

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060222\
 Data File : BF128654.D
 Acq On : 02 Jun 2022 23:10
 Operator : CG\JU
 Sample : N3099-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220426-AMENDED-COMPOSITE-F

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: BF128654.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.416	355	362	365	rBV	1671626	1923047	24.10%	9.151%
2	5.081	458	475	478	rBV	3283585	7978527	100.00%	37.965%
3	6.504	714	717	724	rVB	144143	127651	1.60%	0.607%
4	6.822	767	771	774	rBV	781847	653658	8.19%	3.110%
5	7.387	859	867	870	rBV	1554570	1437950	18.02%	6.842%
6	8.104	984	989	992	rBV	986137	824312	10.33%	3.922%
7	9.181	1167	1172	1176	rVB	2338780	2158094	27.05%	10.269%
8	9.863	1284	1288	1291	rVB	1162285	937348	11.75%	4.460%
9	10.775	1440	1443	1450	rBV2	104676	99957	1.25%	0.476%
10	11.222	1514	1519	1522	rBV4	84333	140904	1.77%	0.670%
11	11.351	1537	1541	1543	rBV	1148214	962977	12.07%	4.582%
12	12.569	1745	1748	1752	rVB	159187	131354	1.65%	0.625%
13	12.792	1781	1786	1789	rBV	122191	115332	1.45%	0.549%
14	12.939	1807	1811	1814	rBV	2315965	2005124	25.13%	9.541%
15	13.992	1985	1990	1993	rBV	744488	727239	9.11%	3.460%
16	14.086	2001	2006	2010	rBV	173397	201346	2.52%	0.958%
17	15.027	2163	2166	2176	rVB	45144	93829	1.18%	0.446%
18	15.457	2234	2239	2243	rBV	424269	497014	6.23%	2.365%

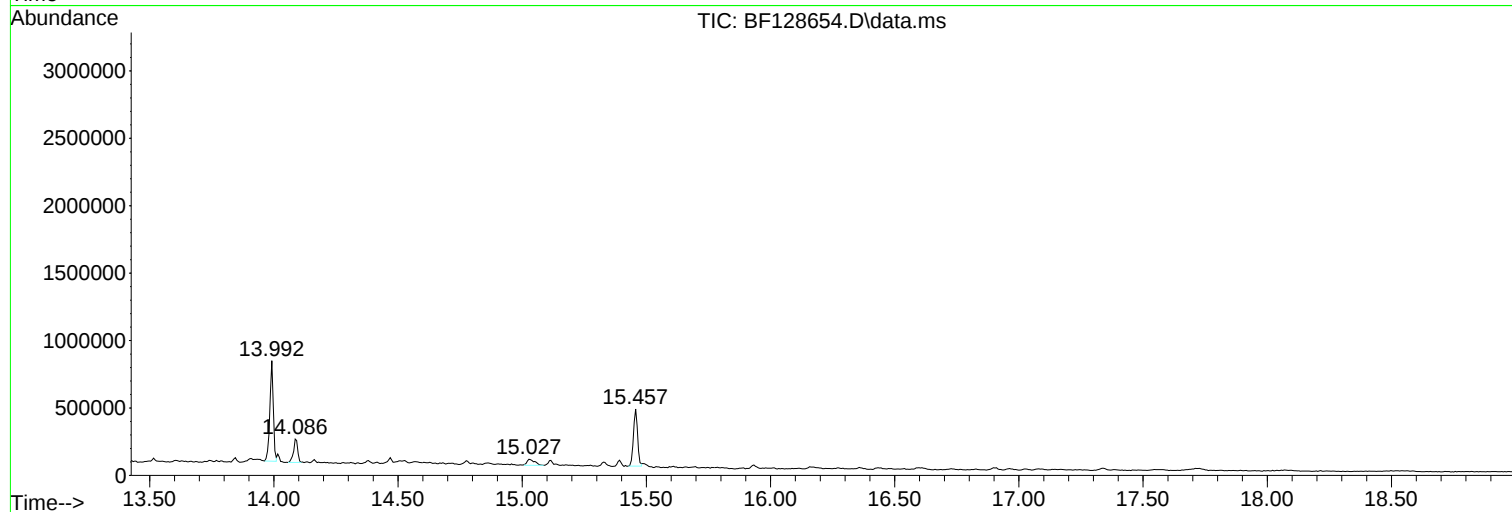
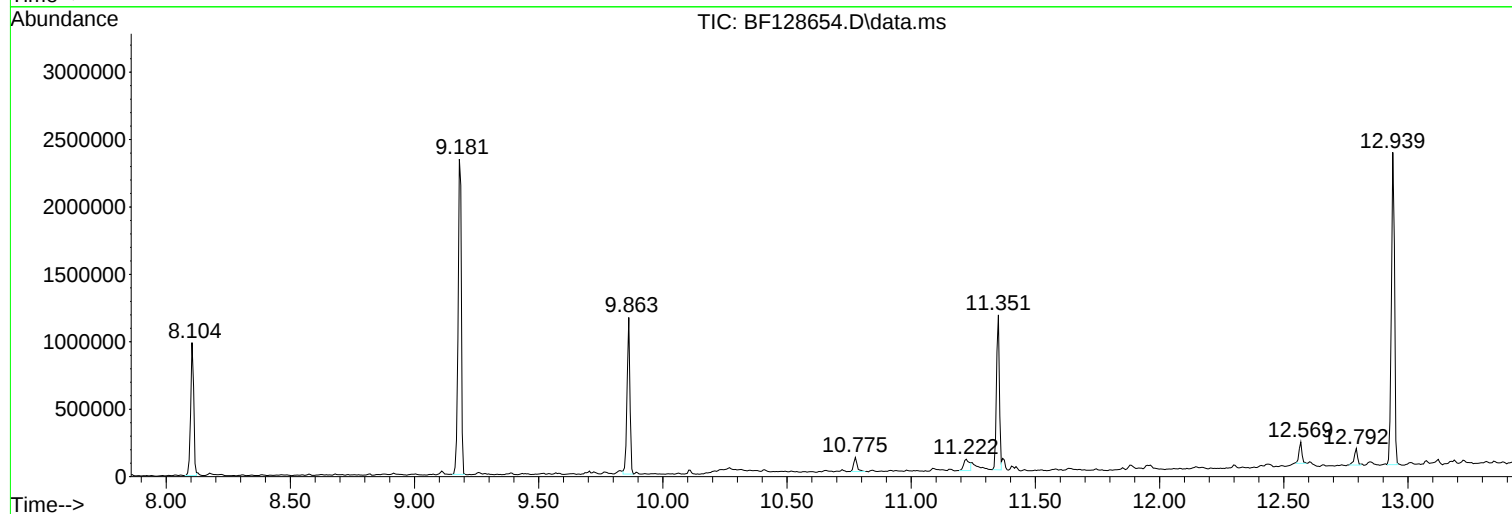
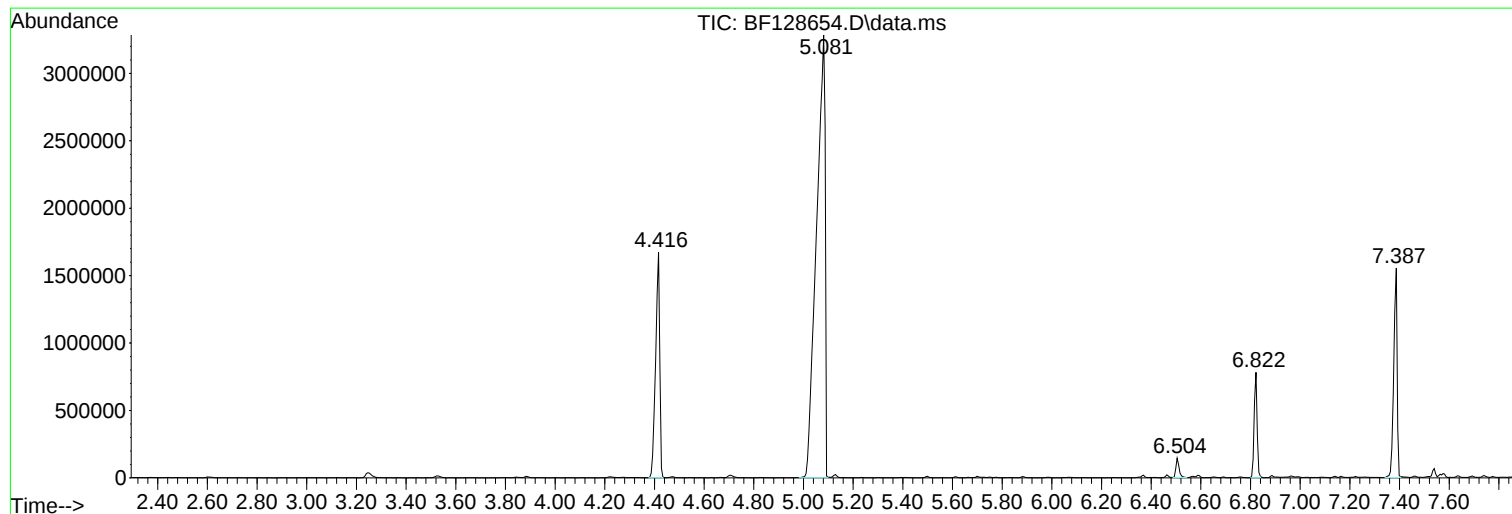
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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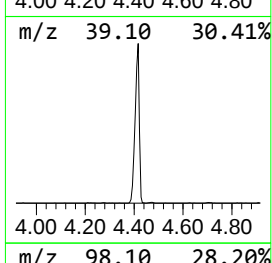
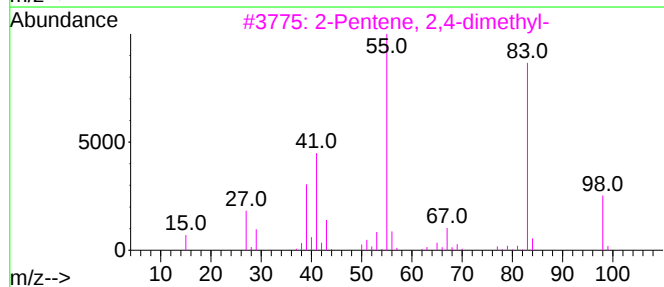
