

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112017\
 Data File : BF100736.D
 Acq On : 20 Nov 2017 18:05
 Operator : SJ/JU
 Sample : PB104390BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB104390BL

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.104	508	513	522	rBB	95043	133374	6.30%	0.759%
2	5.492	574	579	582	rBV	1750506	1665568	78.63%	9.482%
3	6.492	744	749	752	rBV	1581438	1641142	77.48%	9.343%
4	6.639	769	774	777	rBV	1858528	1708112	80.64%	9.724%
5	6.869	809	813	817	rBV	630655	514910	24.31%	2.931%
6	7.028	835	840	843	rBV	1560296	1390269	65.63%	7.915%
7	7.433	903	909	912	rBV	996079	1056983	49.90%	6.017%
8	8.151	1026	1031	1034	rBV	762435	683829	32.28%	3.893%
9	9.227	1208	1214	1217	rBV	2250906	2118225	100.00%	12.059%
10	9.904	1324	1329	1333	rBV	782509	770837	36.39%	4.388%
11	10.698	1459	1464	1467	rBV	1209936	1214052	57.31%	6.912%
12	11.133	1535	1538	1543	rBB2	15976	22243	1.05%	0.127%
13	11.392	1578	1582	1586	rBV	1006499	826387	39.01%	4.705%
14	12.980	1847	1852	1855	rBV	2117755	2098046	99.05%	11.944%
15	13.410	1919	1925	1929	rBV	72700	75549	3.57%	0.430%
16	13.757	1979	1984	1990	rBV	238415	218505	10.32%	1.244%
17	14.027	2026	2030	2034	rBV	794298	716310	33.82%	4.078%
18	14.121	2041	2046	2054	rBV	55678	59459	2.81%	0.338%
19	15.498	2274	2280	2289	rBV2	409645	535098	25.26%	3.046%
20	15.951	2351	2357	2362	rBV2	17392	27537	1.30%	0.157%
21	16.456	2437	2443	2451	rVB2	21013	36085	1.70%	0.205%
22	17.045	2539	2543	2552	rVB4	13279	26435	1.25%	0.150%
23	17.756	2657	2664	2671	rBV7	10785	26606	1.26%	0.151%

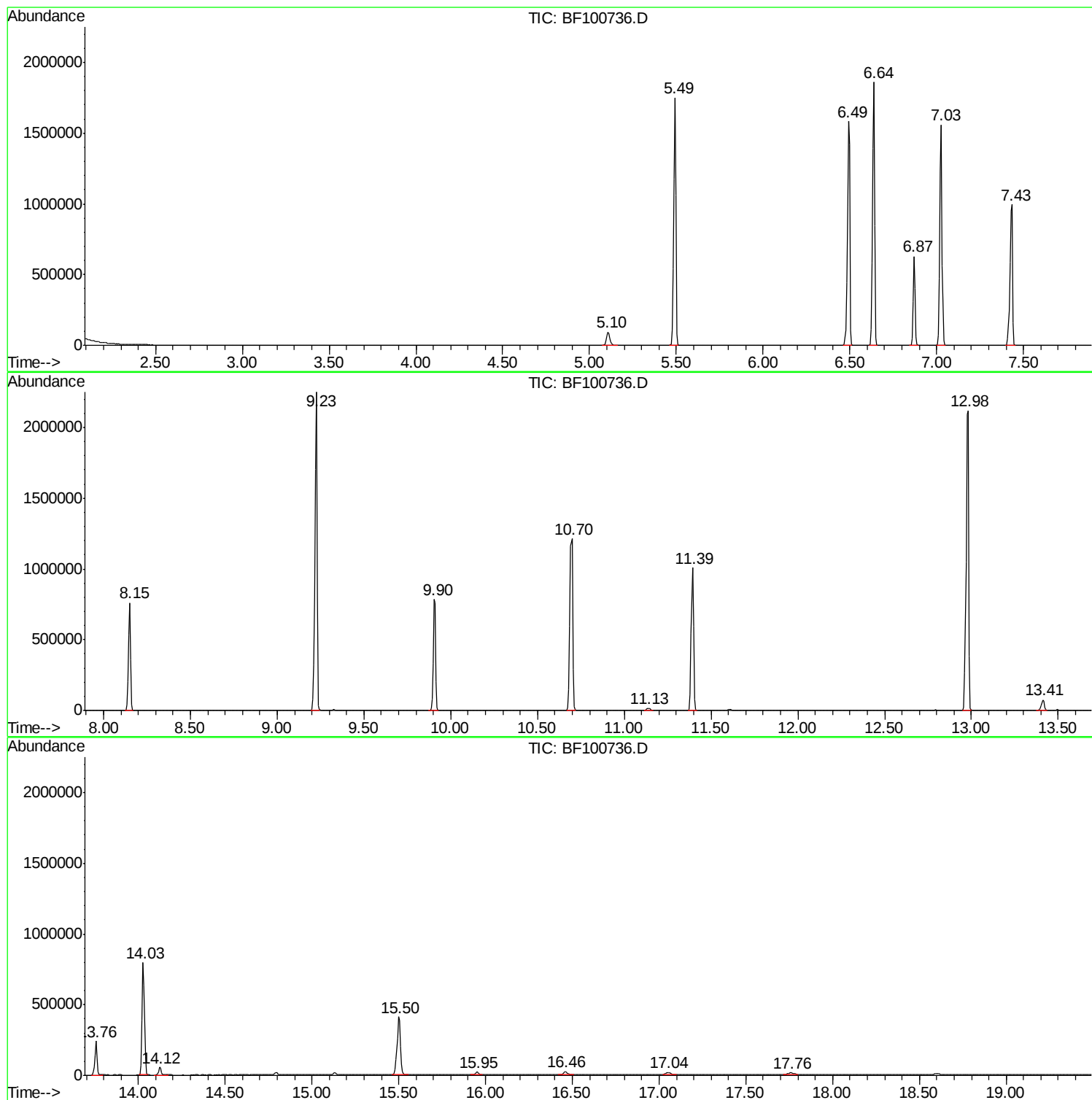
Sum of corrected areas: 17565561

