

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
 Data File : BF136855.D
 Acq On : 30 Dec 2023 05:46
 Operator : CG\JU
 Sample : 05897-15
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GHL-SS-42

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136855.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	493	499	502	rBV	874556	1065897	55.89%	9.455%
2	5.422	564	567	578	rBV	894809	842088	44.15%	7.470%
3	6.428	733	738	752	rBV	1362167	1337964	70.15%	11.868%
4	6.781	794	798	801	rBV	490314	387483	20.32%	3.437%
5	7.339	889	893	904	rBV	981539	923605	48.43%	8.193%
6	8.057	1011	1015	1018	rBV	608165	505740	26.52%	4.486%
7	9.133	1193	1198	1201	rBV	2117372	1872704	98.19%	16.612%
8	9.810	1310	1313	1325	rBV	610816	570034	29.89%	5.056%
9	9.910	1327	1330	1336	rVB2	16173	22045	1.16%	0.196%
10	10.422	1413	1417	1422	rBV2	91378	97539	5.11%	0.865%
11	10.604	1445	1448	1457	rBV	155347	149077	7.82%	1.322%
12	11.304	1563	1567	1575	rBV	704589	588478	30.85%	5.220%
13	11.463	1591	1594	1600	rVB	81311	65496	3.43%	0.581%
14	12.904	1834	1839	1842	rBV	2142859	1907260	100.00%	16.918%
15	13.563	1946	1951	1955	rBV	110958	90623	4.75%	0.804%
16	13.963	2015	2019	2030	rVB	387144	385788	20.23%	3.422%
17	14.433	2094	2099	2104	rVB	25274	24980	1.31%	0.222%
18	14.815	2161	2164	2169	rVB	31608	32455	1.70%	0.288%
19	15.439	2266	2270	2280	rBV	259048	351779	18.44%	3.120%
20	15.680	2307	2311	2318	rBV4	19896	30852	1.62%	0.274%
21	16.751	2487	2493	2499	rVB8	11287	21577	1.13%	0.191%

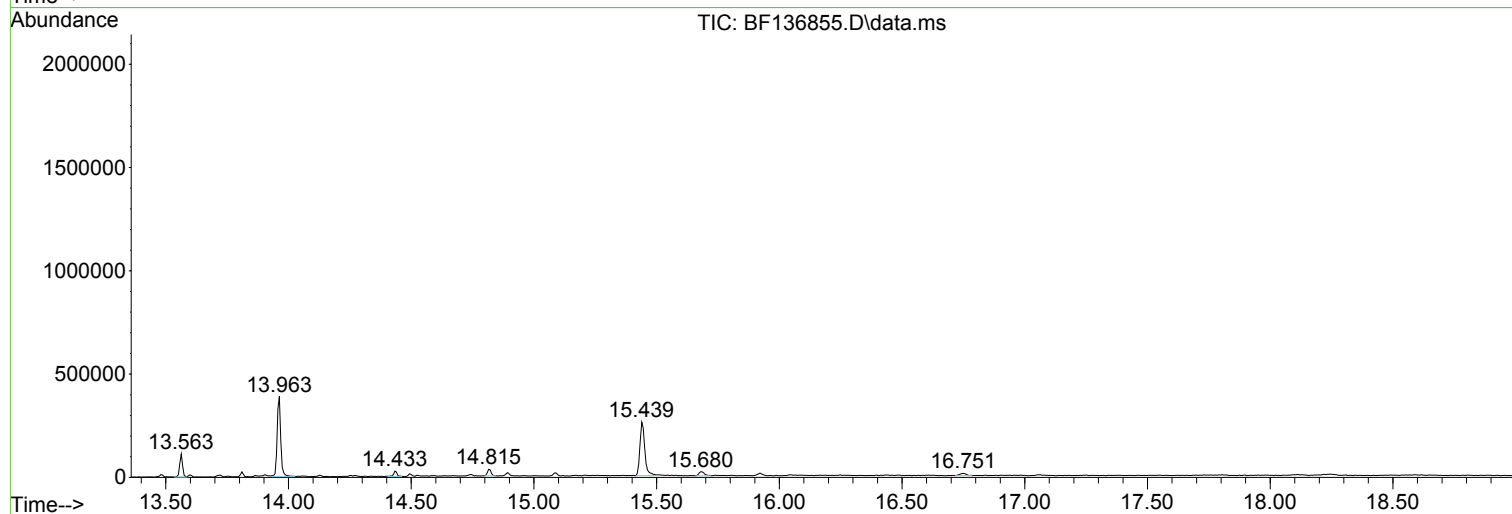
