

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112017\
 Data File : BF100737.D
 Acq On : 20 Nov 2017 18:32
 Operator : SJ/JU
 Sample : PB104343BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB104343BL

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	5.116	510	515	525	rBV	113201	150251	5.57%	0.732%
2	5.498	574	580	583	rBV	2022345	2141138	79.31%	10.429%
3	6.498	744	750	753	rBV	2037866	2084021	77.19%	10.151%
4	6.640	769	774	777	rBV	2173432	2196653	81.36%	10.699%
5	6.869	809	813	817	rBB	598401	468533	17.35%	2.282%
6	7.028	835	840	843	rBV	1983359	1768533	65.50%	8.614%
7	7.434	903	909	912	rBV	1318973	1377725	51.03%	6.711%
8	8.151	1026	1031	1034	rBV	689569	623099	23.08%	3.035%
9	9.228	1208	1214	1217	rBV	2733778	2699859	100.00%	13.150%
10	9.904	1324	1329	1333	rBV2	775390	710827	26.33%	3.462%
11	10.698	1457	1464	1467	rBV	1634184	1571497	58.21%	7.654%
12	11.392	1578	1582	1585	rBV	929426	759490	28.13%	3.699%
13	12.980	1847	1852	1855	rBV	2692466	2625438	97.24%	12.788%
14	13.410	1921	1925	1930	rBV	56297	55406	2.05%	0.270%
15	13.757	1978	1984	1990	rBV	177428	179028	6.63%	0.872%
16	14.027	2026	2030	2034	rBV	720808	629514	23.32%	3.066%
17	14.121	2042	2046	2051	rBV	46778	44888	1.66%	0.219%
18	15.498	2274	2280	2288	rBV	360640	444658	16.47%	2.166%

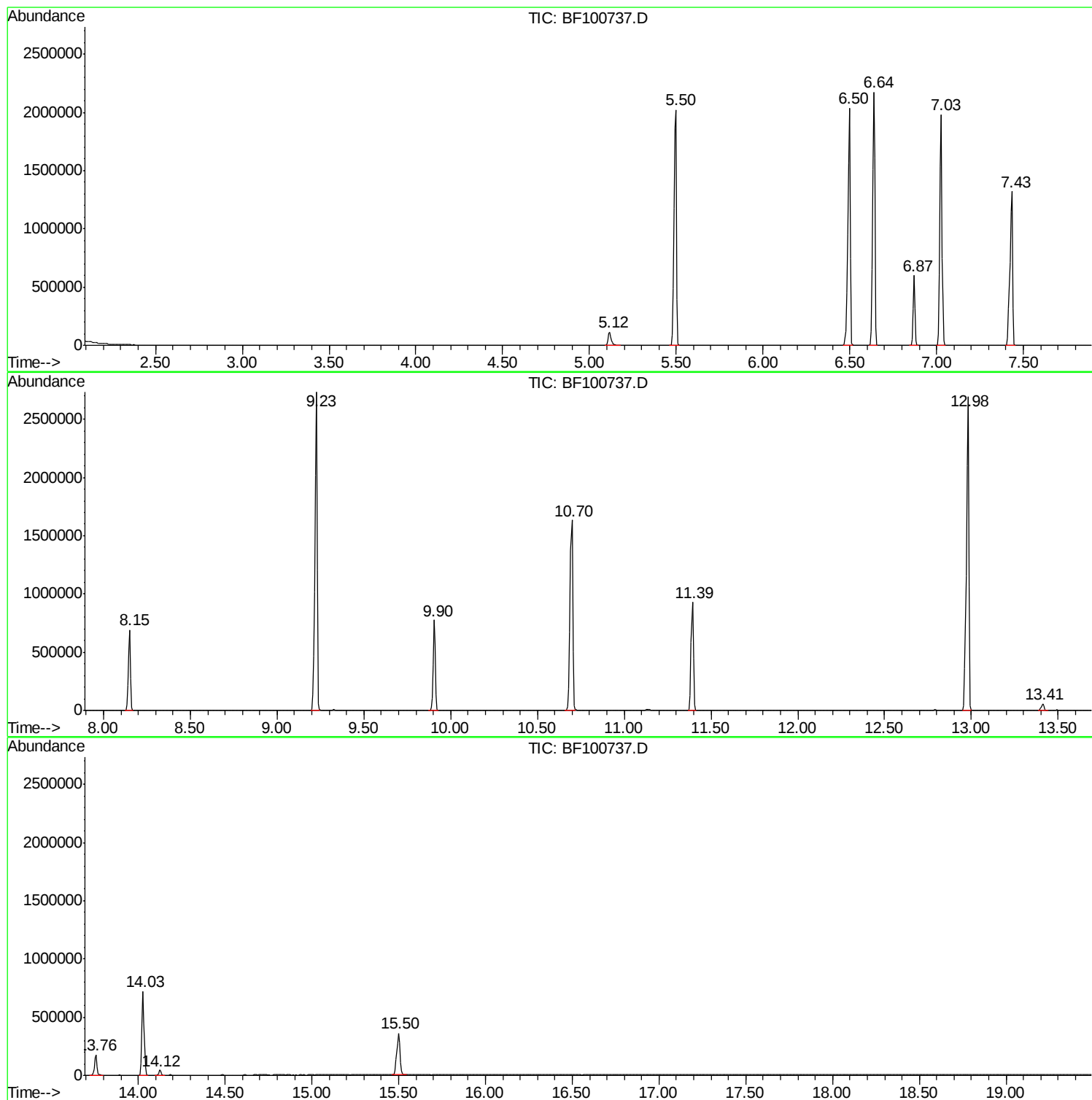
Sum of corrected areas: 20530558

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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



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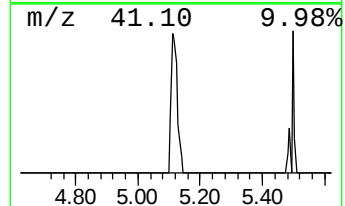
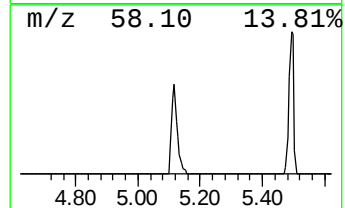
