

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111414\
 Data File : BF075551.D
 Acq On : 15 Nov 2014 20:04
 Operator : TP / JJ
 Sample : F4649-01
 Misc :
 ALS Vial : 49 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S32-FILL04

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-BF111214.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	1.624	44	47	50	rBV	6024012	7012053	100.00%	29.474%
2	1.761	56	59	63	rVB	115619	210219	3.00%	0.884%
3	1.967	74	77	84	rBV2	325943	545111	7.77%	2.291%
4	5.339	370	372	380	rVB	525380	778481	11.10%	3.272%
5	5.842	414	416	419	rBV	1433267	1538446	21.94%	6.467%
6	7.099	523	526	528	rBV	1818507	1622659	23.14%	6.821%
7	7.259	537	540	543	rBV	1689036	1580620	22.54%	6.644%
8	7.545	563	565	568	rBV	233004	297822	4.25%	1.252%
9	7.739	580	582	584	rVB	1337999	1193421	17.02%	5.016%
10	8.242	623	626	628	rVB	1104602	1003502	14.31%	4.218%
11	9.133	701	704	706	rVB	422394	421124	6.01%	1.770%
12	10.471	819	821	824	rBV	1307670	1683840	24.01%	7.078%
13	10.974	863	865	868	rBV	406102	399950	5.70%	1.681%
14	11.305	892	894	897	rBV	350312	463506	6.61%	1.948%
15	12.288	978	980	983	rBV2	943188	1092580	15.58%	4.592%
16	13.157	1054	1056	1059	rVB	493446	497776	7.10%	2.092%
17	14.963	1211	1214	1217	rBV	80733	75280	1.07%	0.316%
18	15.157	1228	1231	1233	rBV	1865156	1940676	27.68%	8.157%
19	16.334	1331	1334	1343	rBV	148704	282000	4.02%	1.185%
20	16.460	1343	1345	1348	rVV	565885	571057	8.14%	2.400%
21	18.243	1498	1501	1504	rBV	449446	580727	8.28%	2.441%

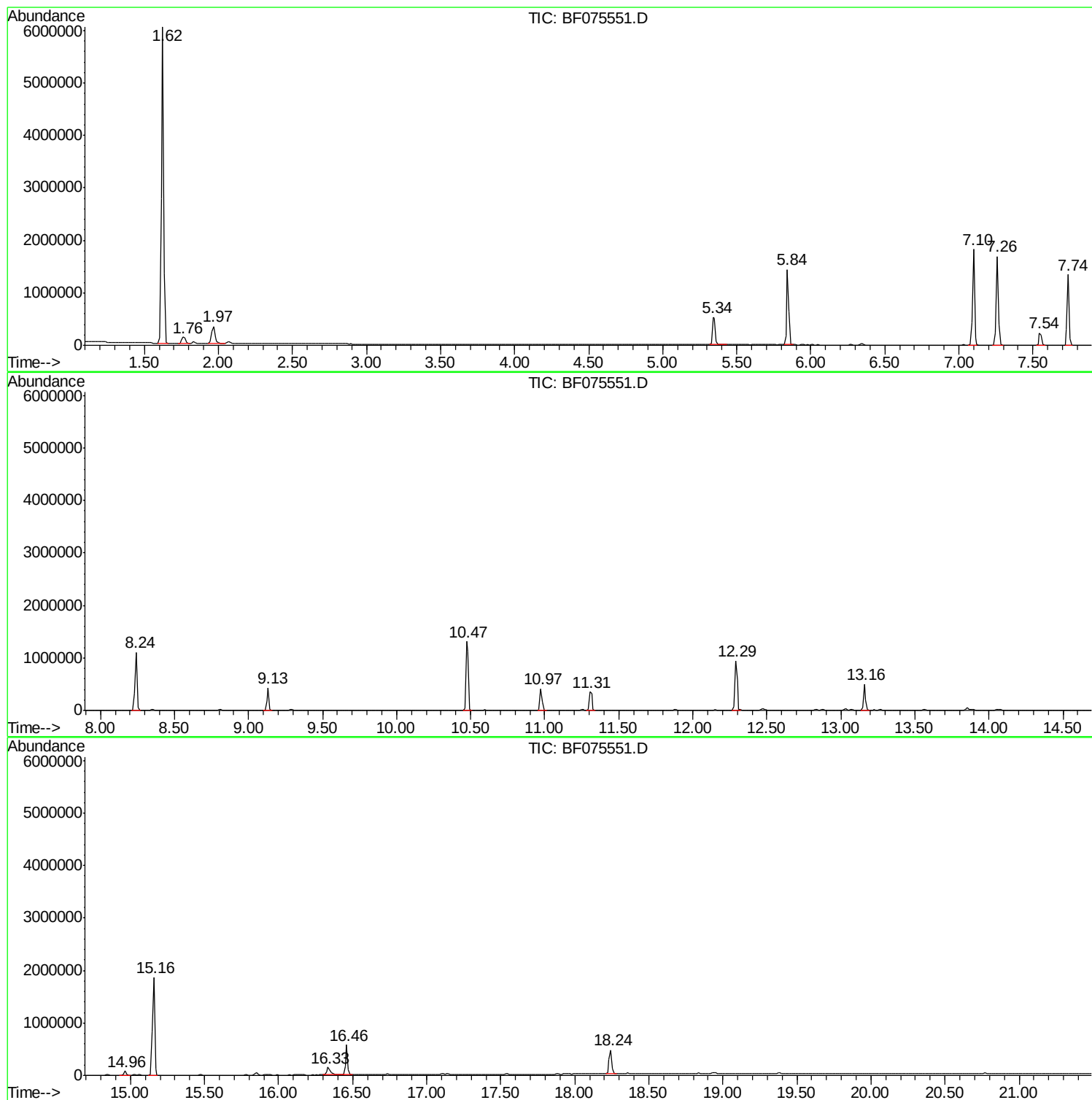
