

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
 Data File : BF082631.D
 Acq On : 31 Oct 2015 19:56
 Operator : UM/IZ
 Sample : PB86353BL
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB86353BL

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_F\METHODS\8270-BF103015.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	2.155	4	6	25	rVB3	109674	415837	6.18%	0.769%
2	5.104	261	264	267	rBV	1839384	2795923	41.53%	5.170%
3	5.516	297	300	303	rBV	4815038	5205203	77.31%	9.625%
4	6.533	386	389	391	rBV	5433471	5662030	84.10%	10.470%
5	6.670	398	401	403	rBV	5807971	5444347	80.87%	10.068%
6	6.899	419	421	423	rVB	1399324	1339657	19.90%	2.477%
7	7.059	432	435	438	rBV	4676553	4240495	62.98%	7.841%
8	7.459	467	470	473	rBV	2698253	3677161	54.62%	6.800%
9	8.190	531	534	536	rBV	2047236	1805637	26.82%	3.339%
10	9.276	625	629	631	rBV	5498374	6732614	100.00%	12.450%
11	9.950	685	688	690	rBV	1819105	1928322	28.64%	3.566%
12	10.728	754	756	759	rBV2	2885109	3962664	58.86%	7.328%
13	11.425	815	817	820	rBV	1479863	1841224	27.35%	3.405%
14	12.854	940	942	944	rBV	263182	210664	3.13%	0.390%
15	13.025	954	957	959	rBV	6526060	6123720	90.96%	11.324%
16	13.562	1002	1004	1006	rBV	169555	141341	2.10%	0.261%
17	14.077	1046	1049	1051	rBV	1331142	1388162	20.62%	2.567%
18	15.540	1174	1177	1180	rBV	906002	1163057	17.27%	2.151%

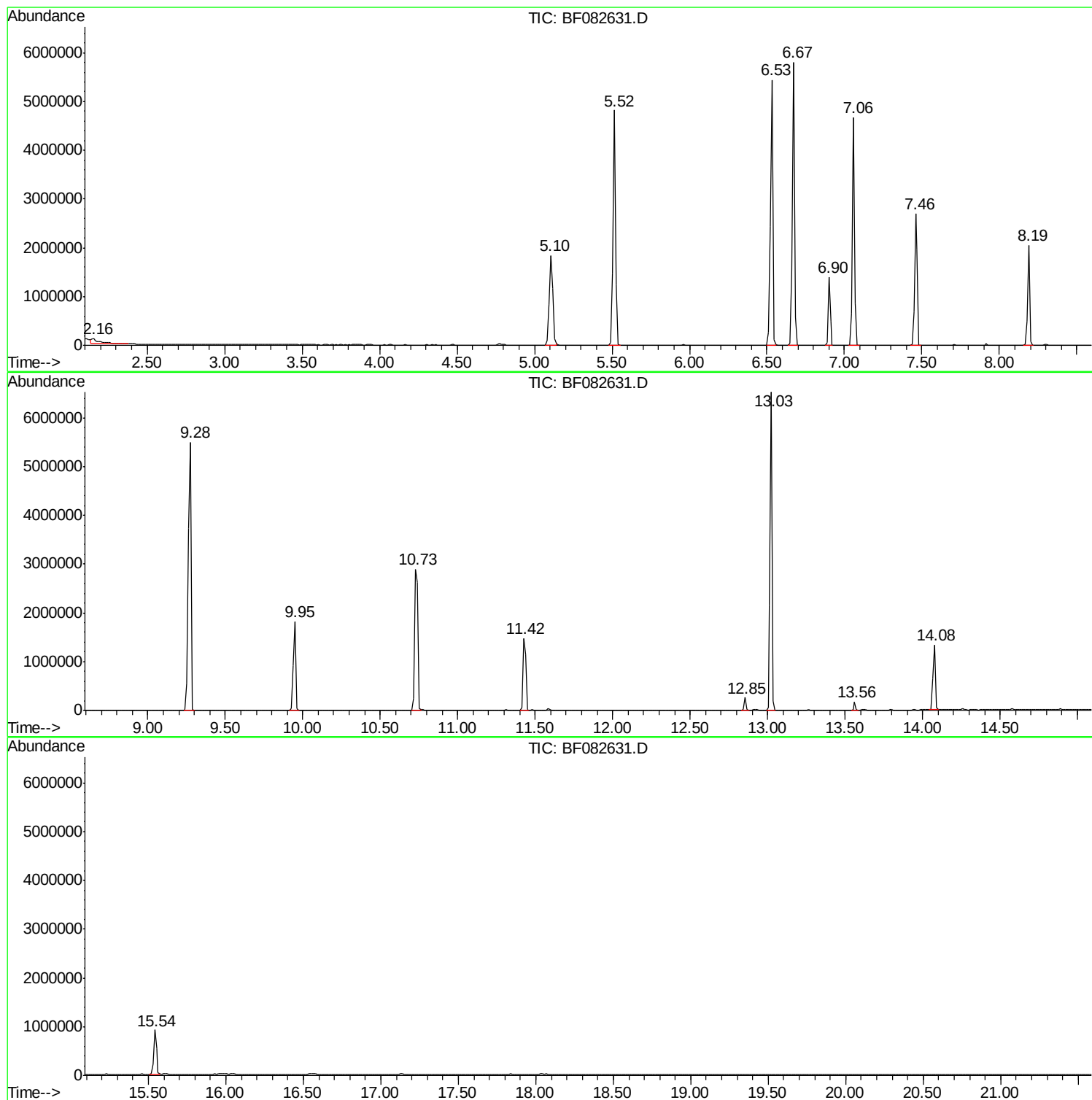
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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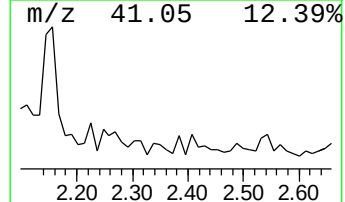
