

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081318\
 Data File : BF108127.D
 Acq On : 13 Aug 2018 20:15
 Operator : JU/SJ
 Sample : J4442-31
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1-4

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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	3.643	219	222	238	rBV	67825	145336	3.05%	0.343%
2	5.260	493	497	509	rVB	739495	941667	19.75%	2.222%
3	5.648	558	563	566	rBV	4665159	4557222	95.57%	10.753%
4	6.642	726	732	735	rBV	4783490	4768322	100.00%	11.251%
5	6.666	735	736	741	rVB	74856	57035	1.20%	0.135%
6	6.795	753	758	761	rBV	5176743	4696564	98.50%	11.082%
7	7.025	793	797	800	rBV	1563792	1240714	26.02%	2.928%
8	7.184	819	824	827	rBV	3959817	3496815	73.33%	8.251%
9	7.584	887	892	895	rBV	3130592	2948663	61.84%	6.958%
10	8.307	1011	1015	1019	rBV	1847988	1506201	31.59%	3.554%
11	9.383	1193	1198	1201	rBV	5474378	4619135	96.87%	10.899%
12	9.772	1260	1264	1269	rBV	495778	387332	8.12%	0.914%
13	10.072	1311	1315	1319	rBV	1606706	1506673	31.60%	3.555%
14	10.866	1446	1450	1454	rBV	2693783	2652187	55.62%	6.258%
15	10.972	1463	1468	1472	rBV	103455	138849	2.91%	0.328%
16	11.442	1545	1548	1554	rVB2	48384	63986	1.34%	0.151%
17	11.572	1566	1570	1574	rBV	1723274	1453158	30.48%	3.429%
18	13.160	1836	1840	1844	rBV	4369888	4177064	87.60%	9.856%
19	14.054	1988	1992	2002	rBV2	189682	430675	9.03%	1.016%
20	14.230	2019	2022	2026	rVB	1364343	1196318	25.09%	2.823%
21	14.360	2042	2044	2048	rVB	73727	61766	1.30%	0.146%
22	14.671	2095	2097	2101	rBV	116337	111591	2.34%	0.263%
23	15.007	2151	2154	2157	rVB	125750	117751	2.47%	0.278%
24	15.377	2214	2217	2221	rVB	161716	177857	3.73%	0.420%
25	15.807	2285	2290	2297	rVB2	634617	927653	19.45%	2.189%