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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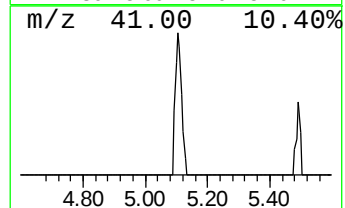
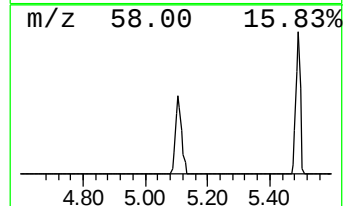
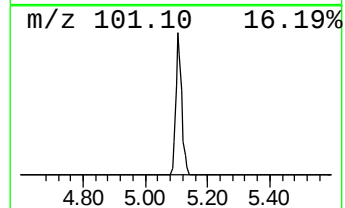
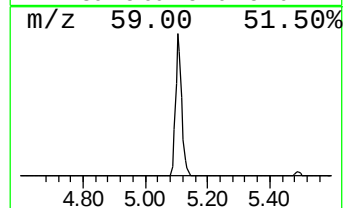
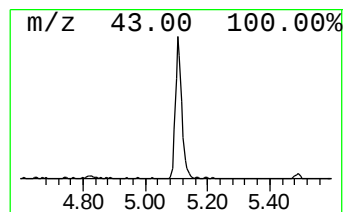
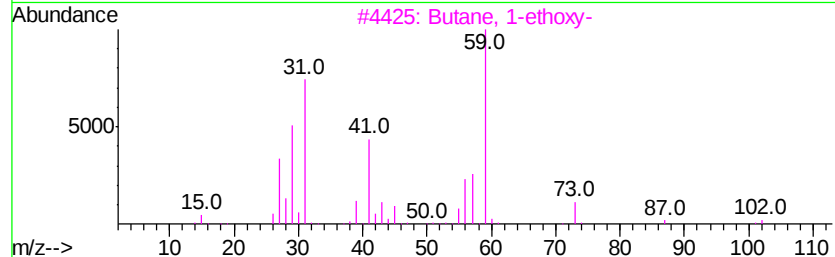
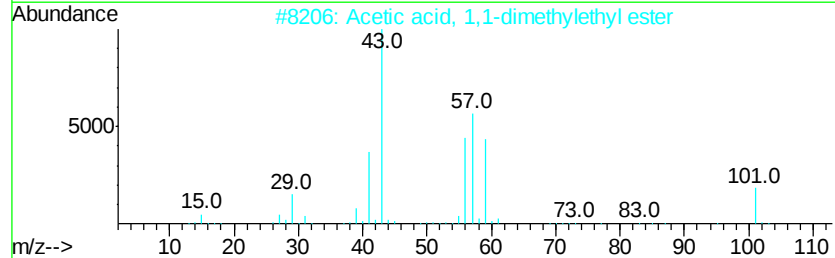
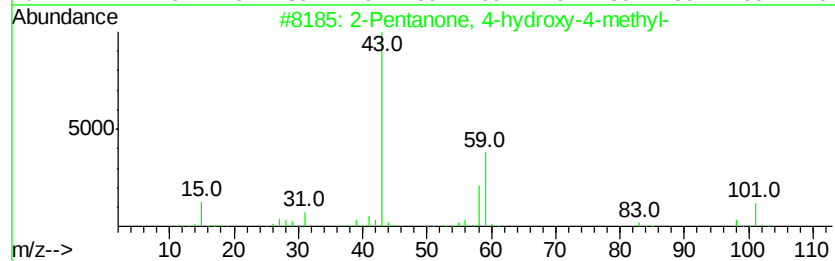
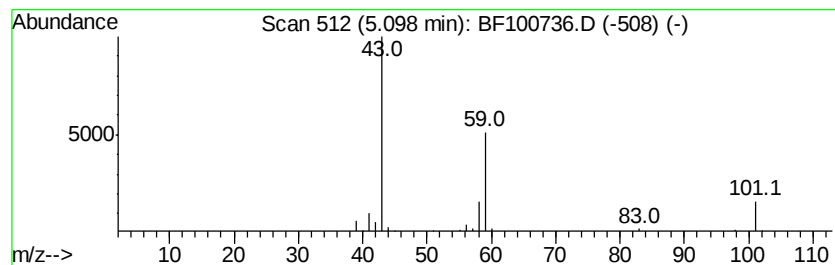
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	5.18 ng	133374	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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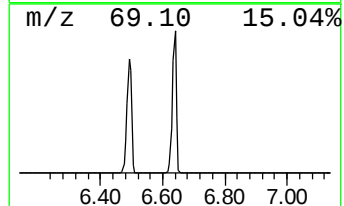
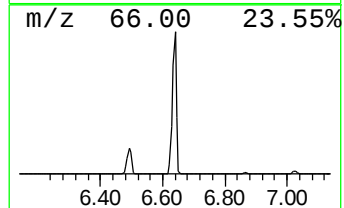
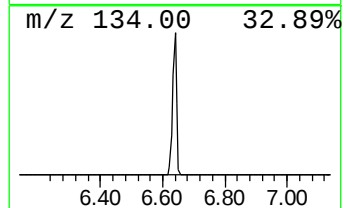
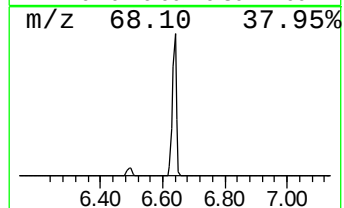