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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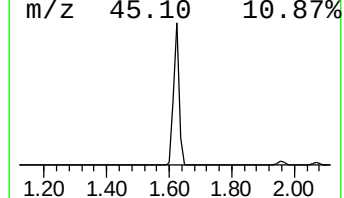
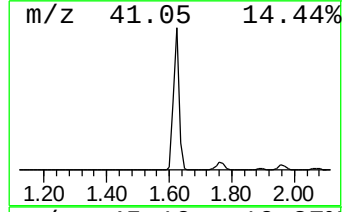
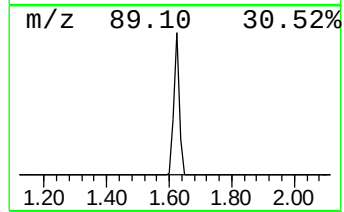
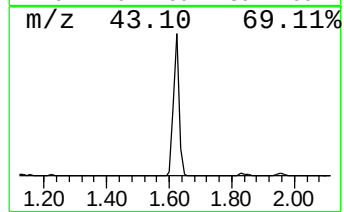
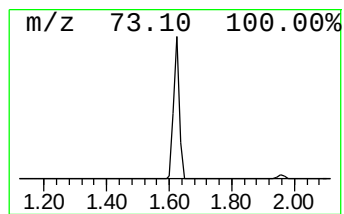
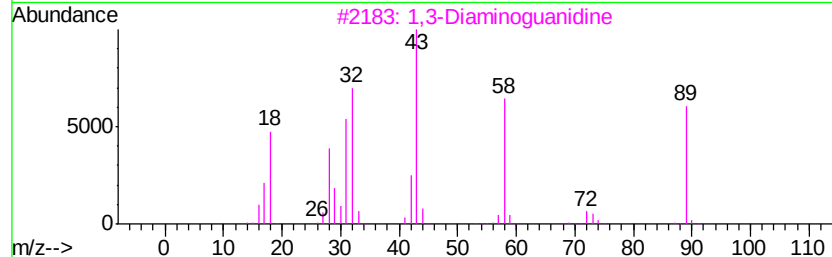
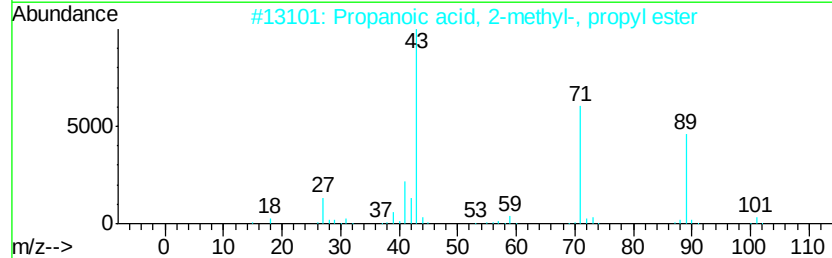
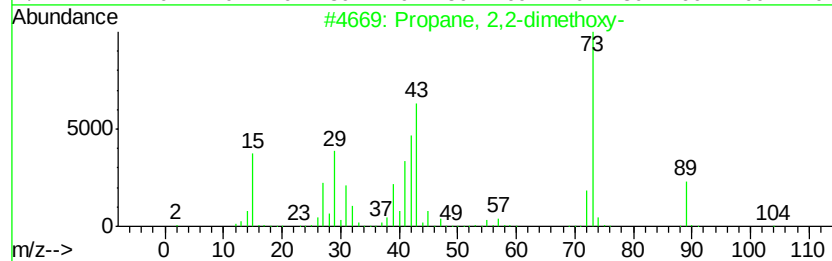
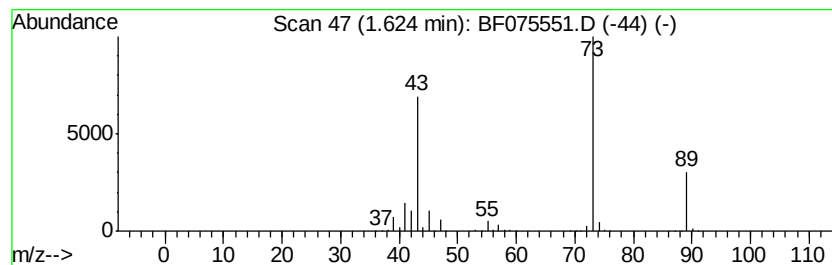
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.62	470.89 ng	7012050	1,4-Dichlorobenzene-d4	7.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	45
2		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	23
3		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



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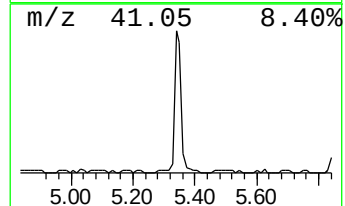
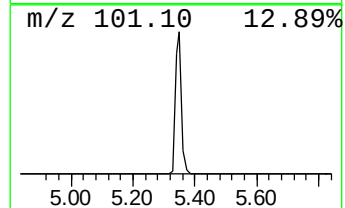
