

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082815\
 Data File : BF081260.D
 Acq On : 28 Aug 2015 3:42
 Operator : UM/IZ
 Sample : G3430-06
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB3(24-25)

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-BF081715.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	3.806	179	181	186	rBB	14156	25044	1.63%	0.180%
2	4.594	247	250	260	rVB	639061	1128727	73.36%	8.111%
3	5.063	289	291	294	rBV	1229970	1328707	86.35%	9.549%
4	5.486	327	328	331	rBV	24289	33613	2.18%	0.242%
5	6.160	384	387	389	rBV	1442815	1538700	100.00%	11.058%
6	6.274	394	397	399	rBV	1233285	1492309	96.99%	10.724%
7	6.503	415	417	419	rBV	324105	258792	16.82%	1.860%
8	6.663	428	431	433	rBV	1105093	1071570	69.64%	7.701%
9	7.075	465	467	470	rBV	876834	857303	55.72%	6.161%
10	7.795	528	530	532	rBV	279167	323366	21.02%	2.324%
11	8.869	622	624	627	rBV	1491907	1375392	89.39%	9.884%
12	9.269	657	659	661	rBV	209976	165642	10.77%	1.190%
13	9.532	680	682	684	rBV	469824	394212	25.62%	2.833%
14	10.321	748	751	753	rBV	828093	1049751	68.22%	7.544%
15	10.458	761	763	768	rVB	25154	28884	1.88%	0.208%
16	10.903	795	802	803	rBV	23819	22447	1.46%	0.161%
17	10.995	808	810	813	rVB	392627	400752	26.04%	2.880%
18	11.555	857	859	863	rBV	55359	80256	5.22%	0.577%
19	12.584	946	949	952	rBV	1492141	1456550	94.66%	10.467%
20	13.498	1026	1029	1036	rBV	103186	180849	11.75%	1.300%
21	13.612	1036	1039	1041	rBV	360141	387737	25.20%	2.786%
22	14.115	1081	1083	1090	rVB4	7290	17336	1.13%	0.125%
23	14.470	1112	1114	1117	rBV	18329	16987	1.10%	0.122%
24	14.938	1152	1155	1157	rBV	191111	262038	17.03%	1.883%
