

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122216\
 Data File : BF091892.D
 Acq On : 22 Dec 2016 18:03
 Operator : UM/SJ
 Sample : H6156-23
 Misc :
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FB121616

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-BF122116.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	4.910	245	247	250	rBV	569657	692583	14.24%	2.237%
2	5.390	287	289	292	rBV	1193599	1737978	35.74%	5.613%
3	6.407	375	378	379	rBV	218454	291953	6.00%	0.943%
4	6.453	379	382	384	rVV	738148	1047966	21.55%	3.384%
5	6.544	387	390	392	rBV	3052472	3550828	73.02%	11.467%
6	6.750	405	408	410	rBV	1031708	897384	18.45%	2.898%
7	6.910	419	422	424	rVB	3647557	3487821	71.72%	11.263%
8	7.322	455	458	460	rBV	2456172	2608200	53.64%	8.423%
9	8.042	518	521	523	rVB	926746	1123222	23.10%	3.627%
10	9.116	612	615	617	rBV	5025358	4862777	100.00%	15.704%
11	9.790	671	674	676	rBV	1233381	1193841	24.55%	3.855%
12	10.579	740	743	746	rBV	1903764	1948760	40.08%	6.293%
13	11.265	801	803	806	rBV	850192	976358	20.08%	3.153%
14	12.614	918	921	925	rBV	72451	96874	1.99%	0.313%
15	12.682	925	927	930	rVB	201152	188989	3.89%	0.610%
16	12.762	930	934	940	rBV	55856	75185	1.55%	0.243%
17	12.854	940	942	945	rBV	3787730	4504443	92.63%	14.547%
18	13.391	987	989	991	rBV	89198	100499	2.07%	0.325%
19	13.905	1031	1034	1036	rBV	786619	831882	17.11%	2.686%
20	15.300	1153	1156	1159	rBV	525938	748220	15.39%	2.416%

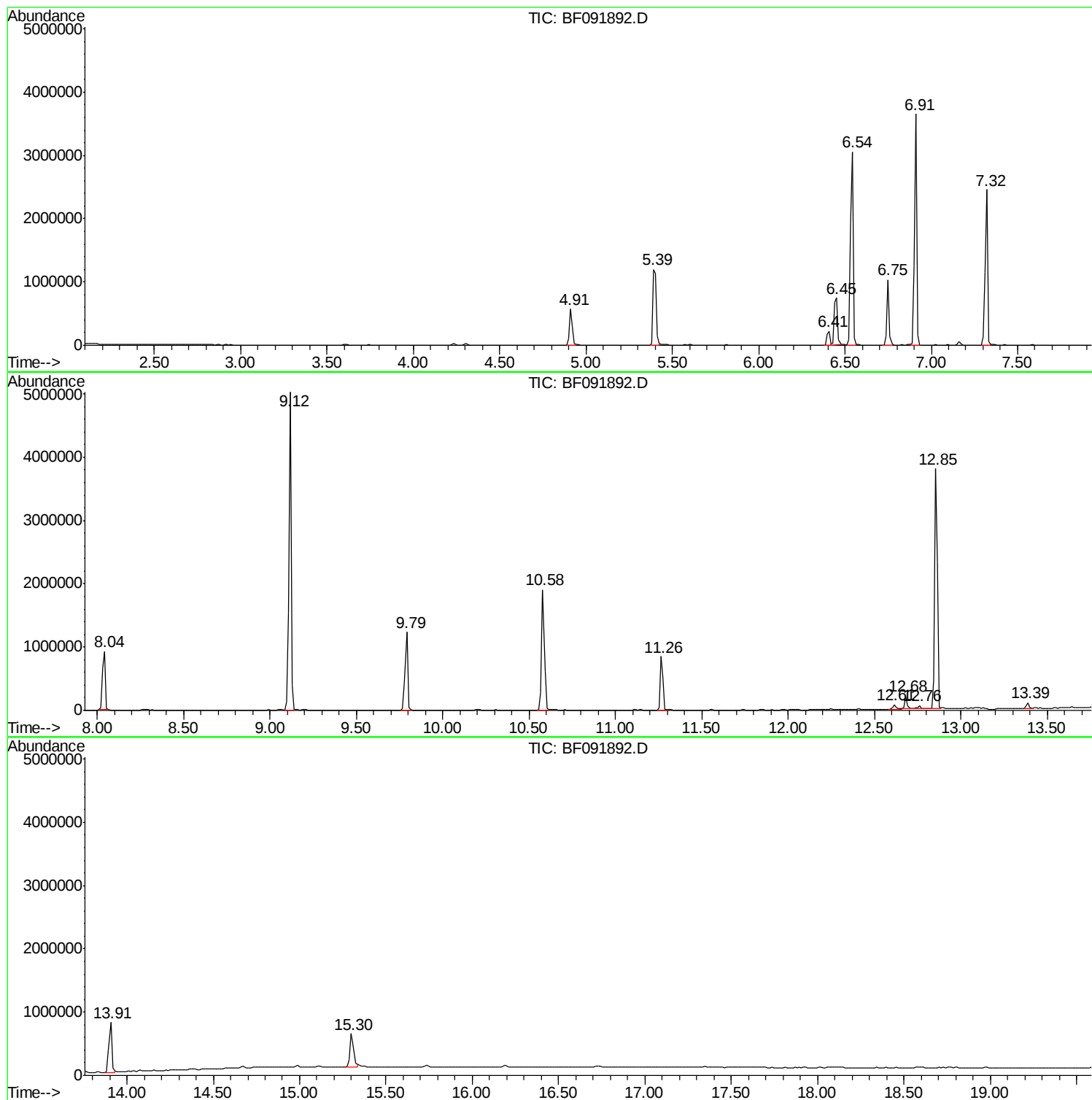
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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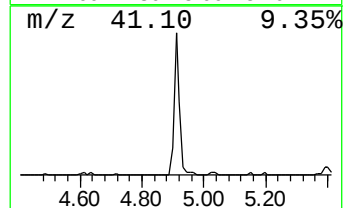