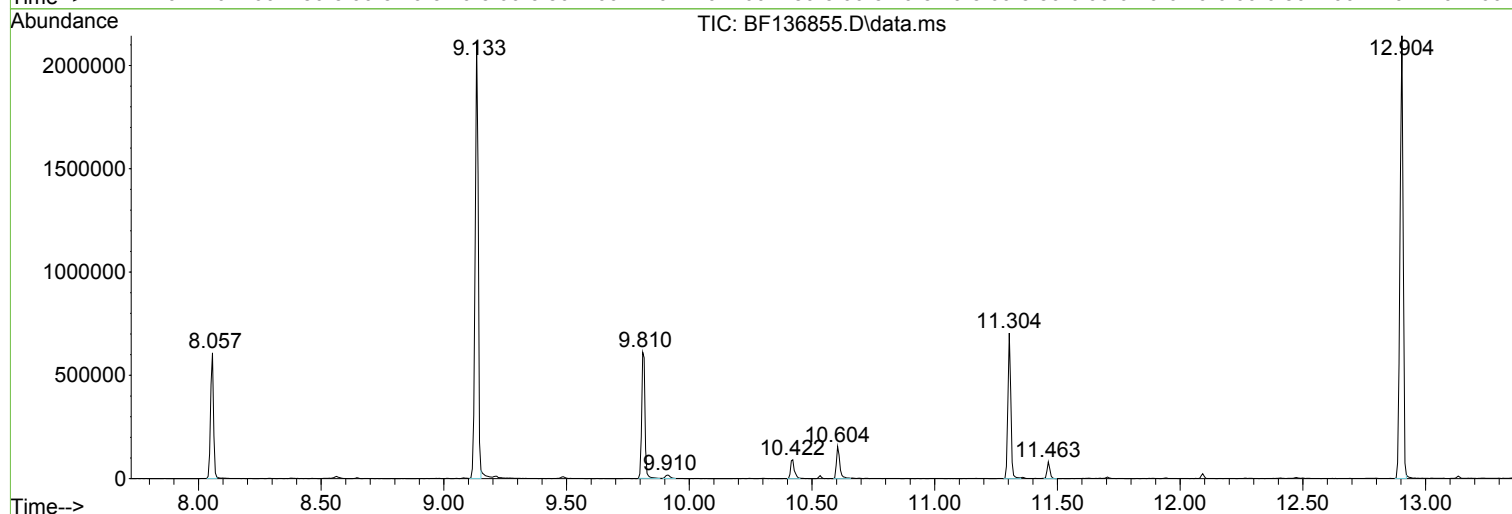
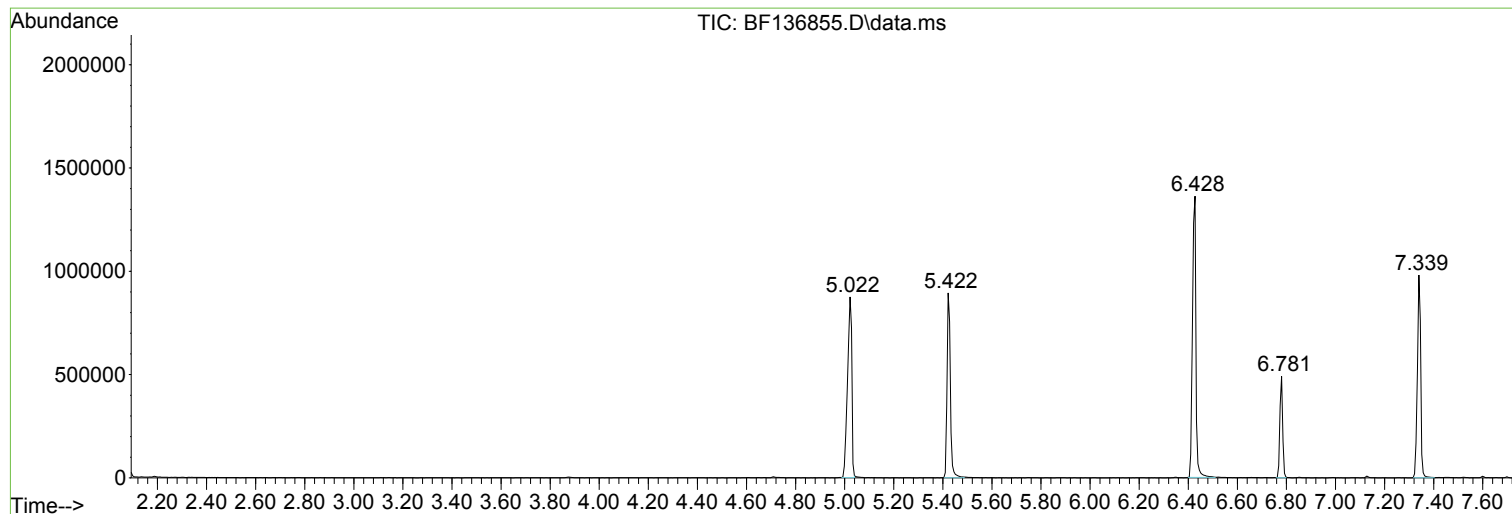
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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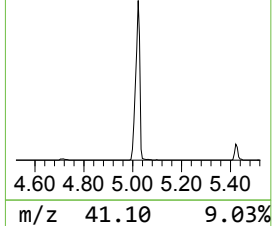
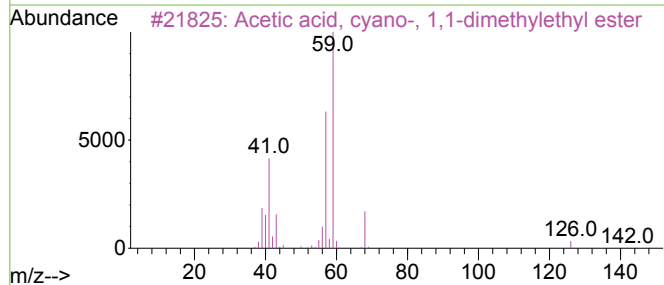
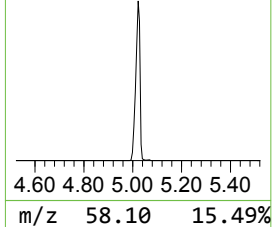
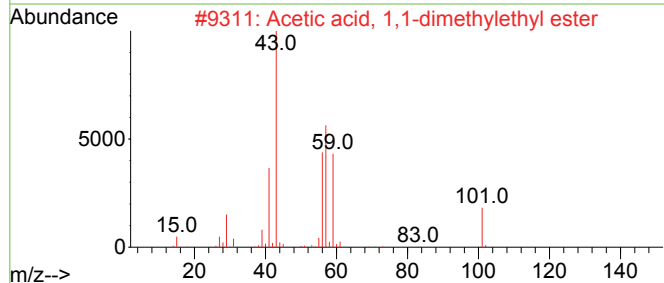
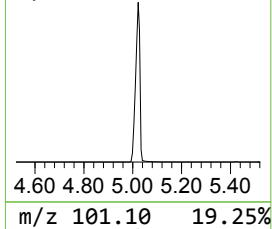
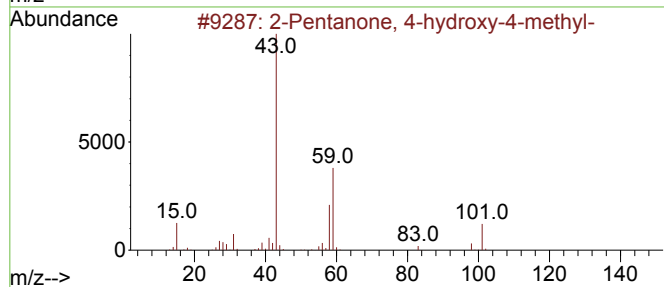
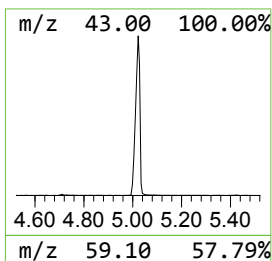
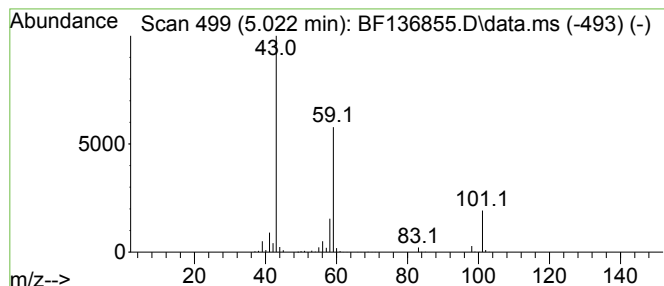
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	55.02 ng	1065900	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9		



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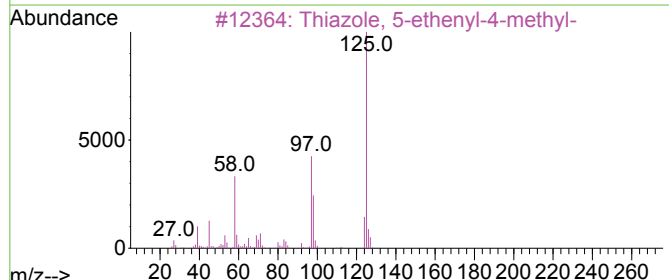
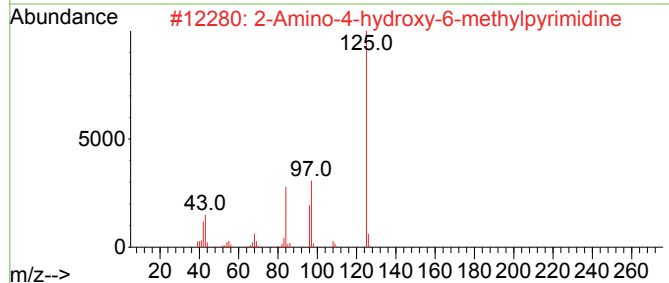
