

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
 Data File : BF089240.D
 Acq On : 23 Jul 2016 16:37
 Operator : UM/SJ
 Sample : H4129-04
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 KSB-10-8.0-10.0

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-BF072016.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	1.713	10	11	30	rVB	866383	1554290	92.47%	10.404%
2	4.707	270	273	280	rBV	43507	76534	4.55%	0.512%
3	5.164	310	313	339	rBV	960255	1416006	84.25%	9.479%
4	6.239	404	407	414	rBV	1172131	1537937	91.50%	10.295%
5	6.342	414	416	435	rVV	933642	1543462	91.83%	10.332%
6	6.582	435	437	448	rVV	190641	269538	16.04%	1.804%
7	6.730	448	450	467	rVB	990032	1031905	61.39%	6.907%
8	7.153	484	487	496	rBV	662919	921338	54.82%	6.167%
9	7.267	496	497	505	rVB	8612	17237	1.03%	0.115%
10	7.862	547	549	560	rBV	345559	376824	22.42%	2.522%
11	8.948	641	644	646	rBV	1296258	1680780	100.00%	11.251%
12	9.336	676	678	681	rBV	173411	239887	14.27%	1.606%
13	9.611	699	702	704	rBV	378661	415366	24.71%	2.780%
14	10.399	768	771	773	rBV	808766	1024658	60.96%	6.859%
15	10.525	781	782	789	rVB	17587	30825	1.83%	0.206%
16	10.971	819	821	826	rBV2	18485	27460	1.63%	0.184%
17	11.085	829	831	835	rBV	382122	424750	25.27%	2.843%
18	11.394	857	858	861	rBV	13275	18044	1.07%	0.121%
19	12.502	953	955	958	rBV	74297	84381	5.02%	0.565%
20	12.662	967	969	972	rBV	1067237	1531738	91.13%	10.253%
21	13.211	1015	1017	1019	rBV	62005	59968	3.57%	0.401%
22	13.577	1046	1049	1058	rBV	48462	93186	5.54%	0.624%
23	13.702	1058	1060	1066	rBV	321573	337909	20.10%	2.262%
24	15.040	1175	1177	1180	rBV	174168	225031	13.39%	1.506%

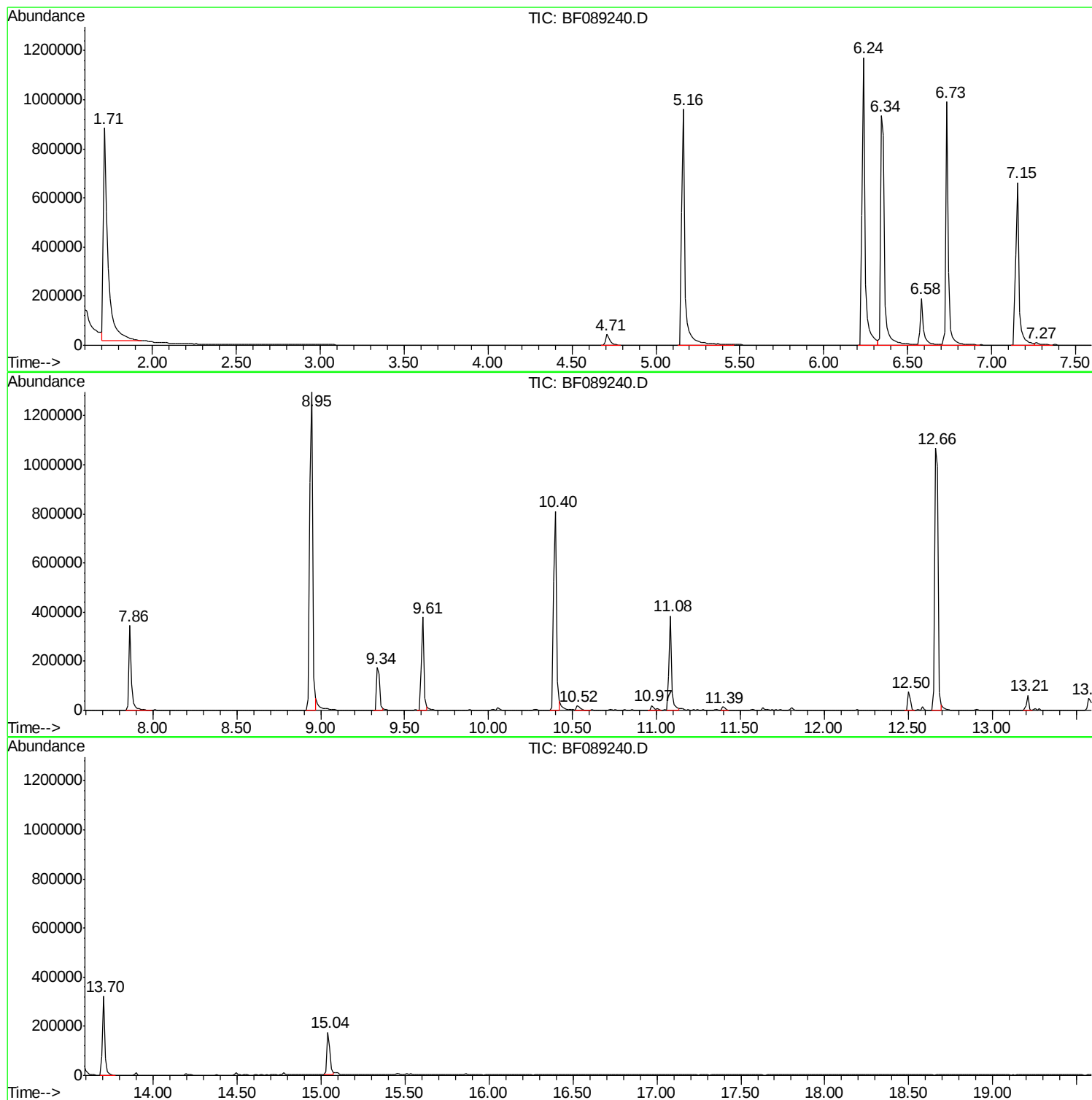
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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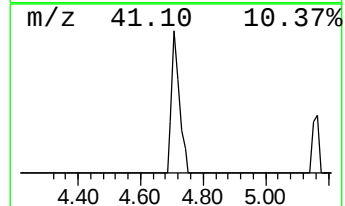