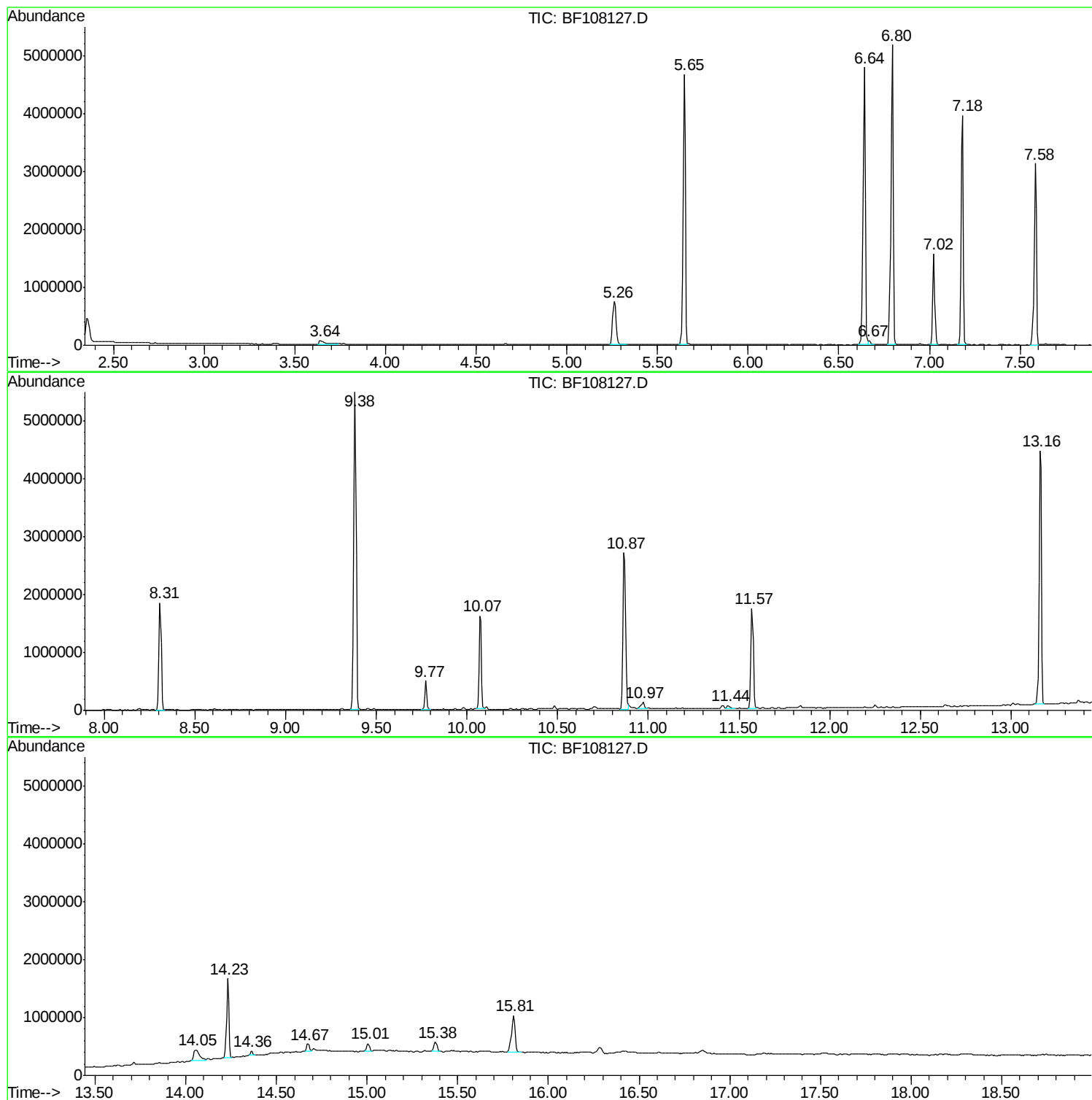
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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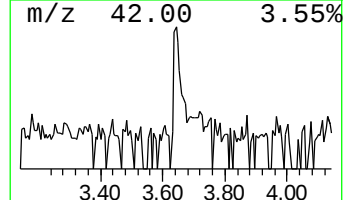
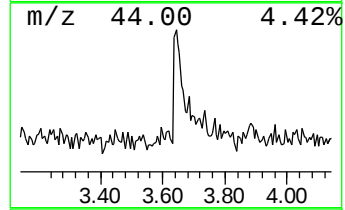
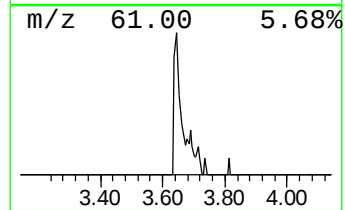
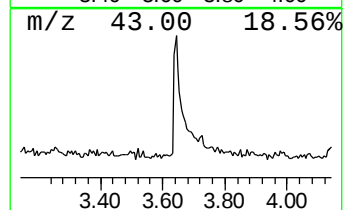
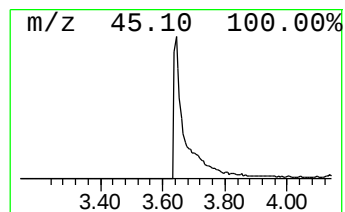
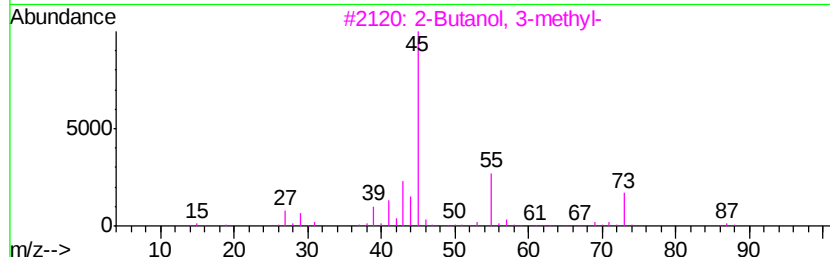
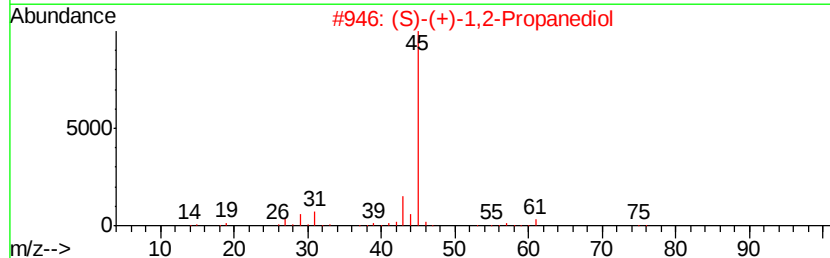
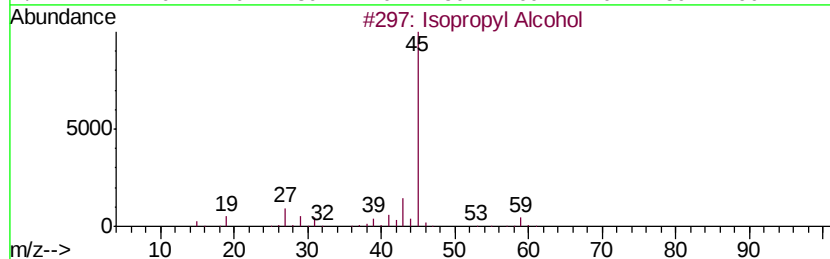
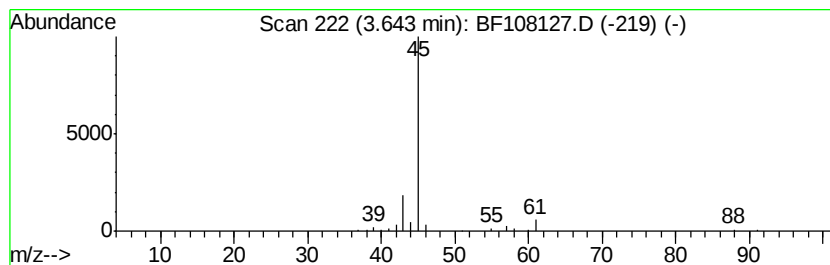
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.64	2.34 ng	145336	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	80
2		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
3		2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9
4		Butane, 1-methoxy-	88	C5H12O	000628-28-4	9
5		2-Methoxyisopropyl cyanoacetate	157	C7H11NO3	032804-79-8	9



