

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062016\
 Data File : BF088192.D
 Acq On : 21 Jun 2016 1:44
 Operator : UM/SJ
 Sample : PB91400BL
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB91400BL

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-BF060716.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	1.655	5	6	14	rVV	204710	316427	13.01%	1.585%
2	1.770	14	16	52	rVB	1006637	1974106	81.15%	9.887%
3	4.113	219	221	233	rVB	41685	76537	3.15%	0.383%
4	4.810	280	282	295	rVB	198679	349534	14.37%	1.751%
5	5.267	319	322	324	rBV	1500452	1865282	76.68%	9.342%
6	6.319	412	414	417	rBV	1518955	1590525	65.38%	7.966%
7	6.433	422	424	427	rBV	1570272	1773358	72.90%	8.882%
8	6.661	442	444	447	rBV	395833	447332	18.39%	2.240%
9	6.822	456	458	460	rBV	1790730	1544583	63.49%	7.736%
10	7.233	492	494	497	rBV	1081180	1081009	44.44%	5.414%
11	7.953	554	557	559	rBV	671443	608810	25.03%	3.049%
12	9.027	648	651	654	rBV	2273748	2202121	90.52%	11.029%
13	9.702	708	710	712	rBV	622205	676726	27.82%	3.389%
14	10.490	776	779	781	rBV2	892463	1125626	46.27%	5.638%
15	11.176	837	839	841	rBV	877967	719797	29.59%	3.605%
16	12.765	975	978	980	rBV	1789577	2432688	100.00%	12.184%
17	13.805	1066	1069	1071	rBV	605243	599795	24.66%	3.004%
18	15.062	1173	1179	1187	rBV2	18043	90810	3.73%	0.455%
19	15.177	1187	1189	1197	rVB	430816	491611	20.21%	2.462%

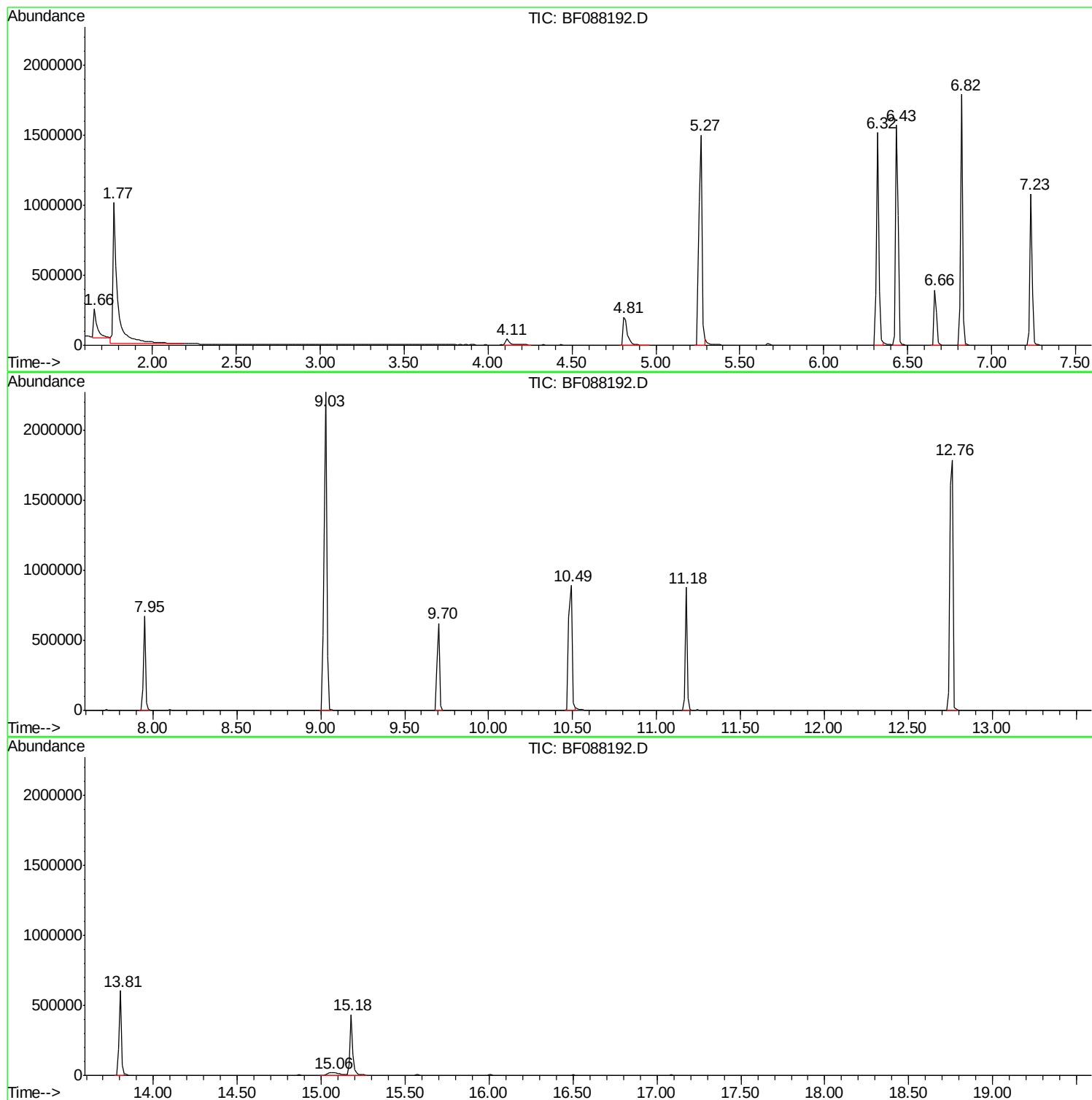
Sum of corrected areas: 19966677

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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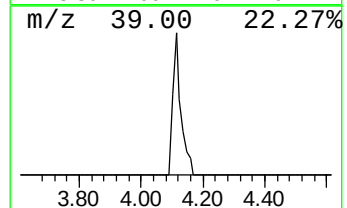