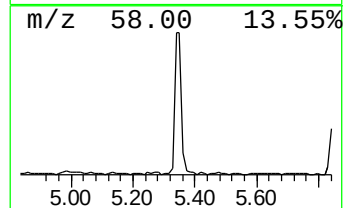
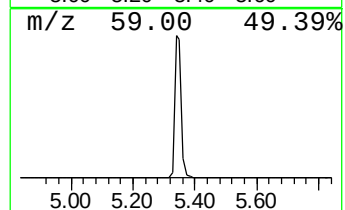
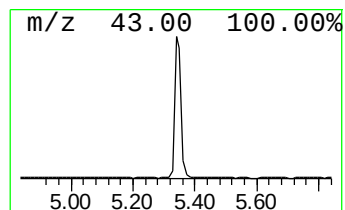
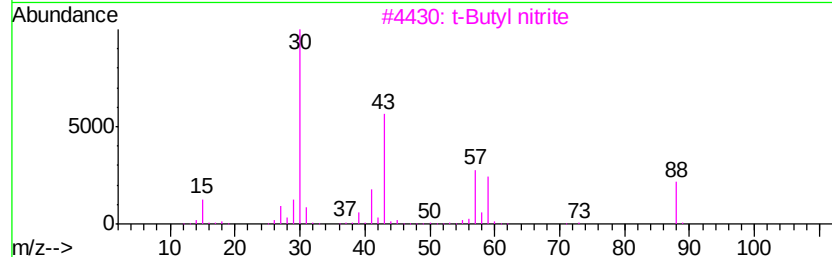
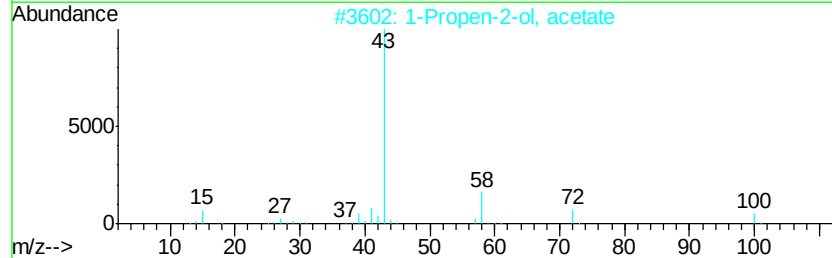
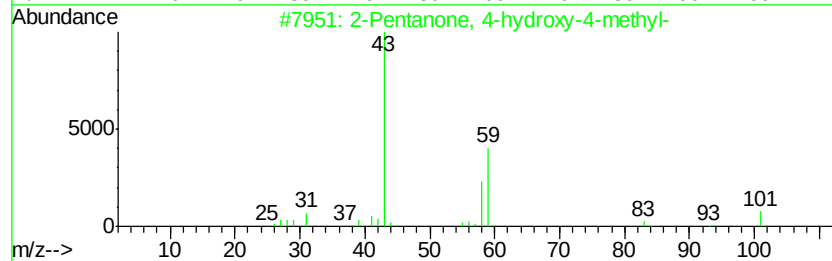
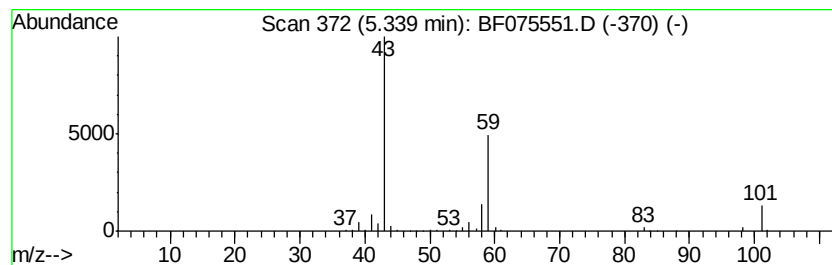
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.34	52.28 ng	778481	1,4-Dichlorobenzene-d4	7.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
3		t-Butyl nitrite	103	C4H9NO2	000540-80-7	9
4		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7
5		Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	7



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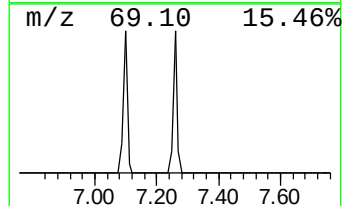
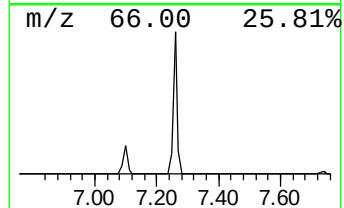
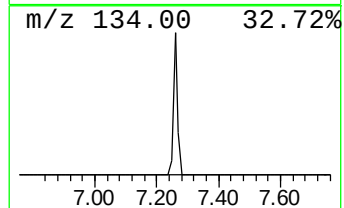