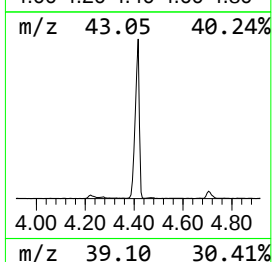
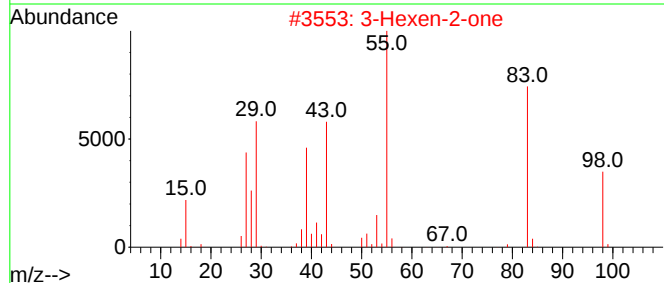
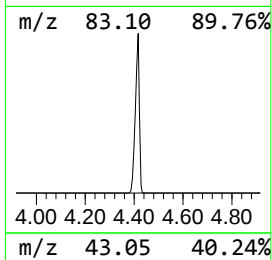
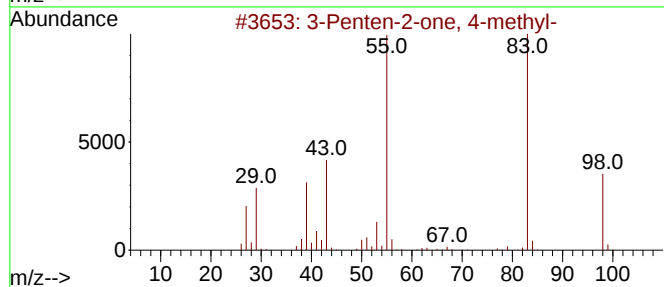
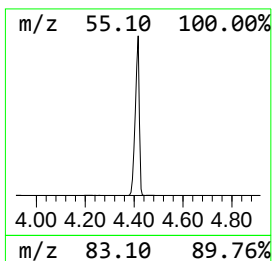
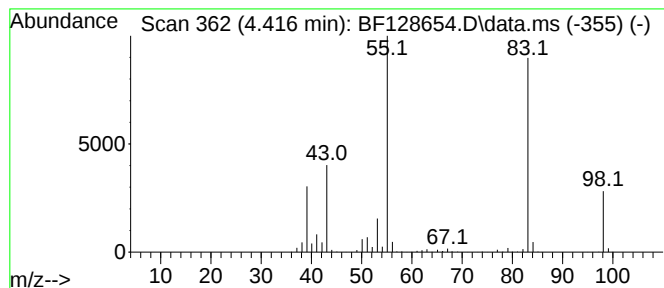
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Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.416	58.84 ng	1923050	1,4-Dichlorobenzene-d4	6.822

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4		2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	78
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78



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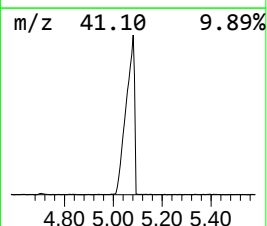
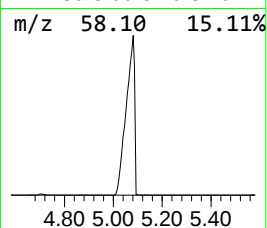
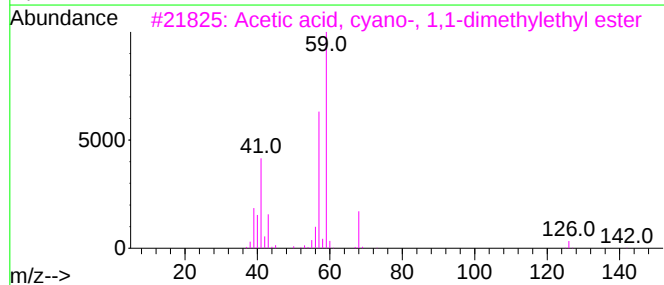
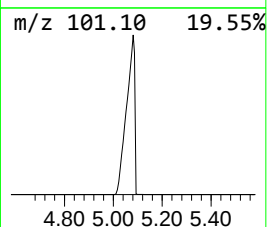
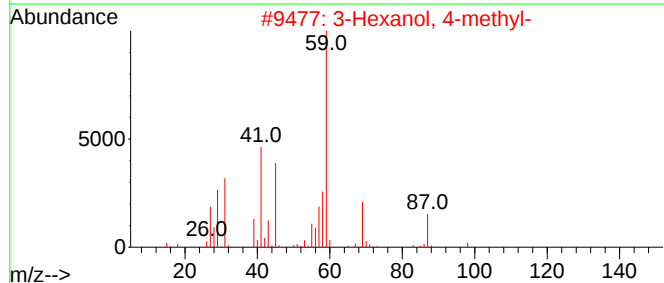