25	15.395	1192	1195	1197	rBV2	7877	18375	1.19%	0.132%

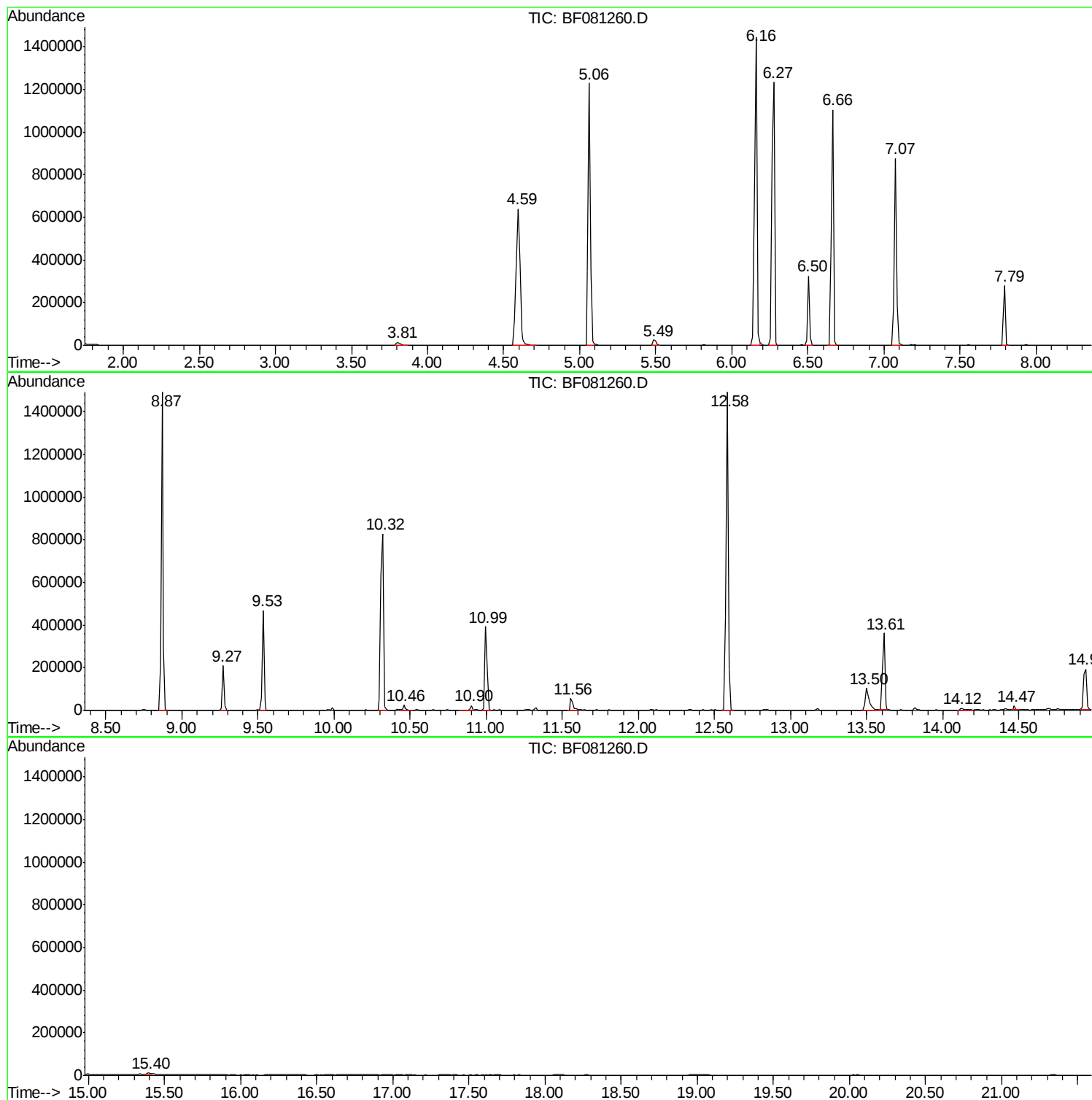
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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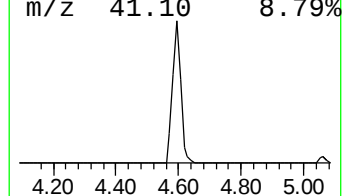
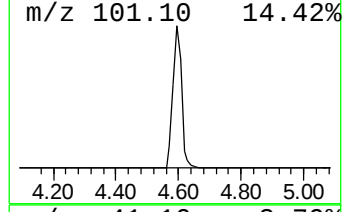
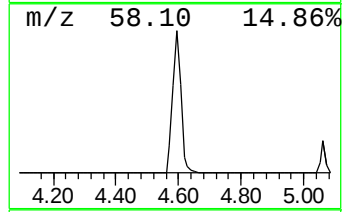
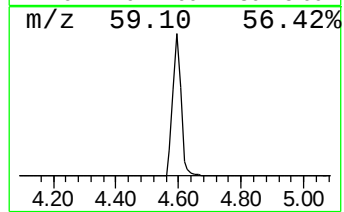
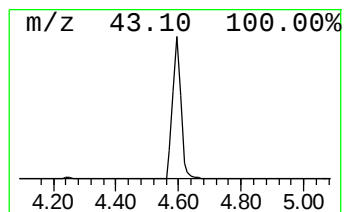
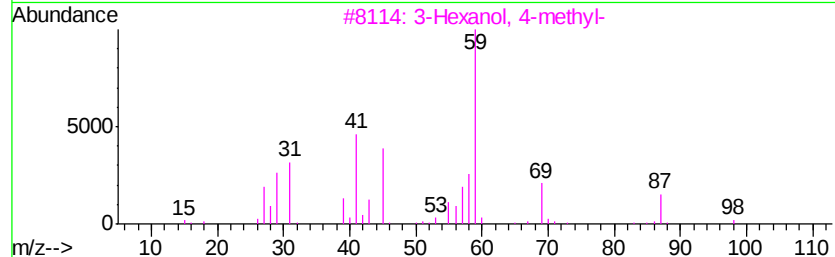
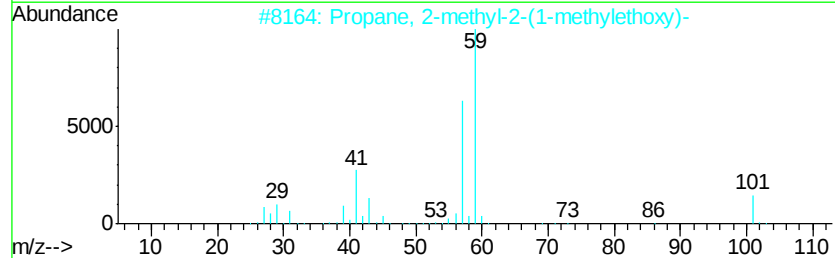
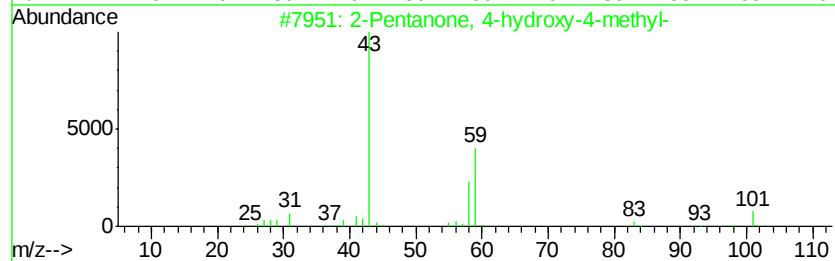
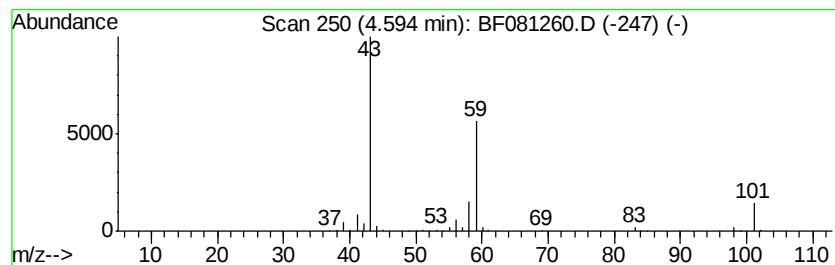
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.59	87.23 ng	1128730	1,4-Dichlorobenzene-d4	6.50

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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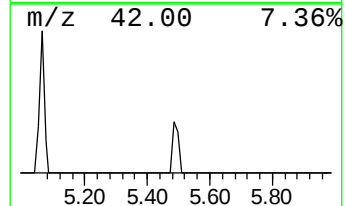