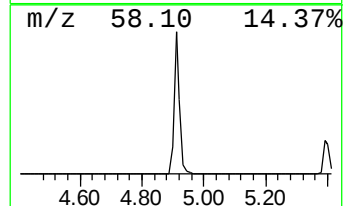
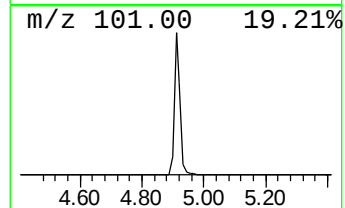
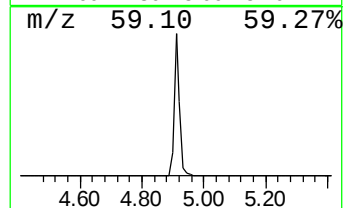
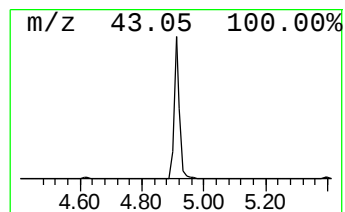
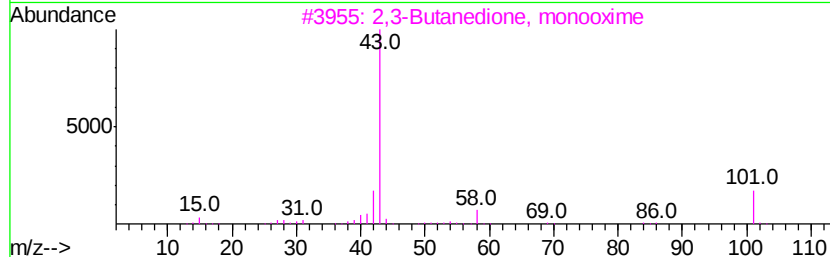
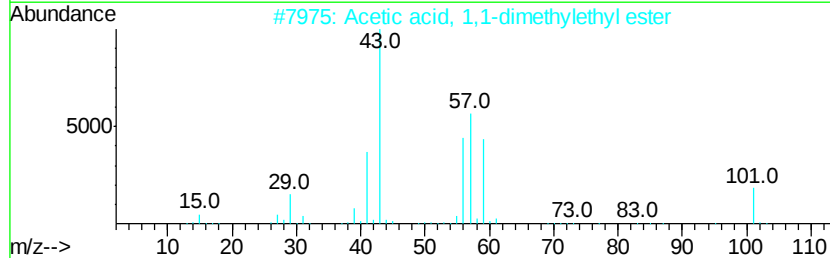
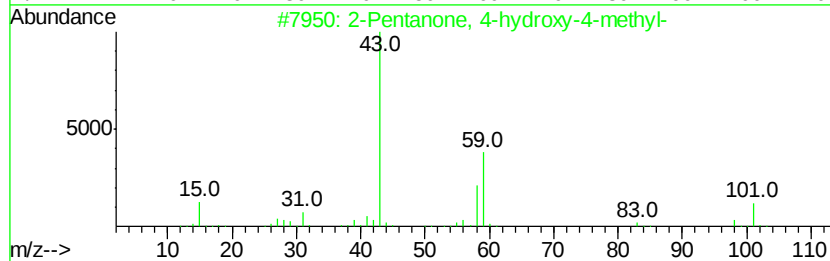
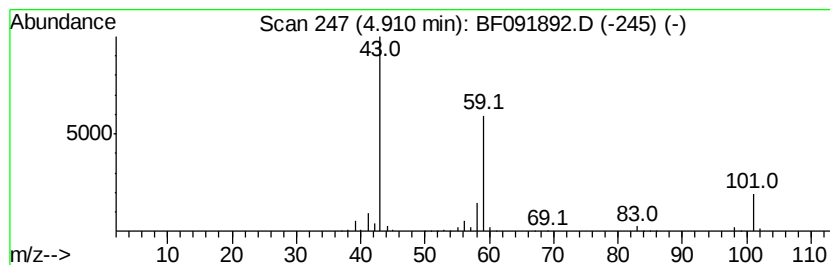
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	15.44 ng	692583	1,4-Dichlorobenzene-d4	6.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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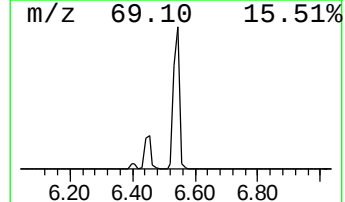
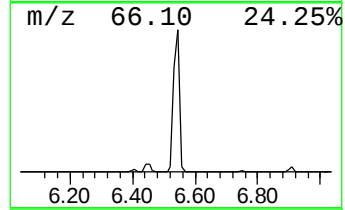
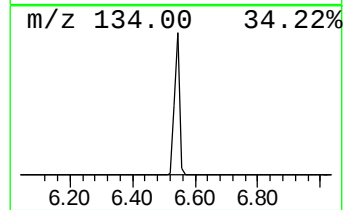
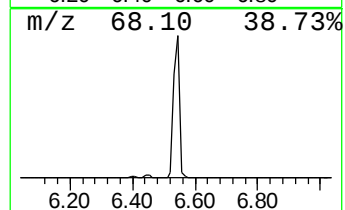
