

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092518\
 Data File : BG036957.D
 Acq On : 25 Sep 2018 20:15
 Operator : JU/SJ
 Sample : J5061-11
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 230-KV-C

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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	4.551	210	215	231	rBV	272270	441833	13.79%	2.520%
2	5.150	311	317	333	rBV	238577	387794	12.10%	2.212%
3	5.614	389	396	411	rBV	644815	1147058	35.80%	6.542%
4	7.201	657	666	697	rBV	656137	1379935	43.07%	7.870%
5	7.577	722	730	747	rBV	637335	1228873	38.35%	7.009%
6	8.041	803	809	825	rVB	134999	261657	8.17%	1.492%
7	8.364	857	864	880	rBV	533732	986741	30.79%	5.628%
8	9.204	999	1007	1027	rBV	404613	856451	26.73%	4.885%
9	10.849	1277	1287	1301	rBV	178405	369693	11.54%	2.109%
10	13.288	1695	1702	1719	rBV	1175007	1982469	61.87%	11.307%
11	14.116	1837	1843	1853	rBV	126012	207299	6.47%	1.182%
12	14.669	1930	1937	1952	rBV2	313767	538776	16.81%	3.073%
13	16.155	2181	2190	2207	rBV	897284	1527705	47.68%	8.713%
14	17.412	2397	2404	2412	rBV	442213	723125	22.57%	4.124%
15	20.021	2841	2848	2860	rBV	2363305	3204269	100.00%	18.275%
16	21.320	3064	3069	3075	rBV3	39409	77262	2.41%	0.441%
17	21.678	3123	3130	3147	rBV2	484156	865855	27.02%	4.938%
18	23.159	3376	3382	3390	rVB2	28844	58529	1.83%	0.334%
19	23.347	3408	3414	3420	rBV3	32067	63920	1.99%	0.365%
20	23.952	3511	3517	3527	rBV2	31317	76120	2.38%	0.434%
21	24.886	3665	3676	3689	rBV2	289478	873463	27.26%	4.982%
22	26.014	3863	3868	3881	rVB5	22820	63572	1.98%	0.363%
23	27.330	4078	4092	4109	rBV8	41895	211057	6.59%	1.204%

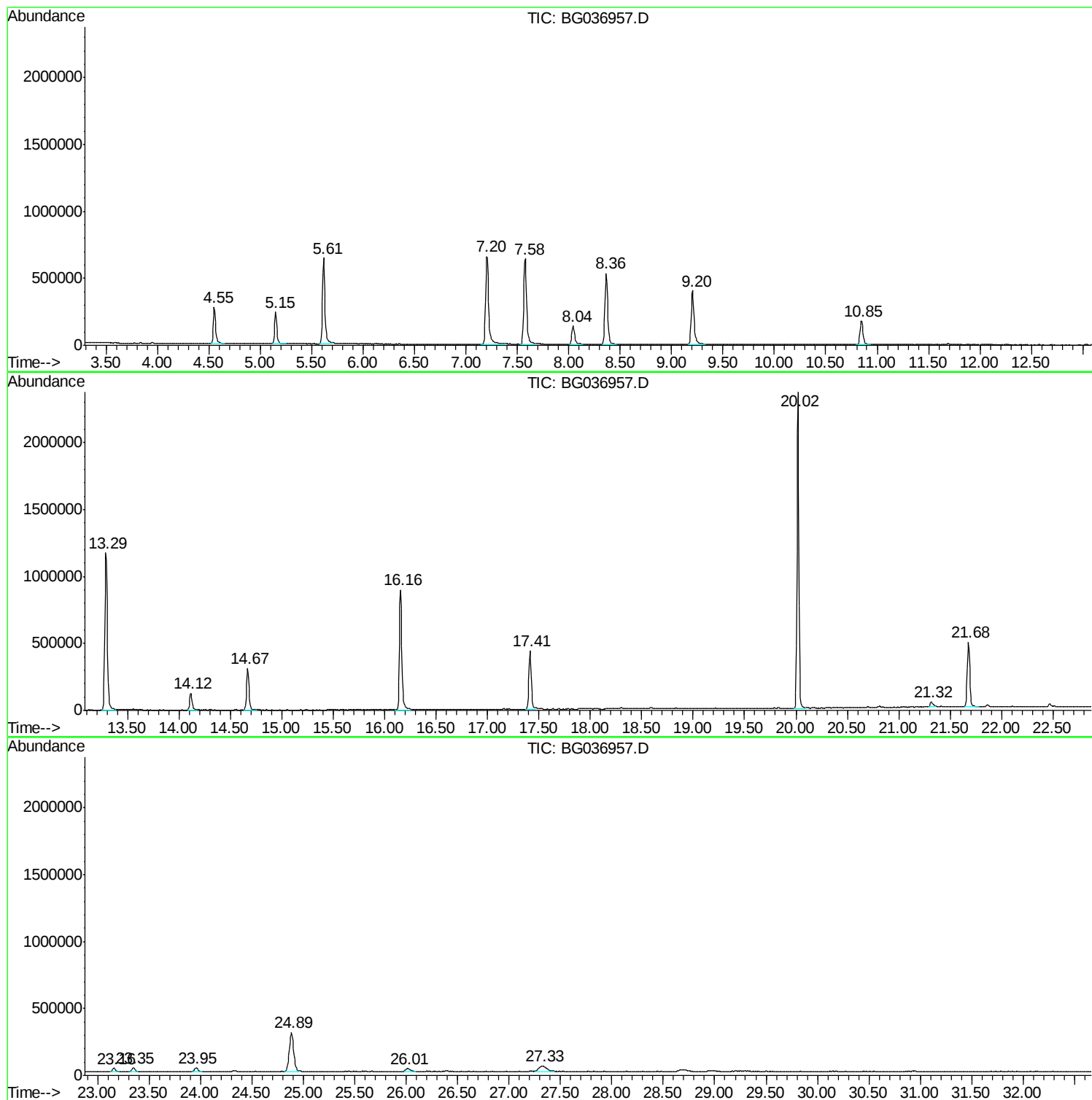
