

Data Path : Z:\HPCHEM1\BNA G\DATA\BG042015\
 Data File : BG016553.D
 Acq On : 20 Apr 2015 16:22
 Operator : TP/IZ
 Sample : G1868-04
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P5-28(0-5)

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:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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	2.746	5	10	19	rVB	116931	180759	4.34%	0.741%
2	2.822	19	23	28	rVB	120609	129888	3.12%	0.532%
3	4.767	348	354	362	rVB	163801	221607	5.32%	0.908%
4	5.243	429	435	450	rBV	1296184	1818744	43.62%	7.455%
5	6.847	696	708	722	rBV	1292223	2043811	49.02%	8.377%
6	7.188	759	766	776	rBV	1303129	2042070	48.98%	8.370%
7	7.652	837	845	854	rBV	264621	408818	9.81%	1.676%
8	7.969	892	899	907	rVB	971453	1498814	35.95%	6.143%
9	8.809	1035	1042	1049	rBV	745011	1191932	28.59%	4.886%
10	10.437	1310	1319	1326	rBV	380531	631815	15.15%	2.590%
11	12.916	1734	1741	1751	rBV	1937798	2909177	69.78%	11.924%
12	13.757	1878	1884	1892	rBV	59175	91905	2.20%	0.377%
13	14.297	1967	1976	1984	rBV2	579015	890550	21.36%	3.650%
14	15.784	2223	2229	2243	rBV	1379115	1973616	47.34%	8.089%
15	16.007	2261	2267	2275	rBV	30823	53155	1.27%	0.218%
16	17.035	2435	2442	2448	rBV2	798462	1104528	26.49%	4.527%
17	17.423	2502	2508	2515	rBV3	23770	43093	1.03%	0.177%
18	17.934	2588	2595	2605	rBV	91759	180796	4.34%	0.741%
19	19.221	2810	2814	2823	rBV2	36793	71913	1.72%	0.295%
20	19.667	2884	2890	2901	rVB	3305865	4169155	100.00%	17.089%
21	20.925	3100	3104	3114	rBV	154942	218575	5.24%	0.896%
22	21.213	3148	3153	3158	rBV	999807	1191002	28.57%	4.882%