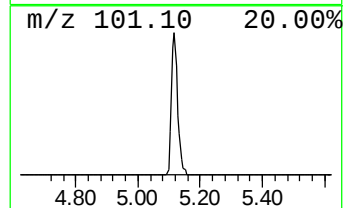
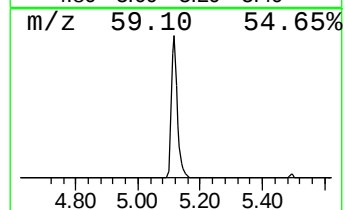
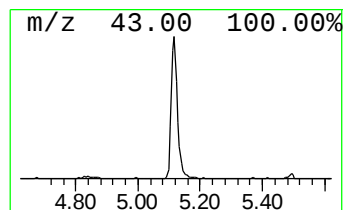
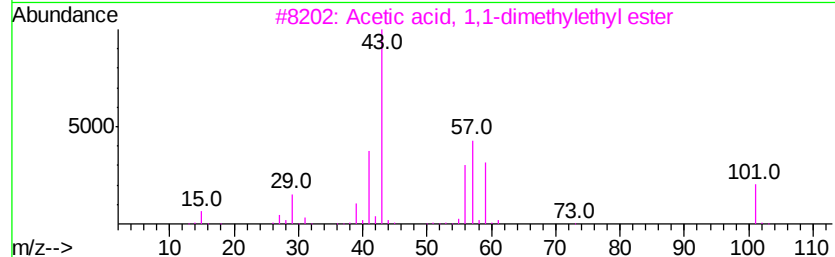
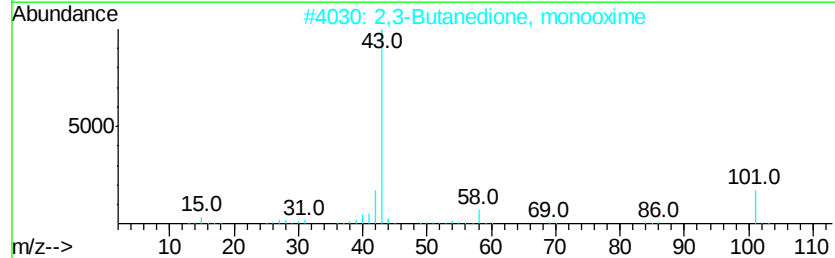
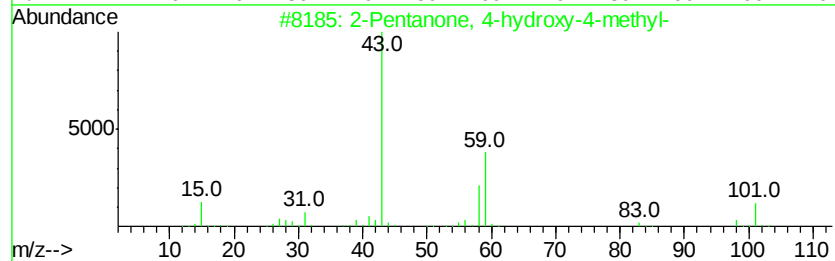
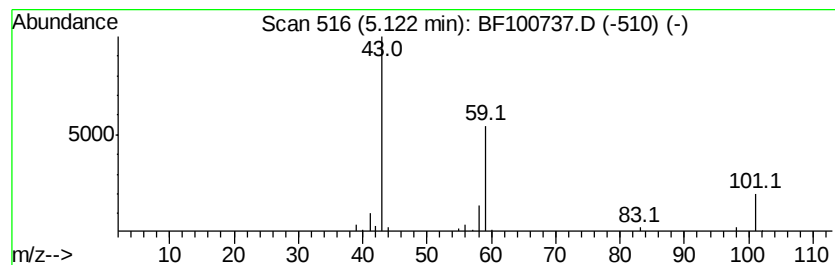
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	6.41 ng	150251	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4		1,2-Butanediol	90	C4H10O2	000584-03-2	9
5		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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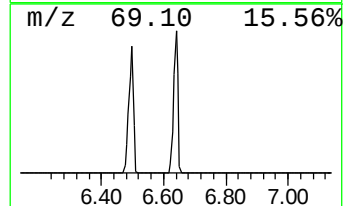
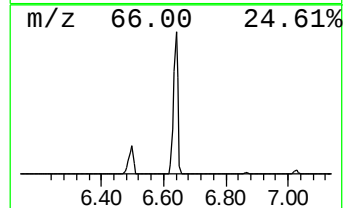
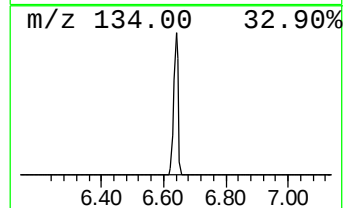
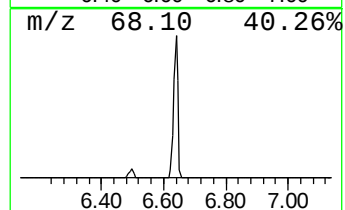
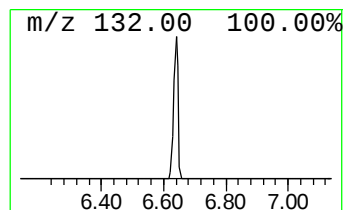
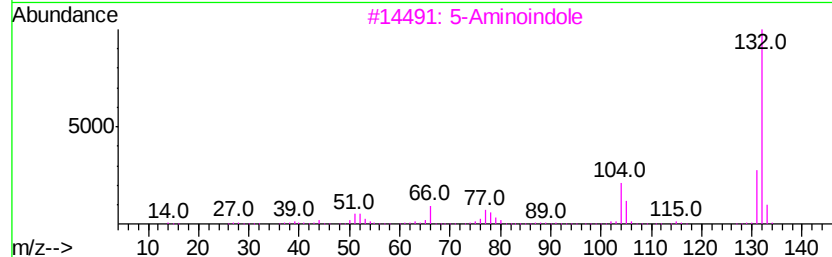
