

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052216\
 Data File : BF087293.D
 Acq On : 22 May 2016 16:19
 Operator : UM/SJ
 Sample : H3172-09
 Misc :
 ALS Vial : 61 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-11

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-BF051716.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	1.701	8	10	64	rVB	3058183	6472278	100.00%	15.994%
2	4.696	270	272	287	rBV	45364	115601	1.79%	0.286%
3	5.142	309	311	335	rBV	1705643	2244196	34.67%	5.546%
4	6.227	405	406	413	rBV	1227041	1550042	23.95%	3.830%
5	6.330	413	415	427	rVB	4011779	3986684	61.60%	9.852%
6	6.559	433	435	440	rBV	665639	850303	13.14%	2.101%
7	6.707	446	448	451	rBV	3353561	3299614	50.98%	8.154%
8	7.142	483	486	488	rBV	2227524	3250106	50.22%	8.031%
9	7.839	545	547	559	rBV2	845661	1189398	18.38%	2.939%
10	8.925	639	642	644	rBV	5456173	5303239	81.94%	13.105%
11	9.336	675	678	681	rBV	49109	76300	1.18%	0.189%
12	9.588	698	700	703	rBV	1386811	1243896	19.22%	3.074%
13	10.033	735	739	741	rBV	79815	81162	1.25%	0.201%
14	10.376	767	769	772	rBV2	2225293	2971289	45.91%	7.342%
15	10.502	778	780	785	rVB	72085	87467	1.35%	0.216%
16	11.062	827	829	832	rBV2	974754	1137784	17.58%	2.812%
17	12.479	951	953	956	rVB	475176	408584	6.31%	1.010%
18	12.651	965	968	970	rBV	4337697	4225544	65.29%	10.442%
19	13.177	1012	1014	1016	rBV	194028	239040	3.69%	0.591%
20	13.554	1044	1047	1054	rBV2	67700	113581	1.75%	0.281%
21	13.691	1057	1059	1066	rBV	710913	828066	12.79%	2.046%
22	14.457	1124	1126	1129	rBV	49087	66944	1.03%	0.165%
23	15.051	1176	1178	1188	rBV	481166	726579	11.23%	1.795%

