

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112817\
 Data File : BF100930.D
 Acq On : 28 Nov 2017 13:35
 Operator : SJ/JU
 Sample : I6594-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 KUSER-CONCRETE

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	5.081	505	509	519	rBV	230092	265426	2.89%	0.747%
2	5.481	572	577	580	rBV	1115485	1013701	11.02%	2.854%
3	6.487	743	748	751	rBV	1294182	1282865	13.95%	3.612%
4	6.628	767	772	775	rBV	1353883	1174886	12.78%	3.308%
5	6.857	807	811	814	rBV	425939	335604	3.65%	0.945%
6	7.016	833	838	841	rBV	1327172	1175936	12.79%	3.311%
7	7.422	902	907	910	rBV	931514	860734	9.36%	2.424%
8	8.139	1025	1029	1032	rBV	522488	445777	4.85%	1.255%
9	9.216	1206	1212	1215	rBV	1929620	1794802	19.52%	5.054%
10	9.892	1323	1327	1336	rVB	588100	528402	5.75%	1.488%
11	10.680	1457	1461	1471	rVB	689804	607957	6.61%	1.712%
12	11.380	1576	1580	1583	rBV	609853	520669	5.66%	1.466%
13	12.963	1845	1849	1852	rBV	1607841	1495713	16.27%	4.212%
14	14.016	2025	2028	2031	rBV	364292	348815	3.79%	0.982%
15	14.610	2098	2129	2133	rBV	1541193	6425013	69.87%	18.091%
16	15.486	2273	2278	2286	rBV	267823	344652	3.75%	0.970%
17	16.674	2444	2480	2483	rBV3	1229994	7697940	83.71%	21.676%
18	19.250	2875	2918	2947	rBV4	948519	9195464	100.00%	25.892%

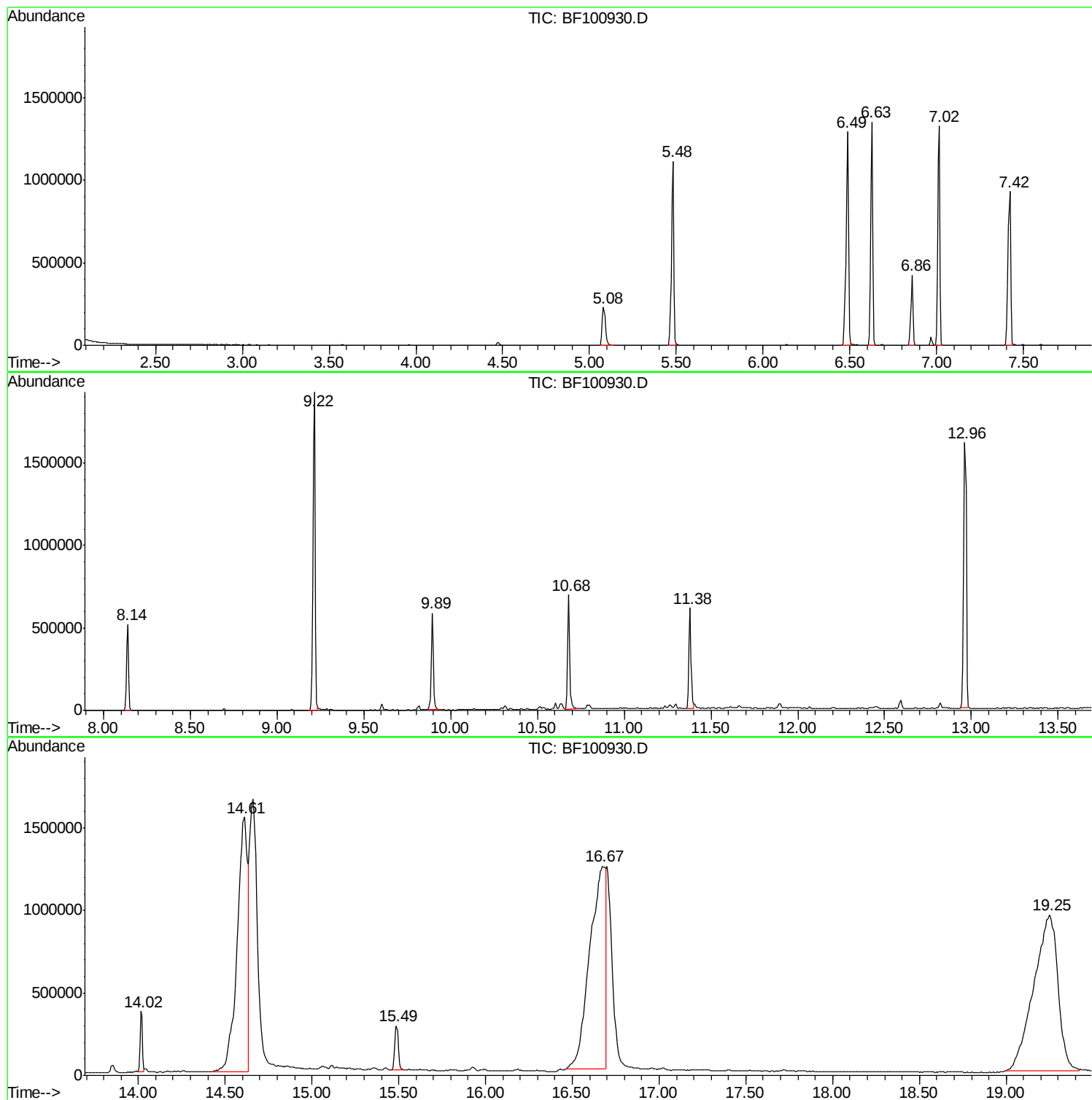
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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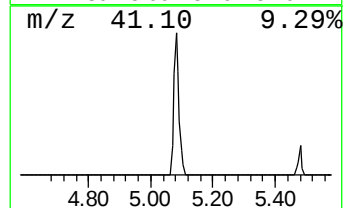
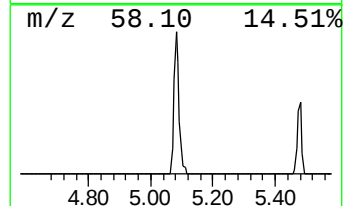
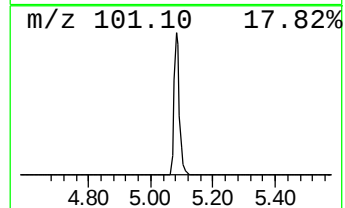