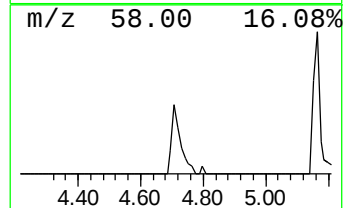
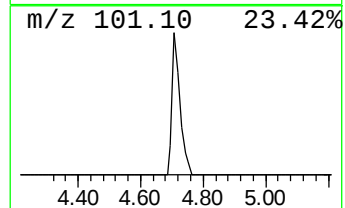
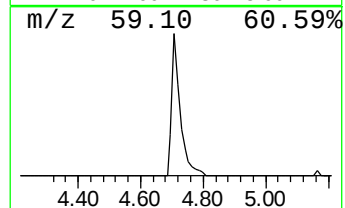
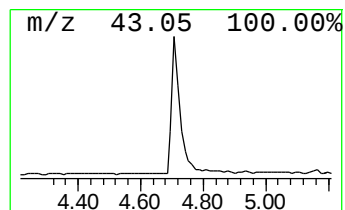
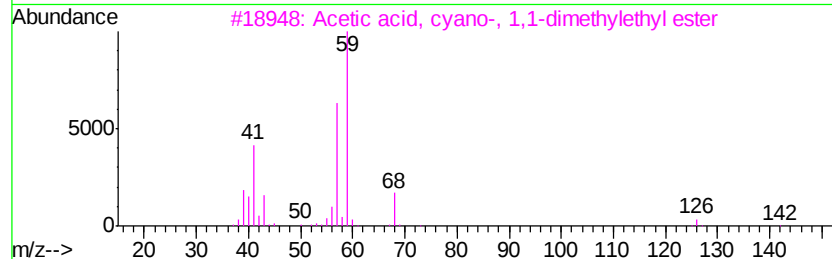
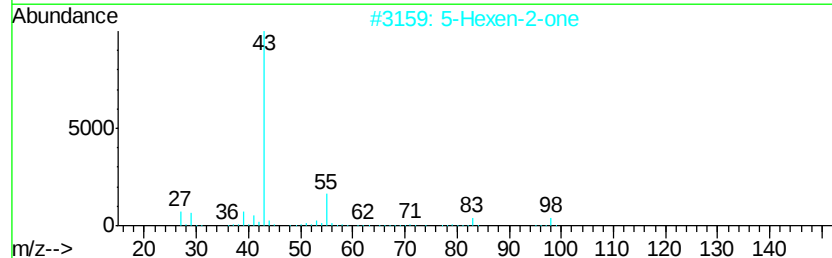
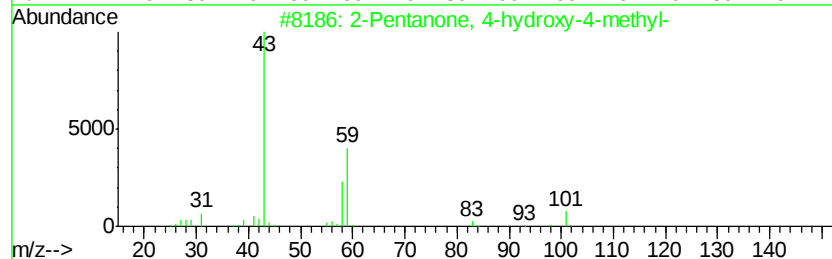
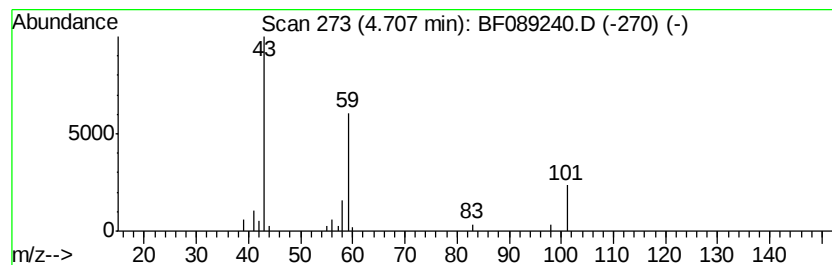
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	5.68 ng	76534	1,4-Dichlorobenzene-d4	6.58

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			5-Hexen-2-one	98	C6H10O	000109-49-9	9
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	9
4			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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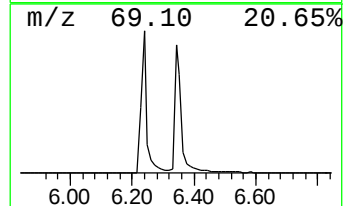
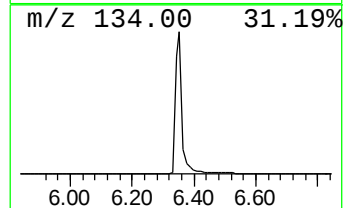
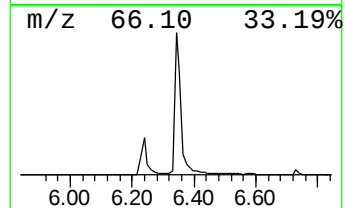