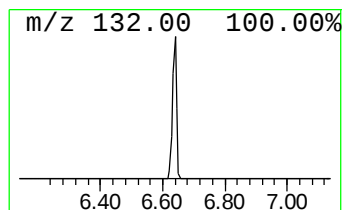
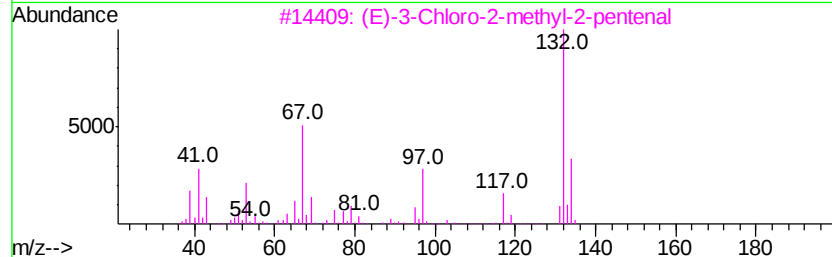
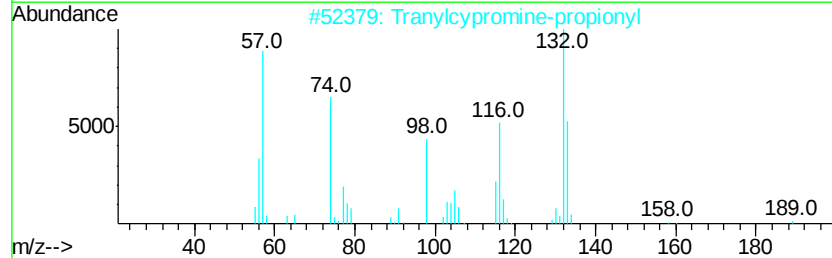
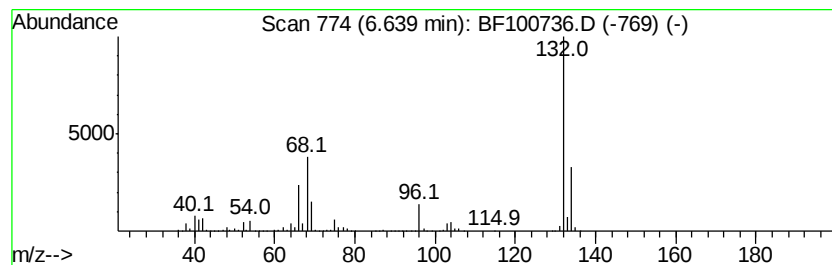
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Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	66.35 ng	1708110	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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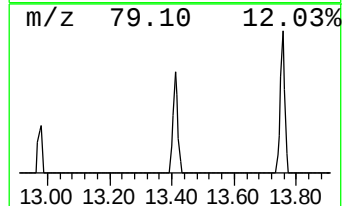
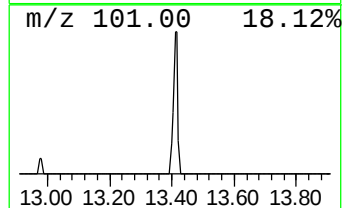
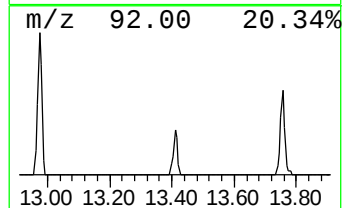
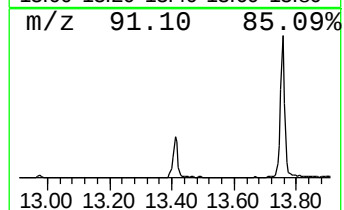
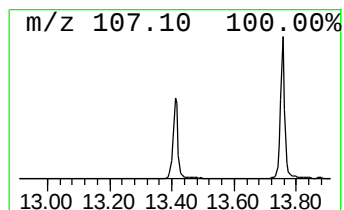
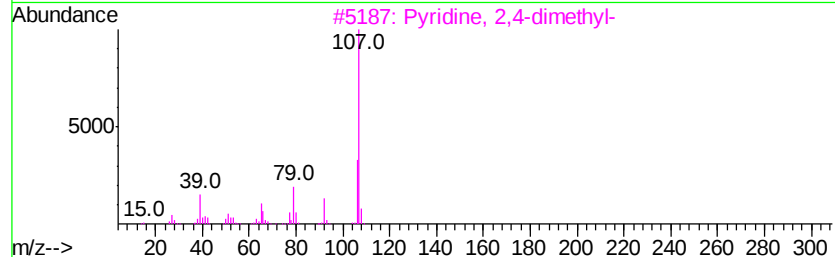
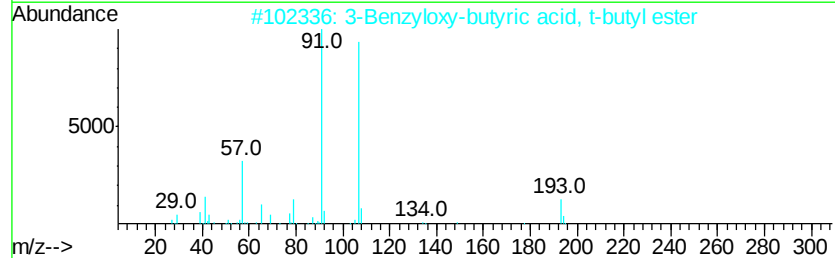
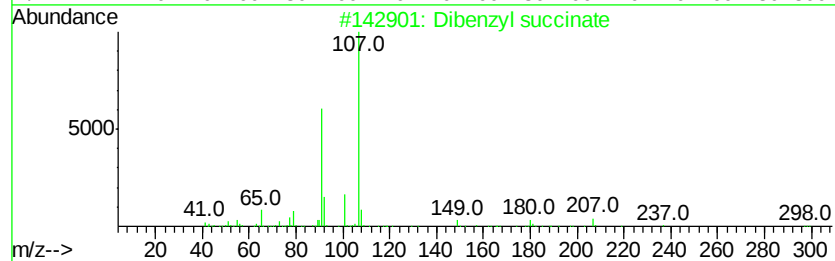
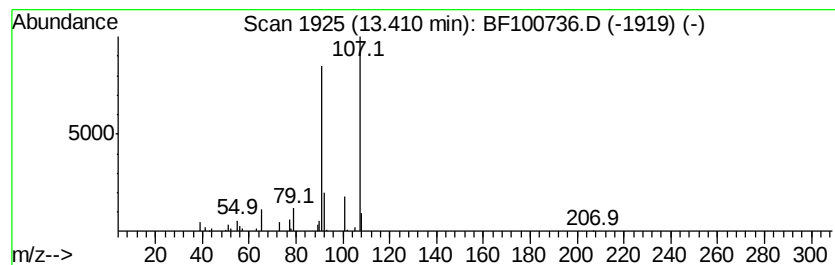
