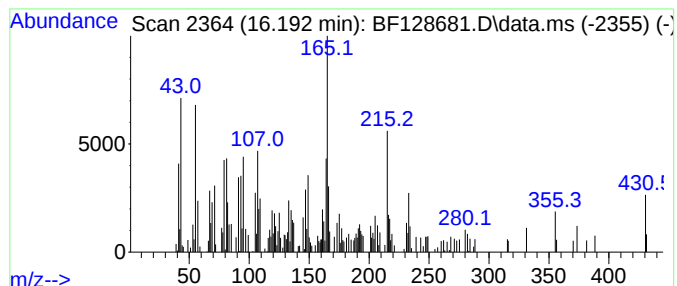
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cholestan-3-ol, (3.alpha.,5... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.192	10.46 ng	229545	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholestan-3-ol, (3.alpha.,5.beta.)-	388	C27H48O	000516-92-7	87
2			3,6-Dimethyl-5-oxo-1,2,3,5-tetra...	165	C8H11N3O	058910-42-2	38
3			Cholestanol	388	C27H48O	000080-97-7	38
4			Cholestan-3-ol	388	C27H48O	027409-41-2	38
5			Cholestan-3-ol, (3.beta.,5.beta.)-	388	C27H48O	000360-68-9	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128681.D
Acq On : 03 Jun 2022 16:08
Operator : CG\JU
Sample : N3170-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220422-AMENDED-COMPOSITE-B

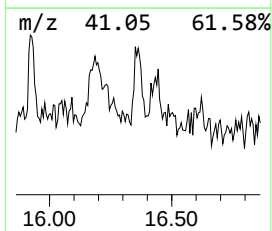
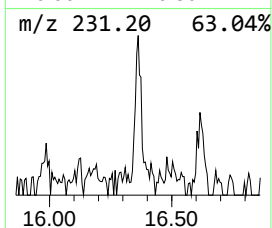
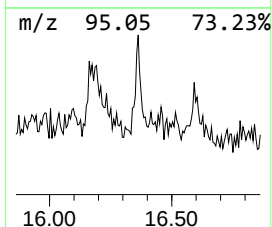
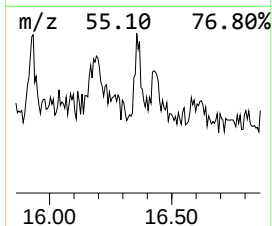
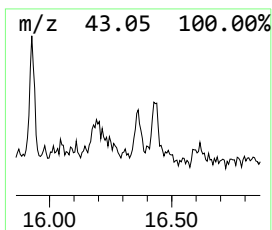
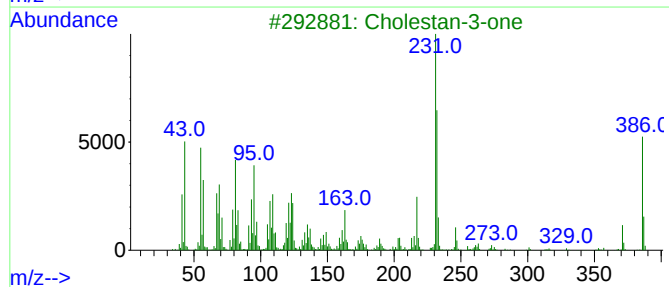
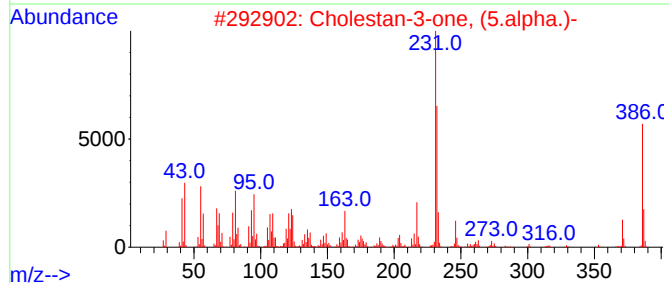
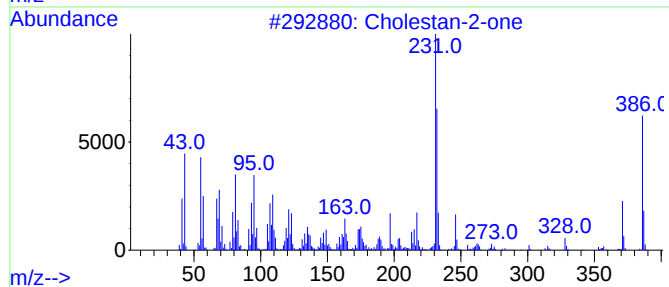
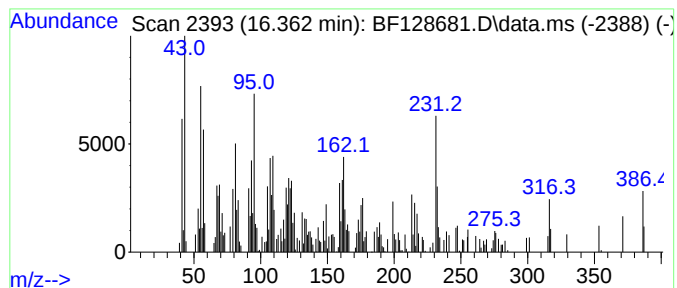
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cholestan-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.362	6.14 ng	134726	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholestan-2-one	386	C27H46O	1010210-43-4	96
2			Cholestan-3-one, (5.alpha.)-	386	C27H46O	000566-88-1	93
3			Cholestan-3-one	386	C27H46O	015600-08-5	86
4			Cholest-4-en-3-ol	386	C27H46O	014597-42-3	83
5			B-Homo-A-norcholestan-6-one, (5....	386	C27H46O	019548-94-8	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128681.D
Acq On : 03 Jun 2022 16:08
Operator : CG\JU
Sample : N3170-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220422-AMENDED-COMPOSITE-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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-...	5.087	360.8	ng	8750730	1	6.822	485144	20.0
1,2,4-Trithiolane	7.539	20.9	ng	609205	2	8.104	581617	20.0
Lenthionine	10.775	4.5	ng	114988	4	11.351	512286	20.0
unknown11.216	11.216	4.2	ng	106178	4	11.351	512286	20.0
unknown11.945	11.945	3.6	ng	92206	4	11.351	512286	20.0
Retene	13.074	3.8	ng	94595	5	13.992	496780	20.0
Triphenylphosph...	14.092	17.6	ng	436783	5	13.992	496780	20.0
Octadecane, 2-m...	15.110	4.6	ng	100385	6	15.457	438739	20.0
Cholestan-3-ol,...	16.192	10.5	ng	229545	6	15.457	438739	20.0
Cholestan-2-one	16.362	6.1	ng	134726	6	15.457	438739	20.0