

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060622\
 Data File : BF128702.D
 Acq On : 06 Jun 2022 17:59
 Operator : CG\JU
 Sample : N3189-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220428-AMENDED-COMPOSITE-H

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: BF128702.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	462	470	473	rVB	1593977	2371789	93.25%	16.529%
2	5.487	541	544	553	rBV	281754	293048	11.52%	2.042%
3	6.463	707	710	712	rBV	110025	91953	3.62%	0.641%
4	6.492	712	715	725	rVV	1265516	1285275	50.53%	8.957%
5	6.563	725	727	730	rVB	41676	28194	1.11%	0.196%
6	6.822	767	771	774	rBV	685920	534234	21.00%	3.723%
7	7.386	861	867	870	rBV	1711631	1525601	59.98%	10.632%
8	7.539	889	893	896	rBV	220619	176609	6.94%	1.231%
9	8.104	985	989	992	rBV	804462	651528	25.62%	4.541%
10	9.180	1167	1172	1175	rBV	2747728	2543465	100.00%	17.726%
11	9.257	1181	1185	1189	rVB2	47606	53103	2.09%	0.370%
12	9.863	1284	1288	1291	rVB	818087	704520	27.70%	4.910%
13	10.374	1370	1375	1378	rBV	36870	31688	1.25%	0.221%
14	10.657	1419	1423	1429	rBV2	168963	234214	9.21%	1.632%
15	10.774	1437	1443	1450	rVB	123084	116013	4.56%	0.809%
16	11.216	1514	1518	1526	rBV6	37332	73013	2.87%	0.509%
17	11.345	1537	1540	1543	rBV	682302	617177	24.27%	4.301%
18	11.416	1547	1552	1556	rVB3	44631	40318	1.59%	0.281%
19	11.880	1628	1631	1637	rBV6	17279	28212	1.11%	0.197%
20	12.792	1778	1786	1788	rBV	23748	32863	1.29%	0.229%
21	12.939	1807	1811	1814	rBV	1905458	1589035	62.48%	11.074%
22	13.862	1961	1968	1980	rBV6	37202	142585	5.61%	0.994%
23	13.992	1985	1990	1993	rBV	519222	480016	18.87%	3.345%
24	14.086	2002	2006	2016	rBV	133611	153896	6.05%	1.073%
25	15.027	2163	2166	2173	rVB3	15294	30143	1.19%	0.210%
26	15.109	2176	2180	2183	rBV2	25691	31318	1.23%	0.218%
27	15.457	2234	2239	2243	rBV	389802	489071	19.23%	3.408%