Sum of corrected areas: 17533456

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



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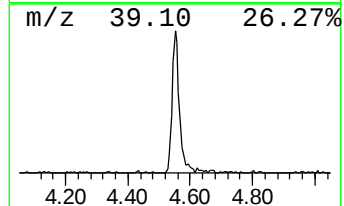
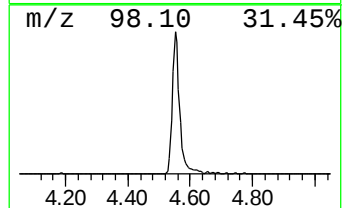
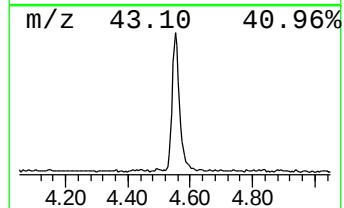
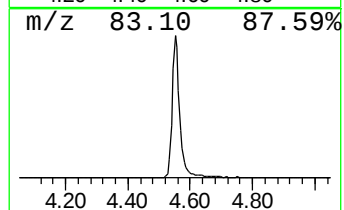
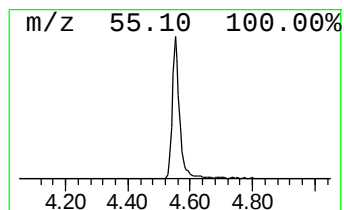
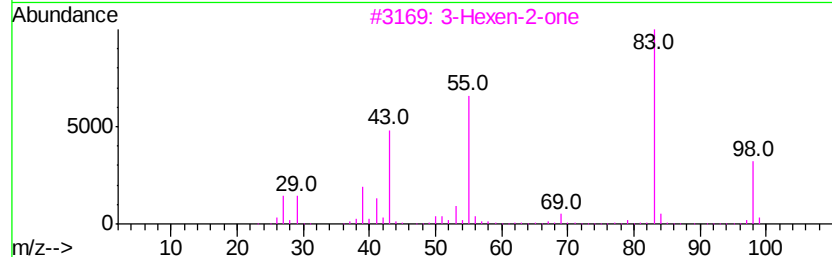
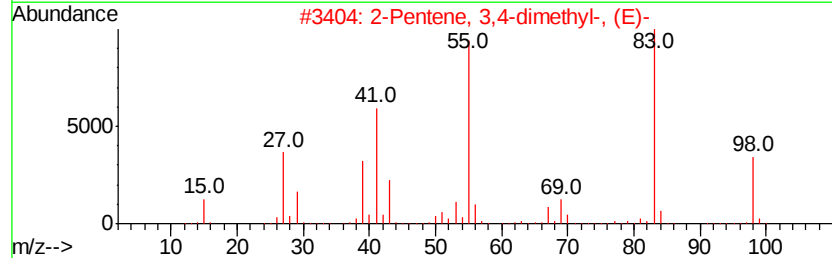
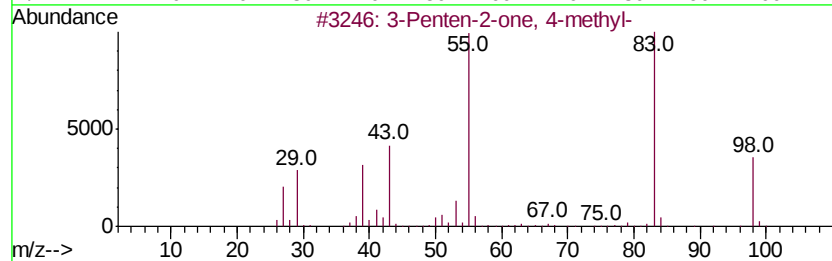
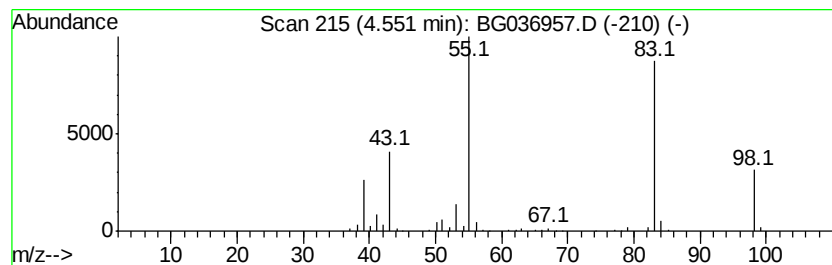
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	33.77 ng	441833	1,4-Dichlorobenzene-d4	8.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3		3-Hexen-2-one	98	C6H10O	000763-93-9	87
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78



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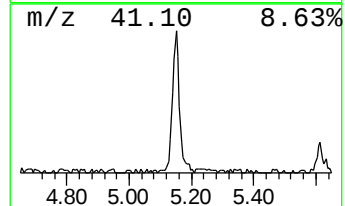