23	21.359	3175	3178	3184	rBV	41519	43130	1.03%	0.177%
24	21.788	3248	3251	3257	rVB2	34430	43008	1.03%	0.176%
25	22.241	3325	3328	3335	rBV2	43065	63060	1.51%	0.258%
26	23.433	3525	3531	3545	rVB	622318	1182352	28.36%	4.846%

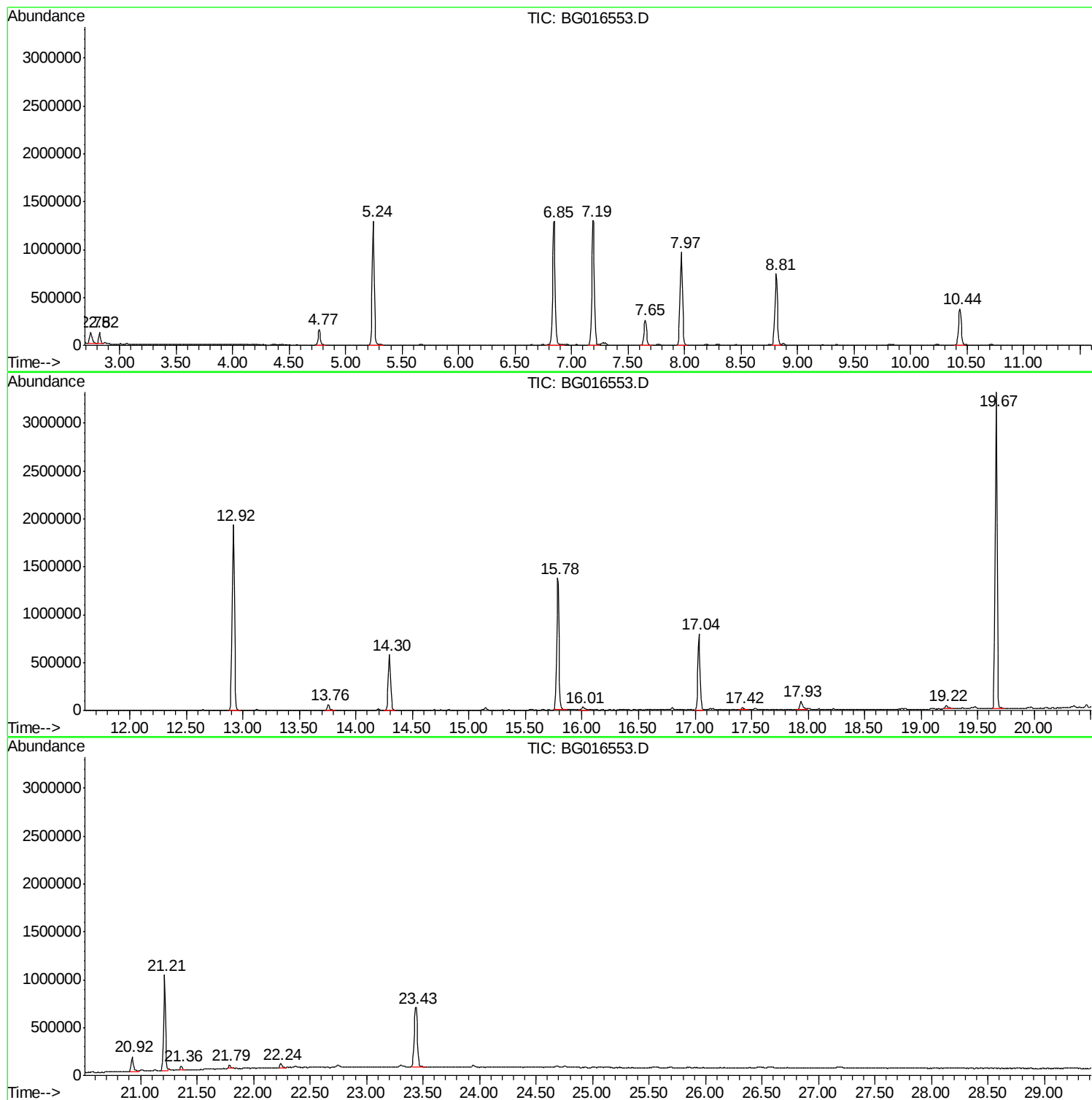
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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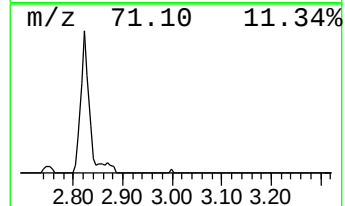
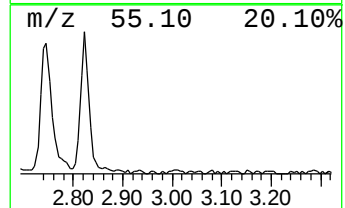
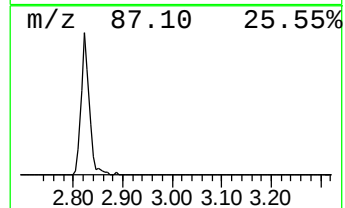
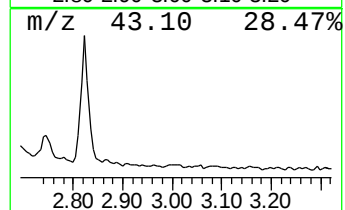
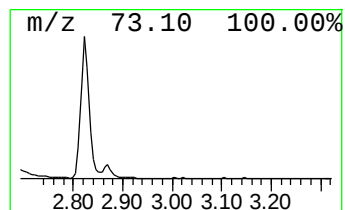
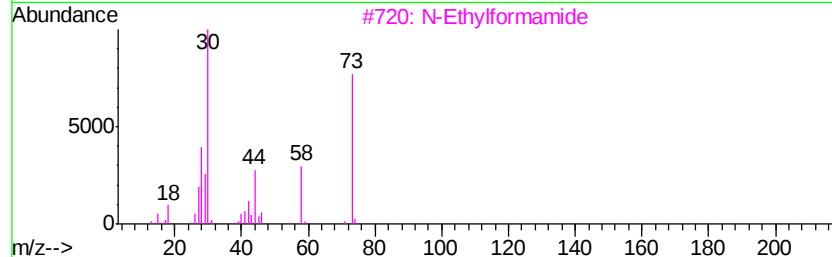
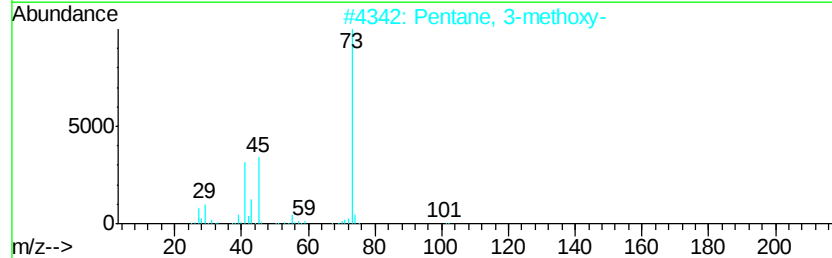
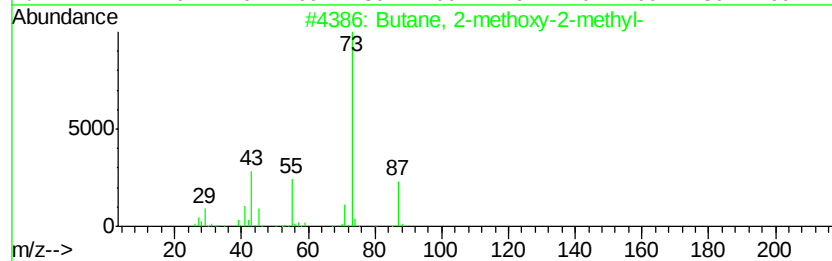
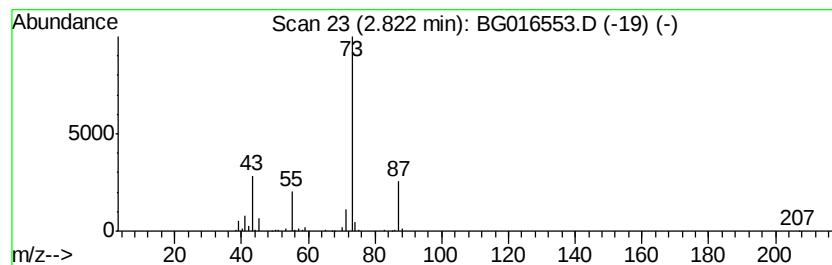