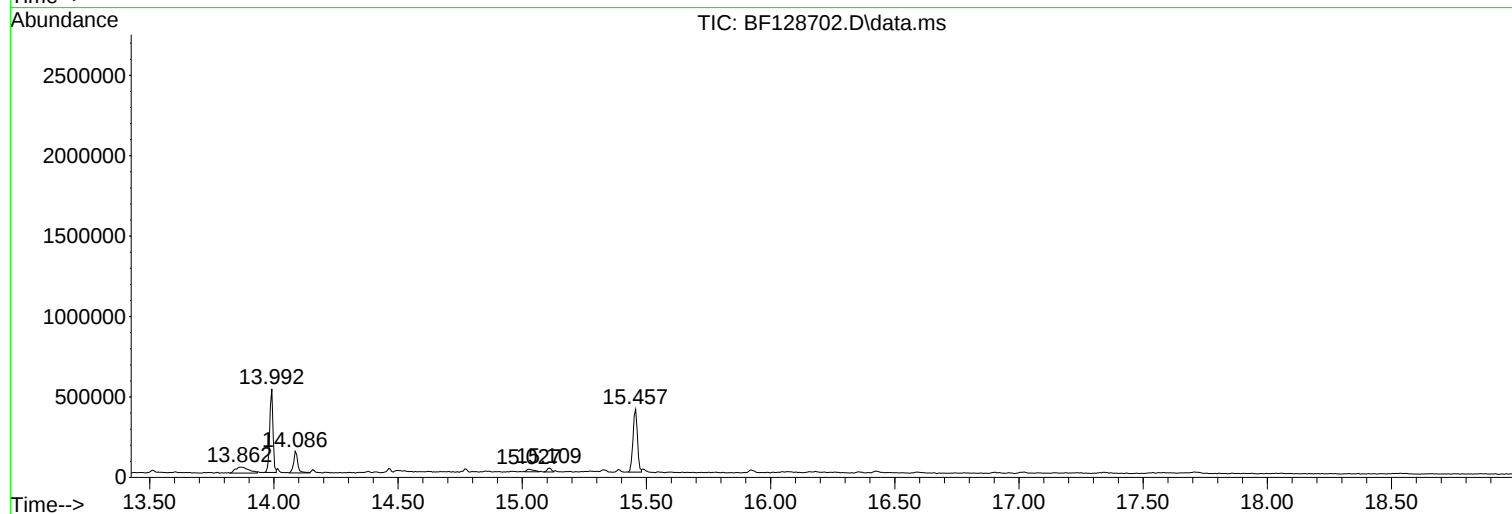
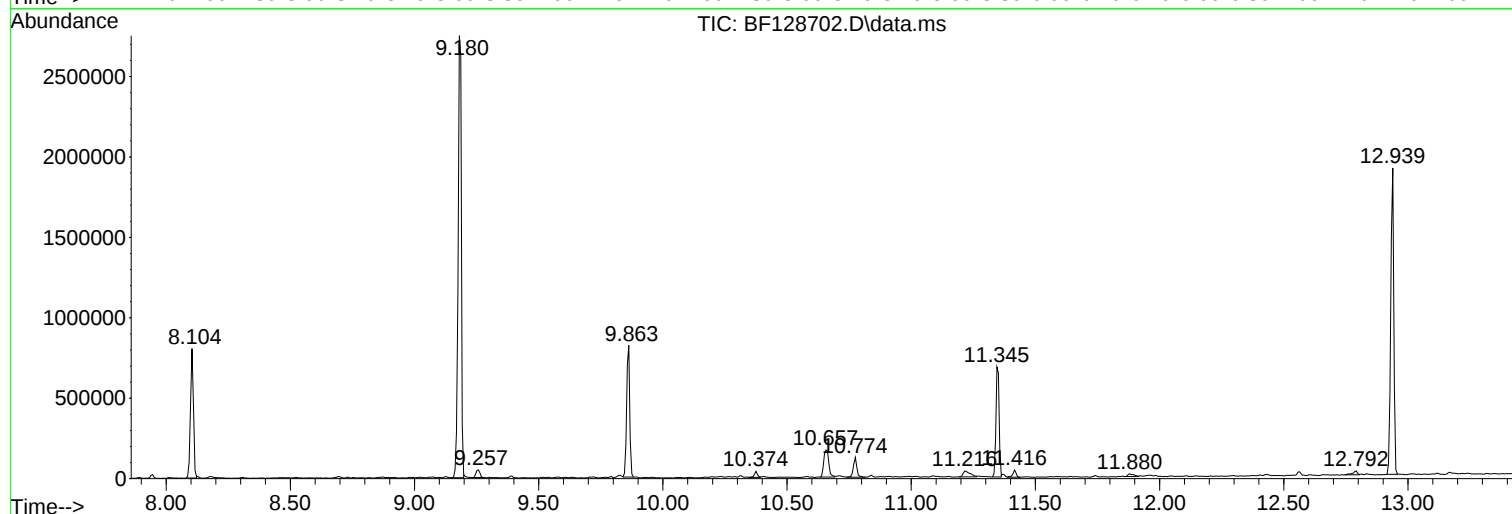
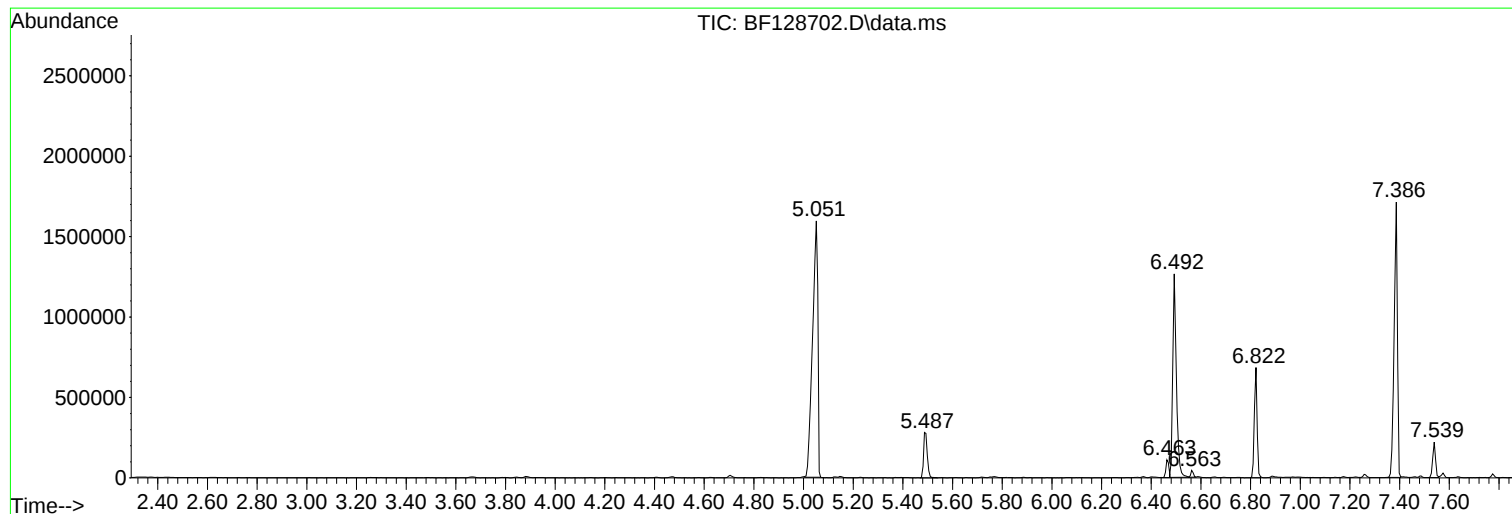
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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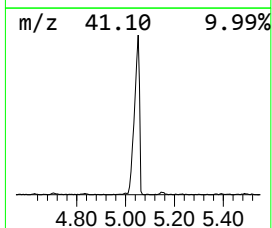
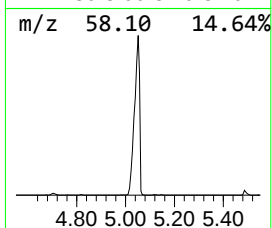
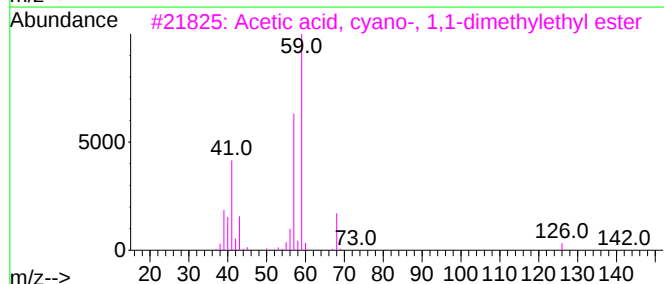
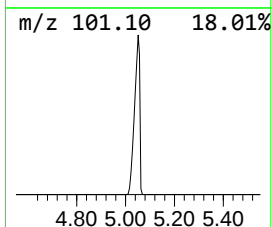
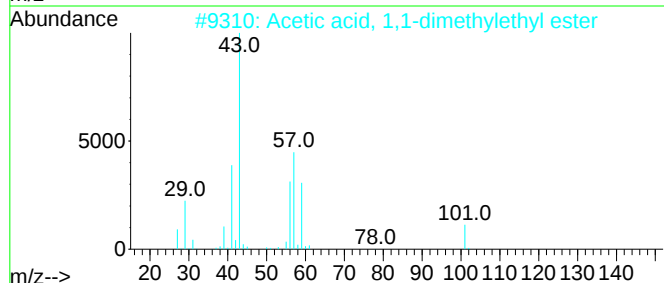
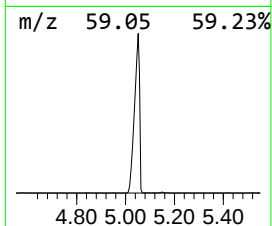
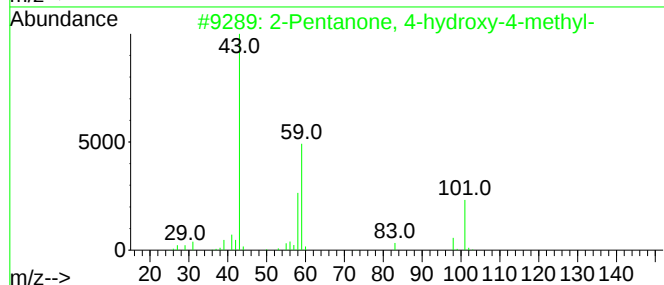
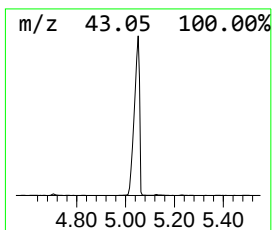
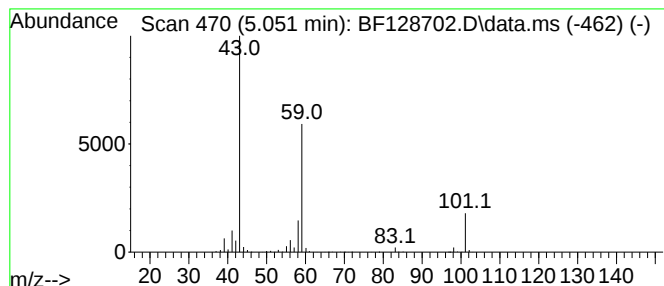
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
5.051	88.79 ng	2371790	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	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		



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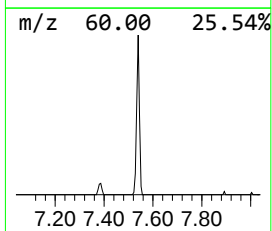
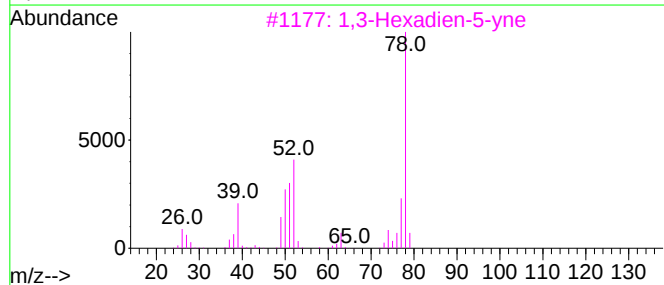