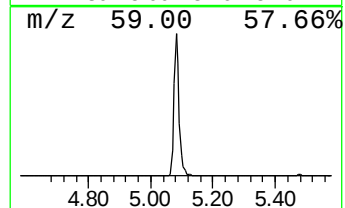
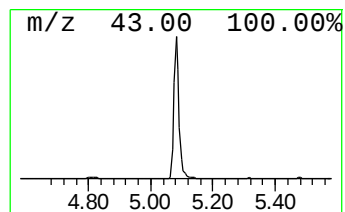
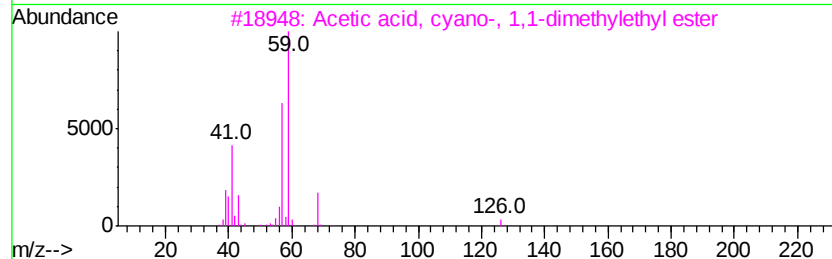
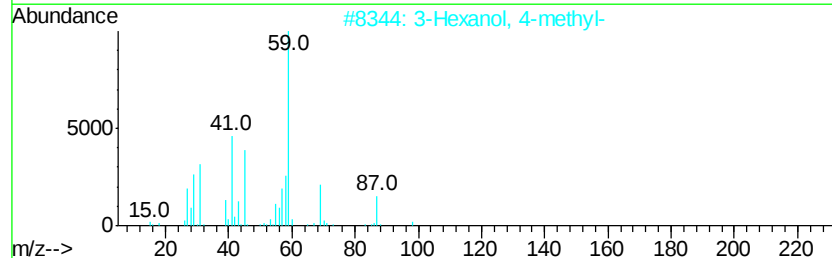
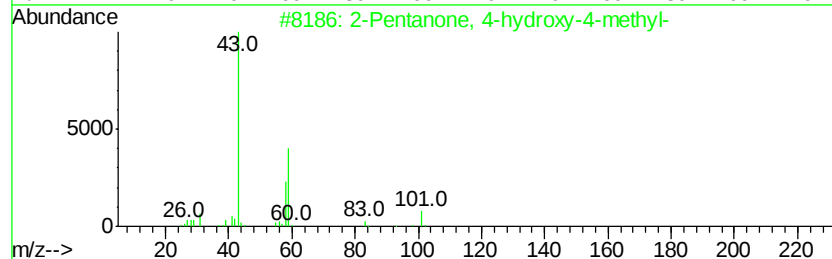
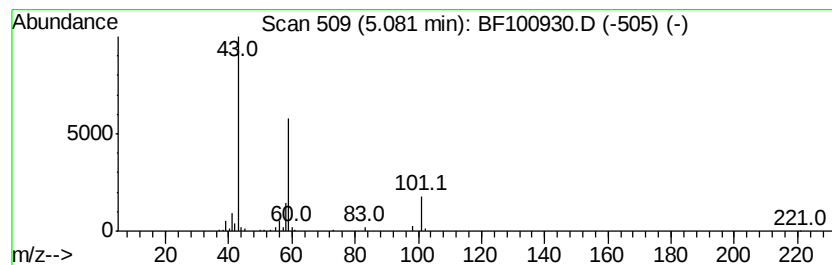
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	15.82 ng	265426	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethyl...	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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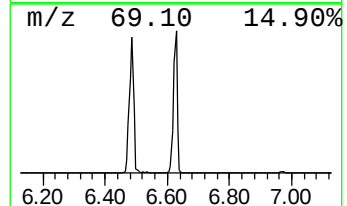
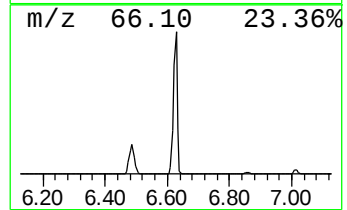
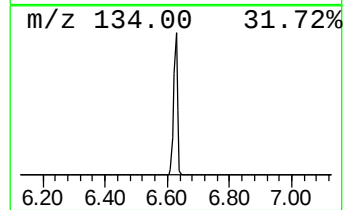
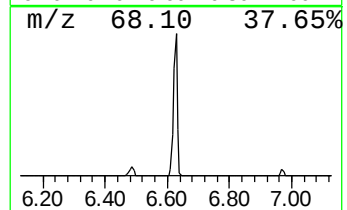
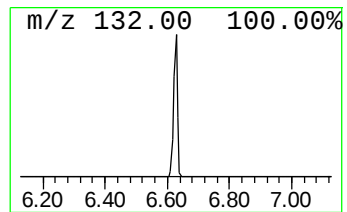
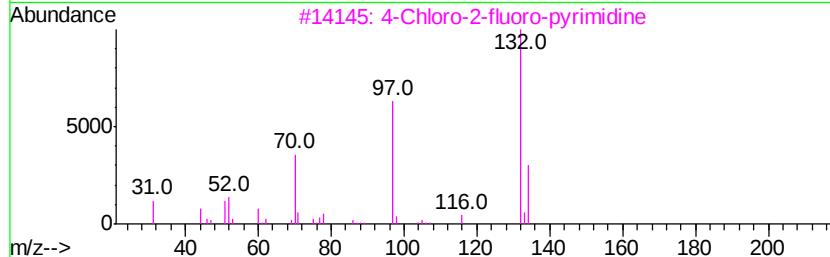
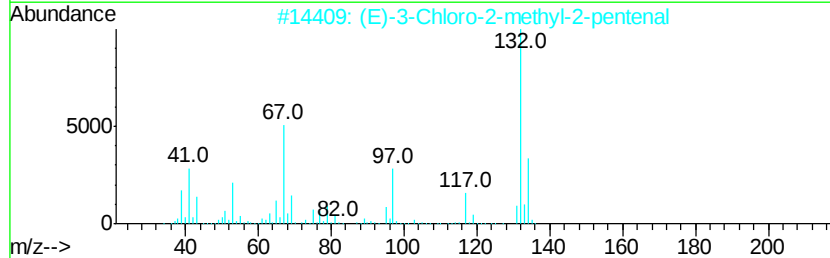
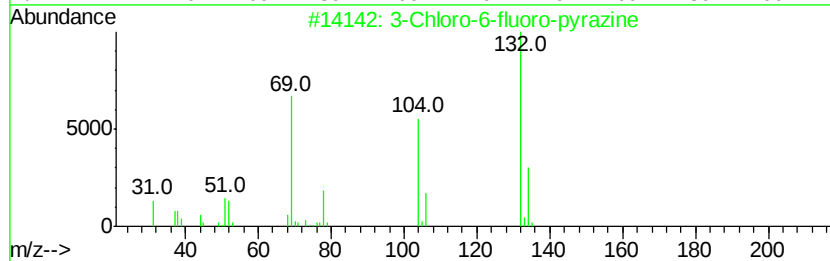