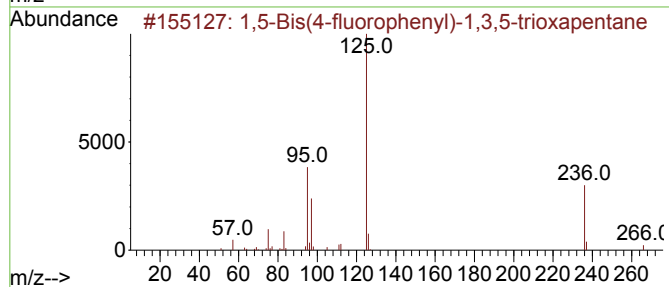
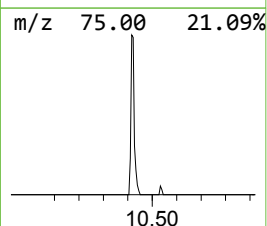
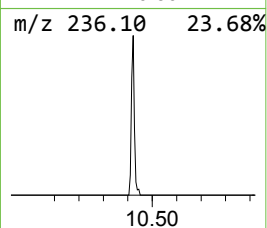
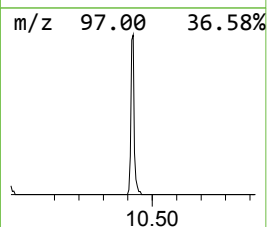
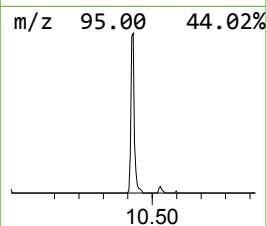
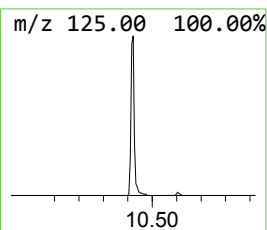
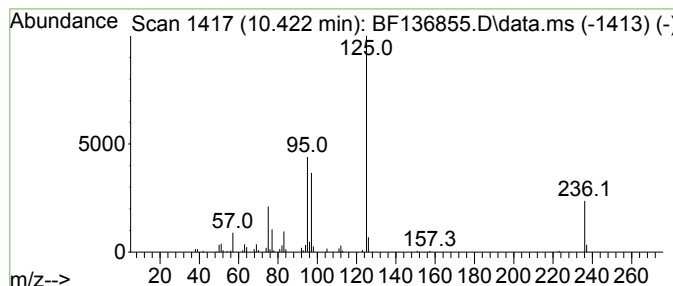
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Peak Number 2 1,5-Bis(4-fluorophenyl)-1,3... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.422	3.42 ng	97539	Acenaphthene-d10	9.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,5-Bis(4-fluorophenyl)-1,3,5-tr...	266	C14H12F2O3	1010280-28-3	59
2			2-Amino-4-hydroxy-6-methylpyrimi...	125	C5H7N3O	003977-29-5	32
3			Thiazole, 5-ethenyl-4-methyl-	125	C6H7NS	001759-28-0	32