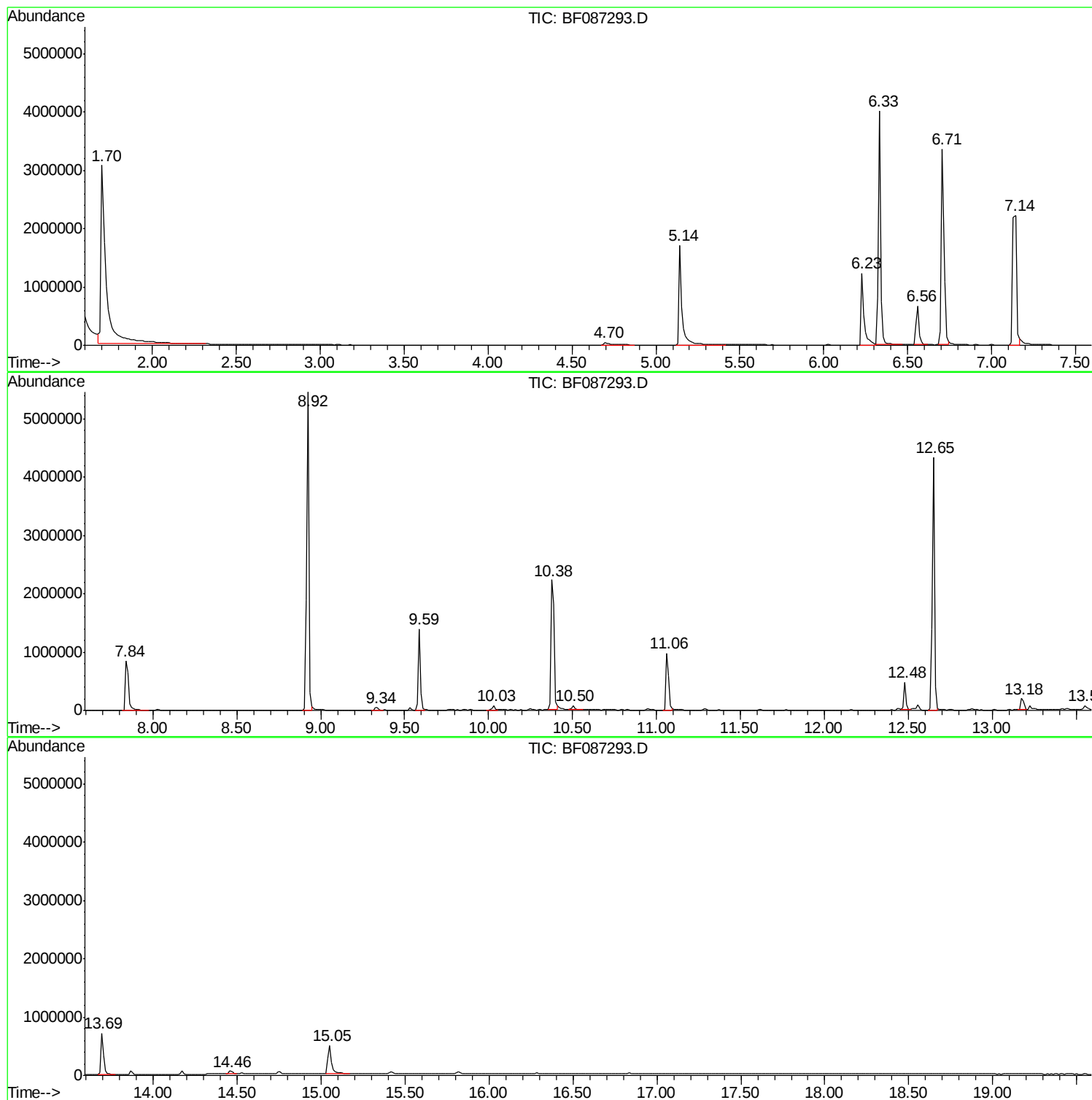
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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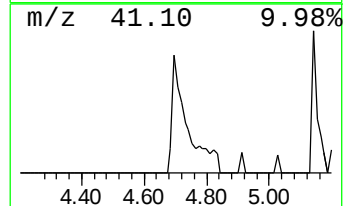
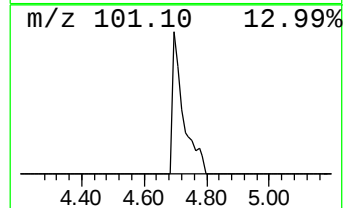
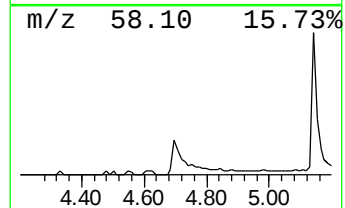
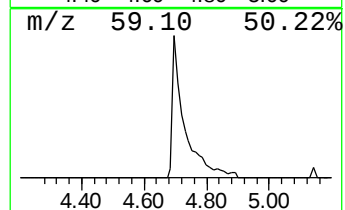
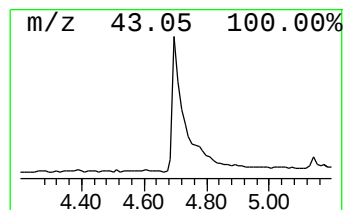
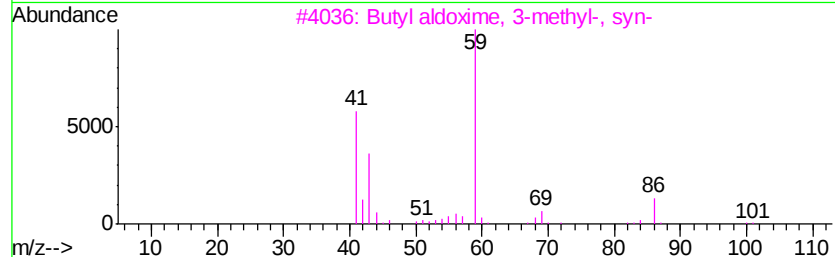
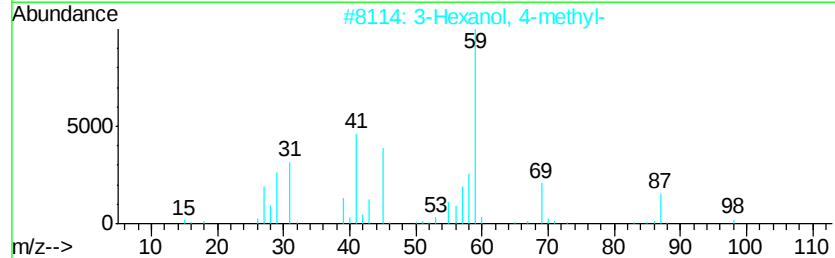
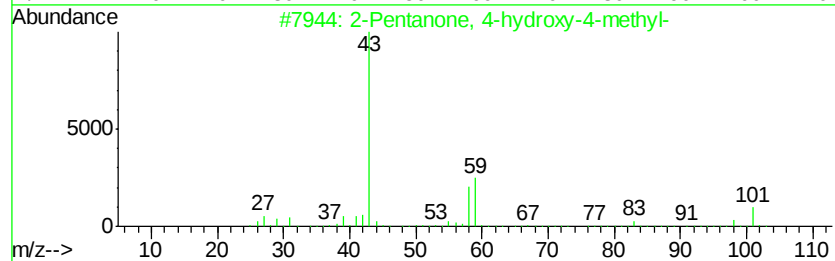
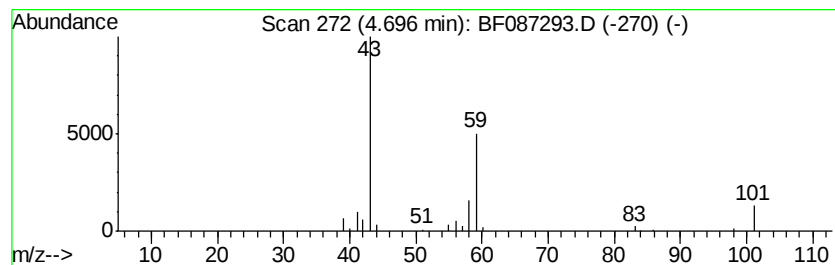
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	2.72 ng	115601	1,4-Dichlorobenzene-d4	6.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4			Diacetamide	101	C4H7NO2	000625-77-4	9
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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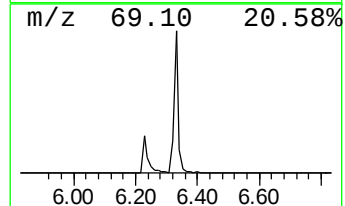