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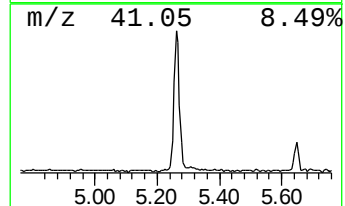
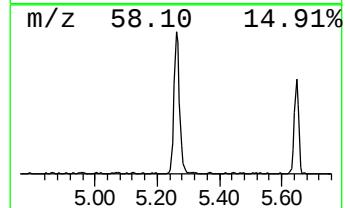
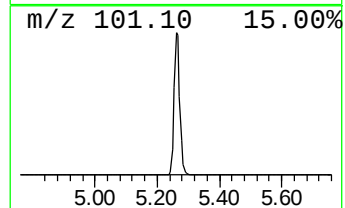
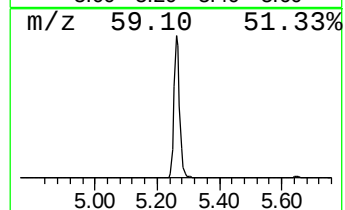
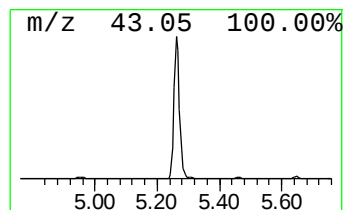
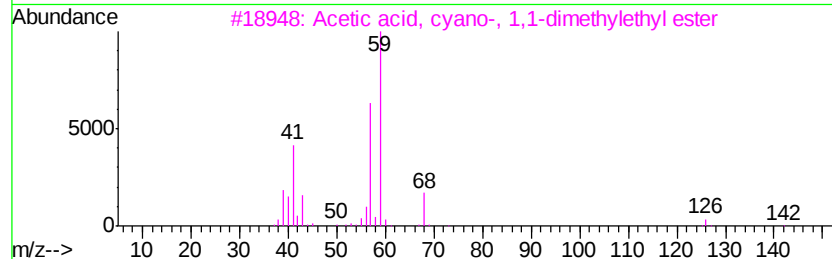
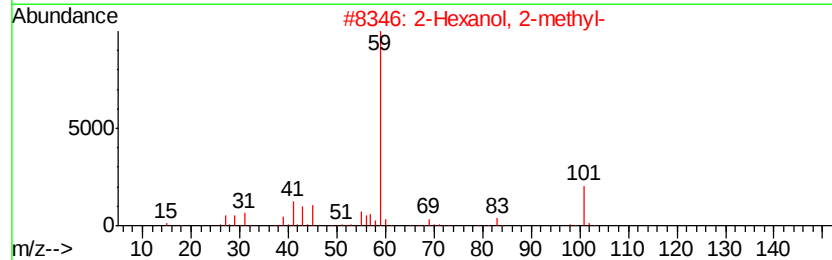
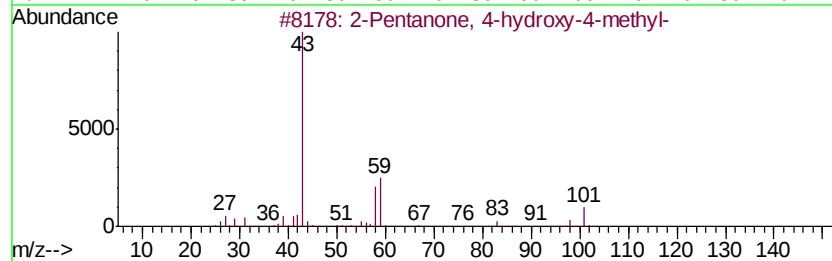
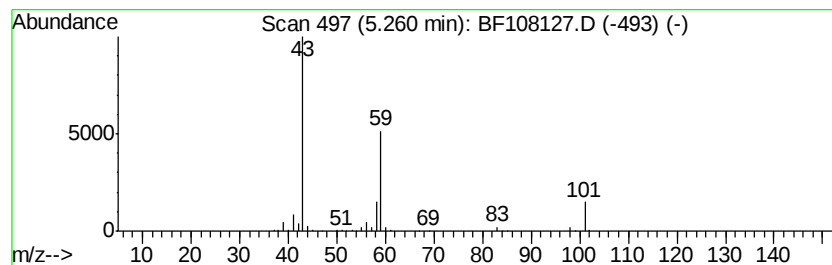
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	15.18 ng	941667	1,4-Dichlorobenzene-d4	7.02

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		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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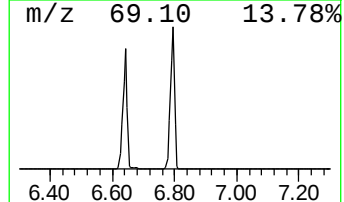
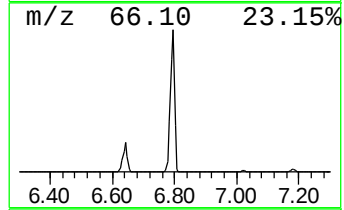
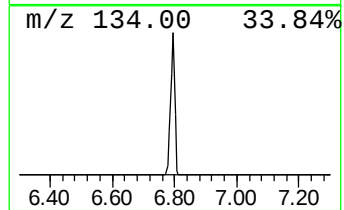
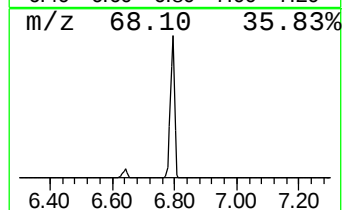