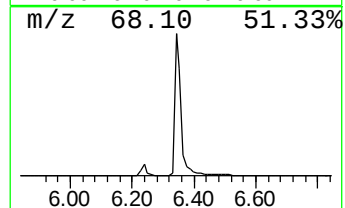
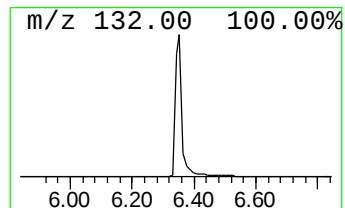
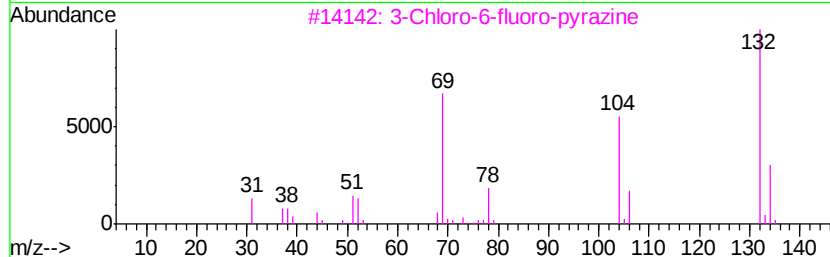
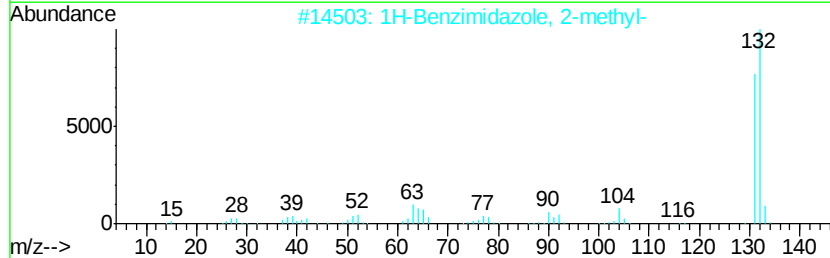
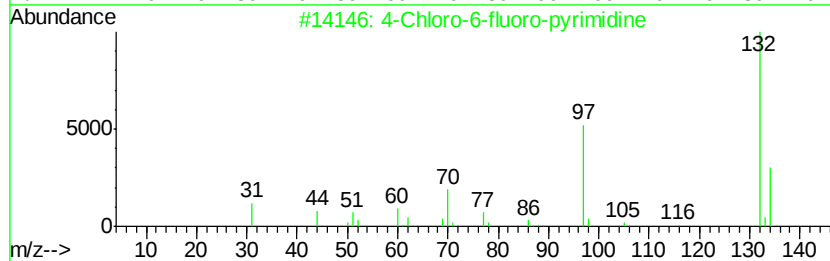
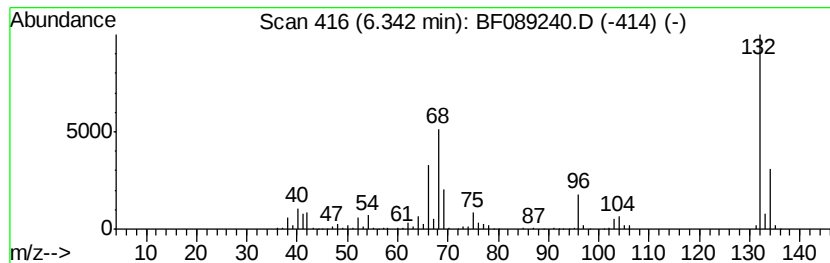
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Peak Number 3 unknown6.34 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	114.53 ng	1543460	1,4-Dichlorobenzene-d4	6.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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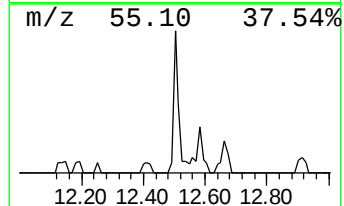
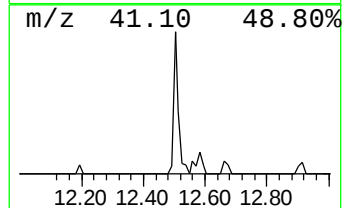
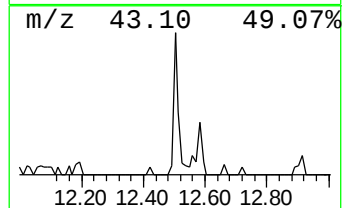
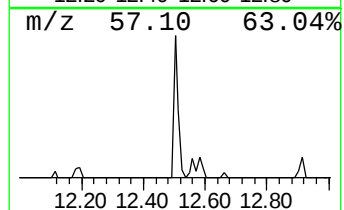
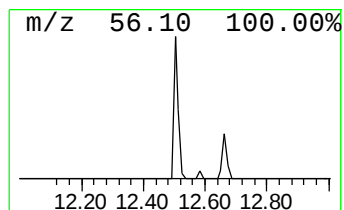
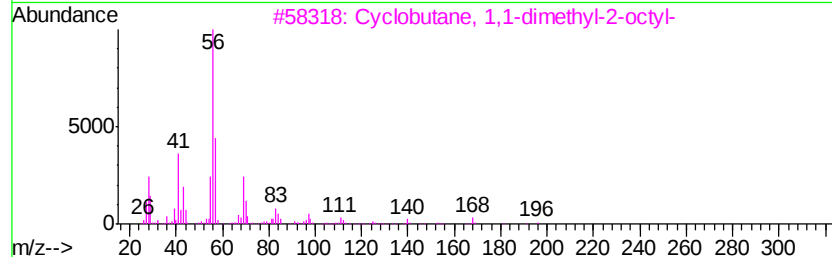
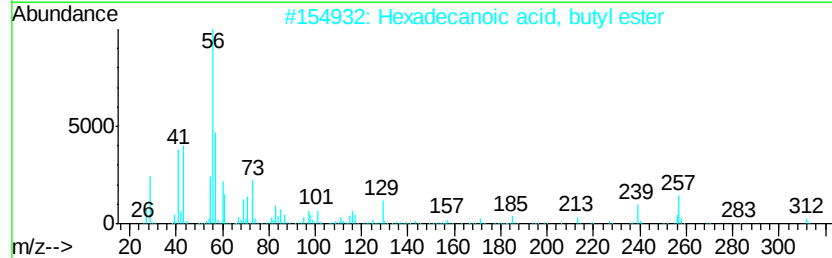
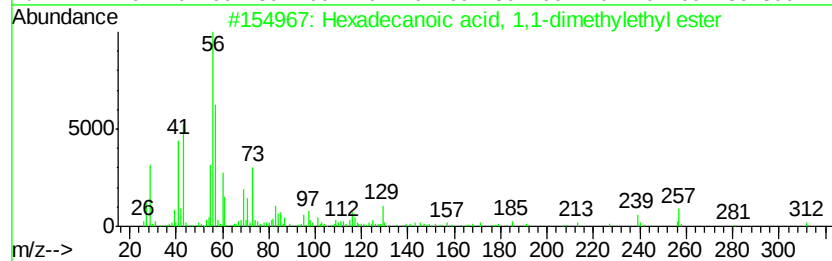