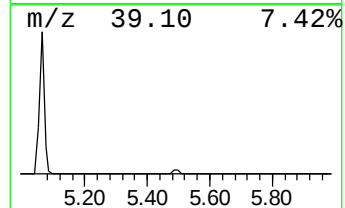
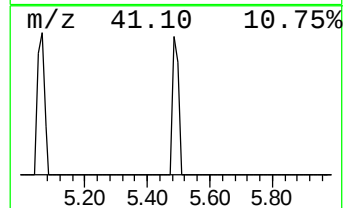
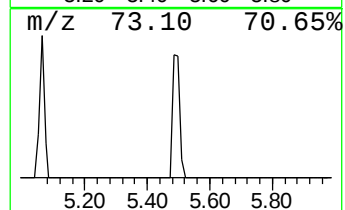
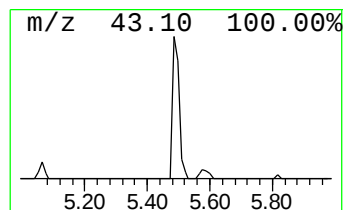
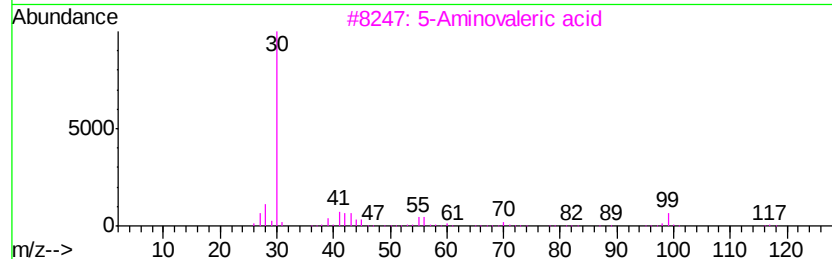
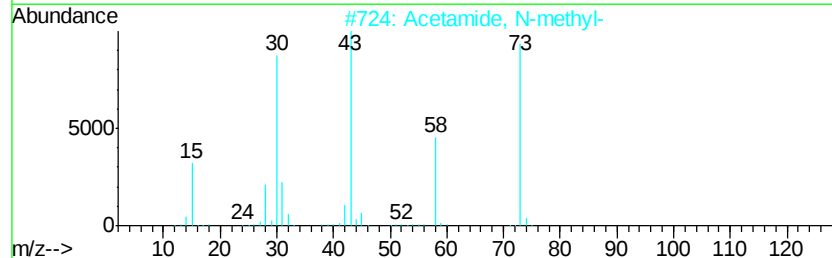
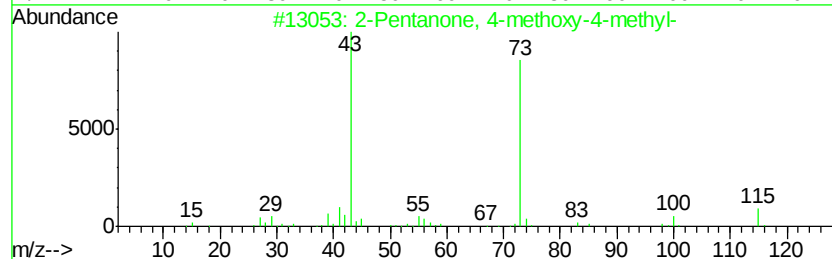
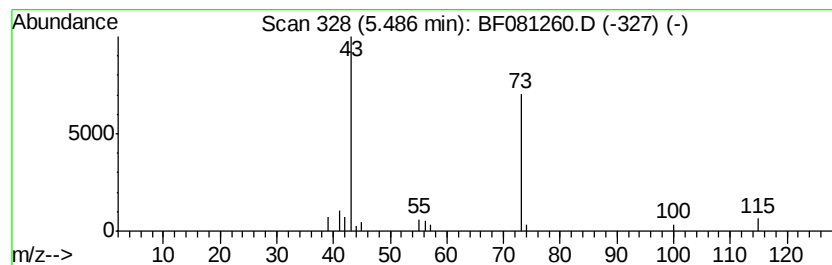
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Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.49	2.60 ng	33613	1,4-Dichlorobenzene-d4	6.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	64
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	58
3		5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	7



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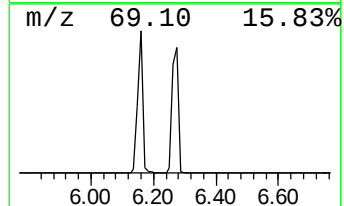
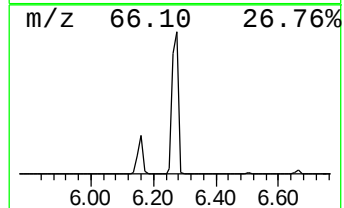