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.82	6.35 ng	129888	1,4-Dichlorobenzene-d4	7.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7



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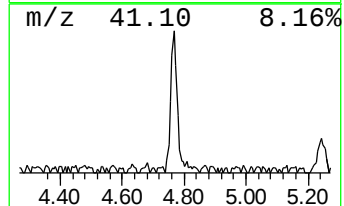
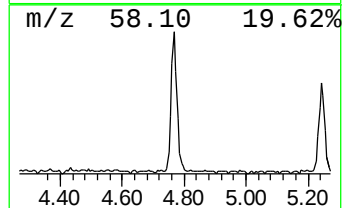
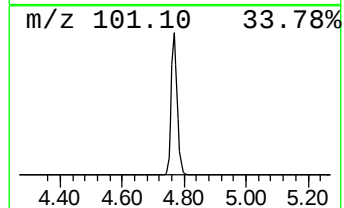
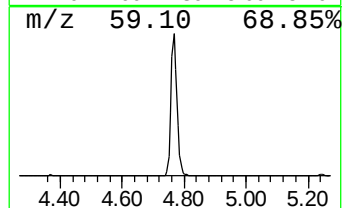
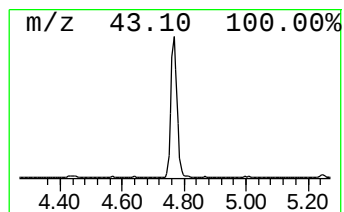
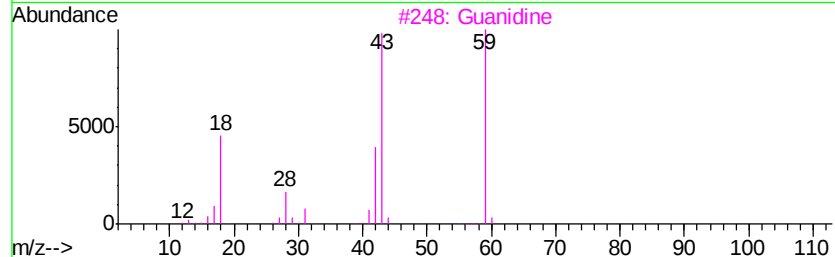
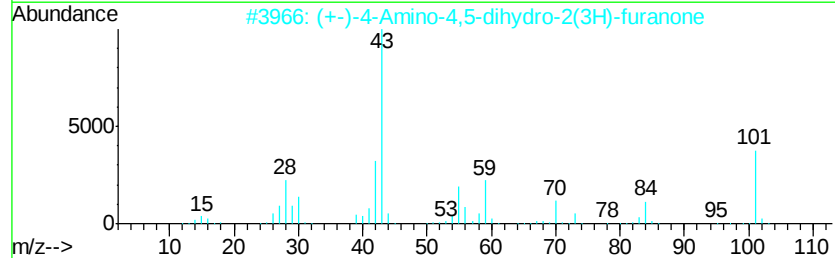
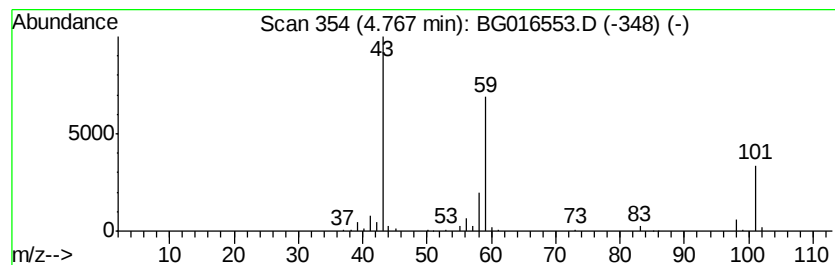
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.77	10.84 ng	221607	1,4-Dichlorobenzene-d4	7.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	38
3		Guanidine	59	CH5N3	000113-00-8	38
4		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	12