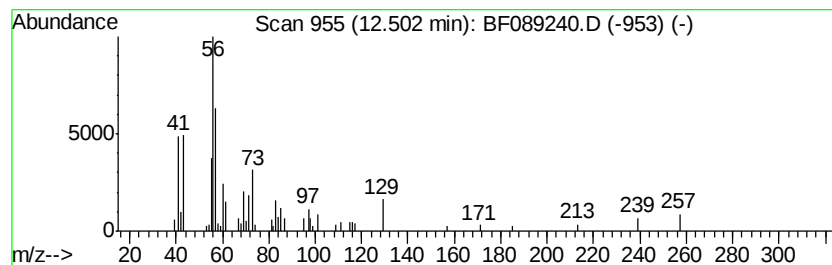
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Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	4.99 ng	84381	Chrysene-d12	13.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	74
3		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	43
4		Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	38
5		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37



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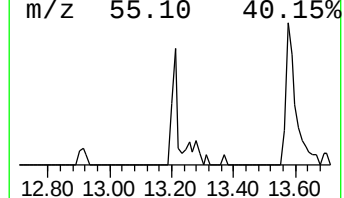
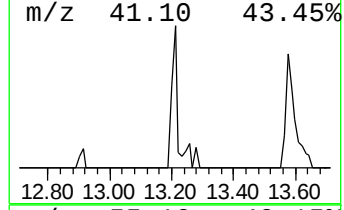
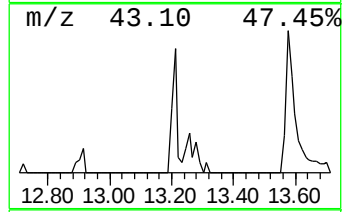
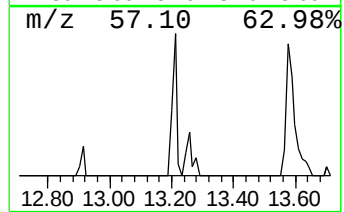
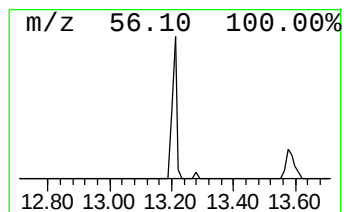
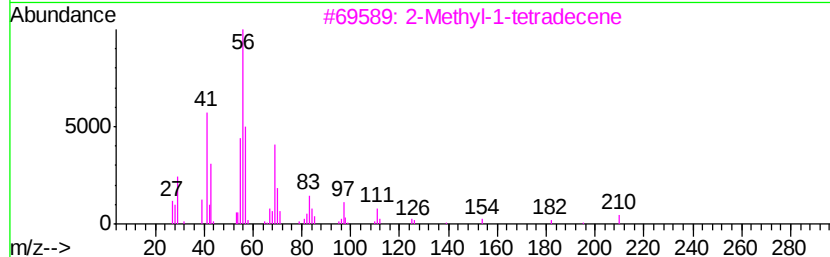
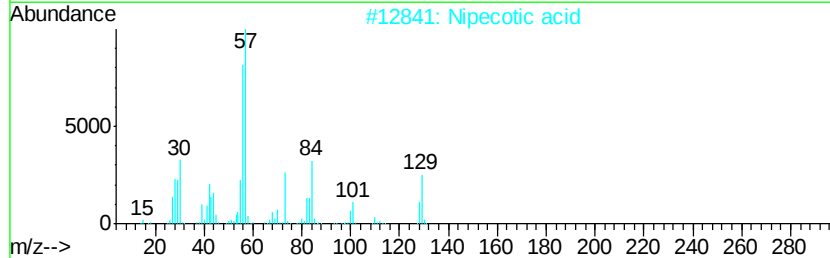
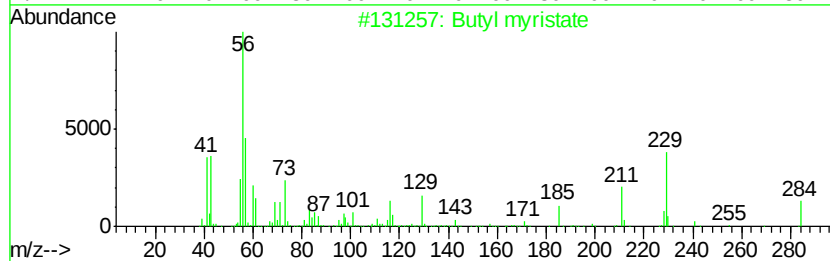
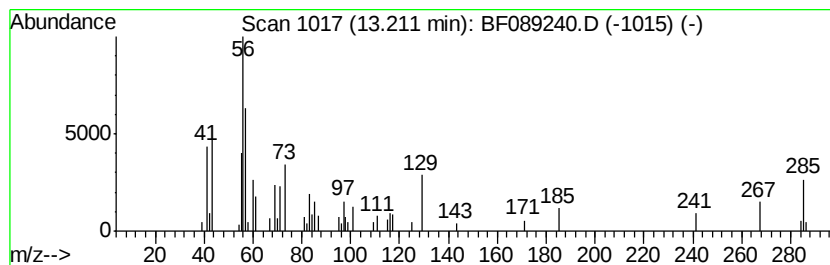