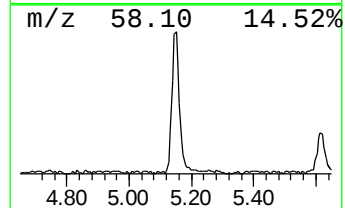
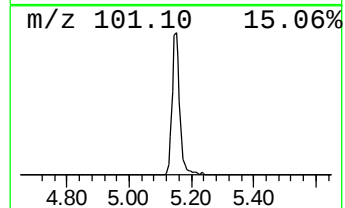
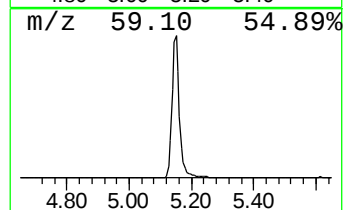
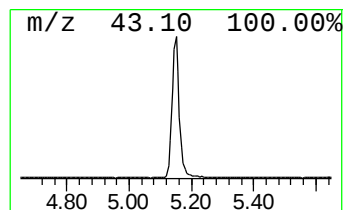
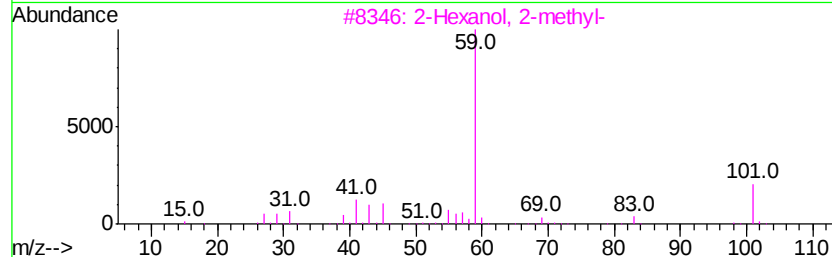
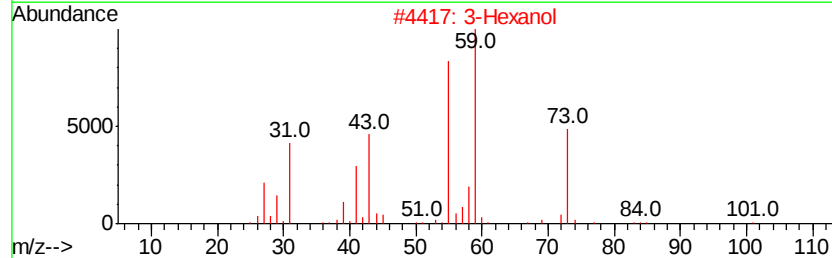
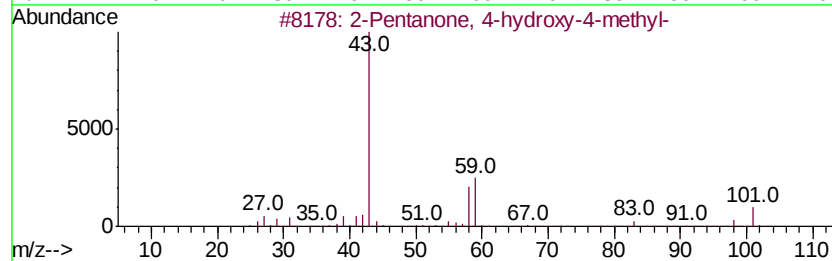
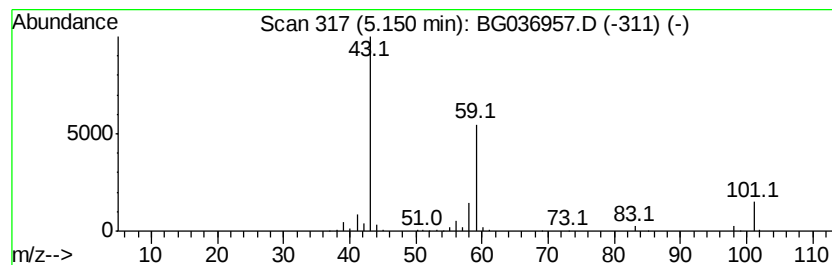
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	29.64 ng	387794	1,4-Dichlorobenzene-d4	8.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		3-Hexanol	102	C6H14O	000623-37-0	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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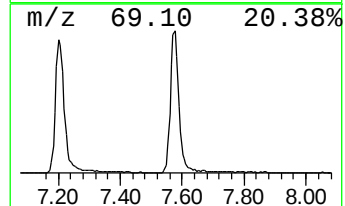
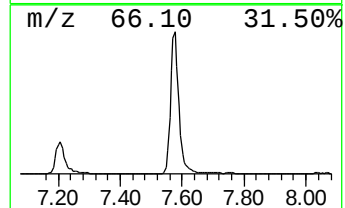
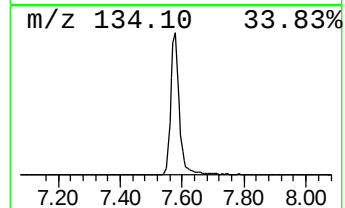
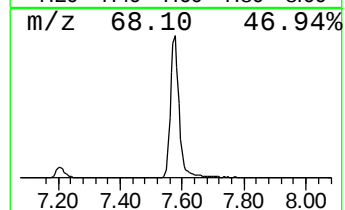
