

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
 Data File : BF092498.D
 Acq On : 26 Jan 2017 1:10
 Operator : SJ/MA
 Sample : I1351-03
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CAS-SB-01-68-70

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-BF012417.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	3.390	112	114	124	rBV	21222	73350	1.43%	0.158%
2	4.818	238	239	246	rVB	33138	53434	1.04%	0.115%
3	5.161	266	269	278	rVB	1501814	2077638	40.63%	4.467%
4	5.561	301	304	307	rBV	3224187	4792453	93.71%	10.305%
5	6.590	391	394	397	rBV	3927814	4729805	92.48%	10.170%
6	6.727	404	406	409	rBV	3320199	4674563	91.40%	10.051%
7	6.967	424	427	429	rBV	1035653	932864	18.24%	2.006%
8	7.127	438	441	443	rVB	3313988	3661826	71.60%	7.874%
9	7.527	473	476	479	rBV	2310010	2981827	58.31%	6.412%
10	8.259	537	540	542	rBV	1348073	1264781	24.73%	2.720%
11	9.345	631	635	637	rBV	4589463	5114147	100.00%	10.997%
12	9.733	666	669	672	rBV	997830	876345	17.14%	1.884%
13	10.019	691	694	697	rBV	1505921	1371538	26.82%	2.949%
14	10.430	728	730	731	rBV	62442	59845	1.17%	0.129%
15	10.453	731	732	734	rVB	85898	66377	1.30%	0.143%
16	10.808	760	763	766	rBV	2302845	2828368	55.30%	6.082%
17	10.933	771	774	778	rVB	78266	145141	2.84%	0.312%
18	11.379	810	813	814	rBV	129594	115651	2.26%	0.249%
19	11.505	822	824	827	rBV	1458722	1371589	26.82%	2.949%
20	11.733	842	844	848	rBV	73922	89339	1.75%	0.192%
21	11.802	848	850	853	rBV	135578	125833	2.46%	0.271%
22	12.042	869	871	872	rBV	56018	65259	1.28%	0.140%
23	12.213	884	886	888	rVB	107200	87648	1.71%	0.188%
24	13.105	961	964	966	rBV	4253873	4978184	97.34%	10.704%
25	13.574	999	1005	1011	rBV2	34709	96955	1.90%	0.208%
26	13.997	1039	1042	1047	rBV	168377	210006	4.11%	0.452%