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Peak Number 4 Dibenzyl succinate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.41	2.11 ng	75549	Chrysene-d12		14.03
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzyl succinate	298	C18H18O4	000103-43-5	90
2	3-Benzyloxy-butyric acid, t-buty...	250	C15H22O3	116761-25-2	64
3	Pyridine, 2,4-dimethyl-	107	C7H9N	000108-47-4	50
4	Pyridine, 2,3-dimethyl-	107	C7H9N	000583-61-9	50
5	Pyridine, 2,5-dimethyl-	107	C7H9N	000589-93-5	49



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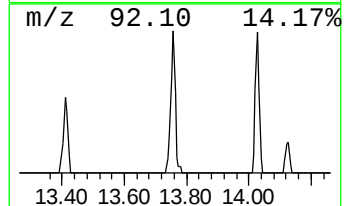
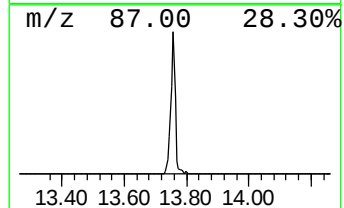
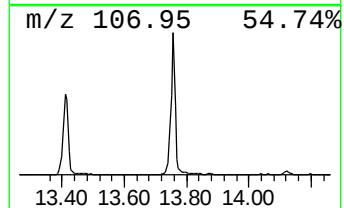
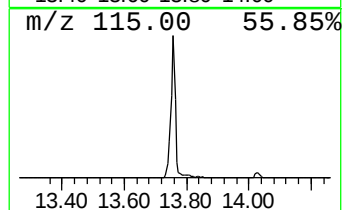
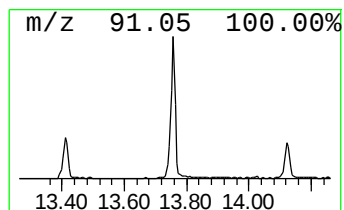
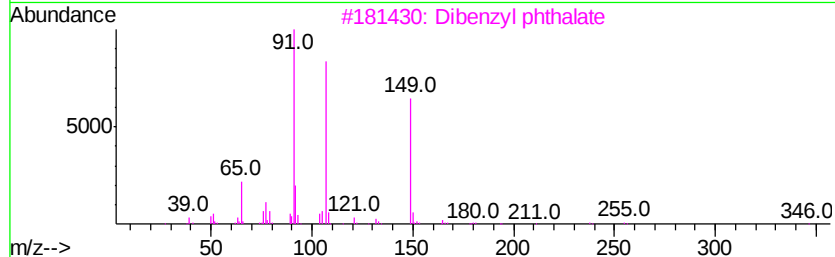
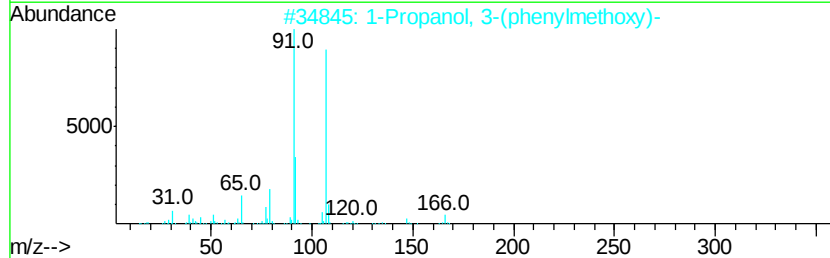
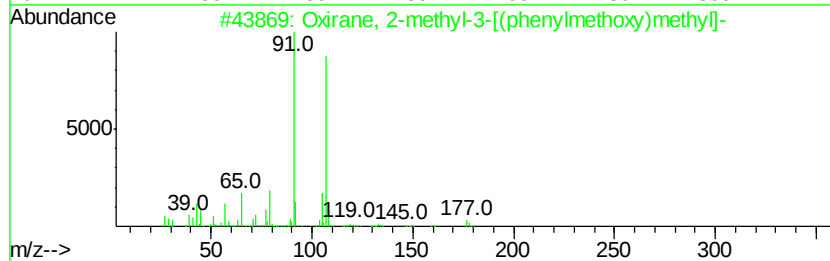