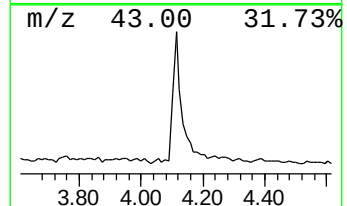
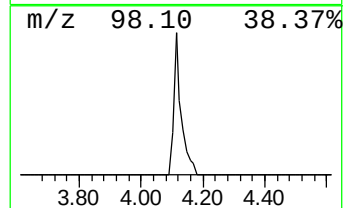
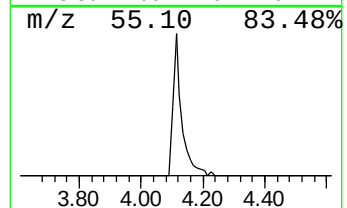
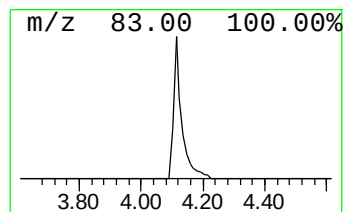
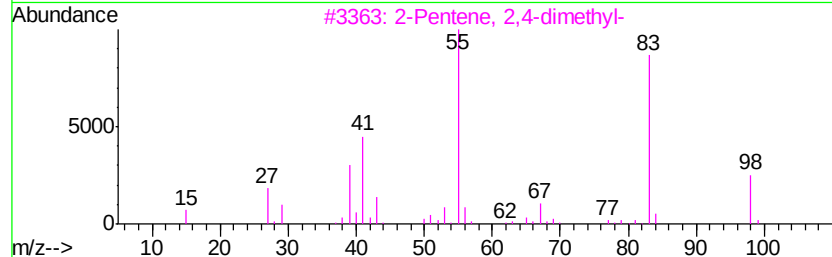
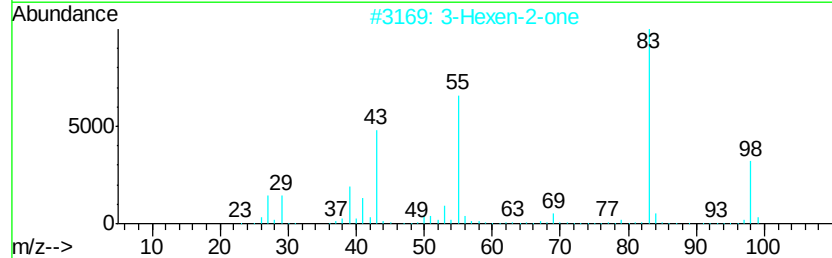
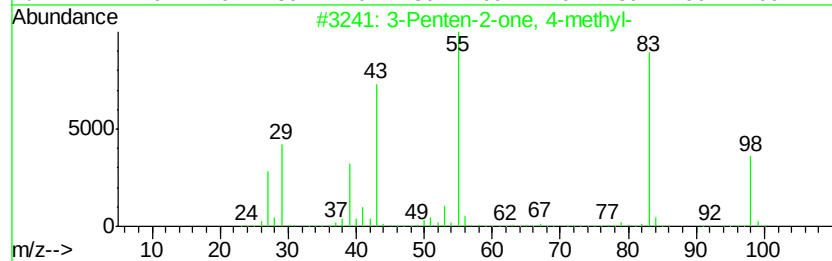
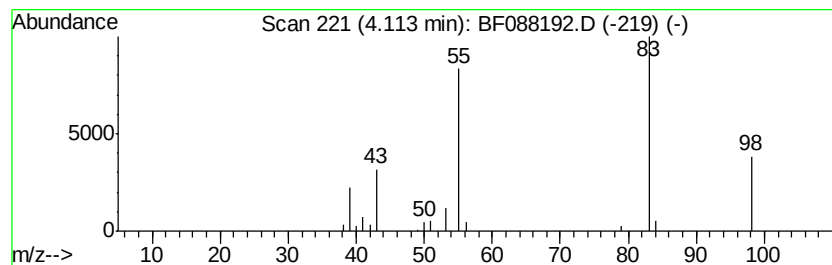
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.11	3.42 ng	76537	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4		2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	80
5		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80



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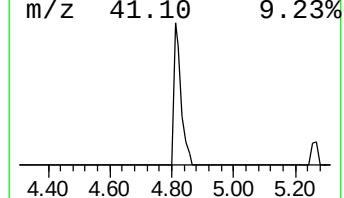
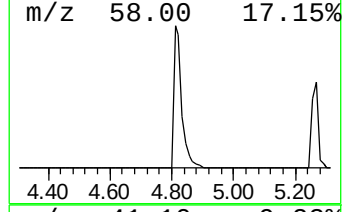
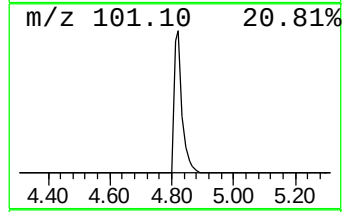
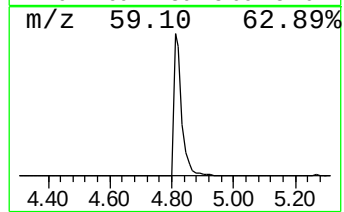