27	14.145	1053	1055	1058	rBV	1547835	1412365	27.62%	3.037%
28	14.625	1093	1097	1104	rBV2	25744	55741	1.09%	0.120%
29	14.911	1120	1122	1129	rBV	727213	899930	17.60%	1.935%
30	15.014	1129	1131	1135	rVB	42008	61177	1.20%	0.132%
31	15.620	1181	1184	1187	rBV	896726	1232320	24.10%	2.650%

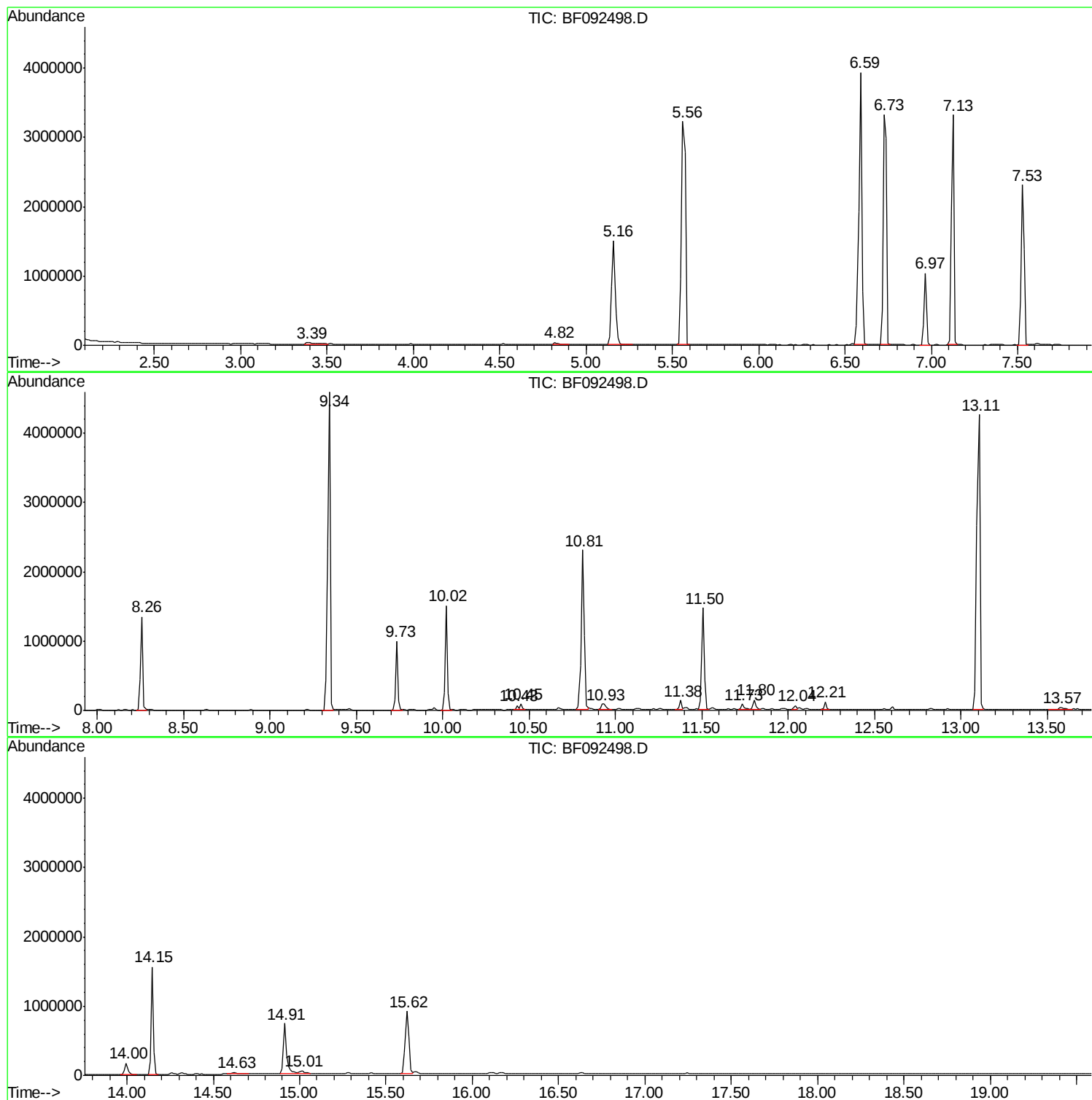
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Instrument :
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ClientSampleId :
CAS-SB-01-68-70

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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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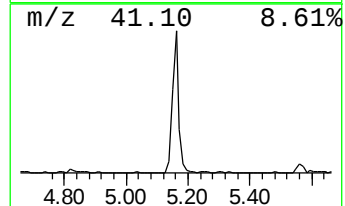
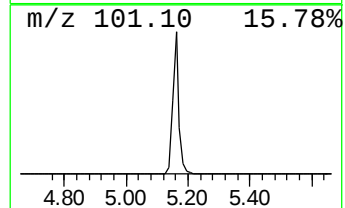
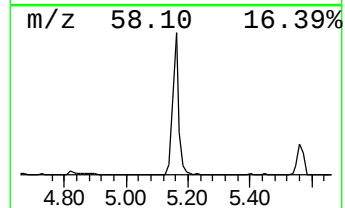
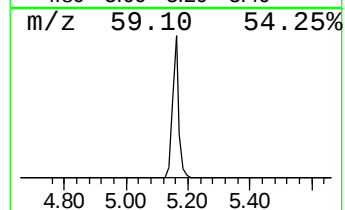
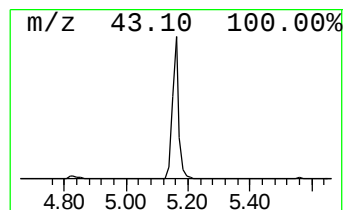
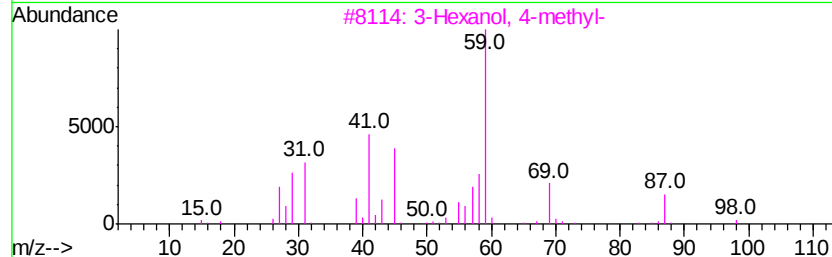