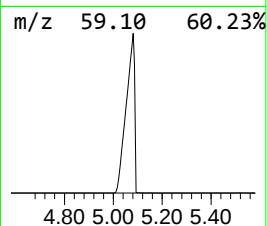
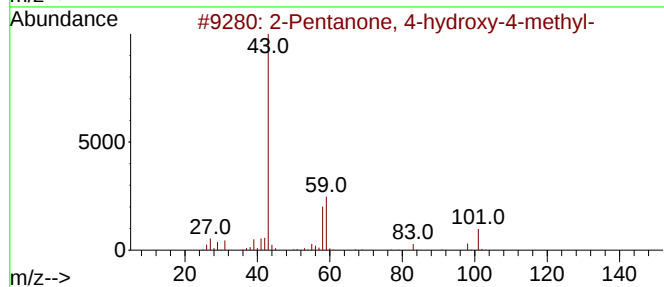
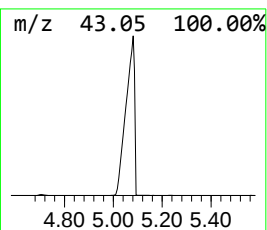
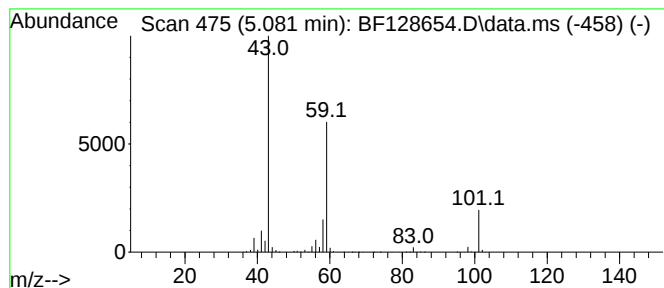
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	244.12 ng	7978530	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	72
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	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	10
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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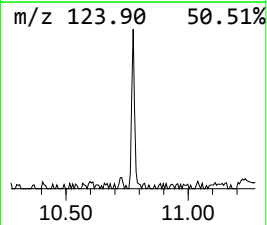
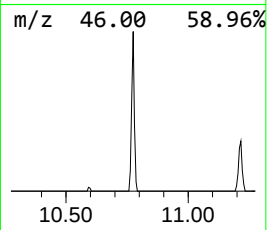
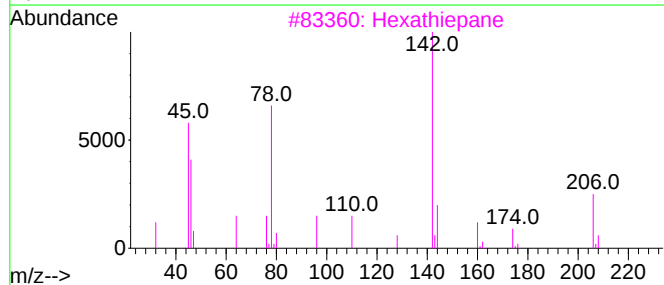
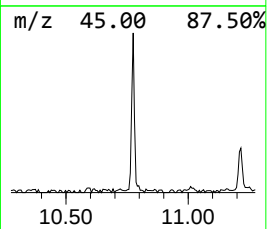
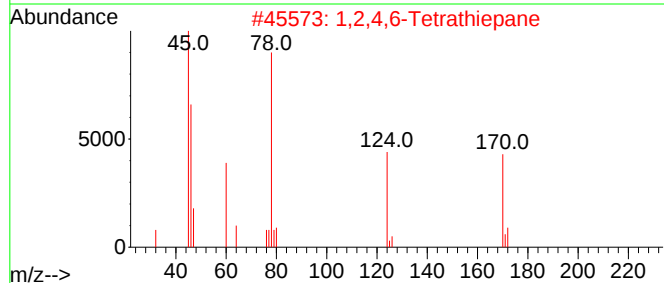
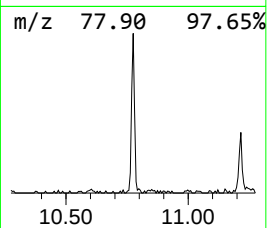
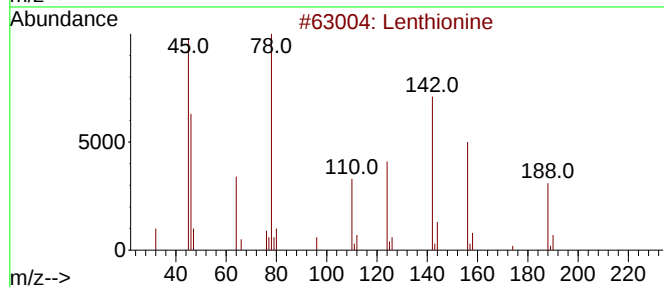
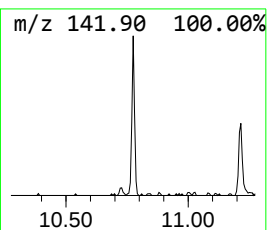