4			4-Fluoromandelic acid	170	C8H7FO3	000395-33-5	28
5			Mandelic acid imine, p-fluoro-	169	C8H8FN02	1000153-29-2	25



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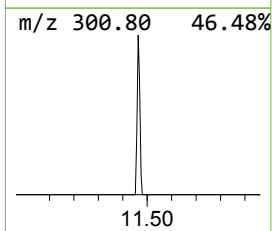
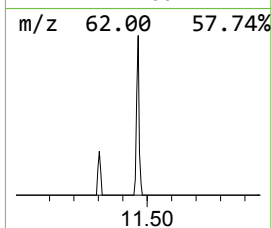
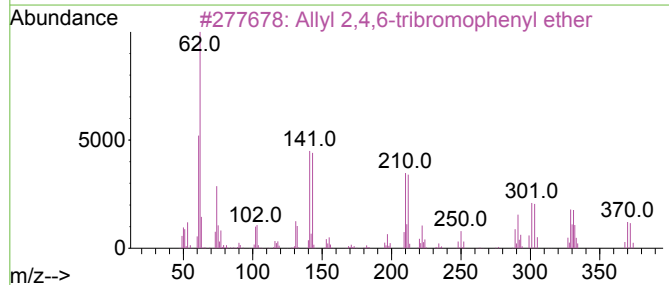
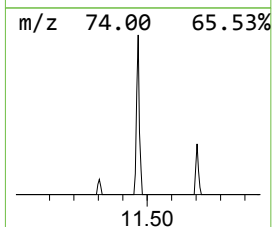
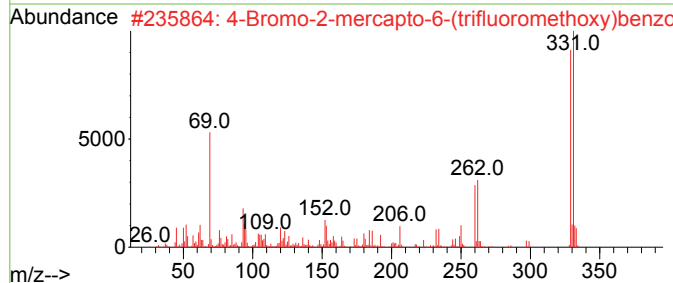
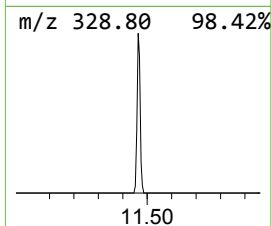
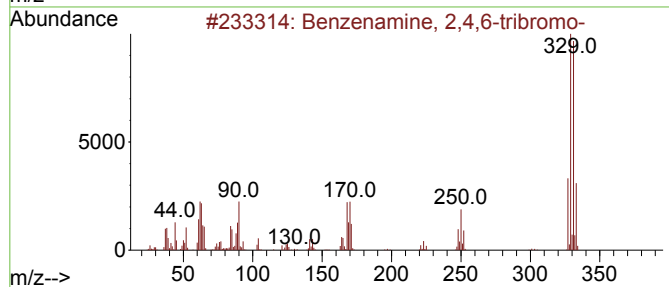
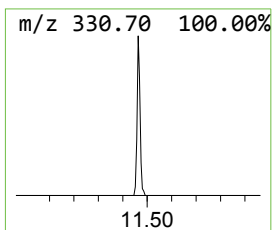
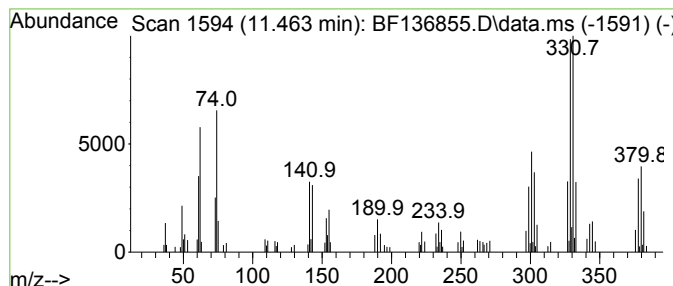
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Peak Number 3 unknown11.463 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.463	2.23 ng	65496	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	43