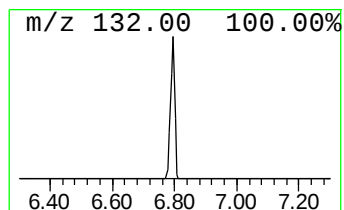
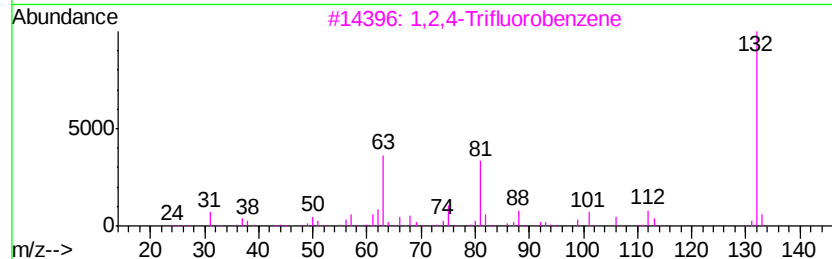
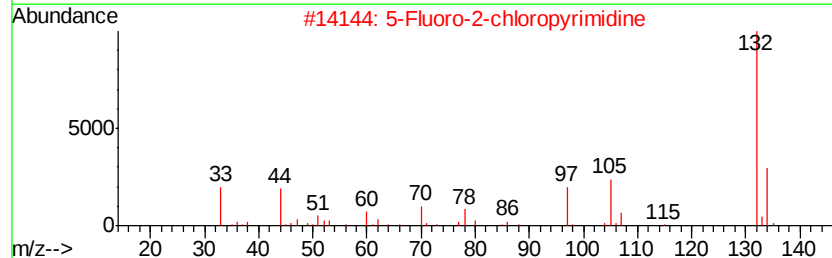
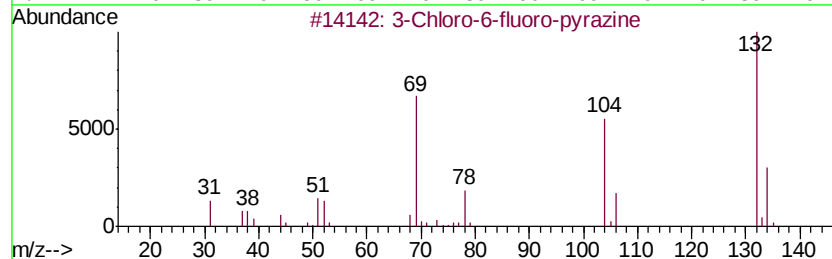
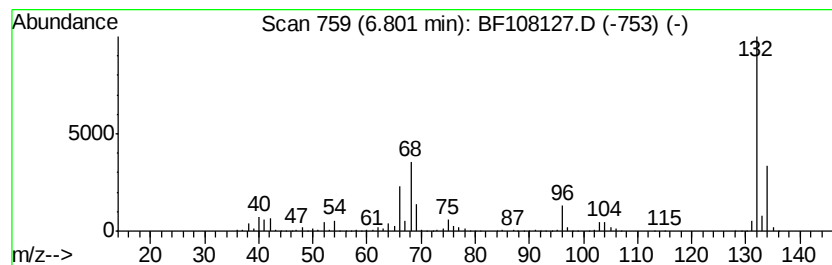
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Peak Number 3 unknown6.80 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.80	75.71 ng	4696560	1,4-Dichlorobenzene-d4	7.02

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		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Xenon	132	Xe	007440-63-3	9



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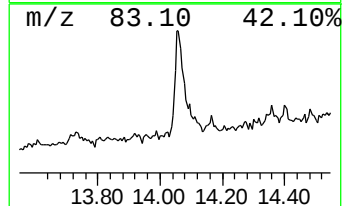
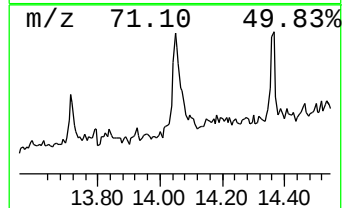
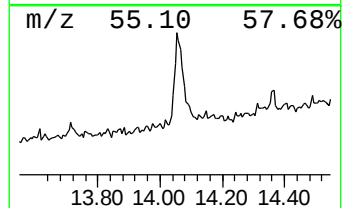
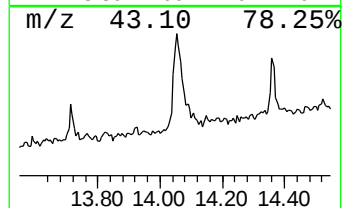
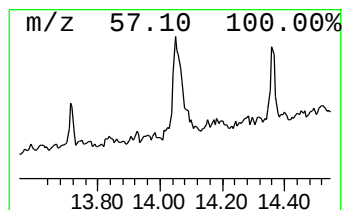
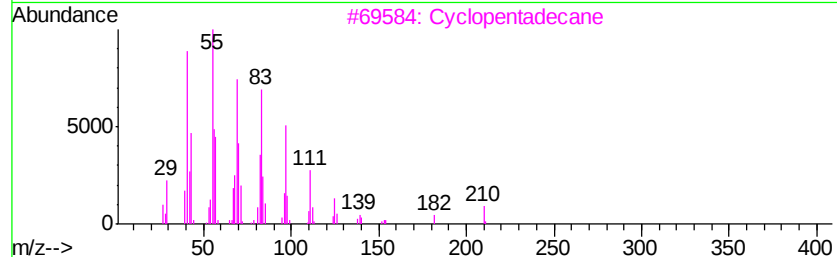
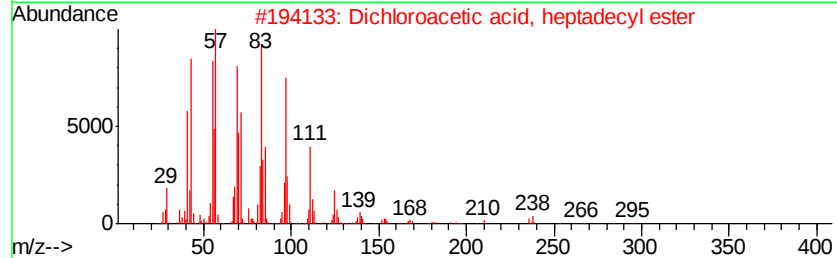