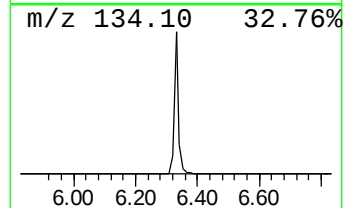
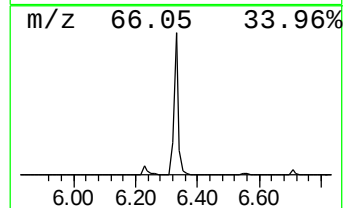
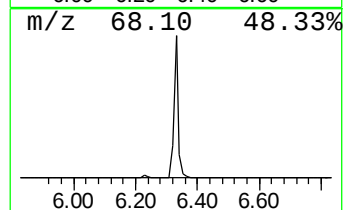
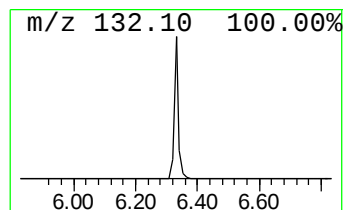
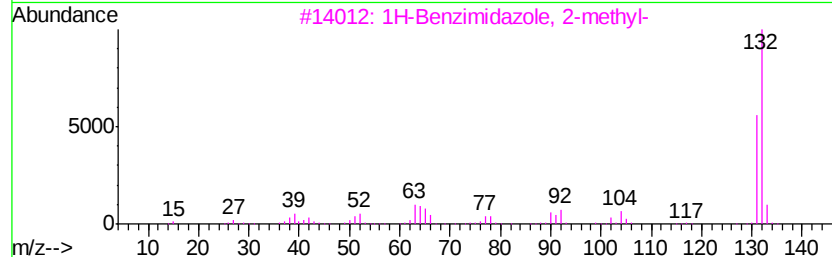
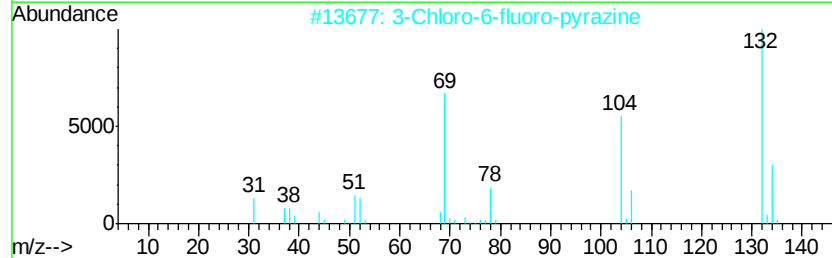
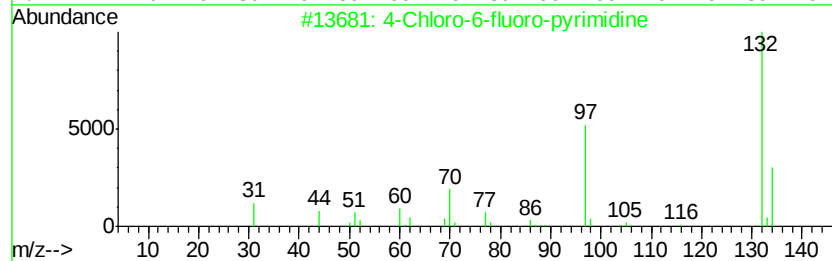
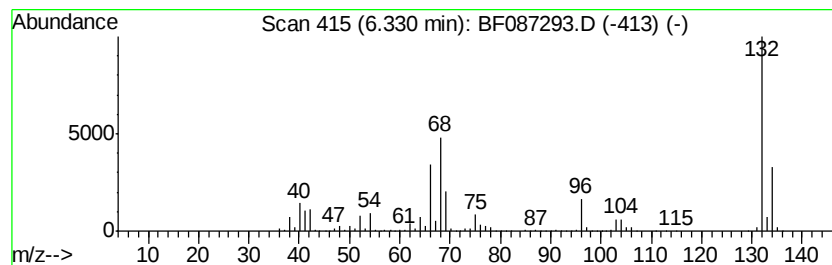
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 unknown6.33 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	93.77 ng	3986680	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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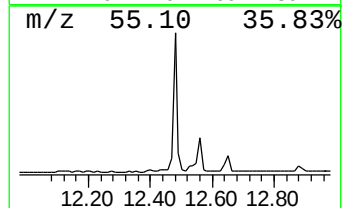
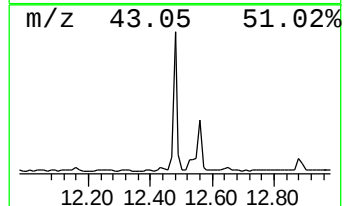
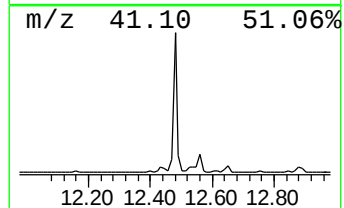
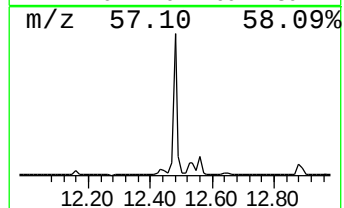