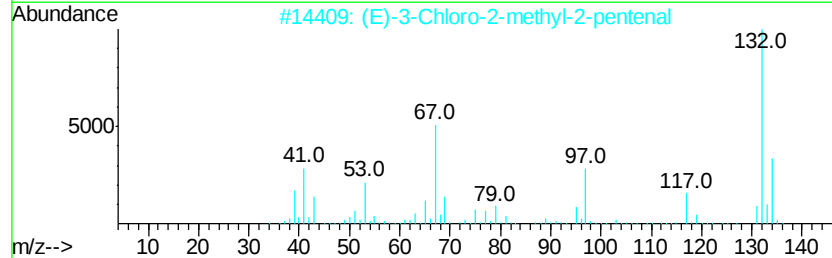
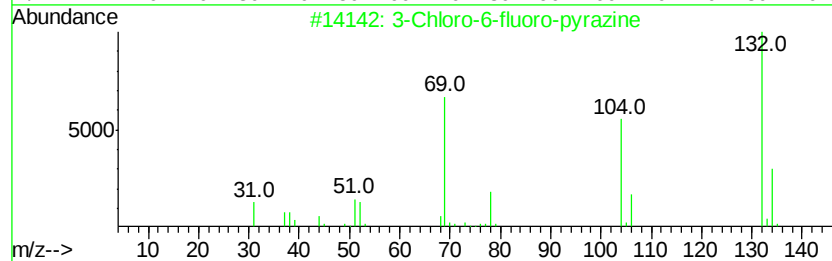
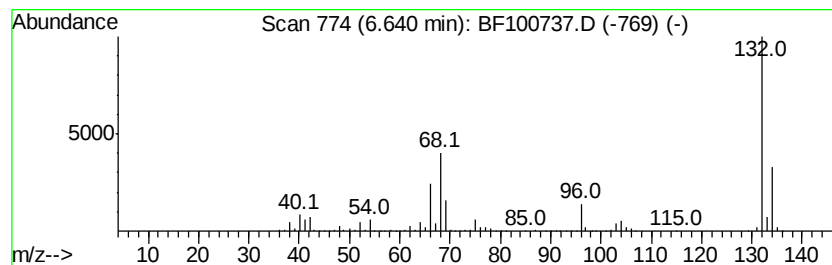
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Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	93.77 ng	2196650	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	16
3	5-Aminoindole			132	C8H8N2	005192-03-0	12
4	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	9
5	4-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-60-2	9



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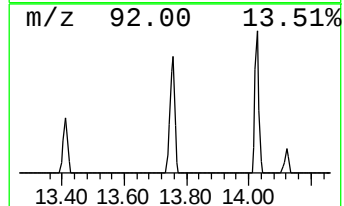
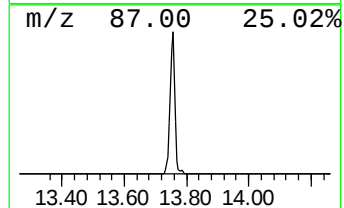
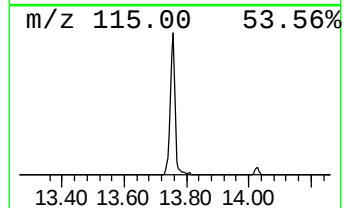
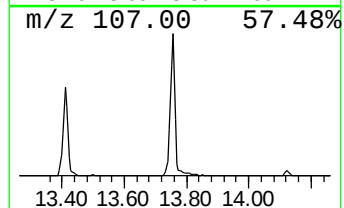
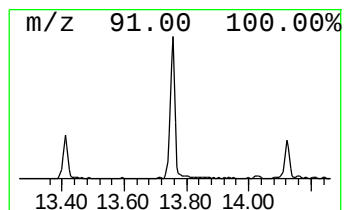
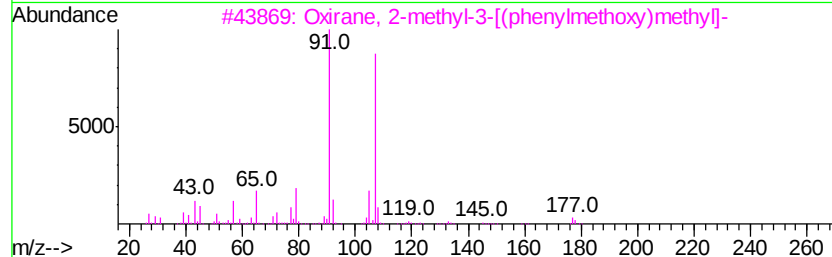
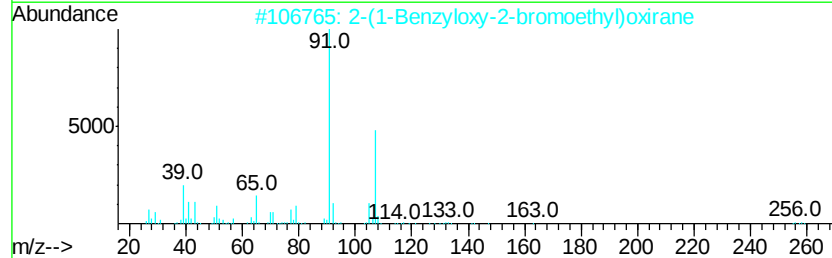