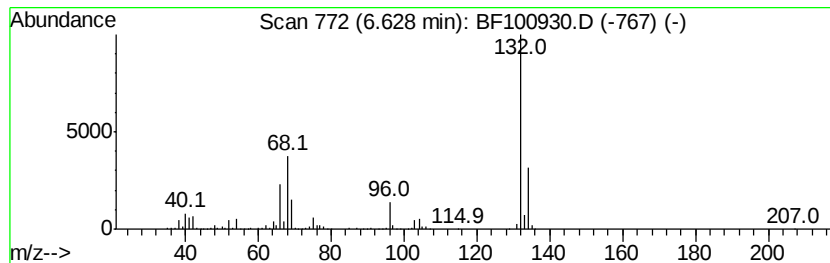
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Peak Number 2 unknown6.63 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	70.02 ng	1174890	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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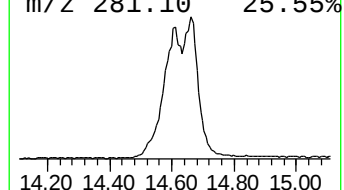
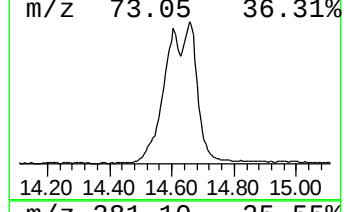
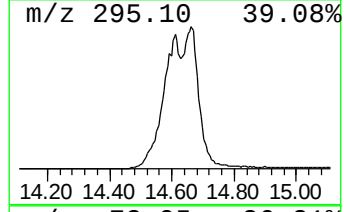
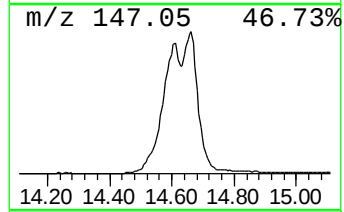
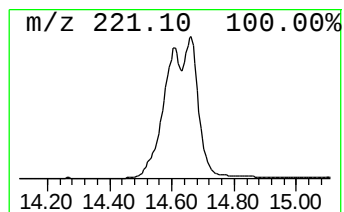
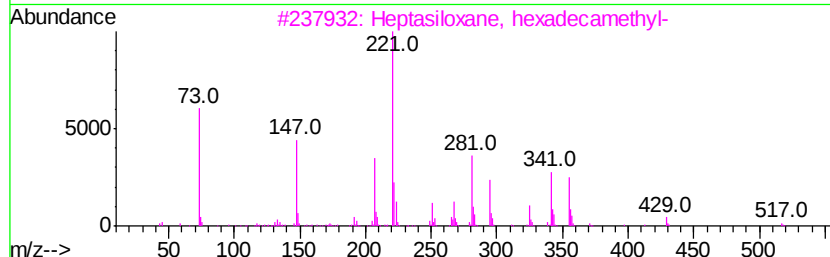
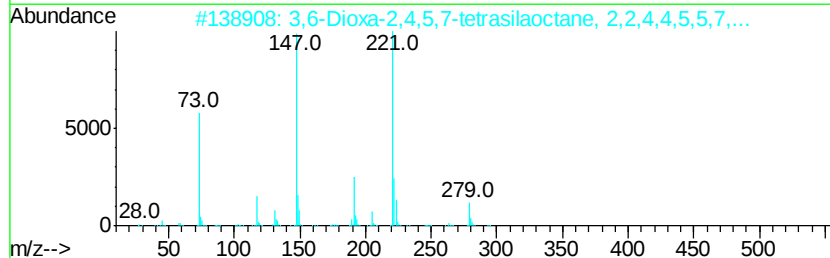
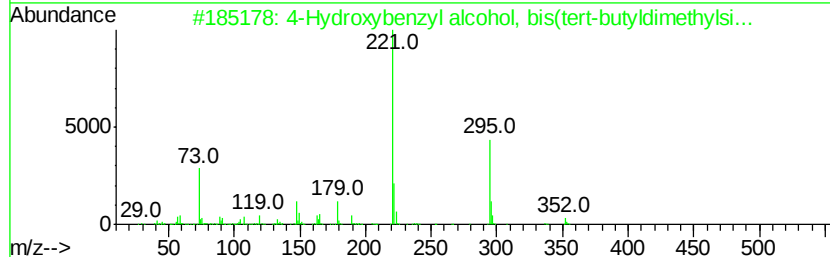
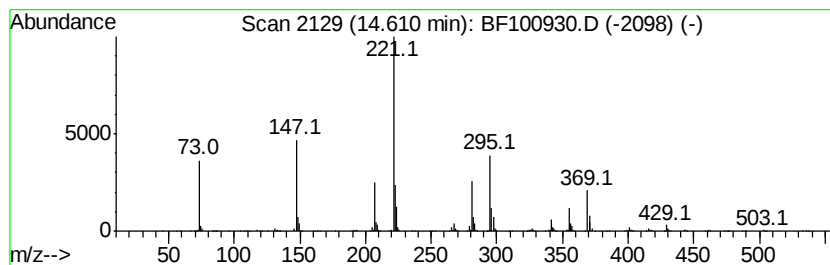