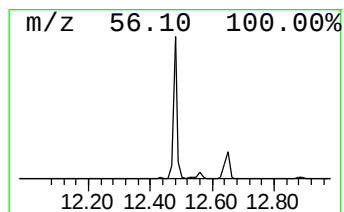
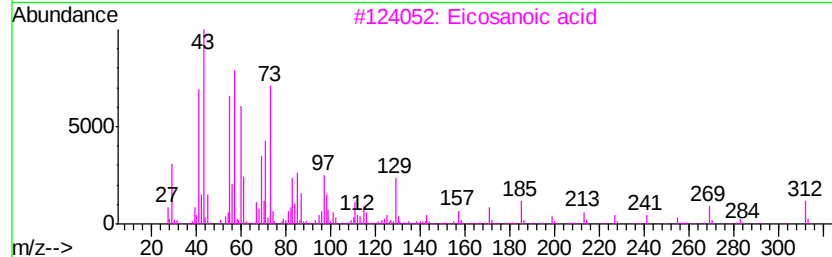
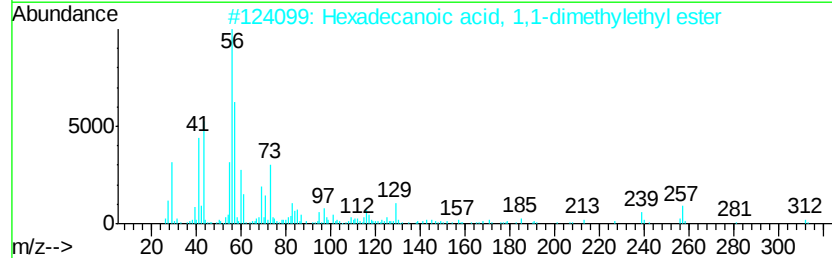
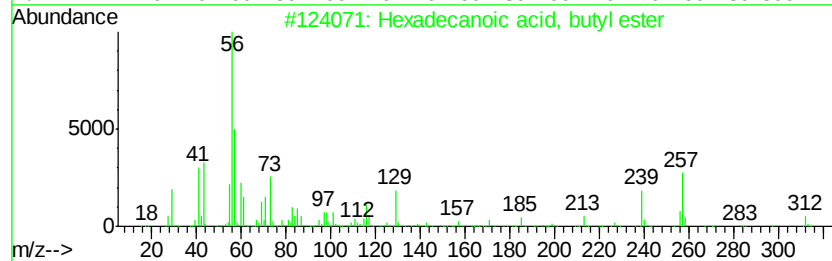
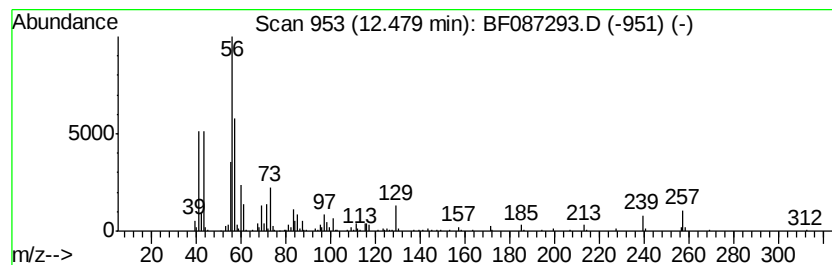
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	9.87 ng	408584	Chrysene-d12	13.69

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	68
3		Eicosanoic acid	312	C20H40O2	000506-30-9	38
4		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35



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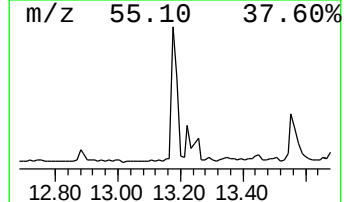
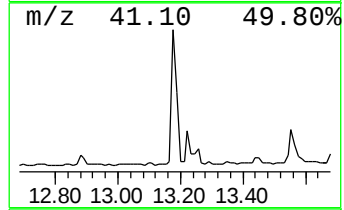
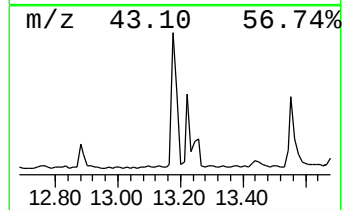
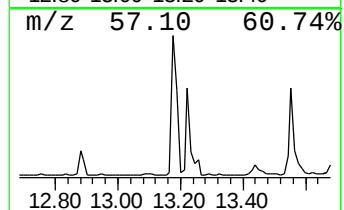
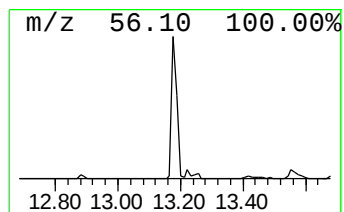
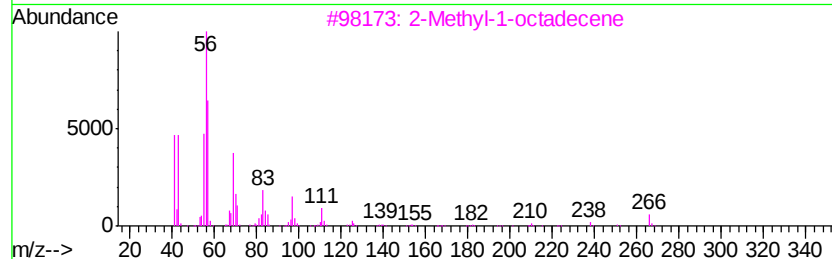
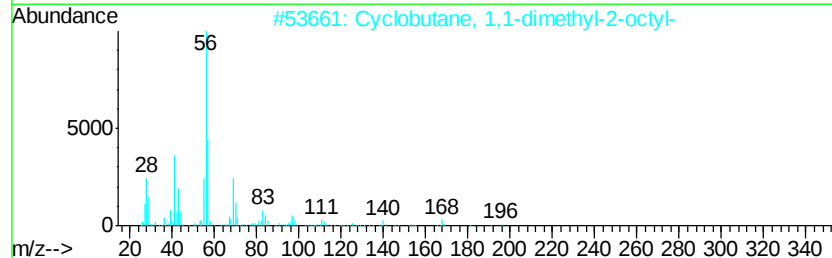