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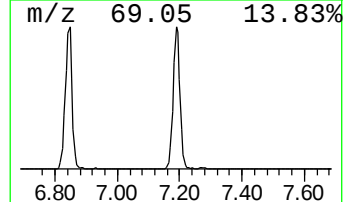
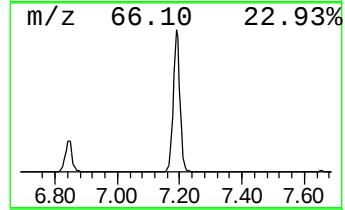
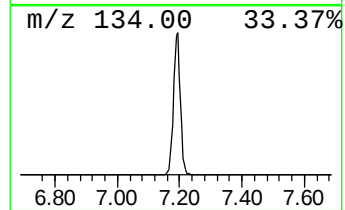
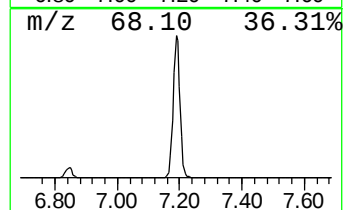
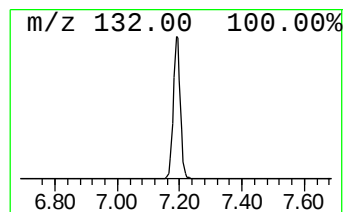
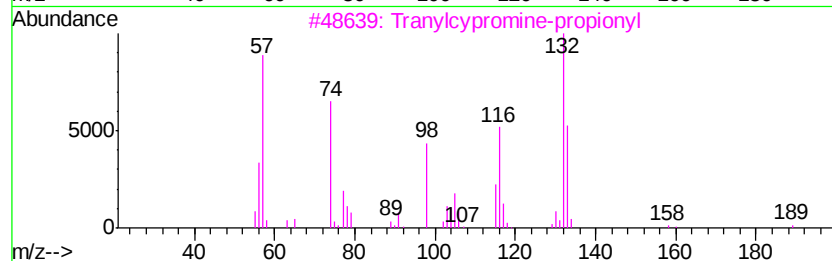
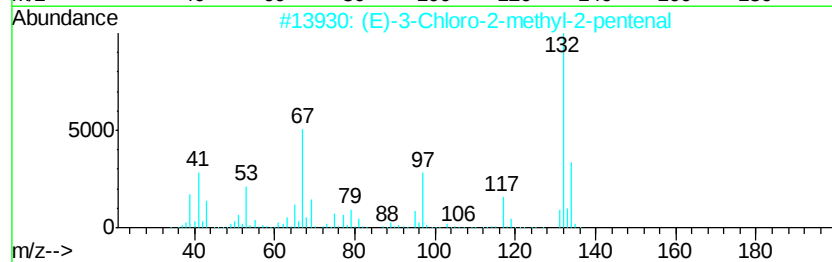
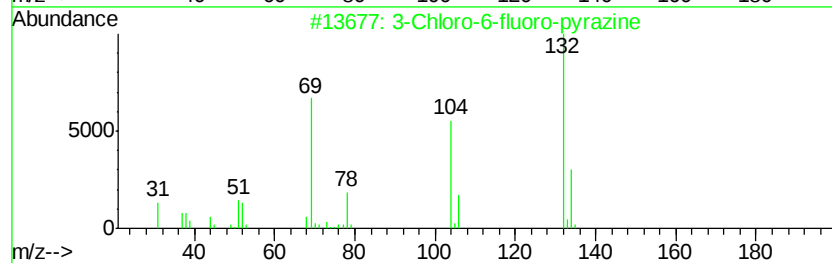
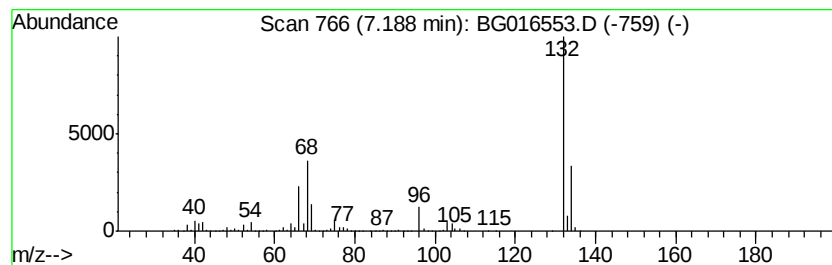
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Peak Number 4 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	99.90 ng	2042070	1,4-Dichlorobenzene-d4	7.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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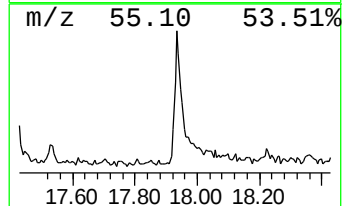
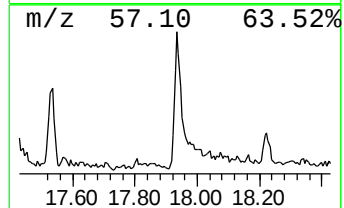
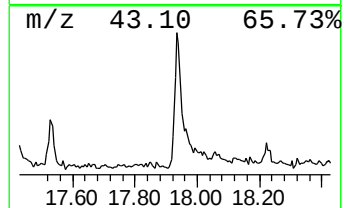