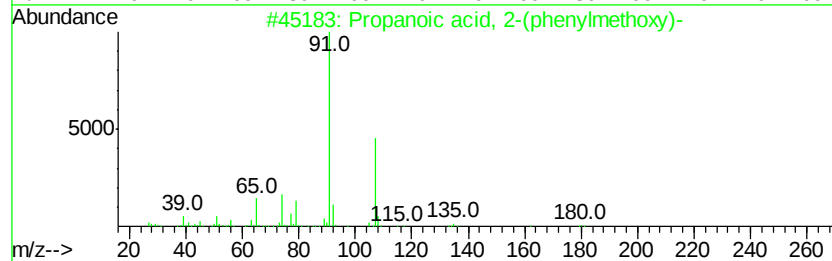
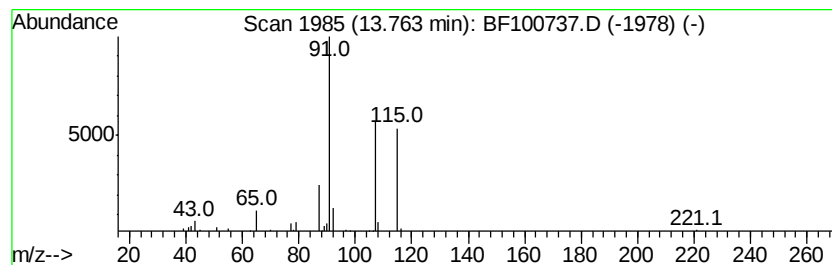
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Peak Number 4 unknown13.76 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	5.69 ng	179028	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-(phenylmethoxy)-	180	C10H12O3	006625-78-1	43
2		2-(1-Benzyloxy-2-bromoethyl)oxirane	256	C11H13BrO2	101514-16-3	43
3		Oxirane, 2-methyl-3-[(phenylmethoxy)methyl]-	178	C11H14O2	116296-88-9	37
4		Benzene, 1,1'-[1,4-butanediylbis(phenyl)]-	270	C18H22O2	006282-65-1	35
5		3-Benzyloxybutanoic acid, methyl ester	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...	5.12	6.4	ng	150251	1	6.87	468533	20.0
unknown6.64	6.64	93.8	ng	2196650	1	6.87	468533	20.0
unknown13.76	13.76	5.7	ng	179028	5	14.03	629514	20.0