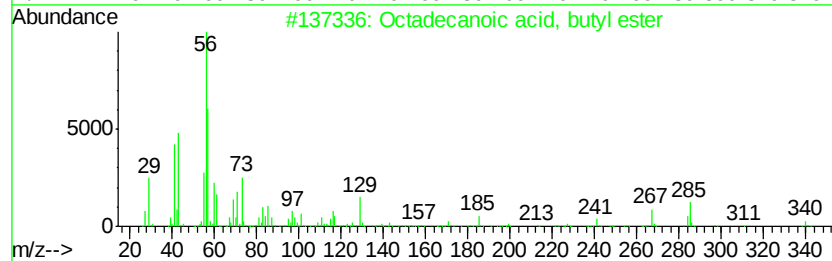
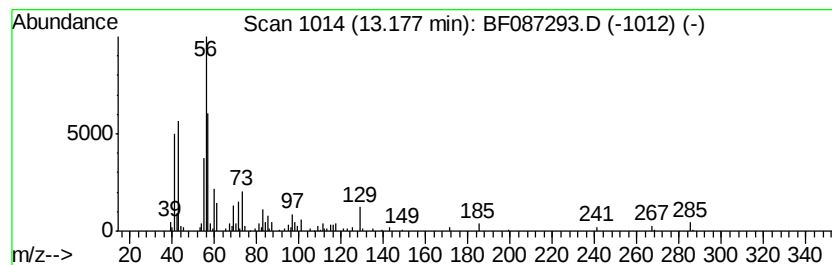
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Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.18	5.77 ng	239040	Chrysene-d12	13.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
3		2-Methyl-1-octadecene	266	C19H38	061868-20-0	38
4		Chloromethyl 2-chloroundecanoate	268	C12H22Cl2O2	080418-88-8	37
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35



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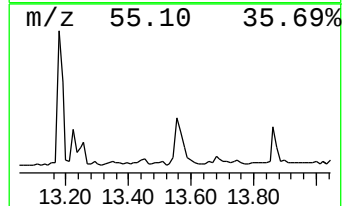
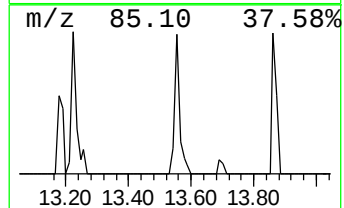
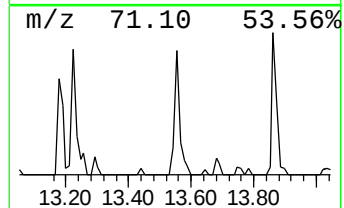
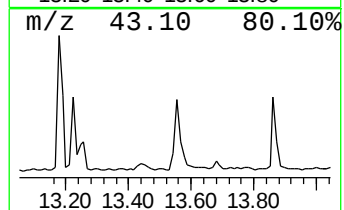
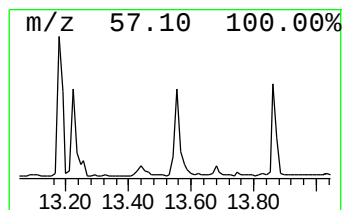
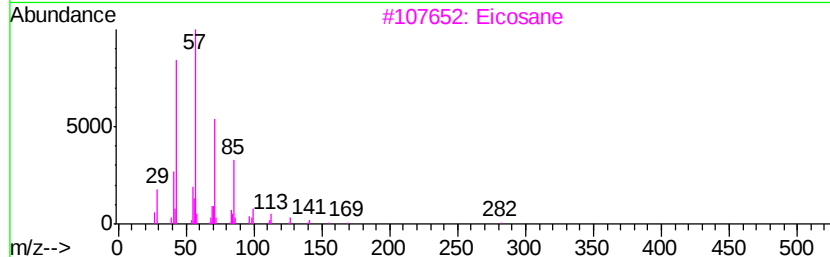
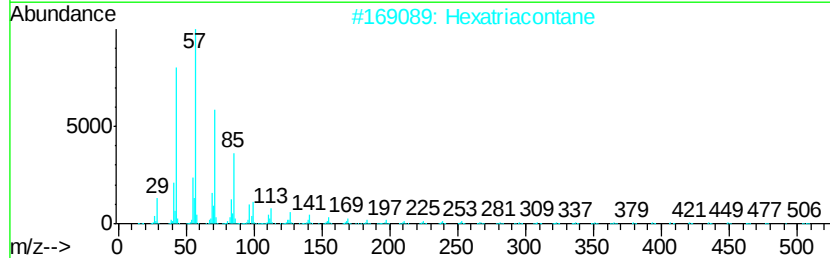