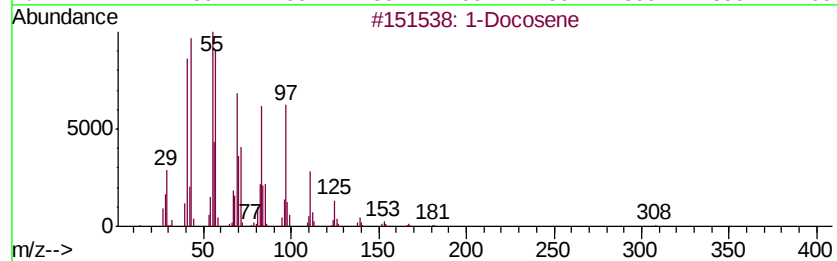
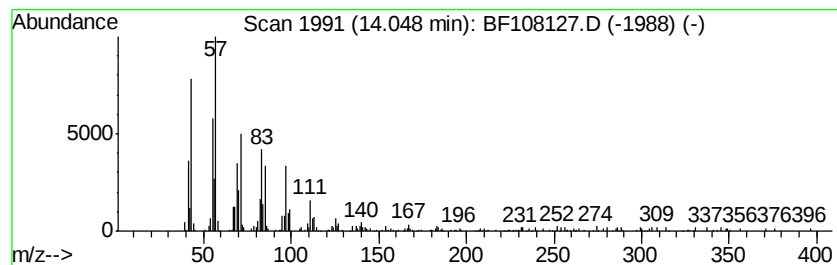
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Peak Number 5 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.05	7.20 ng	430675	Chrysene-d12	14.23
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosene		308 C22H44	001599-67-3 94
2	Dichloroacetic acid, heptadecyl ...		366 C19H36Cl2O2	1000282-98-2 94
3	Cyclopentadecane		210 C15H30	000295-48-7 93
4	Bromoacetic acid, octadecyl ester		390 C20H39BrO2	018992-03-5 93
5	Heptadecyl heptafluorobutyrate		452 C21H35F7O2	959085-66-6 91



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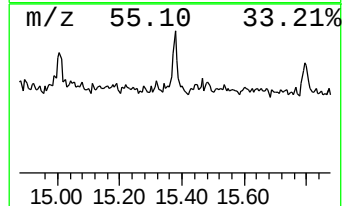
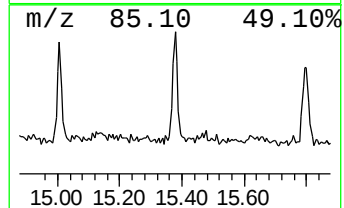
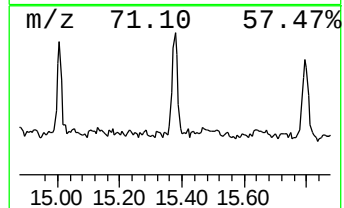
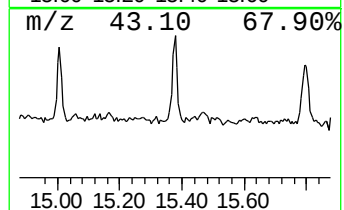
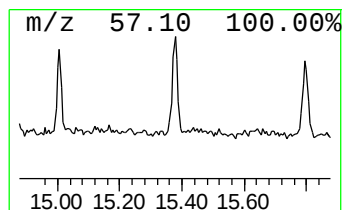
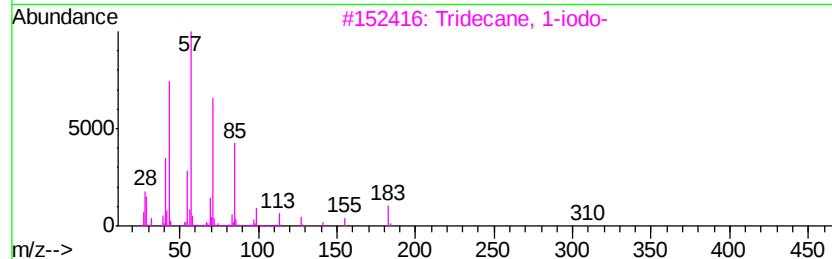