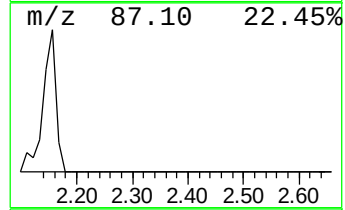
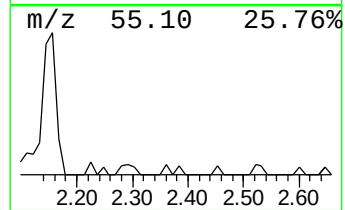
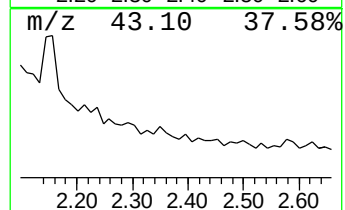
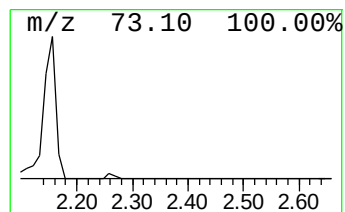
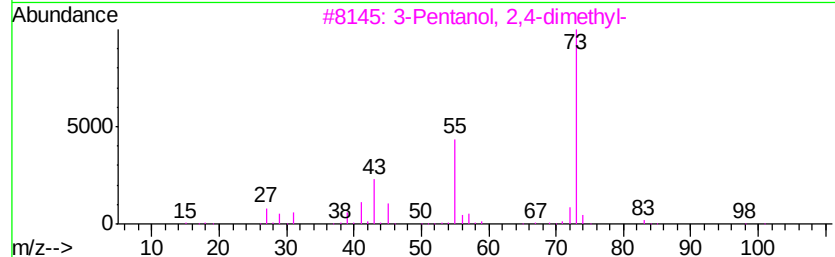
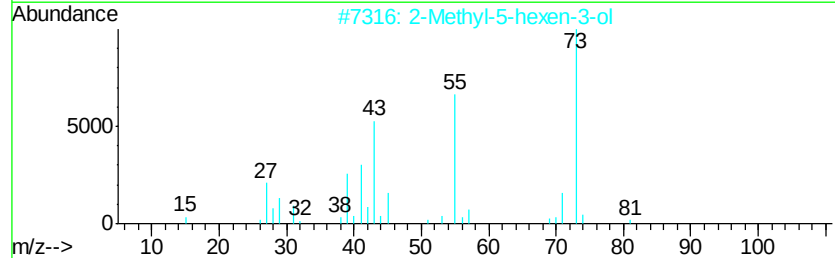
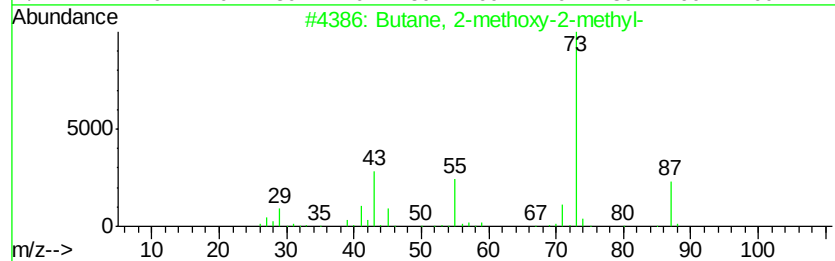
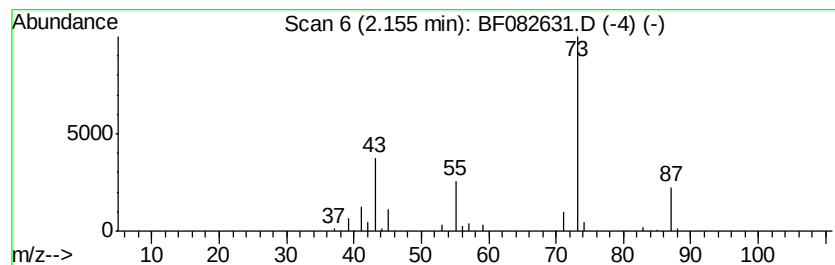
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	6.21 ng	415837	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	40
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	32
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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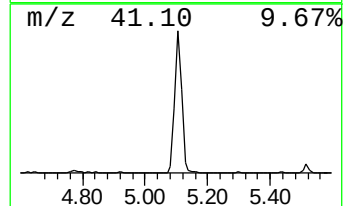
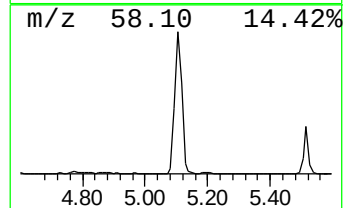