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Peak Number 4 4-Hydroxybenzyl alcohol, bi... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	368.39 ng	6425010	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Hydroxybenzyl alcohol, bis(ter...	352	C19H36O2Si2	1000364-43-9	50
2		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	49
3		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	42
4		2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	35
5		3-Oxobutan-2-yl trimethylsilyl p...	308	C15H20O5Si	1000373-49-5	27



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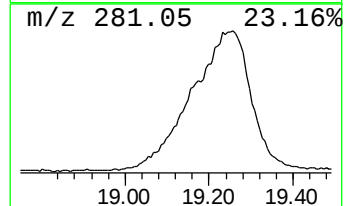
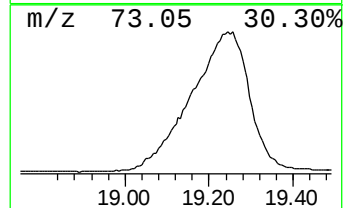
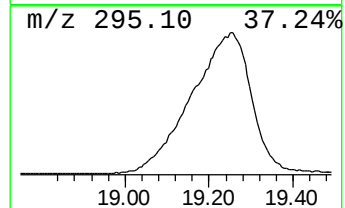
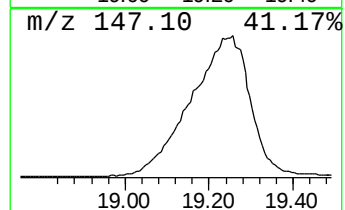
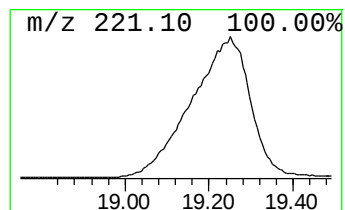
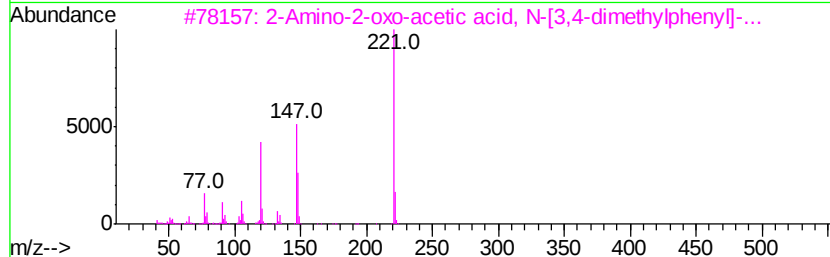
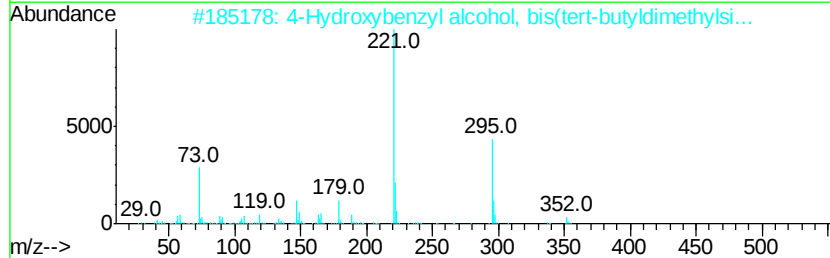