2			4-Bromo-2-mercapto-6-(trifluoromethoxy)benzoic acid	329	C8H3BrF3NOS2	1000502-92-7	30
3			Allyl 2,4,6-tribromophenyl ether	368	C9H7Br3O	003278-89-5	22
4			6-Chloro-4-phenyl-2-(p-tolyl)quinoline	329	C22H16ClN	021923-41-1	10
5			Glutaric acid, 2,2,3,3,4,4,5,5-octabromo-	490	C16H12Cl2F8O4	1010392-05-1	10



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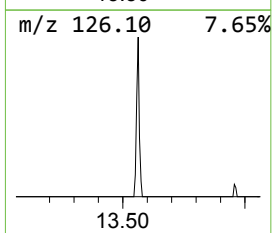
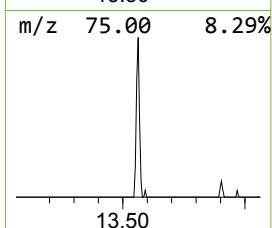
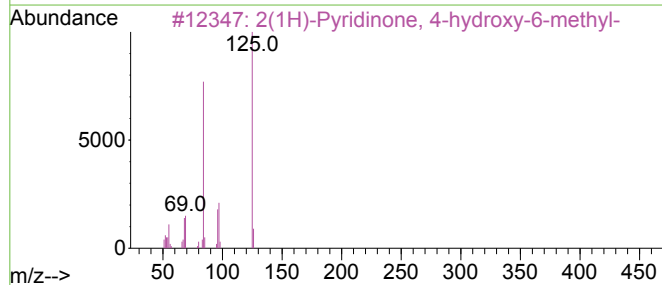
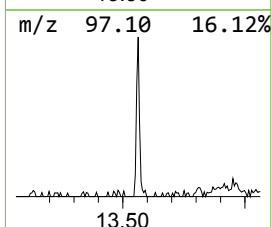
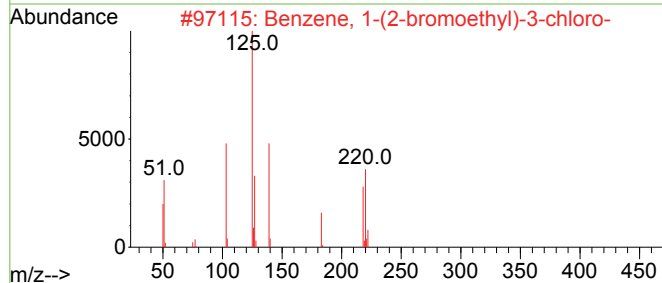
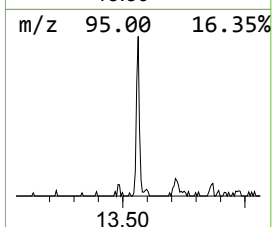
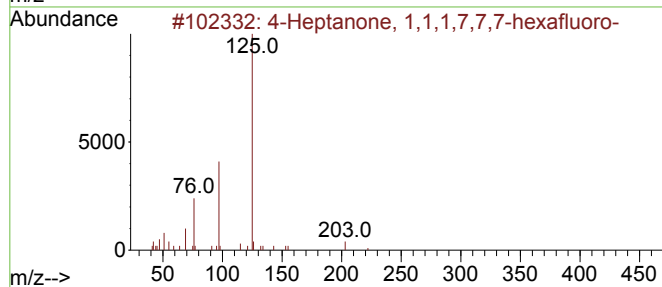
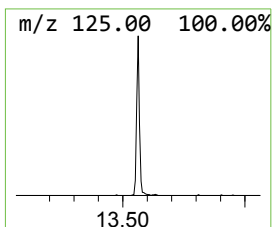
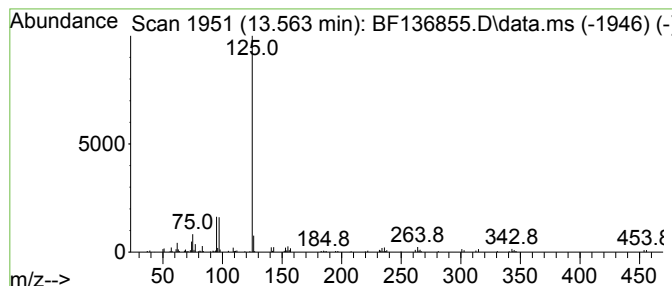
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Peak Number 4 4-Heptanone, 1,1,1,7,7,7-he... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.563	4.70 ng	90623	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 1,1,1,7,7,7-hexaflu...	222	C7H8F6O	000332-86-5	59
2			Benzene, 1-(2-bromoethyl)-3-chloro-	218	C8H8BrCl	016799-05-6	50
3			2(1H)-Pyridinone, 4-hydroxy-6-me...	125	C6H7NO2	003749-51-7	45
4			1-Oxaspiro[4.5]decan-2-one, 6-is...	208	C13H20O2	1010157-58-3	40
5			Glycine, N-[(5-methyl-3-thienyl)...]	323	C12H12F3NO4S	1000511-01-1	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.022	55.0	ng	1065900	1	6.781	387483	20.0
1,5-Bis(4-fluor...	10.422	3.4	ng	97539	3	9.810	570034	20.0
unknown11.463	11.463	2.2	ng	65496	4	11.304	588478	20.0
4-Heptanone, 1,...	13.563	4.7	ng	90623	5	13.963	385788	20.0