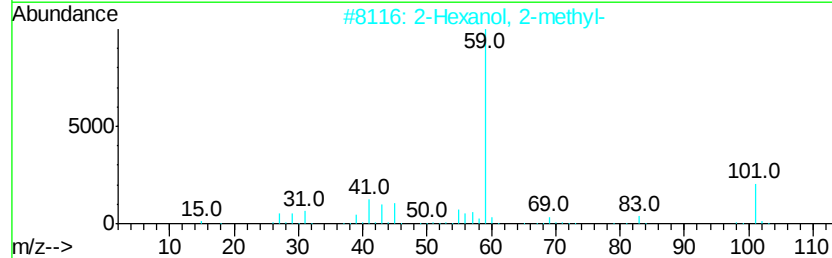
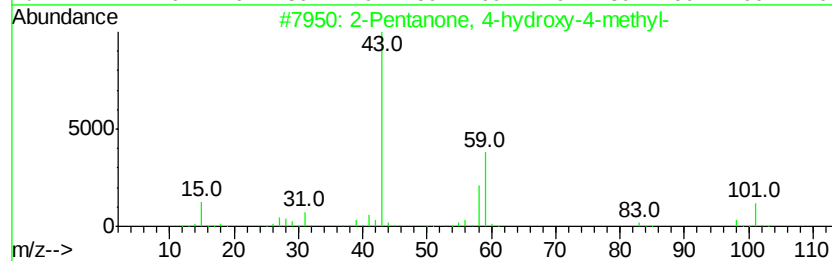
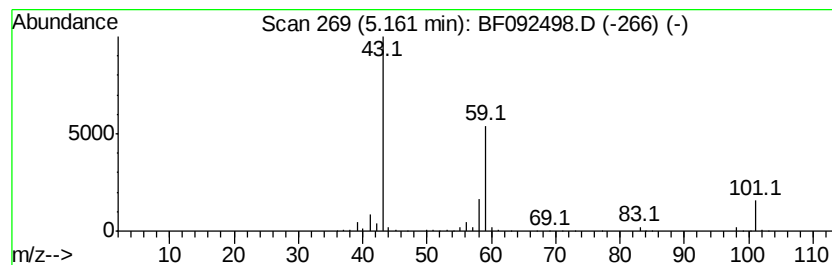
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.16	44.54 ng	2077640	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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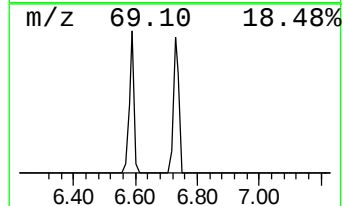
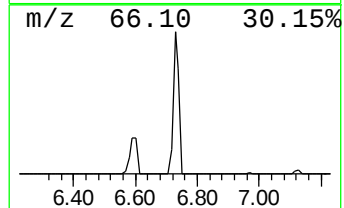
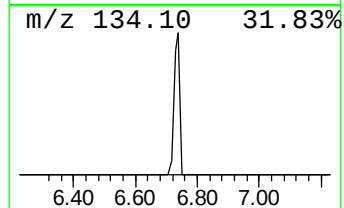
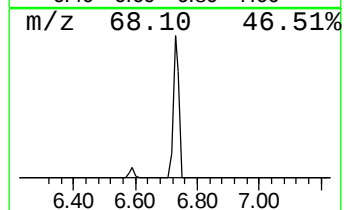
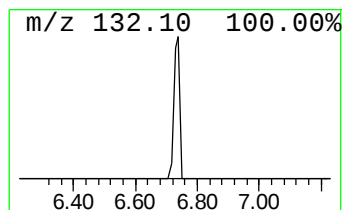
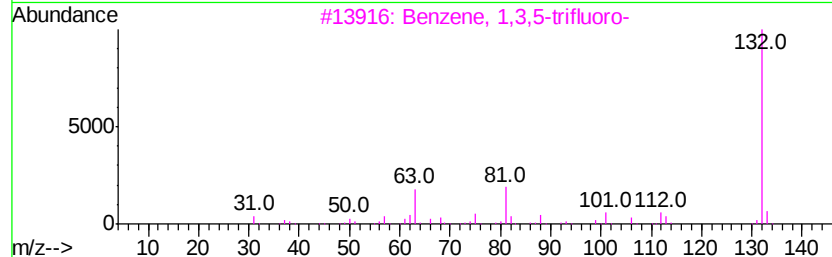
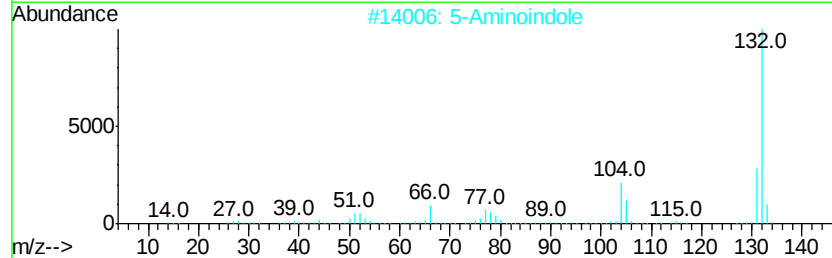
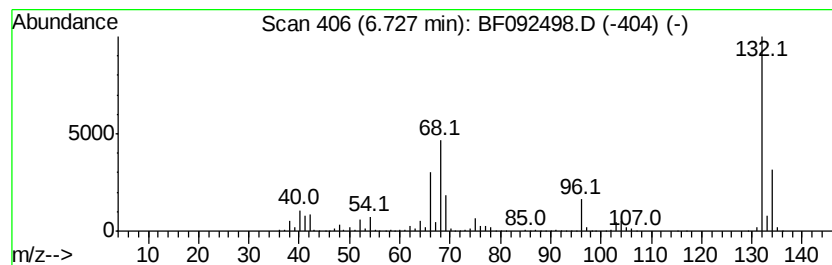
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Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	100.22 ng	4674560	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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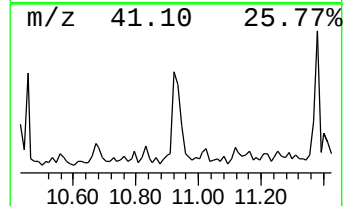