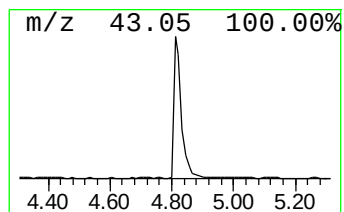
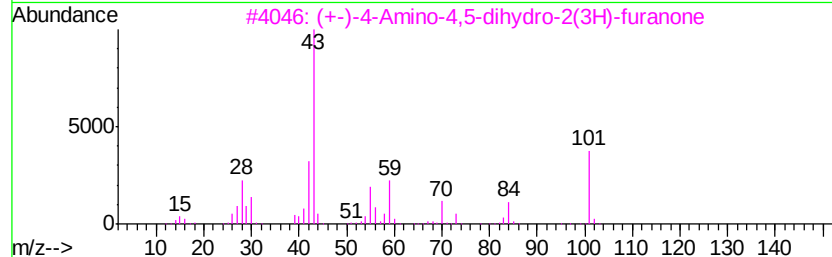
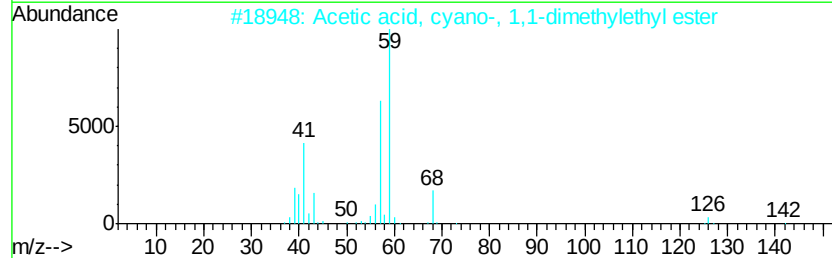
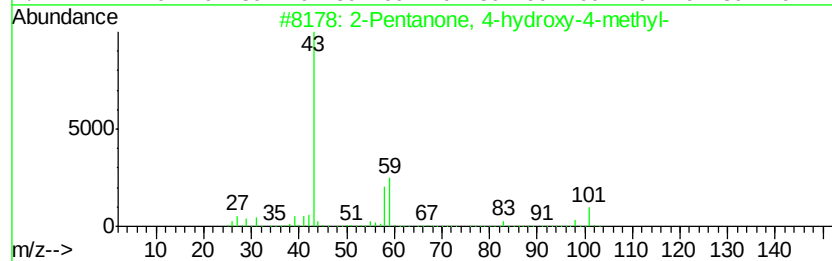
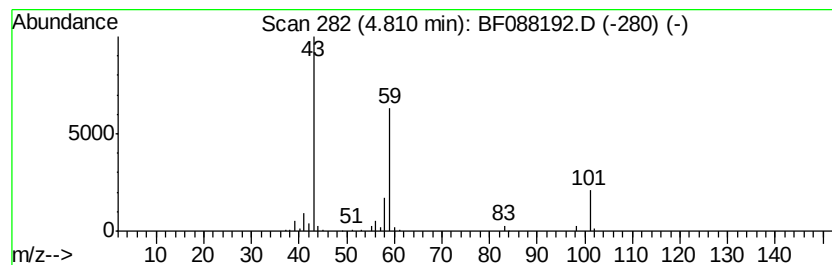
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	15.63 ng	349534	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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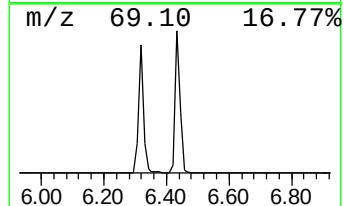
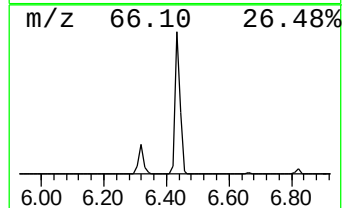
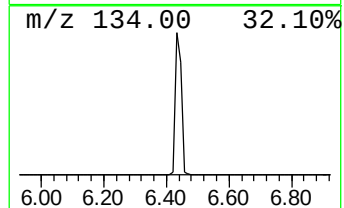
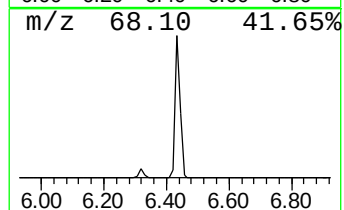
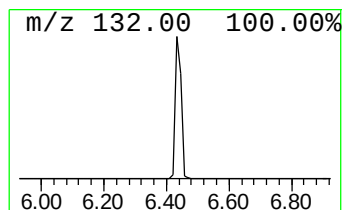
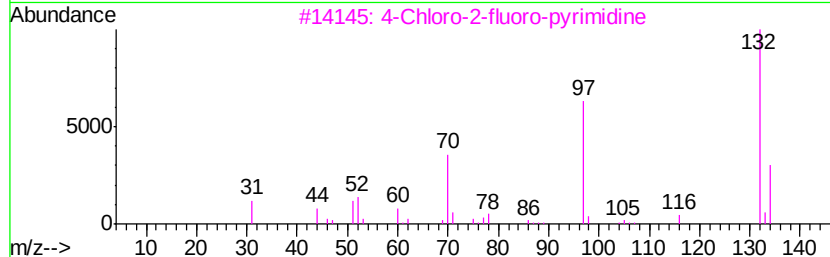
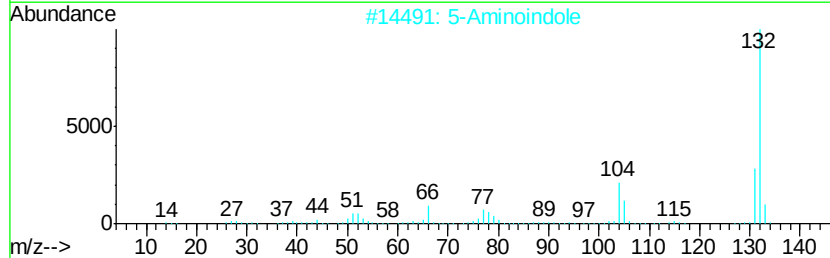
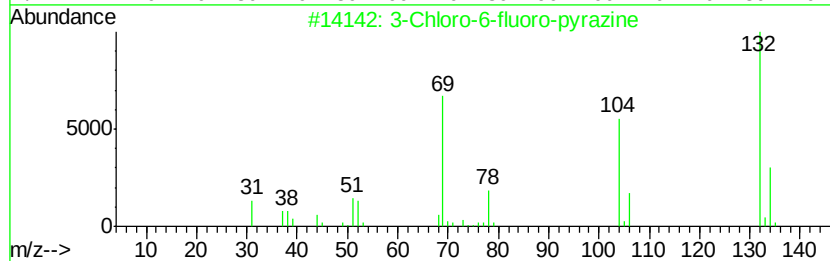
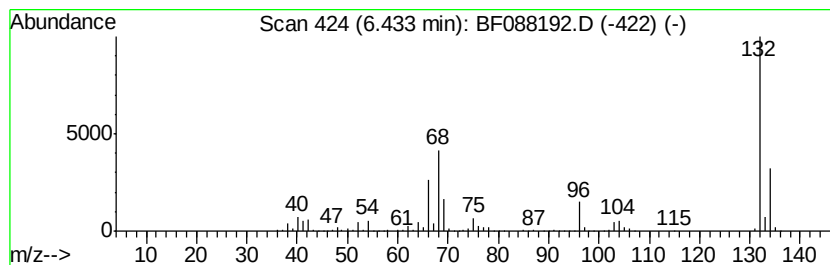