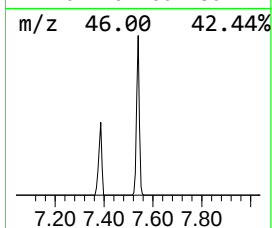
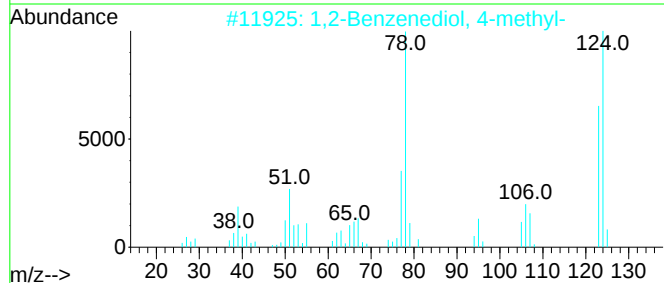
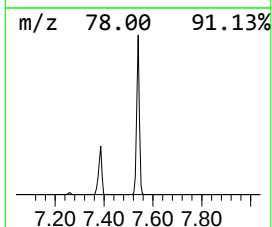
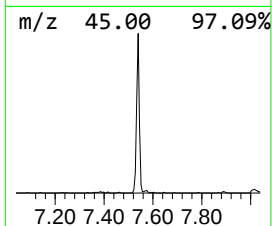
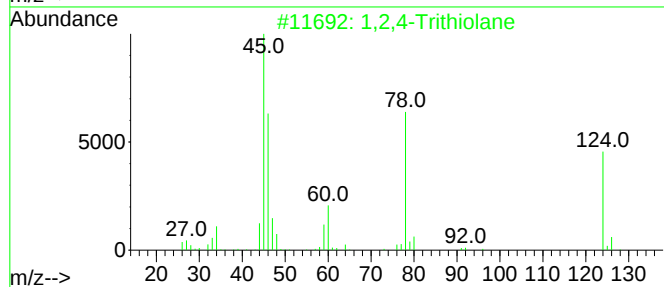
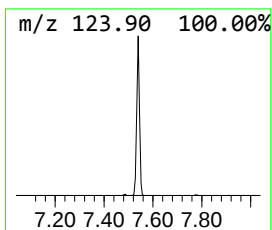
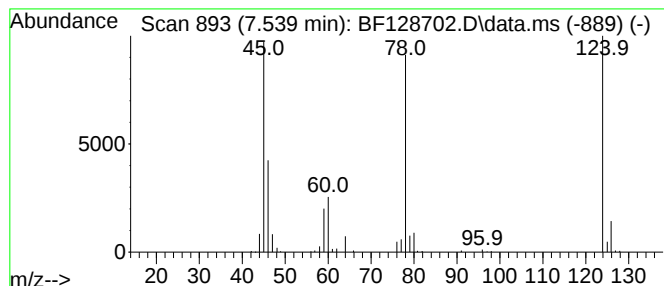
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Peak Number 2 unknown7.539 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.539	5.42 ng	176609	Naphthalene-d8	8.104

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,2,4-Trithiolane	124	C2H4S3	000289-16-7	43
2		1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	42
3		1,3-Hexadien-5-yne	78	C6H6	010420-90-3	25
4		Benzene	78	C6H6	000071-43-2	9
5		2,4-Hexadiyne	78	C6H6	002809-69-0	9



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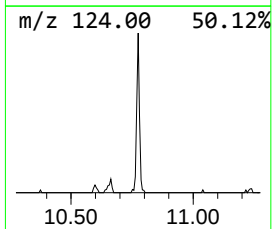
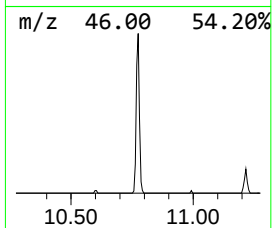
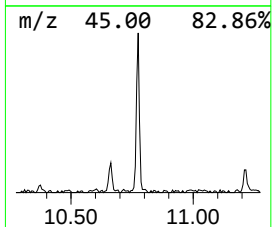