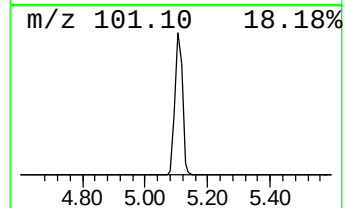
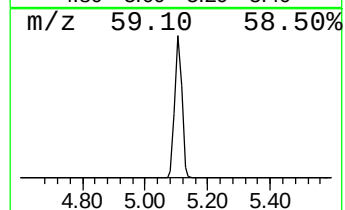
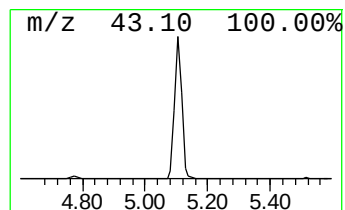
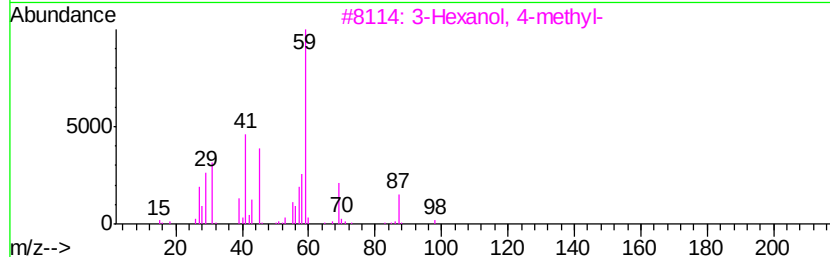
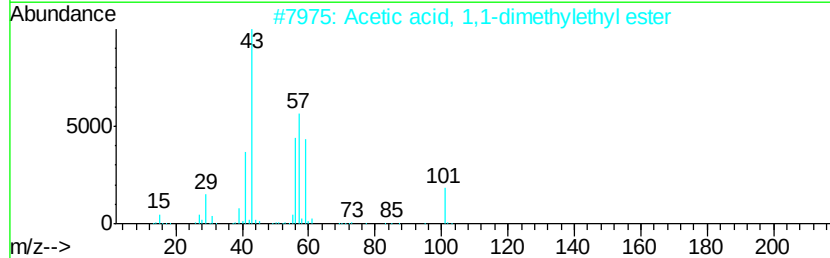
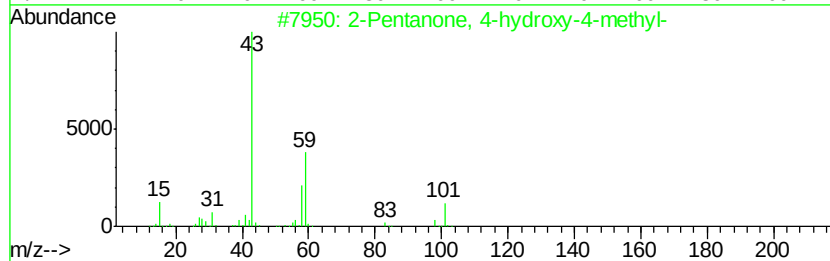
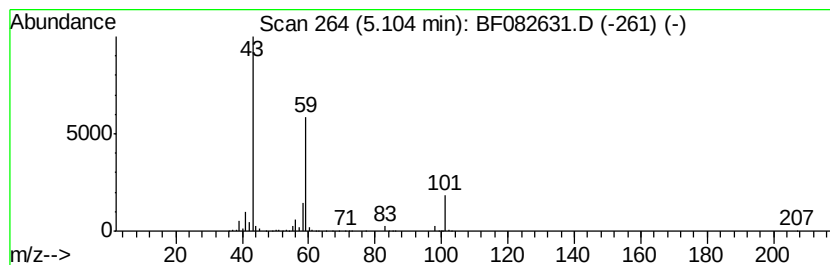
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	41.74 ng	2795920	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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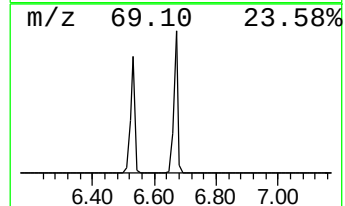
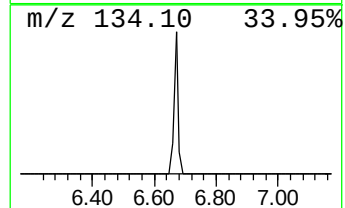
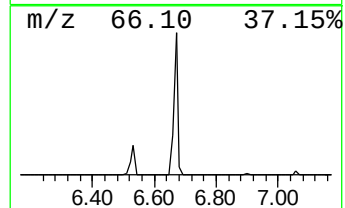
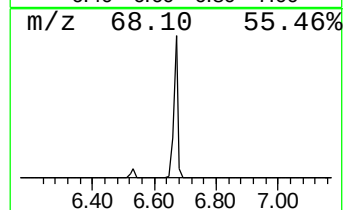
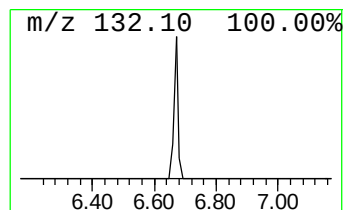
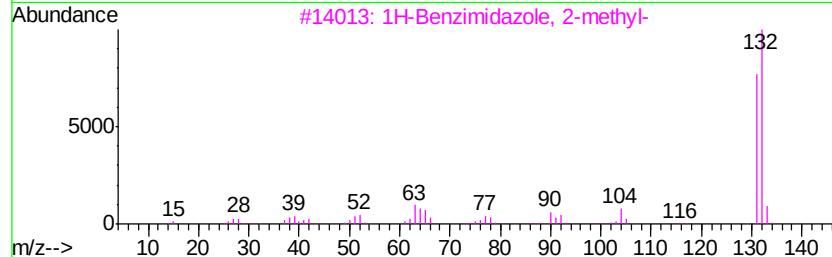