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Peak Number 6 Butyl myristate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	3.55 ng	59968	Chrysene-d12	13.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butyl myristate	284	C18H36O2	000110-36-1	58
2		Nipecotic acid	129	C6H11NO2	000498-95-3	38
3		2-Methyl-1-tetradecene	210	C15H30	052254-38-3	27
4		2-Methyl-1-octadecene	266	C19H38	061868-20-0	27
5		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27



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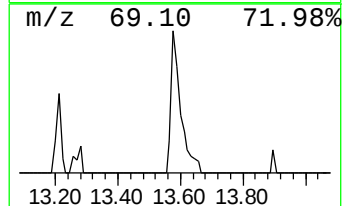
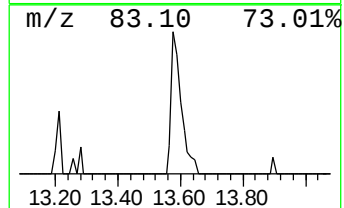
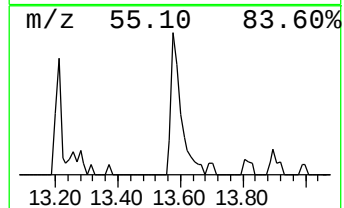
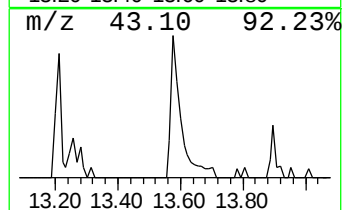
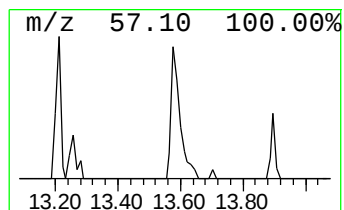
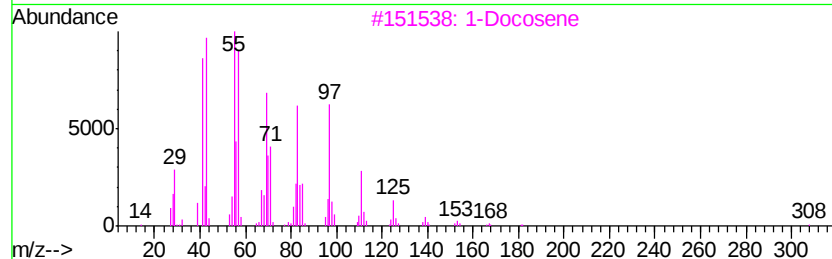
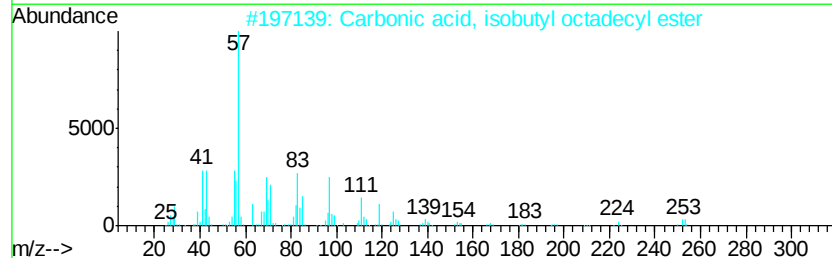
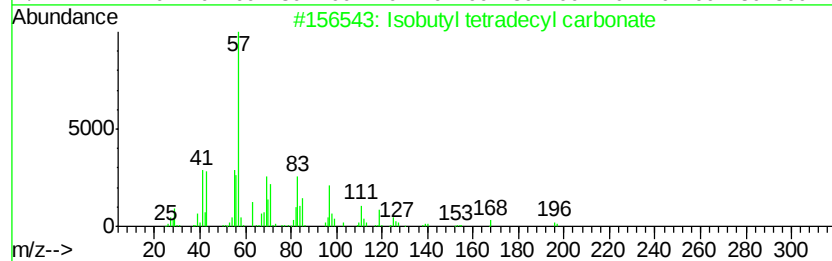
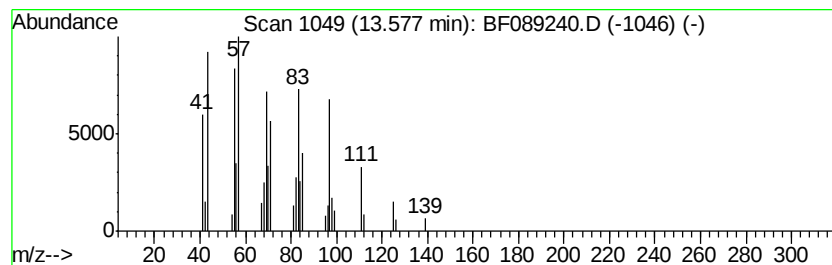
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Peak Number 7 Isobutyl tetradecyl carbonate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.58	5.52 ng	93186	Chrysene-d12	13.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	91
2		Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	91
3		1-Docosene	308	C22H44	001599-67-3	81
4		17-Pentatriacontene	491	C35H70	006971-40-0	72
5		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	72



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TIC Library : C:\Database\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.71	5.7	ng	76534	1	6.58	269538	20.0
unknown6.34	6.34	114.5	ng	1543460	1	6.58	269538	20.0
Hexadecanoic acid...	12.50	5.0	ng	84381	5	13.70	337909	20.0
Butyl myristate	13.21	3.5	ng	59968	5	13.70	337909	20.0
Isobutyl tetradec...	13.58	5.5	ng	93186	5	13.70	337909	20.0