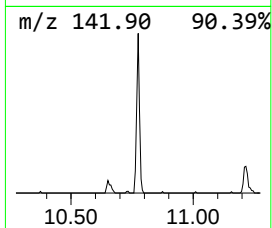
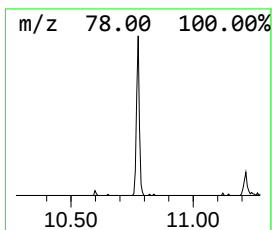
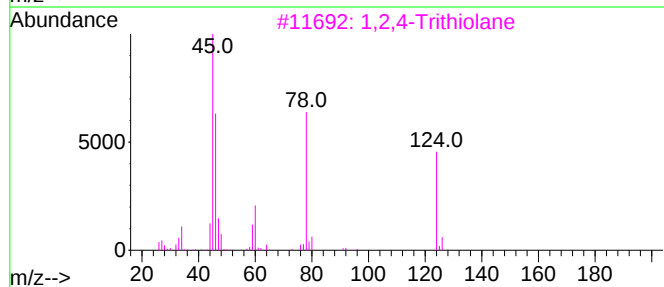
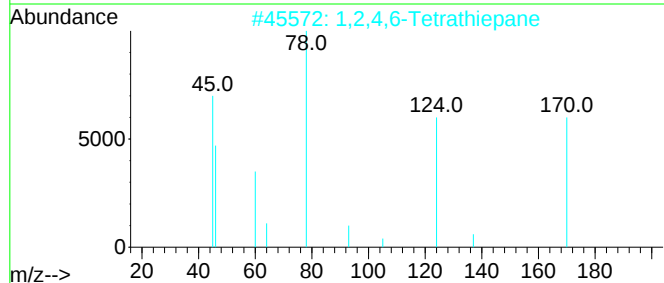
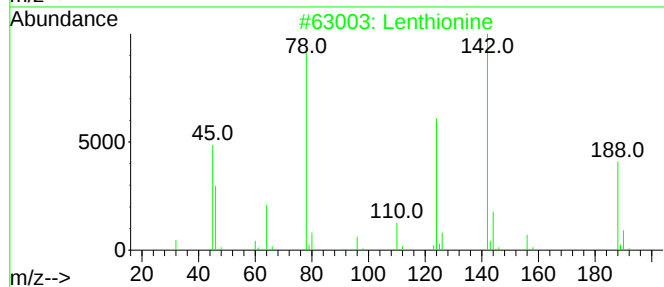
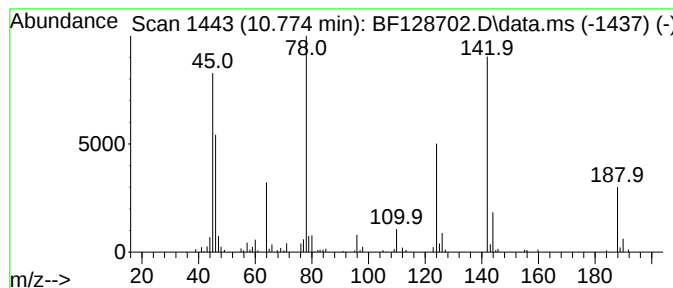
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Lenthionine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.775	3.76 ng	116013	Phenanthrene-d10	11.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lenthionine	188	C2H4S5	000292-46-6	94
2			1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	45
3			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	38
4			Methylthiophosphonamidic acid, S...	125	C2H8NOPS	1000306-03-2	28
5			Benzene	78	C6H6	000071-43-2	9



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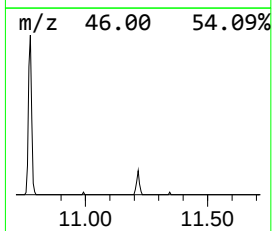
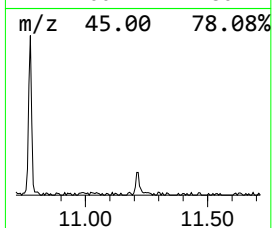
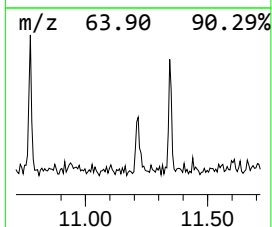
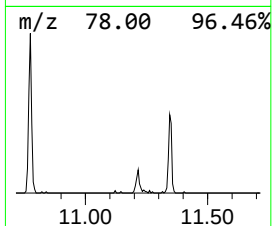