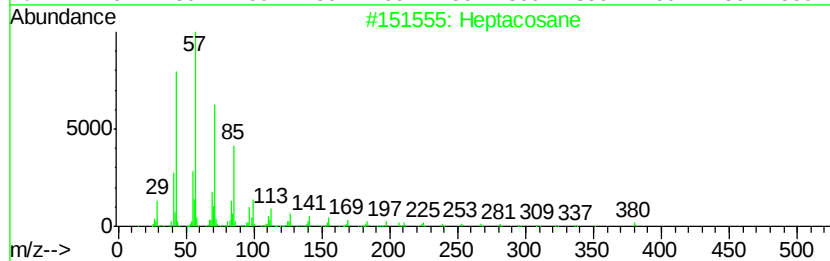
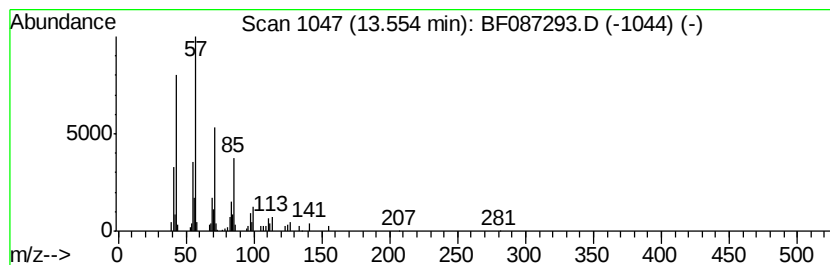
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Peak Number 7 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	2.74 ng	113581	Chrysene-d12	13.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Hexatriacontane		507	C36H74	000630-06-8	91
3	Eicosane		282	C20H42	000112-95-8	91
4	Tetratetracontane		619	C44H90	007098-22-8	91
5	10-Methylnonadecane		282	C20H42	056862-62-5	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.70	2.7	ng	115601	1	6.56	850303	20.0
unknown6.33	6.33	93.8	ng	3986680	1	6.56	850303	20.0
Hexadecanoic acid...	12.48	9.9	ng	408584	5	13.69	828066	20.0
Octadecanoic acid...	13.18	5.8	ng	239040	5	13.69	828066	20.0
Heptacosane	13.55	2.7	ng	113581	5	13.69	828066	20.0