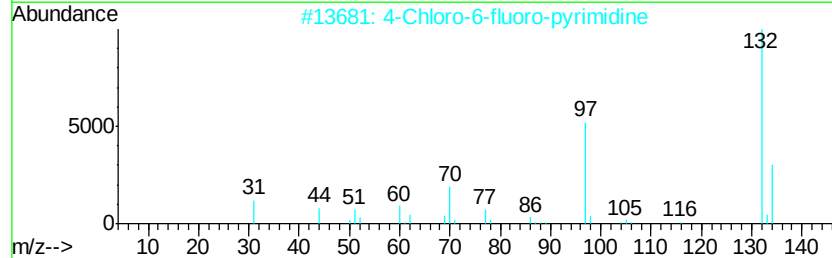
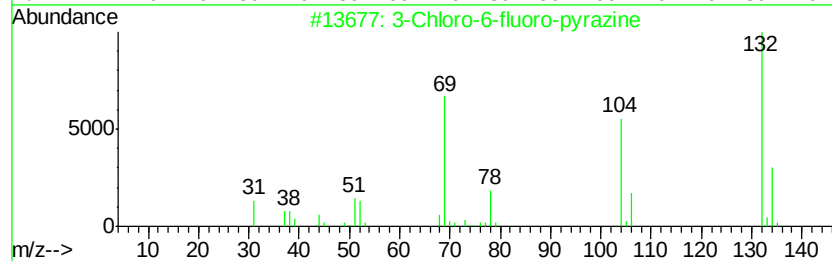
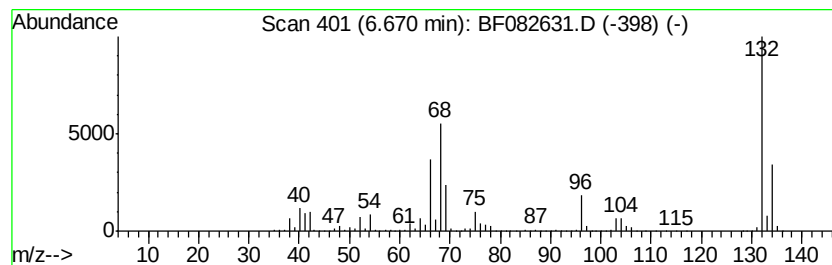
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Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	81.28 ng	5444350	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5			Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12



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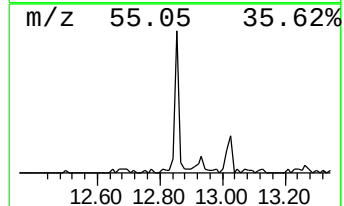
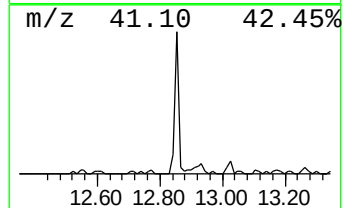
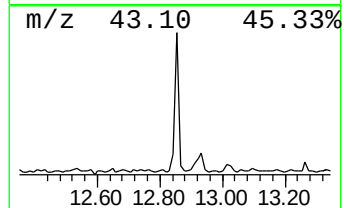
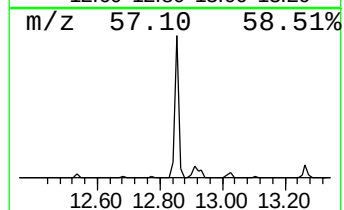
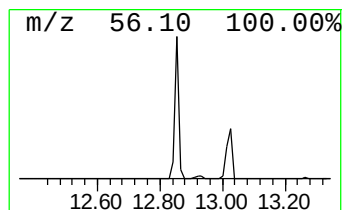
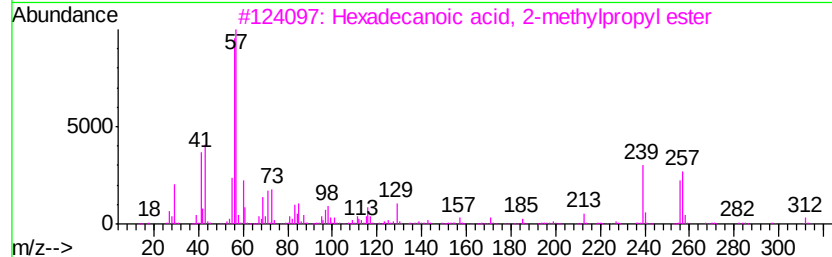
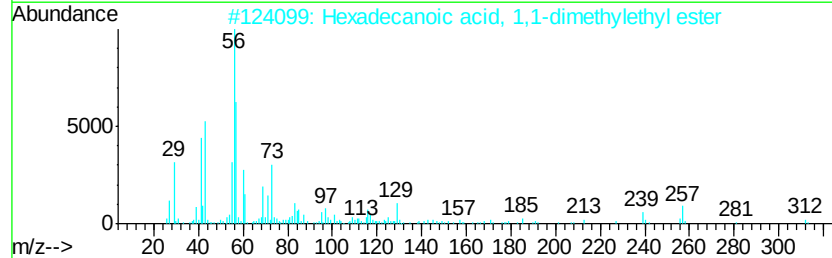
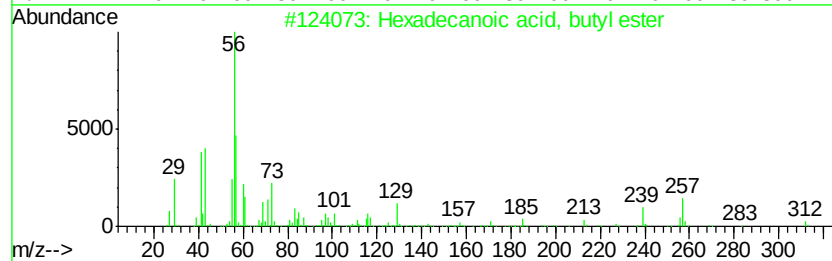