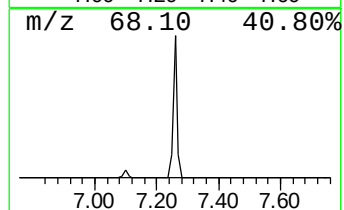
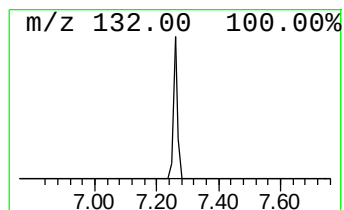
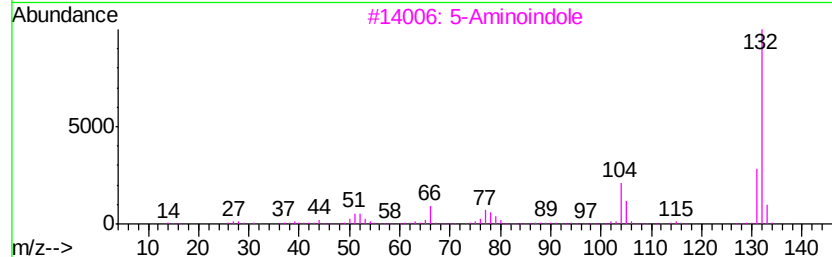
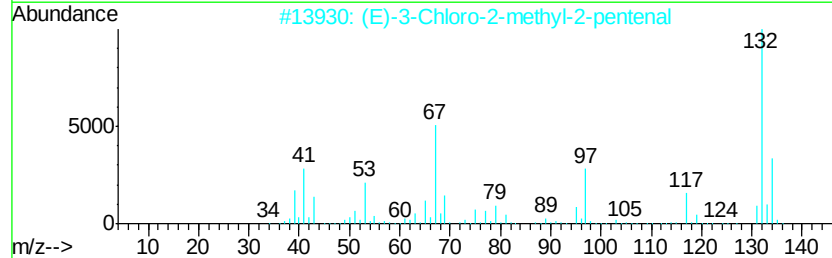
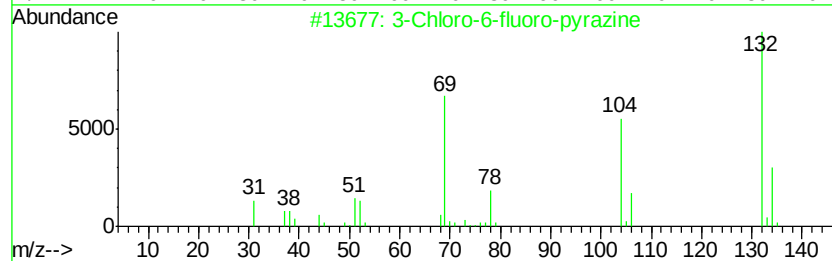
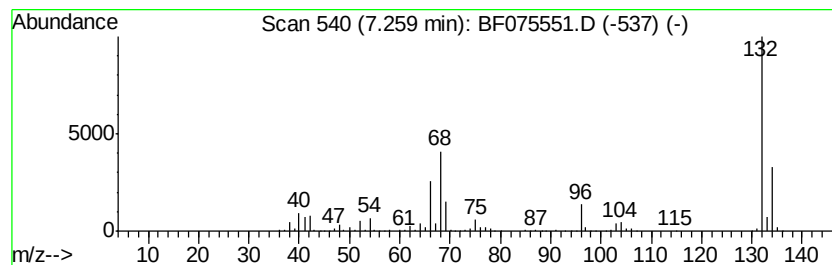
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Peak Number 5 unknown7.26 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.26	106.15 ng	1580620	1,4-Dichlorobenzene-d4	7.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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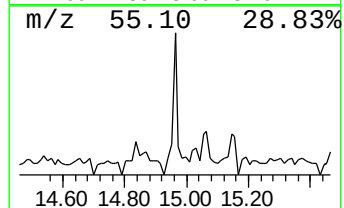
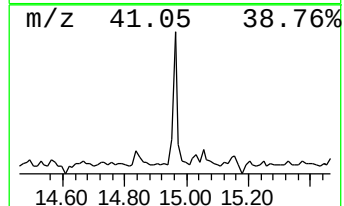
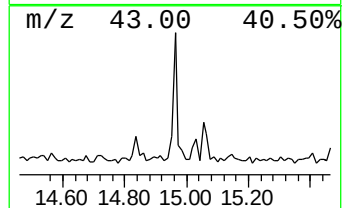
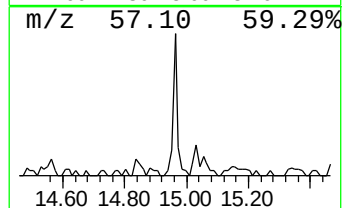
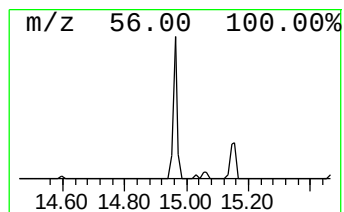
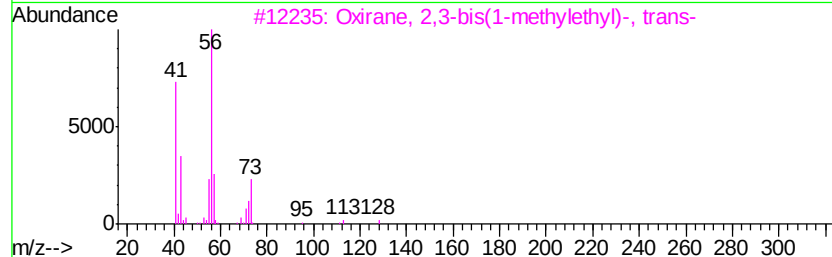
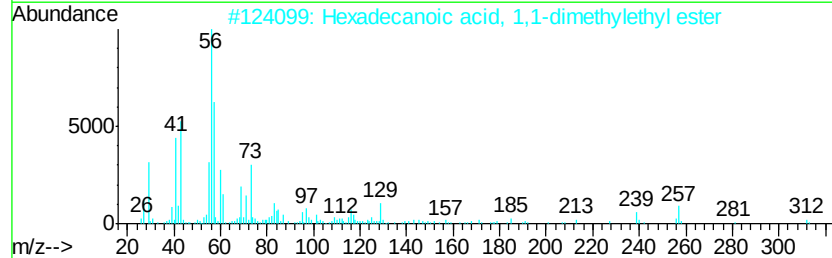