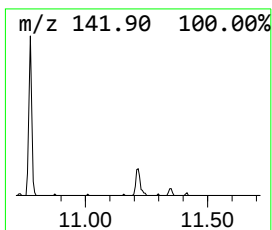
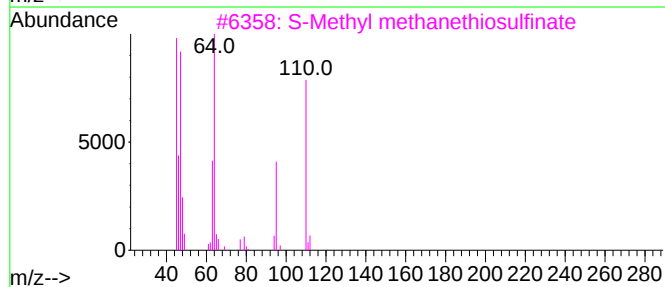
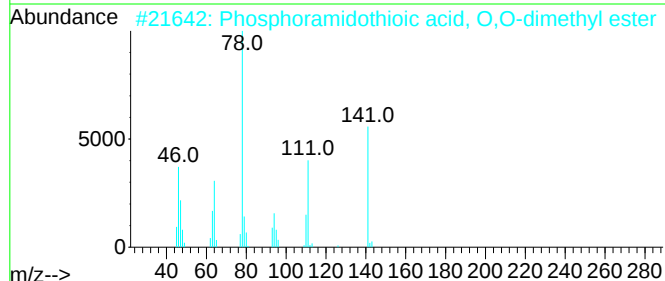
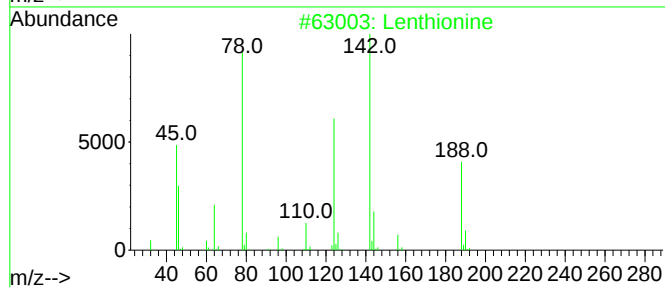
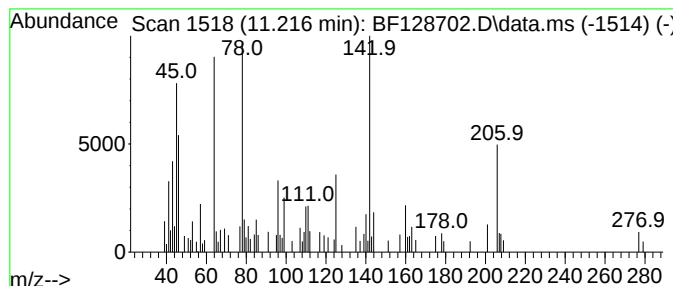
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Peak Number 4 unknown11.216 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.216	2.37 ng	73013	Phenanthrene-d10	11.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lenthionine	188	C2H4S5	000292-46-6	32
2			Phosphoramidothioic acid, O,O-di...	141	C2H8N02PS	017321-47-0	27
3			S-Methyl methanethiosulfinate	110	C2H6OS2	013882-12-7	25
4			Thiosulfuric acid (H2S2O3), S-(...	288	C11H16N2O3S2	063869-36-3	22
5			Thiosulfuric acid (H2S2O3), S-(2...	320	C11H16N2O3S3	040284-00-2	22



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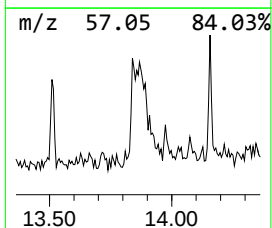
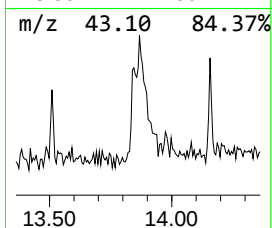
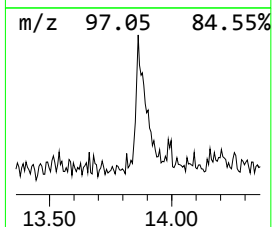