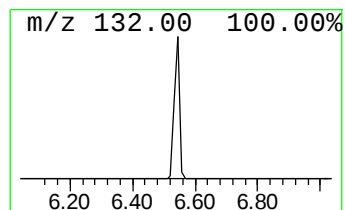
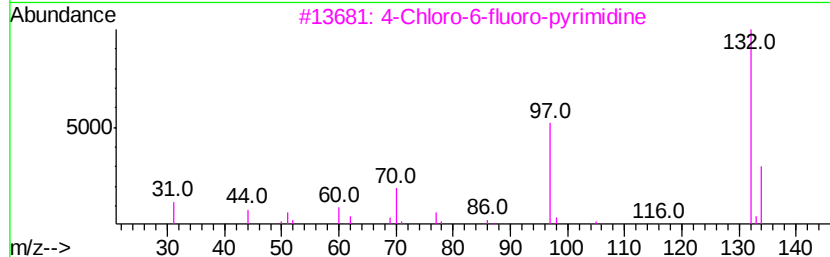
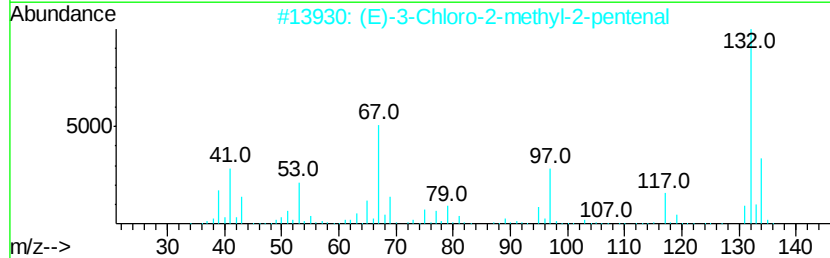
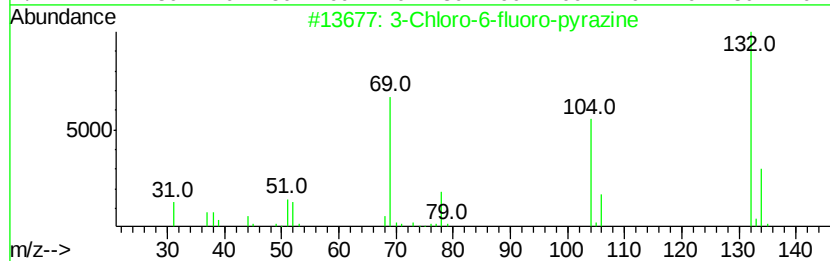
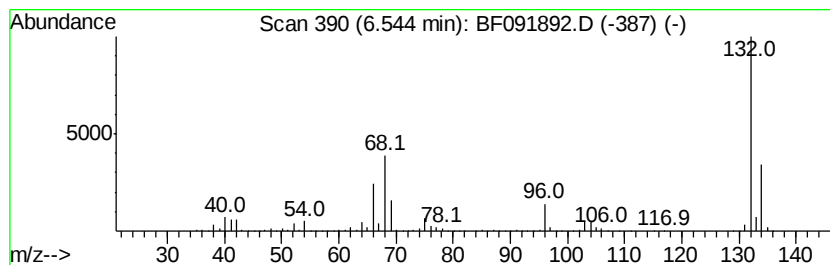
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Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	79.14 ng	3550830	1,4-Dichlorobenzene-d4	6.75

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		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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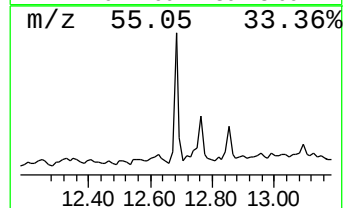
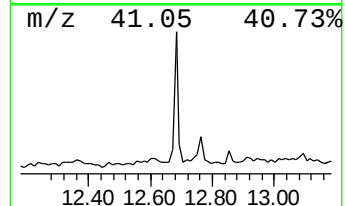
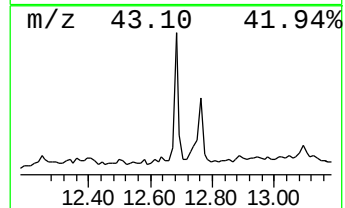
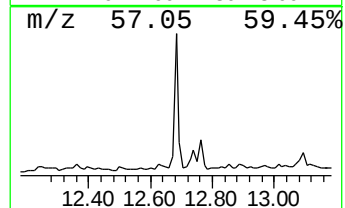
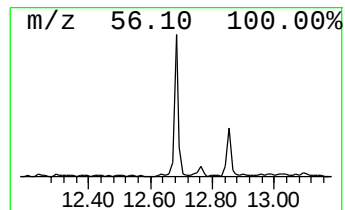
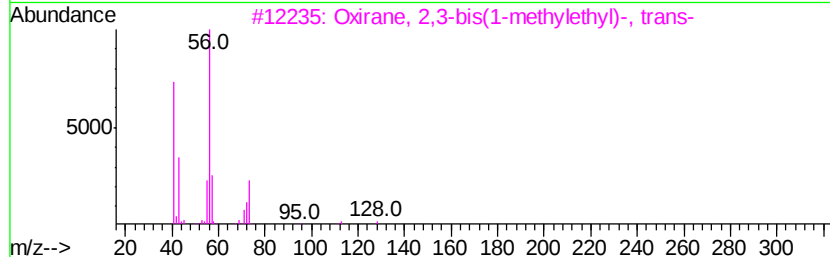