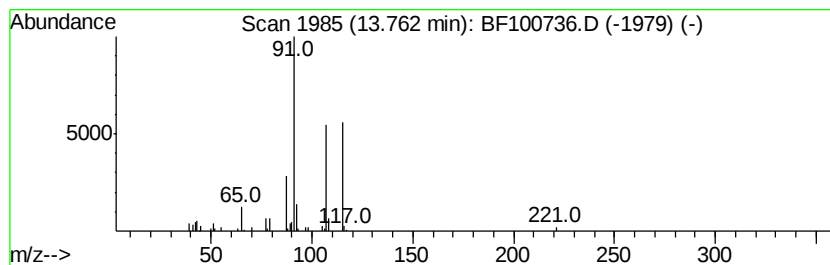
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Peak Number 5 unknown13.76 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	6.10 ng	218505	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, 2-methyl-3-[(phenylmeth...	178	C11H14O2	116296-88-9	43
2		1-Propanol, 3-(phenylmethoxy)-	166	C10H14O2	004799-68-2	38
3		Dibenzyl phthalate	346	C22H18O4	000523-31-9	38
4		.beta.-Alanine, N-benzylloxycarbo...	313	C18H19NO4	1000328-66-7	32
5		3-Benzyloxybutanoic acid, methyl...	208	C12H16O3	116761-24-1	32



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.10	5.2	ng	133374	1	6.87	514910	20.0
unknown6.64	6.64	66.3	ng	1708110	1	6.87	514910	20.0
Dibenzyl succinate	13.41	2.1	ng	75549	5	14.03	716310	20.0
unknown13.76	13.76	6.1	ng	218505	5	14.03	716310	20.0