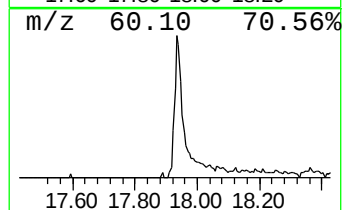
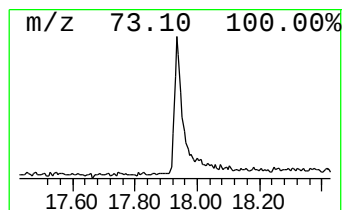
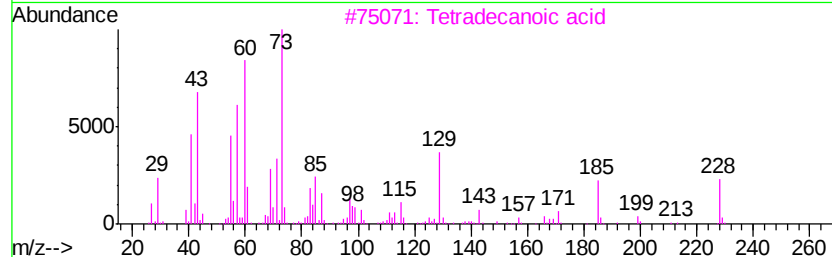
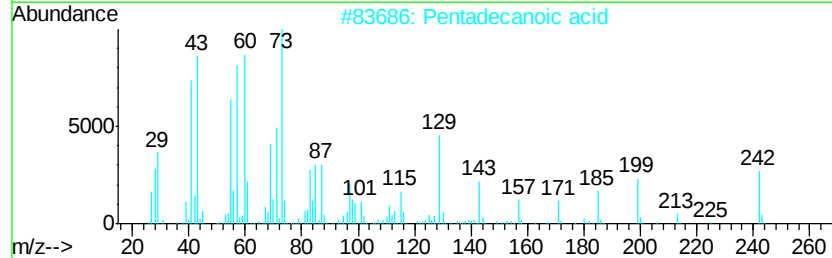
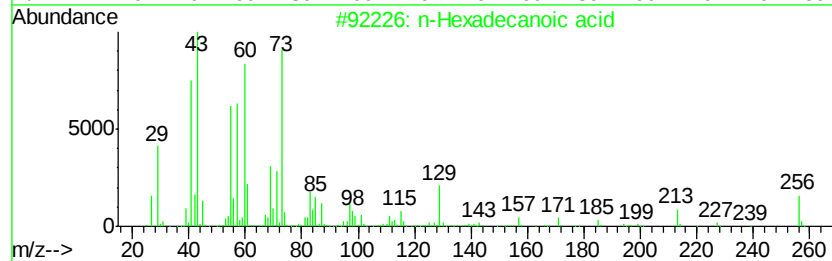
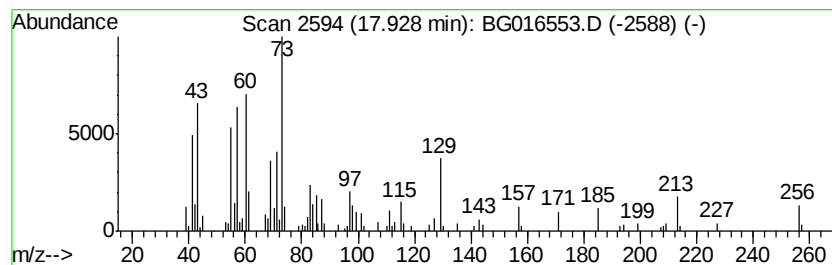
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.93	3.27 ng	180796	Phenanthrene-d10	17.04

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4		Tridecanoic acid	214	C13H26O2	000638-53-9	70
5		n-Decanoic acid	172	C10H20O2	000334-48-5	62



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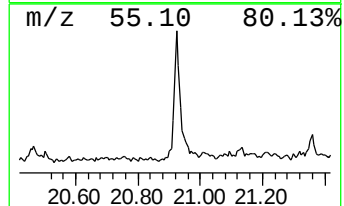
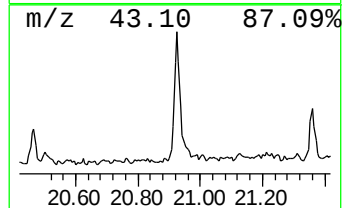
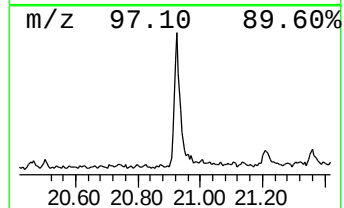
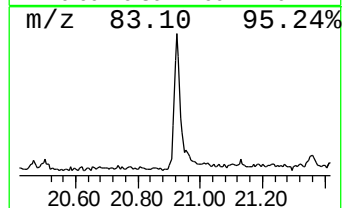
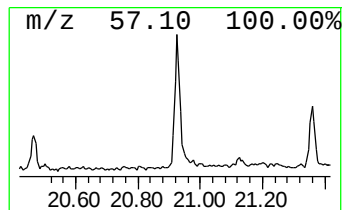
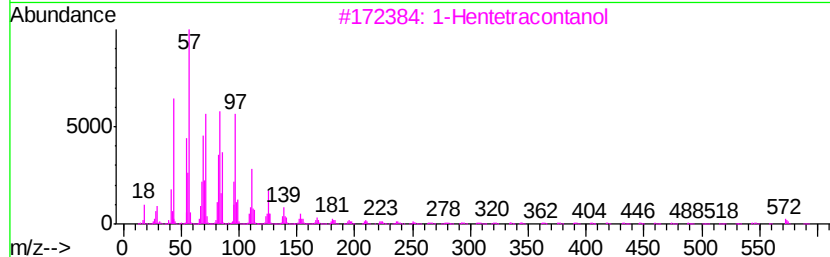