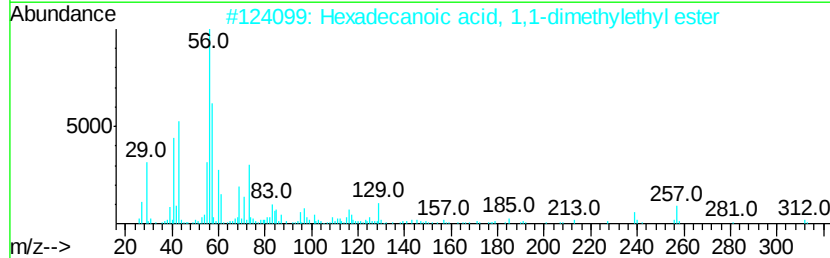
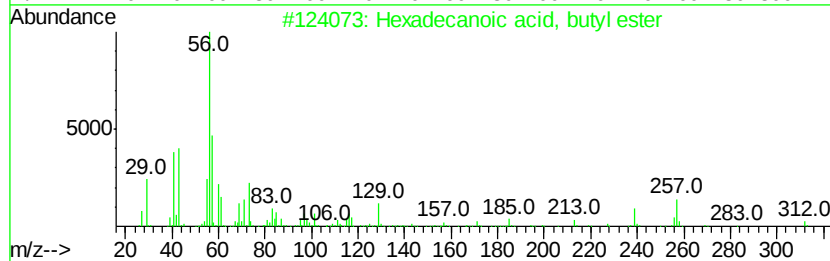
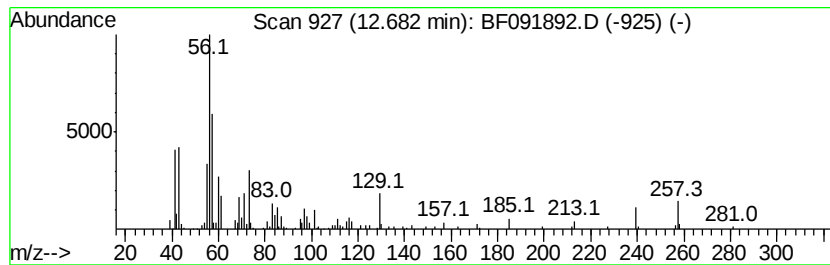
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	4.54 ng	188989	Chrysene-d12	13.91

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	91
3		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	38
4		Oxan-4-one, 2-trifluoromethyl-2-...	212	C8H11F3O3	212615-80-0	38
5		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35



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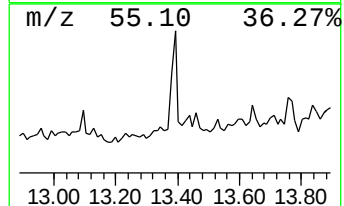
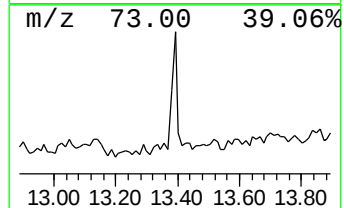
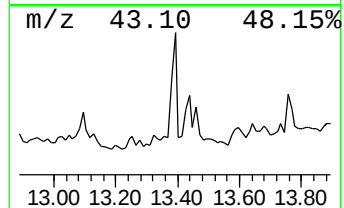
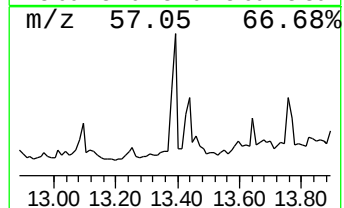
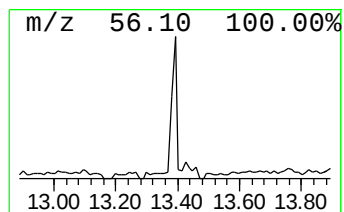
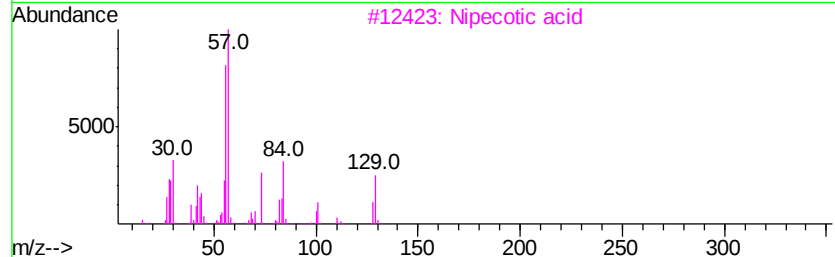
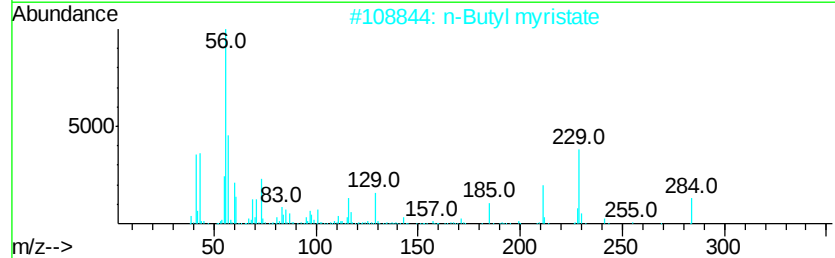