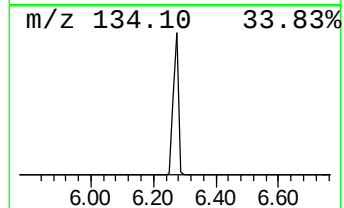
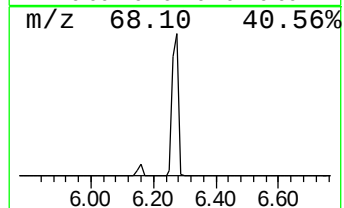
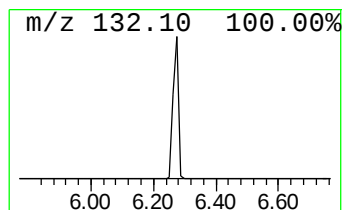
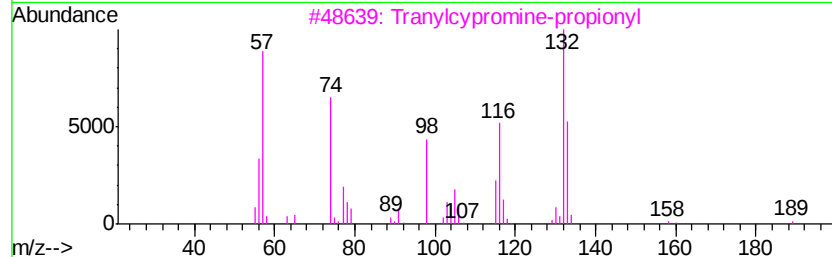
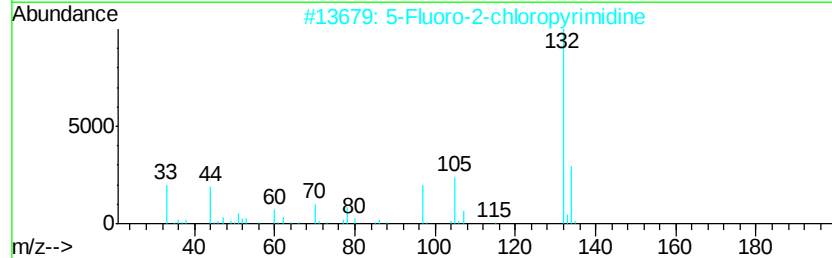
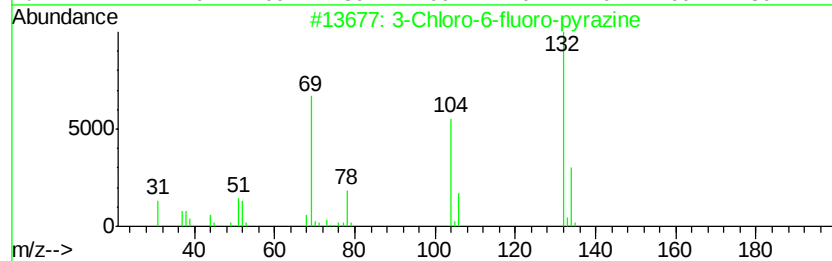
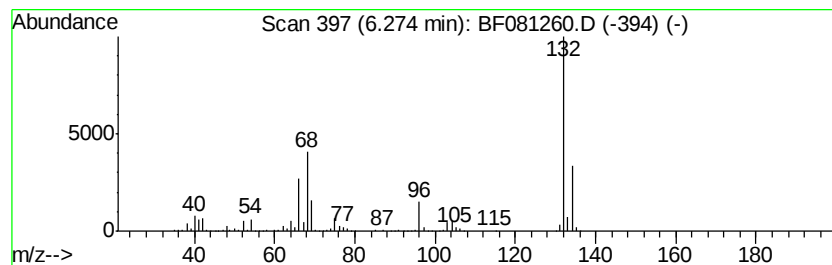
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	115.33 ng	1492310	1,4-Dichlorobenzene-d4	6.50

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	16
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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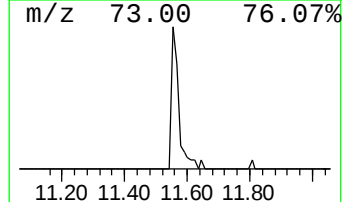
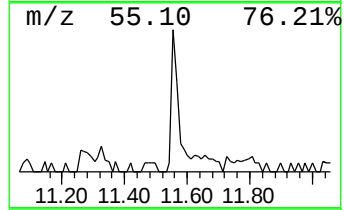
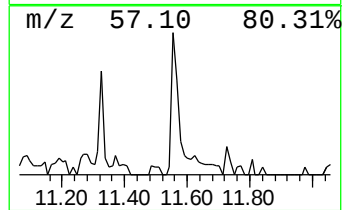
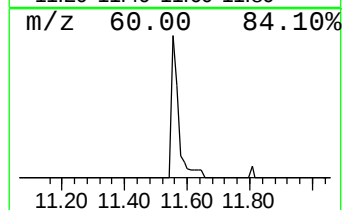
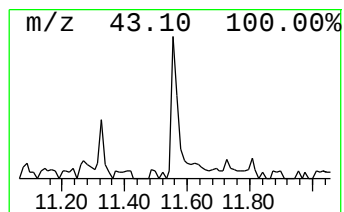
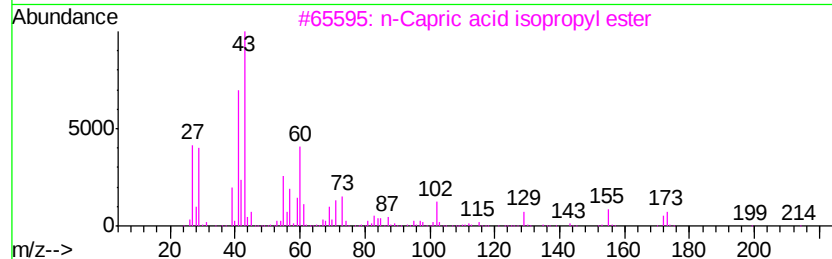