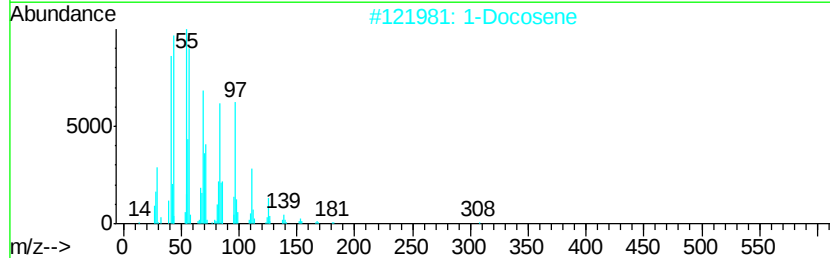
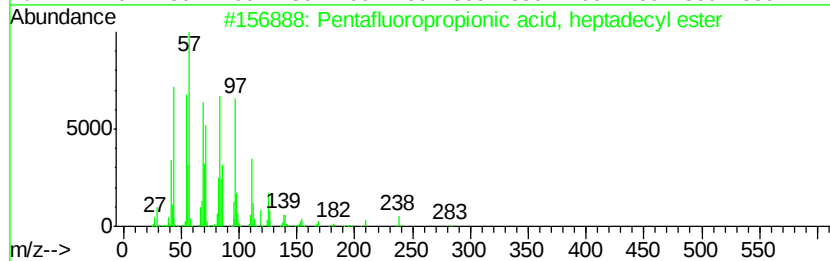
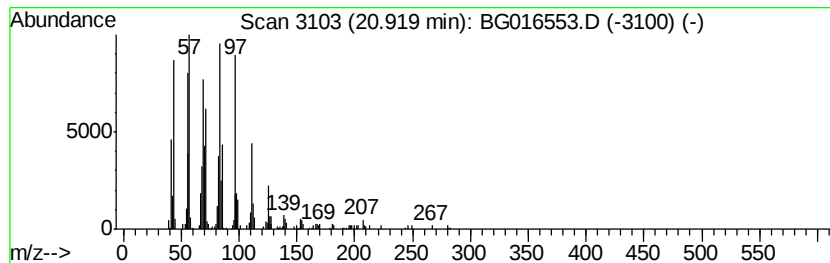
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Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.92	3.67 ng	218575	Chrysene-d12	21.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	90
2		1-Docosene	308	C22H44	001599-67-3	90
3		1-Hentetracontanol	593	C41H84O	040710-42-7	90
4		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87
5		Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.82	6.3	ng	129888	1	7.65	408818	20.0
2-Pentanone, 4-hy...	4.77	10.8	ng	221607	1	7.65	408818	20.0
unknown7.19	7.19	99.9	ng	2042070	1	7.65	408818	20.0
n-Hexadecanoic acid	17.93	3.3	ng	180796	4	17.04	1104530	20.0
Pentafluoropropio...	20.92	3.7	ng	218575	5	21.21	1191000	20.0