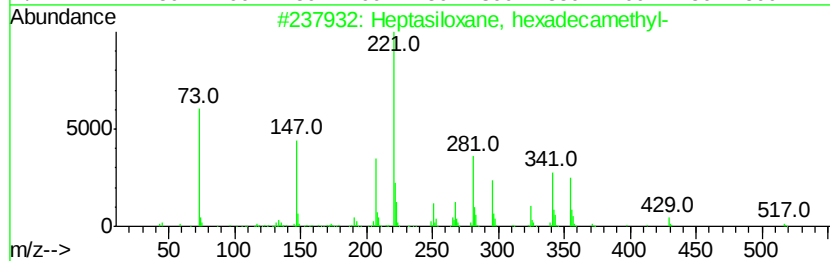
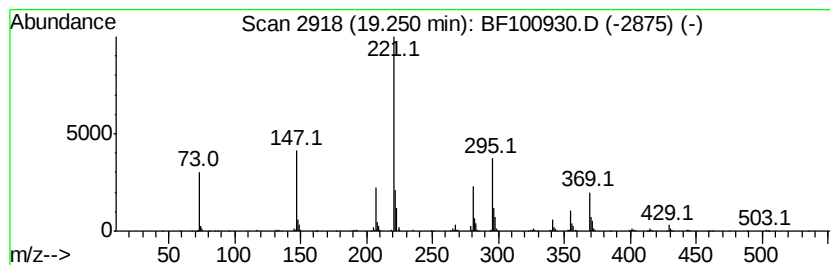
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Peak Number 6 unknown19.25 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.25	533.61 ng	9195460	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	42
2		4-Hydroxybenzyl alcohol, bis(ter...	352	C19H36O2Si2	1000364-43-9	38
3		2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15N03	024451-17-0	32
4		Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	32
5		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.08	15.8	ng	265426	1	6.86	335604	20.0
unknown6.63	6.63	70.0	ng	1174890	1	6.86	335604	20.0
4-Hydroxybenzyl a...	14.61	368.4	ng	6425010	5	14.02	348815	20.0
unknown19.25	19.25	533.6	ng	9195460	6	15.49	344652	20.0