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Peak Number 5 unknown6.43 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	79.29 ng	1773360	1,4-Dichlorobenzene-d4	6.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5		Aminoindole	132	C8H8N2	005192-03-0	12
3	4		Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	9
5	1-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-59-9	9



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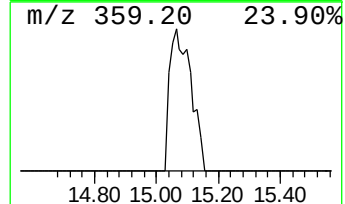
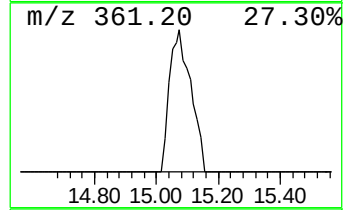
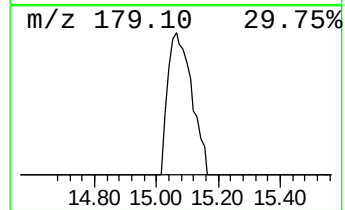
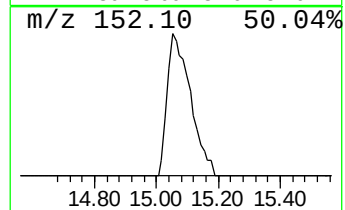
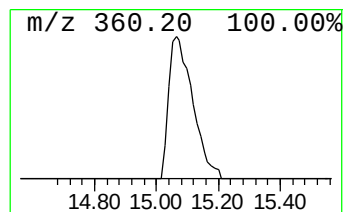
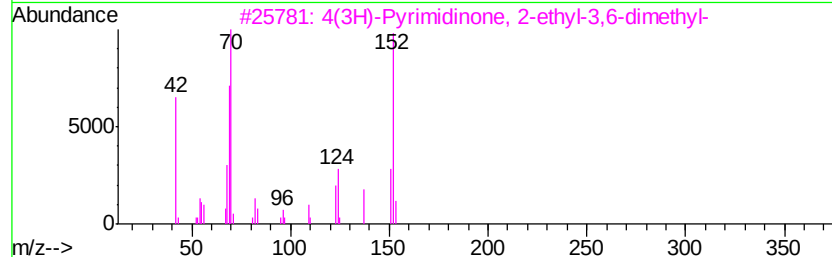
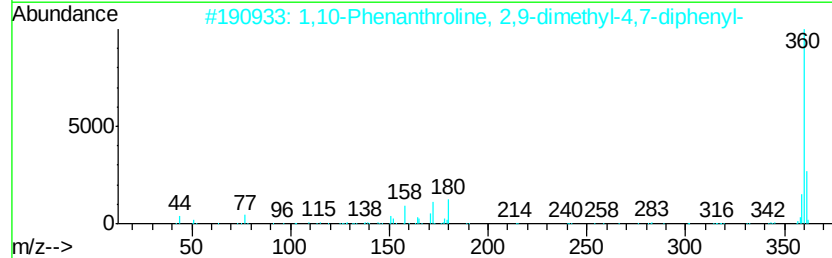
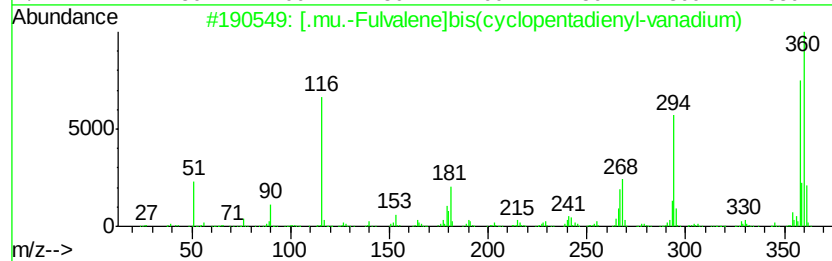
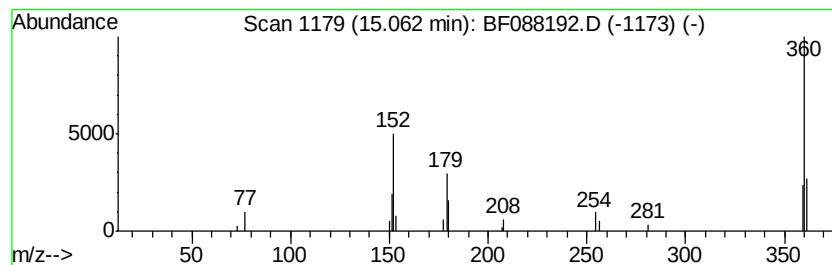
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Peak Number 7 unknown15.06 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	3.69 ng	90810	Perylene-d12	15.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	[.mu.-Fulvalene]bis(cyclopentadi...	360	C20H18V2	1000163-45-2	38
2		1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	9
3		4(3H)-Pyrimidinone, 2-ethyl-3,6-...	152	C8H12N2O	032363-54-5	9
4		2-Fluoro-1,3-dimethyl-1,3,2-diaz...	152	C4H10FN2OP	1000305-90-9	7
5		[2-(3,4-Dimethoxy-phenyl)-ethyl]...	223	C13H21N02	1000300-71-5	7



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.11	3.4	ng	76537	1	6.66	447332	20.0
2-Pentanone, 4-hy...	4.81	15.6	ng	349534	1	6.66	447332	20.0
unknown6.43	6.43	79.3	ng	1773360	1	6.66	447332	20.0
unknown15.06	15.06	3.7	ng	90810	6	15.18	491611	20.0