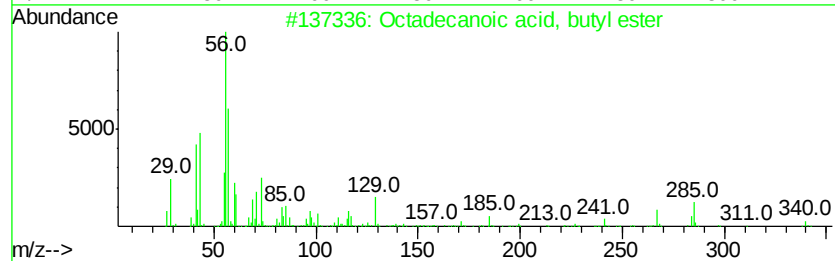
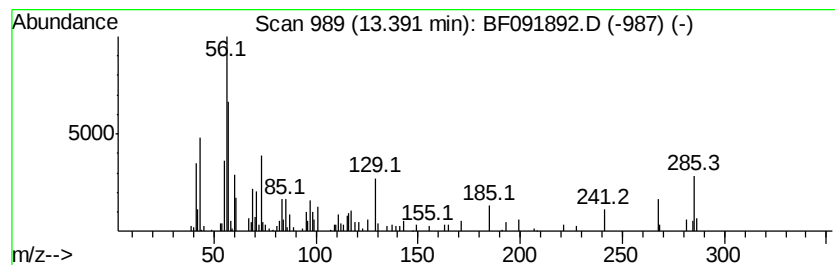
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Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.39	2.42 ng	100499	Chrysene-d12	13.91

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		n-Butyl myristate	284	C18H36O2	000110-36-1	47
3		Nipecotic acid	129	C6H11NO2	000498-95-3	43
4		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	38
5		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	35



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.91	15.4	ng	692583	1	6.75	897384	20.0
unknown6.54	6.54	79.1	ng	3550830	1	6.75	897384	20.0
Hexadecanoic acid...	12.68	4.5	ng	188989	5	13.91	831882	20.0
Octadecanoic acid...	13.39	2.4	ng	100499	5	13.91	831882	20.0