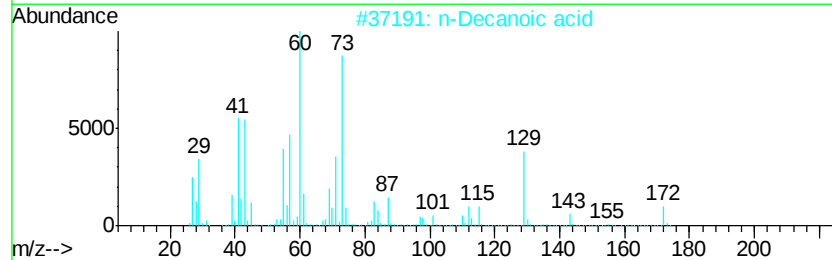
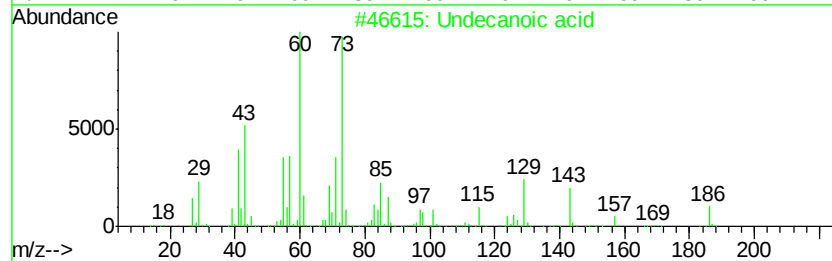
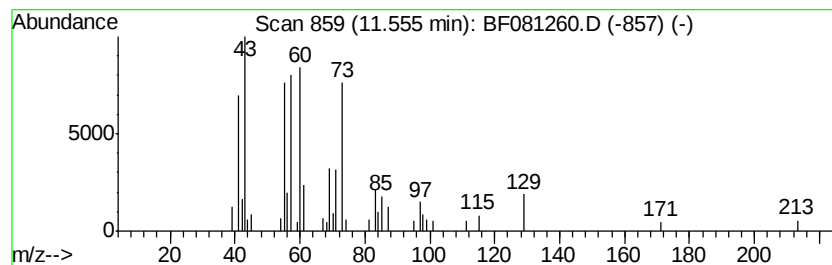
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Peak Number 5 Undecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	4.01 ng	80256	Phenanthrene-d10	10.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Undecanoic acid	186	C11H22O2	000112-37-8	80
2		n-Decanoic acid	172	C10H20O2	000334-48-5	59
3		n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	56
4		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	53
5		.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	47



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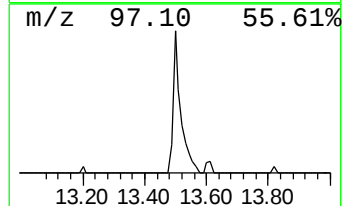
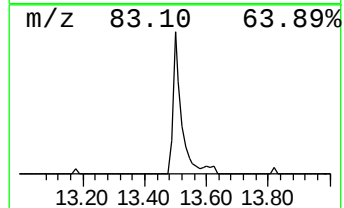
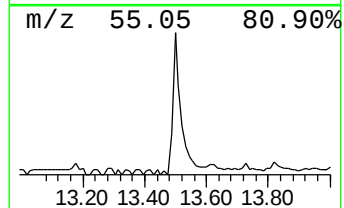
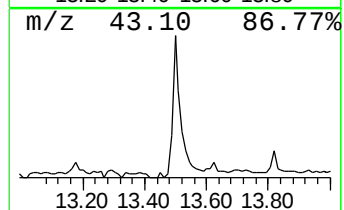