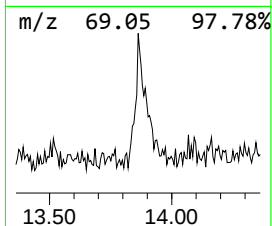
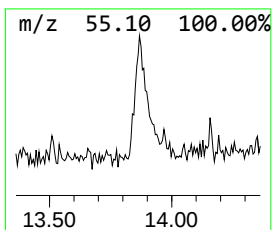
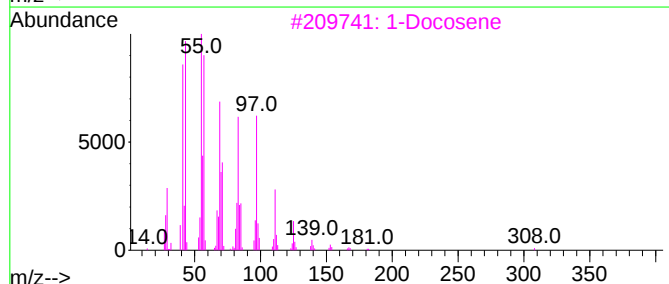
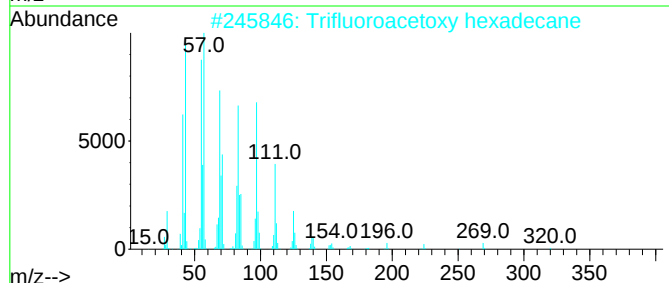
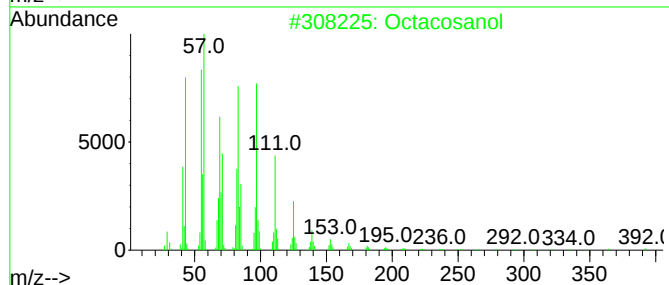
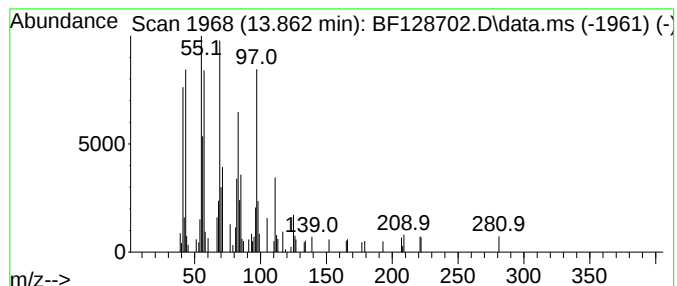
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Peak Number 5 Octacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	5.94 ng	142585	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosanol	410	C28H58O	000557-61-9	70
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	62
3			1-Docosene	308	C22H44	001599-67-3	62
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	58
5			1-Hexacosene	364	C26H52	018835-33-1	58



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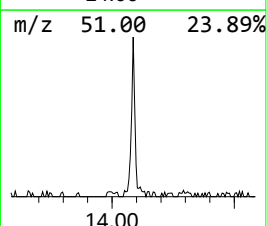
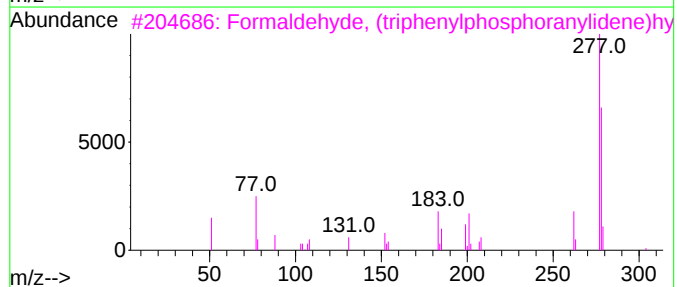
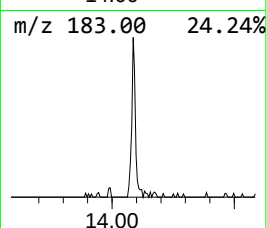
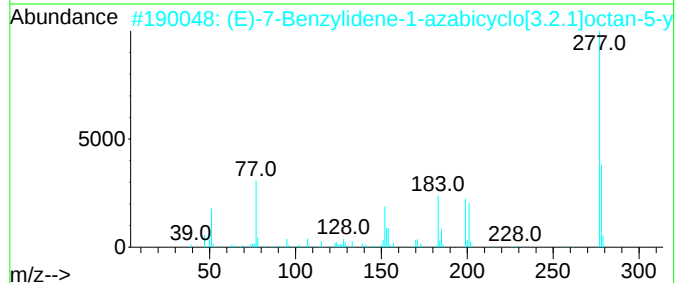