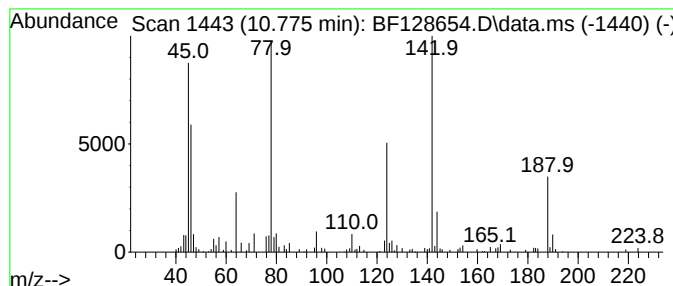
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Peak Number 3 Lenthionine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.775	2.08 ng	99957	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lenthionine	188	C2H4S5	000292-46-6	91
2			1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	59
3			Hexathiepane	206	CH2S6	017233-71-5	56
4			2-Pyridinesulfonylacetonitrile	182	C7H6N2O2S	170449-34-0	32
5			Salicyl alcohol	124	C7H8O2	000090-01-7	23



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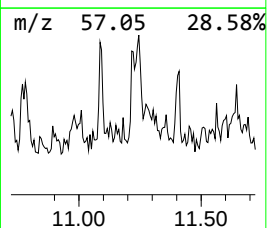
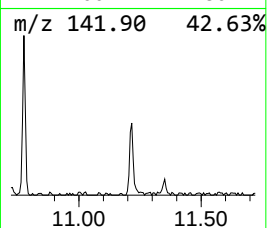
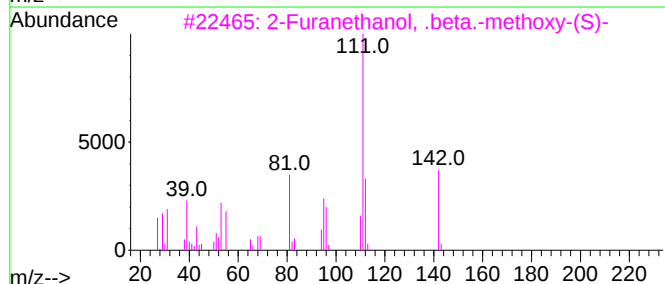
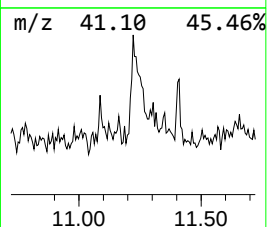
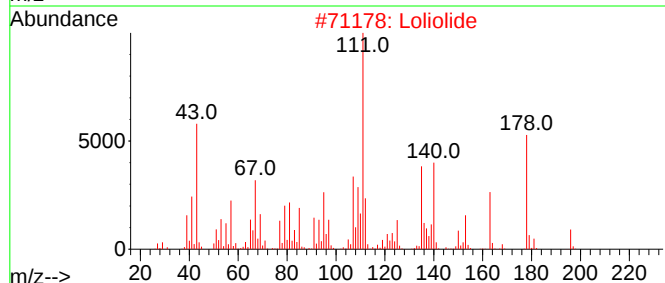
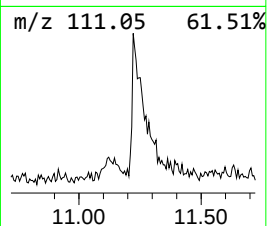
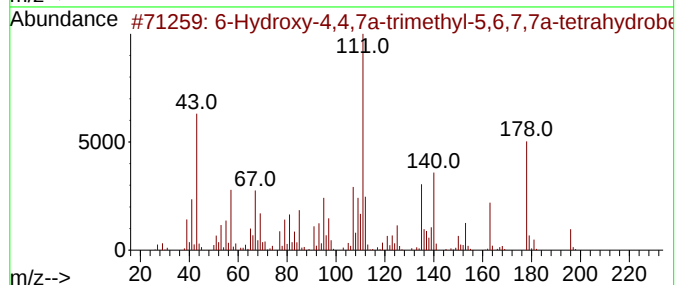