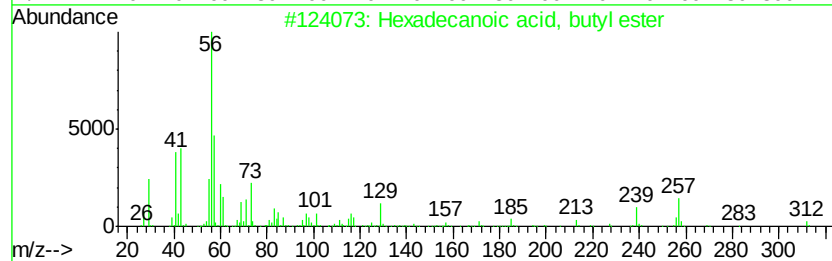
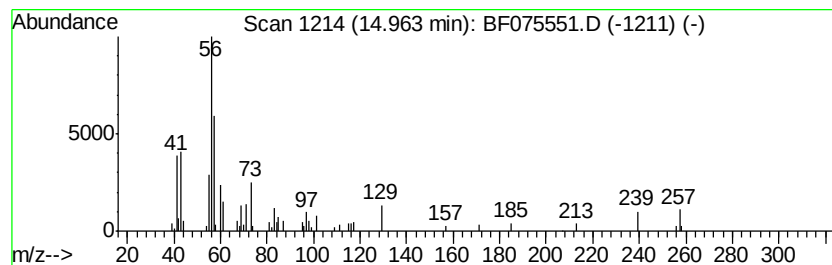
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Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.64 ng	75280	Chrysene-d12	16.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	62
3		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	37
4		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	35
5		Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	35



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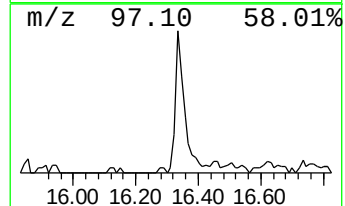
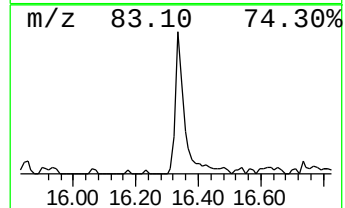
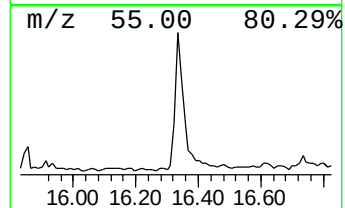
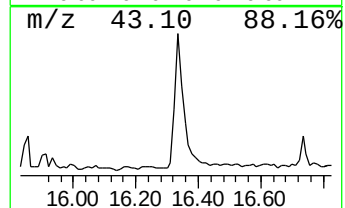
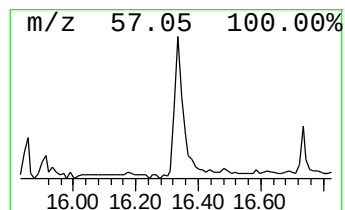
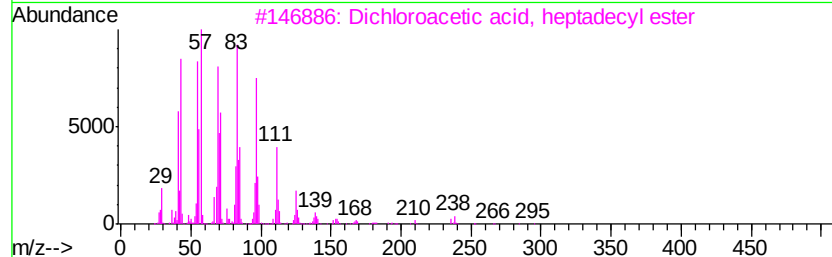
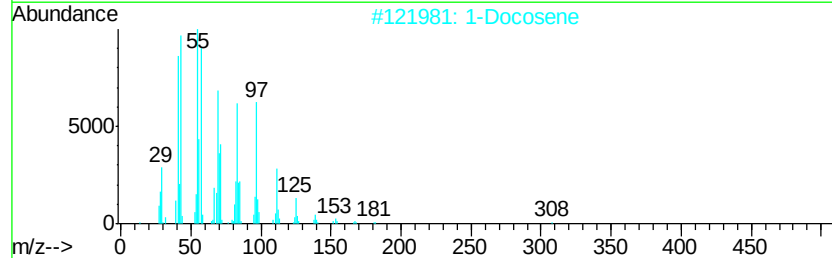