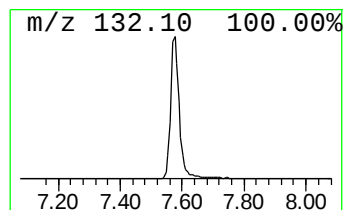
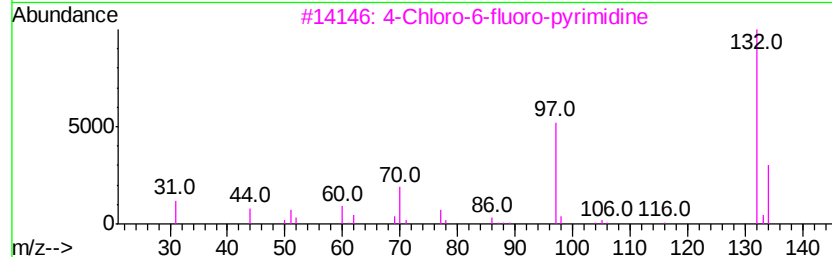
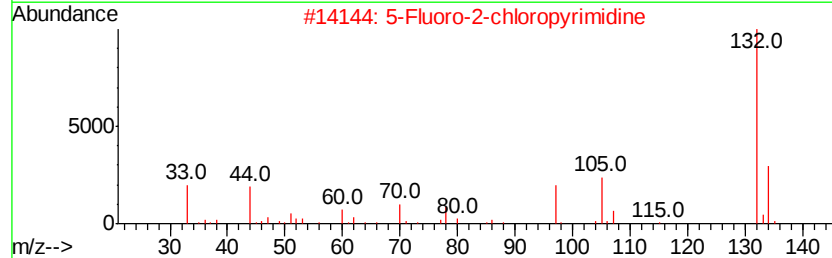
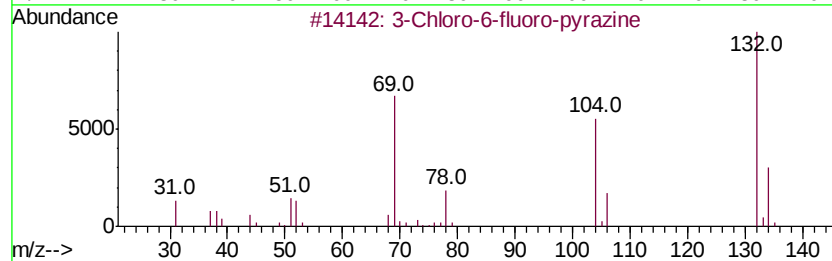
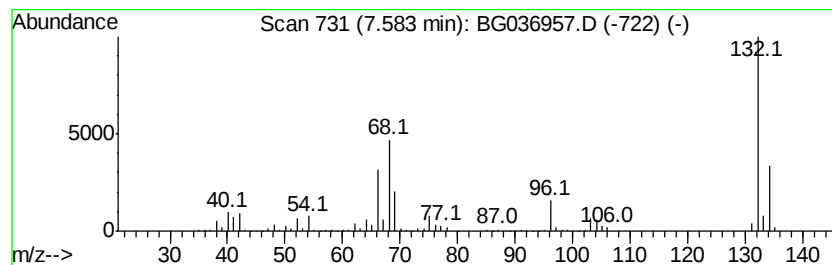
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Peak Number 3 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	93.93 ng	1228870	1,4-Dichlorobenzene-d4	8.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		5-Aminoindole	132	C8H8N2	005192-03-0	22



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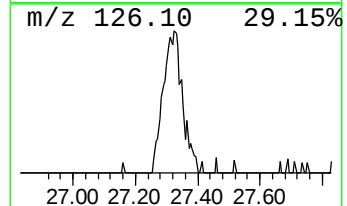
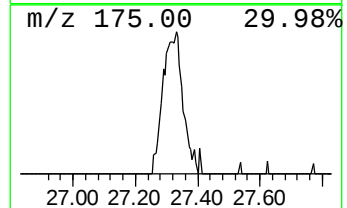
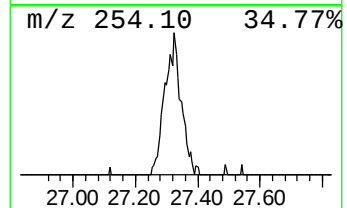
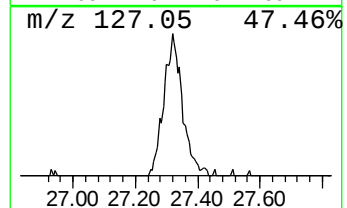
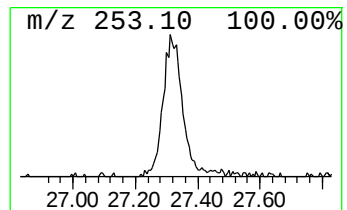
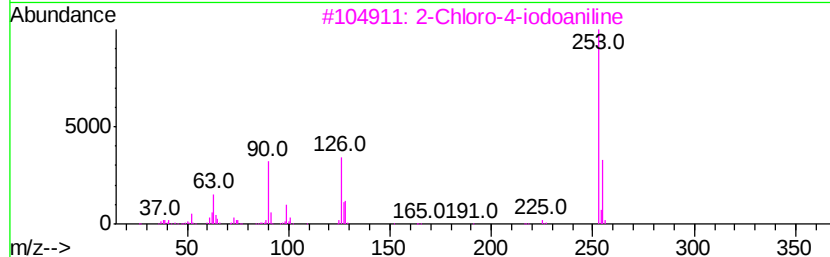
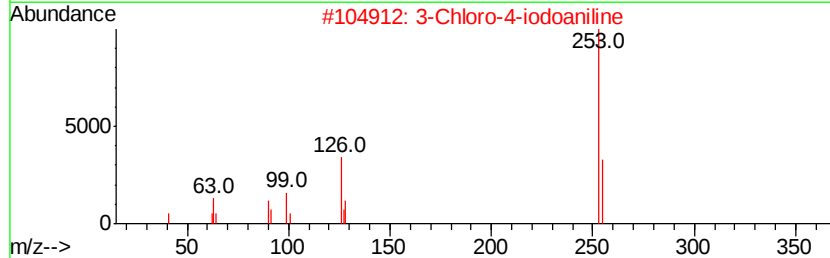
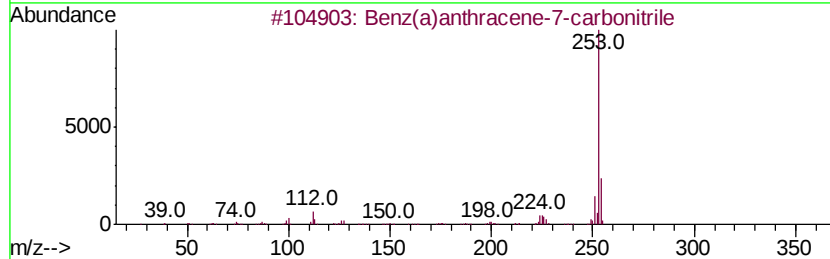