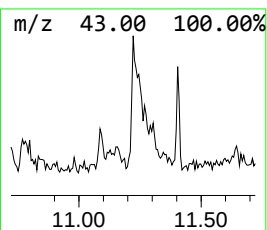
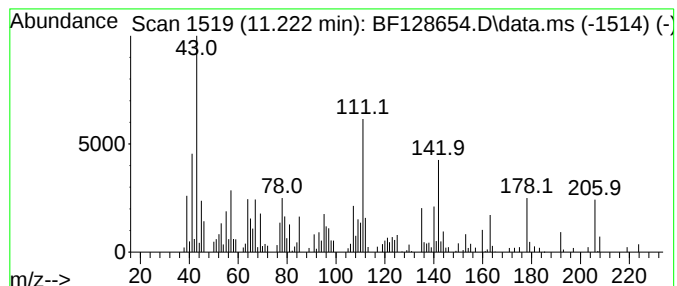
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Peak Number 4 unknown11.222 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.222	2.93 ng	140904	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Hydroxy-4,4,7a-trimethyl-5,6,7...	196	C11H16O3	073410-02-3	49		
2	Loliolide	196	C11H16O3	005989-02-6	27		
3	2-Furanethanol, .beta.-methoxy-(S)-	142	C7H10O3	101996-92-3	22		
4	5-Amino-3H-[1,2,3]triazole-4-car...	142	C3H6N6O	1000318-26-9	22		
5	2H-Pyran-2-methanol, 3,4-dihydro...	142	C8H14O2	054004-34-1	22		



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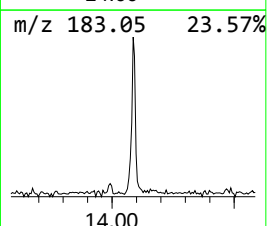
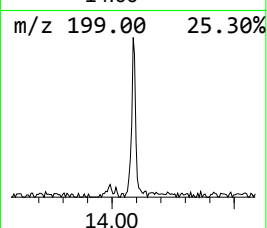
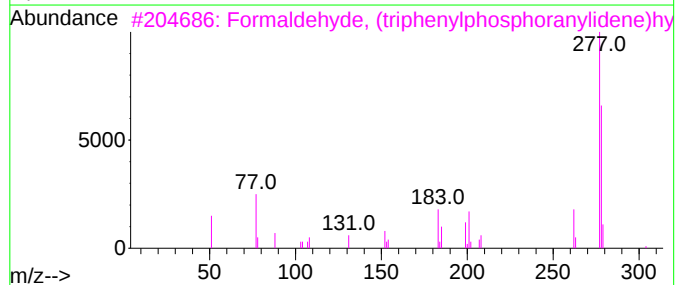
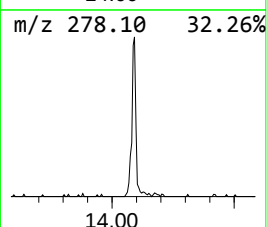