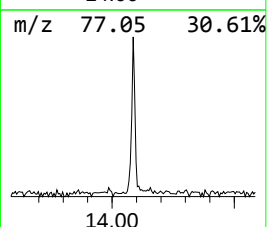
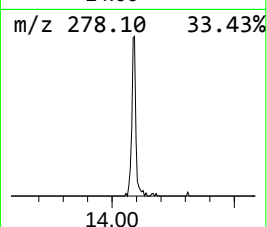
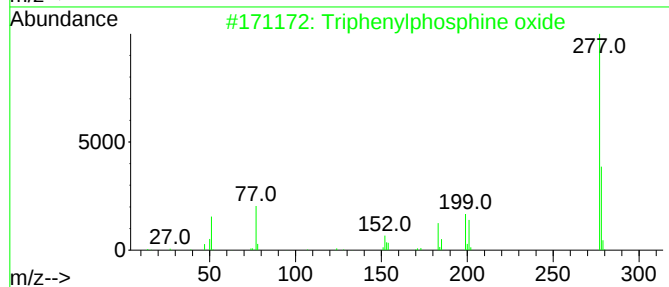
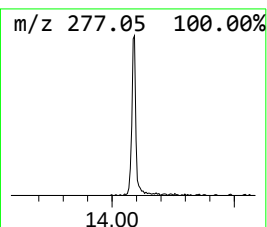
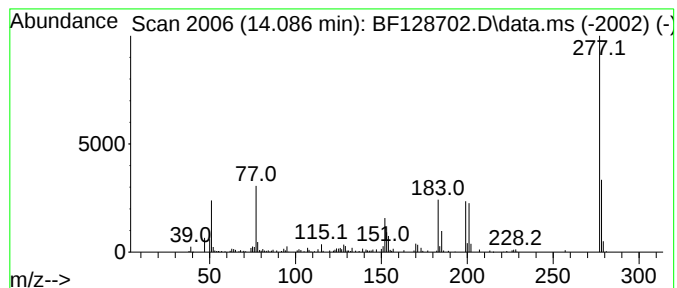
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	6.41 ng	153896	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	43
5			3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060622\
Data File : BF128702.D
Acq On : 06 Jun 2022 17:59
Operator : CG\JU
Sample : N3189-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220428-AMENDED-COMPOSITE-H

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.051	88.8	ng	2371790	1	6.822	534234	20.0
unknown7.539	7.539	5.4	ng	176609	2	8.104	651528	20.0
Lenthionine	10.775	3.8	ng	116013	4	11.345	617177	20.0
unknown11.216	11.216	2.4	ng	73013	4	11.345	617177	20.0
Octacosanol	13.863	5.9	ng	142585	5	13.992	480016	20.0
Triphenylphosph...	14.086	6.4	ng	153896	5	13.992	480016	20.0