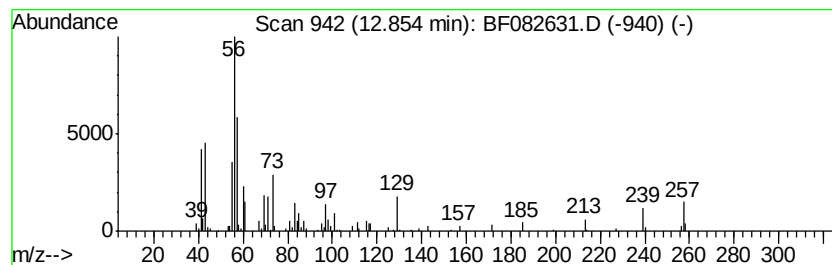
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	3.04 ng	210664	Chrysene-d12	14.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	86
3		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	50
4		1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	37
5		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37



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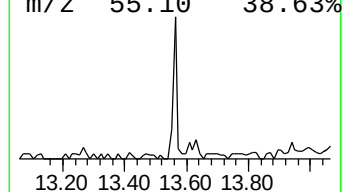
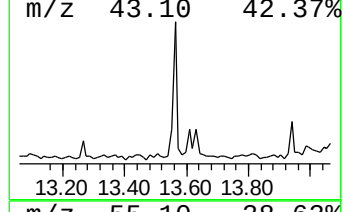
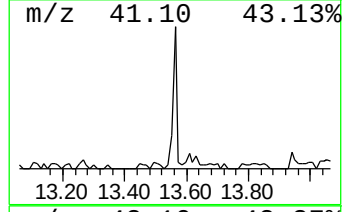
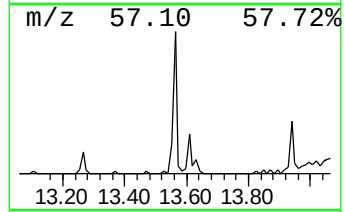
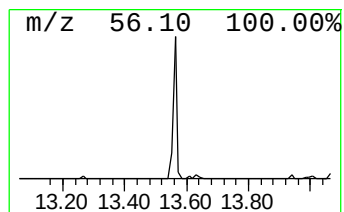
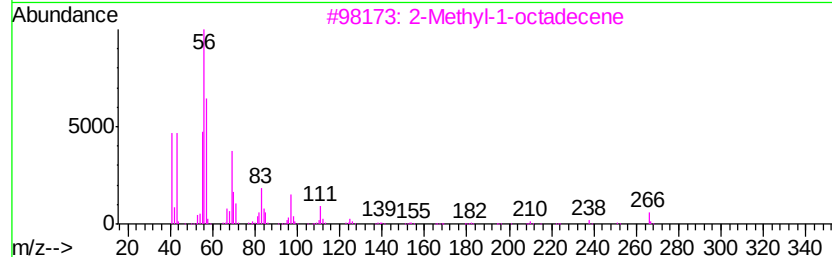
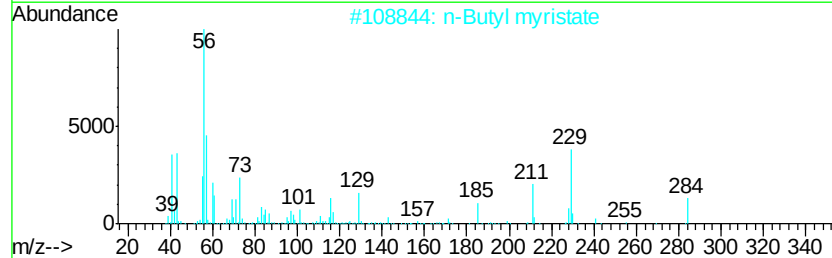
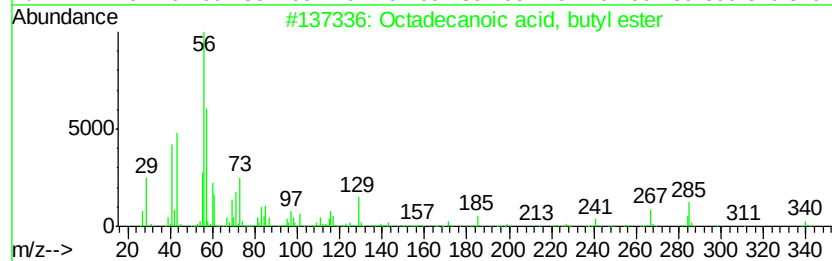