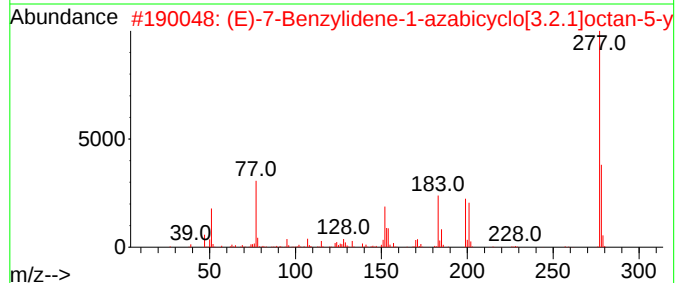
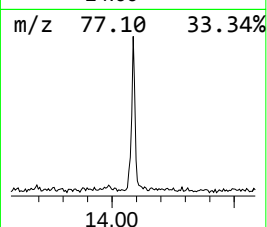
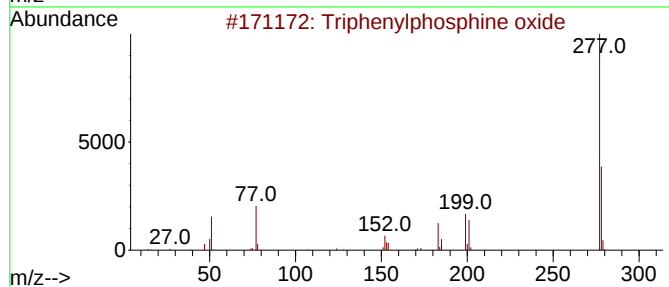
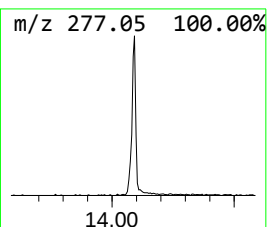
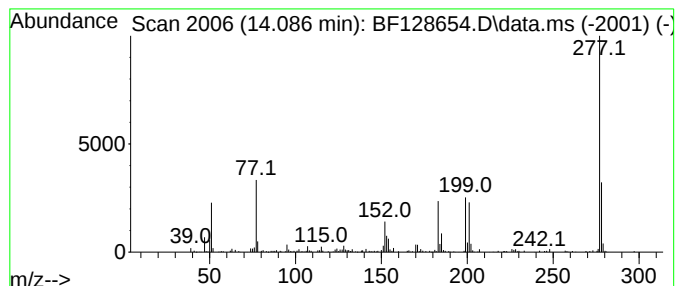
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	5.54 ng	201346	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	90
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	39
4			4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	38
5			Vanadium, cycloheptatrienyl-(pen...]	277	C17H22V	1000155-20-5	37



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.416	58.8	ng	1923050	1	6.822	653658	20.0
2-Pentanone, 4-...	5.081	244.1	ng	7978530	1	6.822	653658	20.0
Lenthionine	10.775	2.1	ng	99957	4	11.351	962977	20.0
unknown11.222	11.222	2.9	ng	140904	4	11.351	962977	20.0
Triphenylphosph...	14.086	5.5	ng	201346	5	13.992	727239	20.0