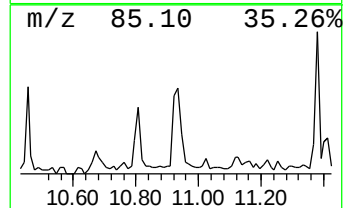
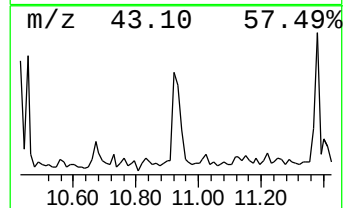
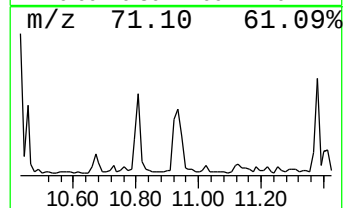
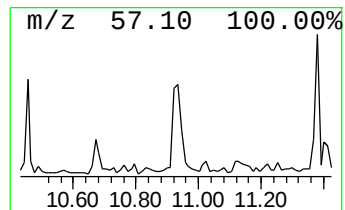
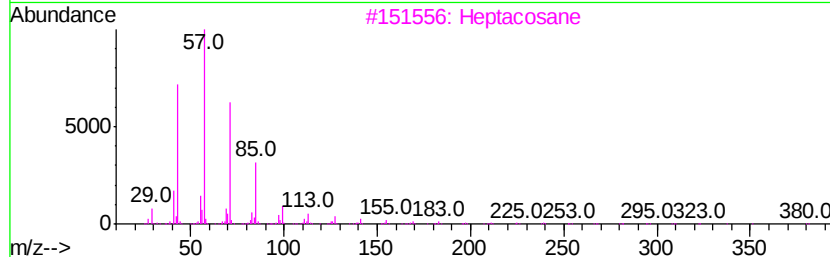
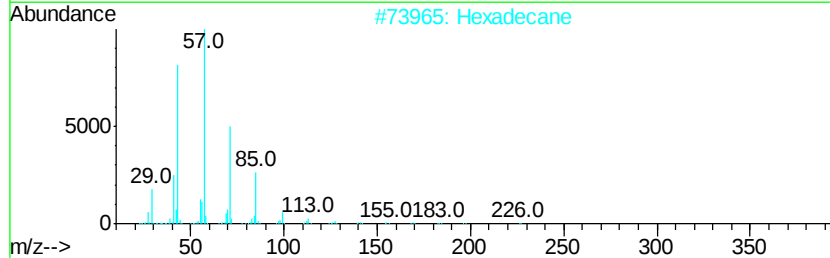
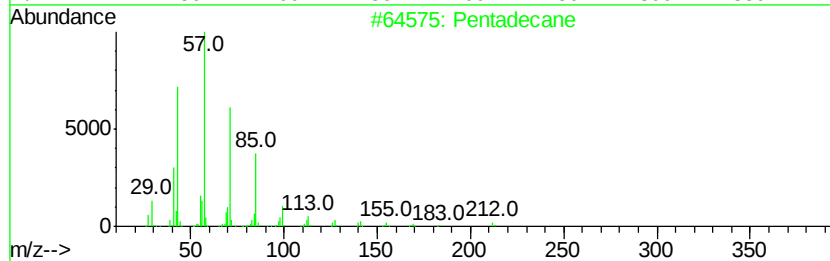
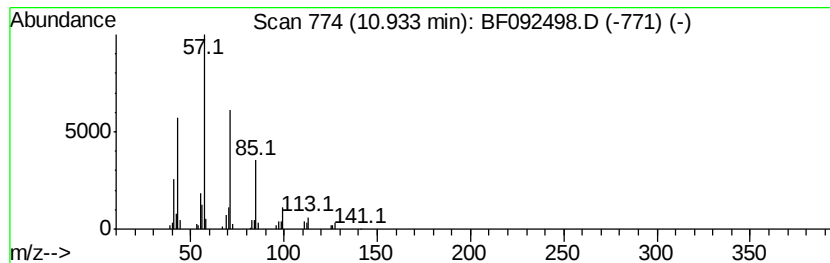
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Peak Number 4 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.93	2.12 ng	145141	Phenanthrene-d10	11.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	86
2	Hexadecane	226	C16H34	000544-76-3	86
3	Heptacosane	380	C27H56	000593-49-7	83
4	Eicosane	282	C20H42	000112-95-8	80
5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	64



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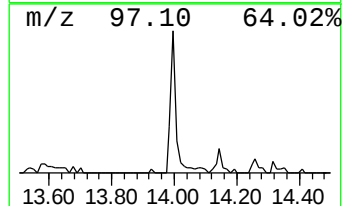
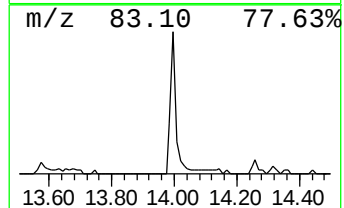