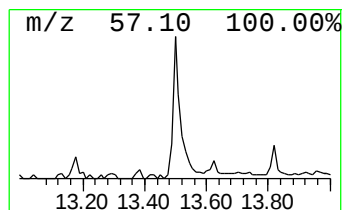
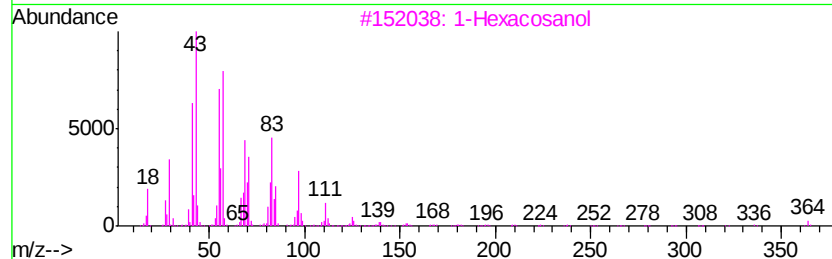
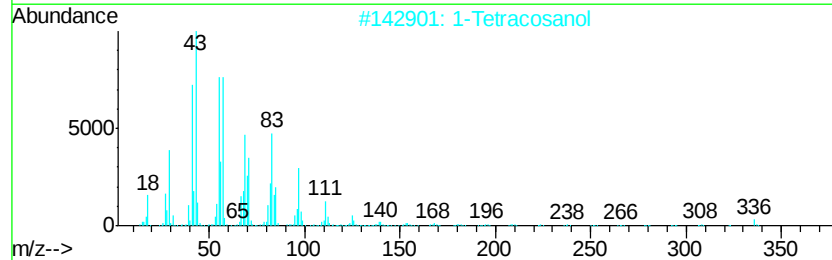
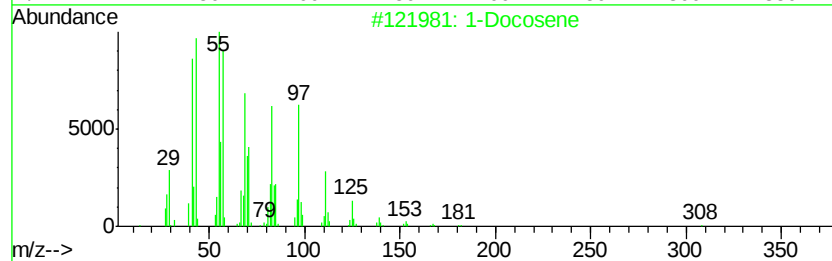
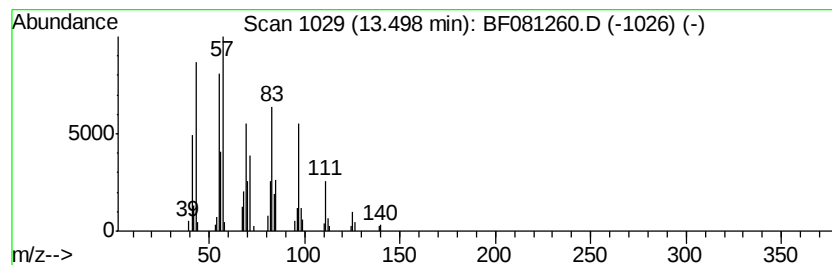
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	9.33 ng	180849	Chrysene-d12	13.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	91
2		1-Tetracosanol	354	C24H50O	000506-51-4	83
3		1-Hexacosanol	382	C26H54O	000506-52-5	83
4		17-Pentatriacontene	491	C35H70	006971-40-0	74
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.59	87.2	ng	1128730	1	6.50	258792	20.0
2-Pentanone, 4-me...	5.49	2.6	ng	33613	1	6.50	258792	20.0
unknown6.27	6.27	115.3	ng	1492310	1	6.50	258792	20.0
Undecanoic acid	11.56	4.0	ng	80256	4	10.99	400752	20.0
1-Docosene	13.50	9.3	ng	180849	5	13.61	387737	20.0