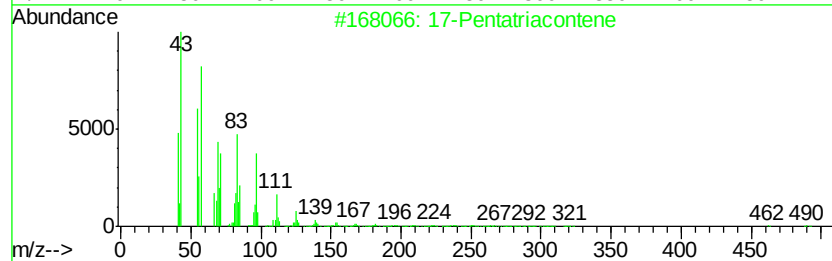
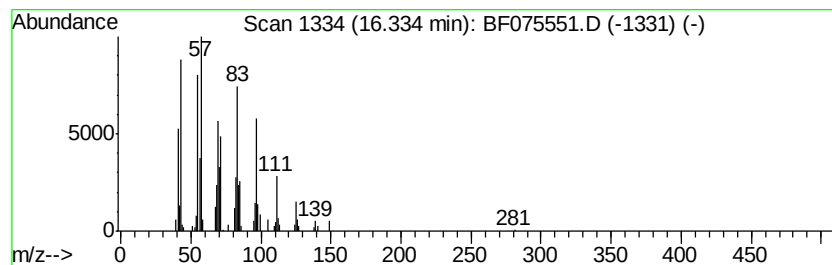
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Peak Number 8 17-Pentatriacontene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.33	9.88 ng	282000	Chrysene-d12	16.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-Pentatriacontene	491	C35H70	006971-40-0	91
2		1-Docosene	308	C22H44	001599-67-3	91
3		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
5		Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.62	1.62	470.9	ng	7012050	1	7.56	297822	20.0
2-Pentanone, 4-hy...	5.34	52.3	ng	778481	1	7.56	297822	20.0
unknown7.26	7.26	106.2	ng	1580620	1	7.56	297822	20.0
Hexadecanoic acid...	14.96	2.6	ng	75280	5	16.46	571057	20.0
17-Pentatriacontene	16.33	9.9	ng	282000	5	16.46	571057	20.0