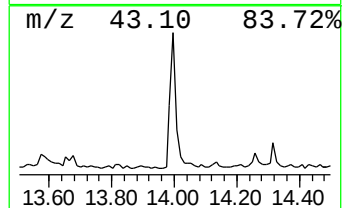
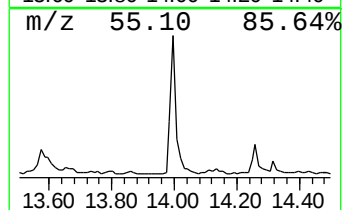
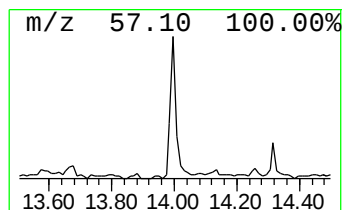
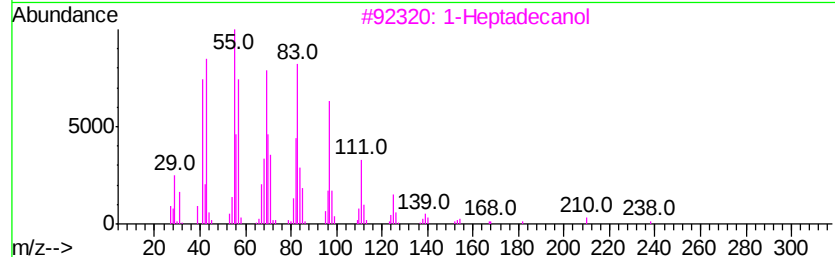
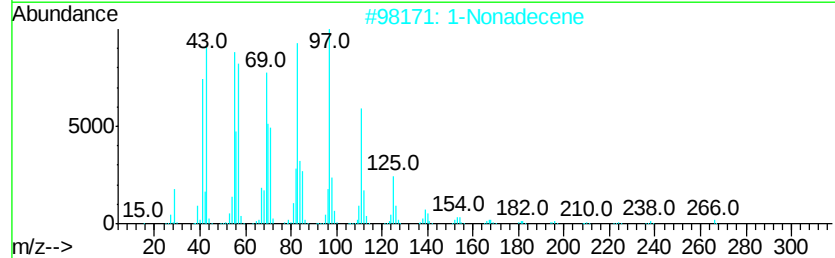
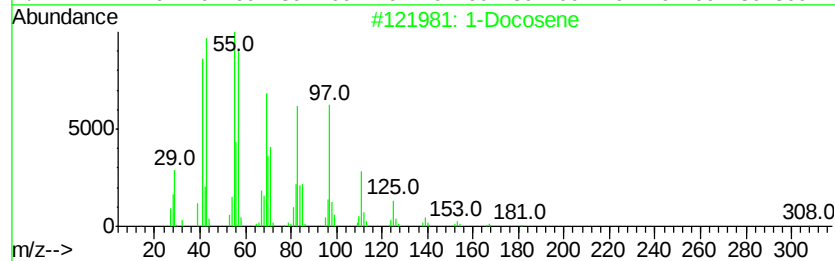
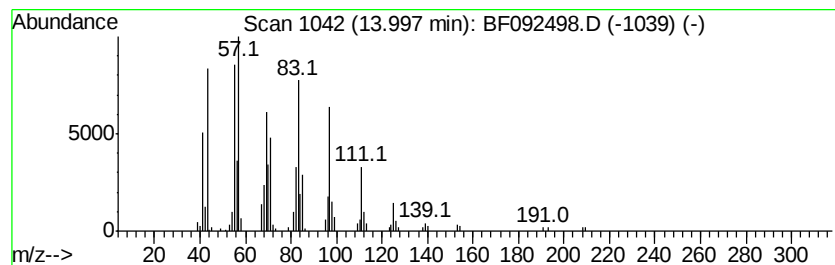
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Peak Number 5 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.00	2.97 ng	210006	Chrysene-d12		14.15
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	1-Nonadecene	266	C19H38	018435-45-5	83
3	1-Heptadecanol	256	C17H36O	001454-85-9	83
4	1-Tetracosanol	354	C24H50O	000506-51-4	80
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	80



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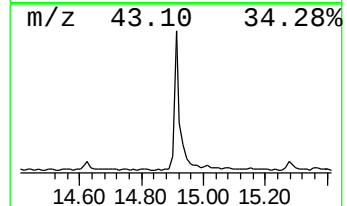
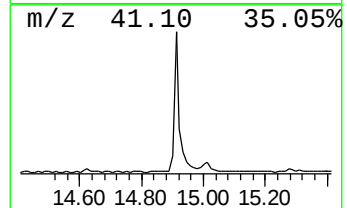
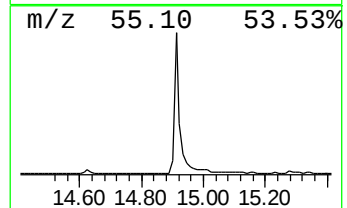