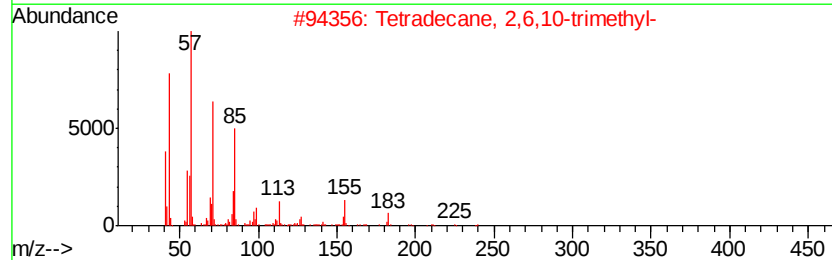
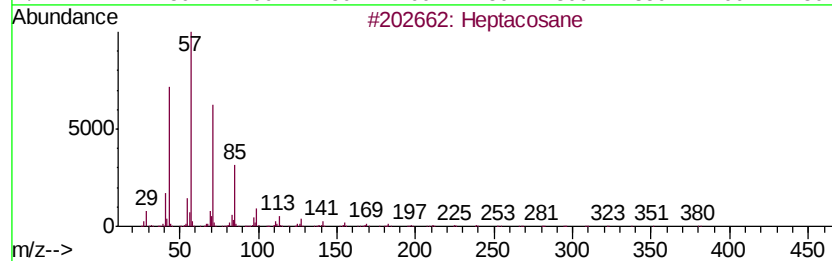
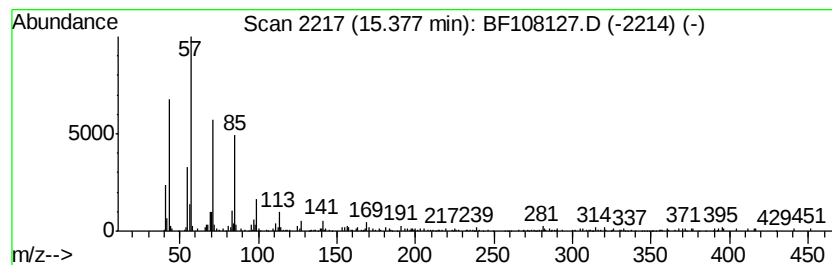
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Peak Number 6 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.38	3.83 ng	177857	Perylene-d12	15.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	96
2	Tetradecane, 2,6,10-trimethyl-		240	C17H36	014905-56-7	89
3	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	81
4	Docosane		310	C22H46	000629-97-0	72
5	Heptadecane		240	C17H36	000629-78-7	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	3.64	2.3	ng	145336	1	7.02	1240710	20.0
2-Pentanone, 4-hy...	5.26	15.2	ng	941667	1	7.02	1240710	20.0
unknown6.80	6.80	75.7	ng	4696560	1	7.02	1240710	20.0
1-Docosene	14.05	7.2	ng	430675	5	14.23	1196320	20.0
Heptacosane	15.38	3.8	ng	177857	6	15.81	927653	20.0