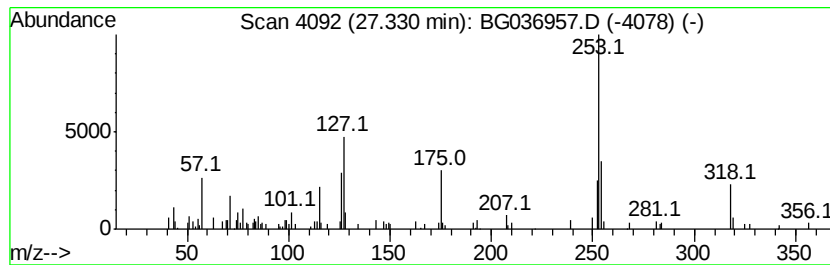
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Peak Number 5 unknown27.33 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.33	4.83 ng	211057	Perylene-d12	24.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benz(a)anthracene-7-carbonitrile	253	C19H11N	007476-08-6	35
2		3-Chloro-4-iodoaniline	253	C6H5ClIN	135050-44-1	17
3		2-Chloro-4-iodoaniline	253	C6H5ClIN	042016-93-3	17
4		1H-Indene, 1,1'-(1,2-ethanedivli...	254	C20H14	072088-04-1	10
5		cis-2,4,5-Trimethoxy-.beta.-meth...	253	C12H15NO5	017231-84-4	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.55	33.8	ng	441833	1	8.04	261657	20.0
2-Pentanone, 4-hy...	5.15	29.6	ng	387794	1	8.04	261657	20.0
unknown7.58	7.58	93.9	ng	1228870	1	8.04	261657	20.0
unknown27.33	27.33	4.8	ng	211057	6	24.88	873463	20.0