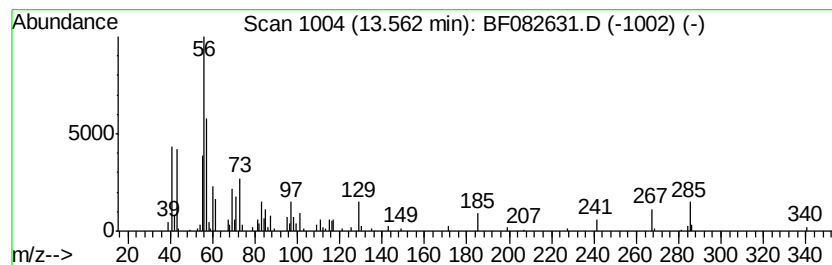
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Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.56	2.04 ng	141341	Chrysene-d12	14.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	95
2		n-Butyl myristate	284	C18H36O2	000110-36-1	80
3		2-Methyl-1-octadecene	266	C19H38	061868-20-0	38
4		3-Amino-2,2-dimethyl-1-propanol	103	C5H13NO	026734-09-8	38
5		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.16	6.2	ng	415837	1	6.90	1339660	20.0
2-Pentanone, 4-hy...	5.10	41.7	ng	2795920	1	6.90	1339660	20.0
unknown6.67	6.67	81.3	ng	5444350	1	6.90	1339660	20.0
Hexadecanoic acid...	12.85	3.0	ng	210664	5	14.08	1388160	20.0
Octadecanoic acid...	13.56	2.0	ng	141341	5	14.08	1388160	20.0