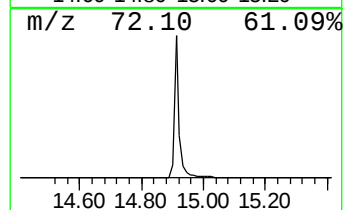
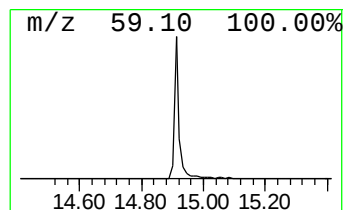
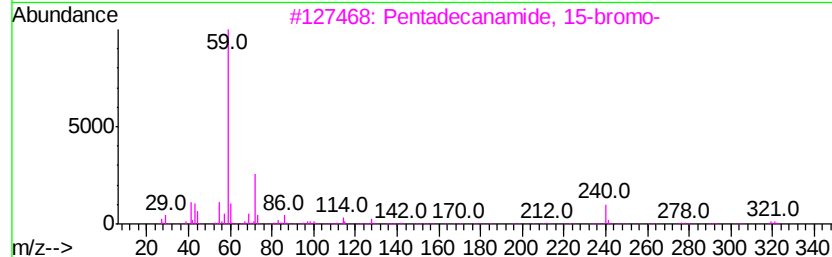
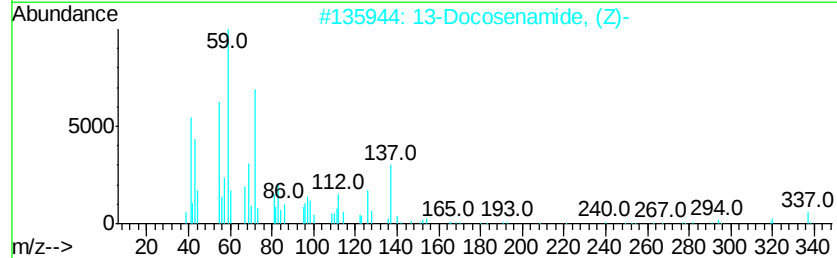
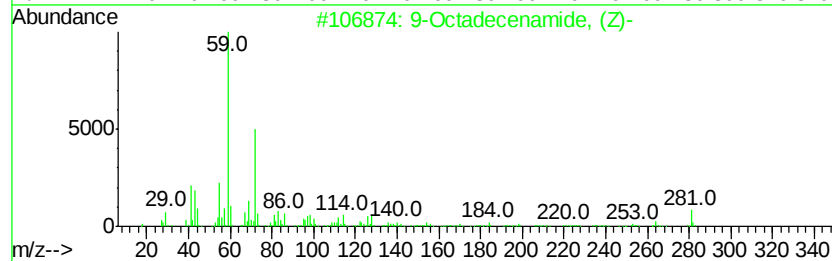
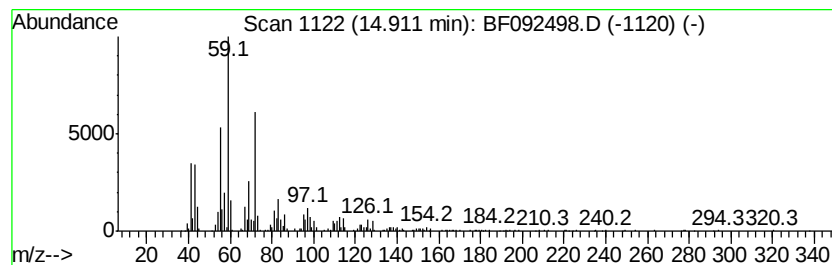
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Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	14.61 ng	899930	Perylene-d12	15.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	78
3		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	64
4		7-Nonenamide	155	C9H17NO	090949-53-4	64
5		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.16	44.5	ng	2077640	1	6.97	932864	20.0
unknown6.73	6.73	100.2	ng	4674560	1	6.97	932864	20.0
Pentadecane	10.93	2.1	ng	145141	4	11.50	1371590	20.0
1-Docosene	14.00	3.0	ng	210006	5	14.15	1412370	20.0
9-Octadecenamide,...	14.91	14.6	ng	899930	6	15.62	1232320	20.0