

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040618\
 Data File : BF104355.D
 Acq On : 7 Apr 2018 13:21
 Operator : JU/SJ
 Sample : J2255-10
 Misc :
 ALS Vial : 49 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 040418-DBRI-E-U-B

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-BF040618.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	4.998	491	495	500	rVB	162954	162494	3.90%	0.668%
2	5.404	559	564	567	rBV	1282920	1102228	26.45%	4.533%
3	6.416	732	736	747	rVB	862255	708379	17.00%	2.913%
4	6.569	757	762	765	rBV	2193400	2090934	50.18%	8.599%
5	6.804	798	802	807	rVB	942907	874887	21.00%	3.598%
6	6.963	824	829	832	rBV	3042857	3001521	72.04%	12.343%
7	7.369	892	898	901	rBV	2416874	2396875	57.53%	9.857%
8	8.086	1016	1020	1023	rVB	1334491	1103020	26.47%	4.536%
9	9.163	1198	1203	1206	rBV	3991430	4166535	100.00%	17.134%
10	9.551	1266	1269	1273	rBV	191158	175439	4.21%	0.721%
11	9.769	1303	1306	1309	rBV	102228	79584	1.91%	0.327%
12	9.839	1313	1318	1322	rVB2	1369895	1171501	28.12%	4.818%
13	10.269	1384	1391	1394	rBV	114611	103904	2.49%	0.427%
14	10.627	1447	1452	1455	rBV	1666564	1427872	34.27%	5.872%
15	10.745	1469	1472	1482	rVB	100274	99409	2.39%	0.409%
16	11.327	1567	1571	1574	rBV	1109728	902045	21.65%	3.710%
17	12.739	1808	1811	1815	rVB	159047	117419	2.82%	0.483%
18	12.921	1837	1842	1845	rBV	2844751	2867720	68.83%	11.793%
19	13.445	1928	1931	1934	rBV	96592	73756	1.77%	0.303%
20	13.810	1990	1993	2003	rBV	190260	204140	4.90%	0.839%
21	13.968	2016	2020	2023	rBV	907070	784489	18.83%	3.226%
22	15.421	2262	2267	2271	rBV	591420	702952	16.87%	2.891%

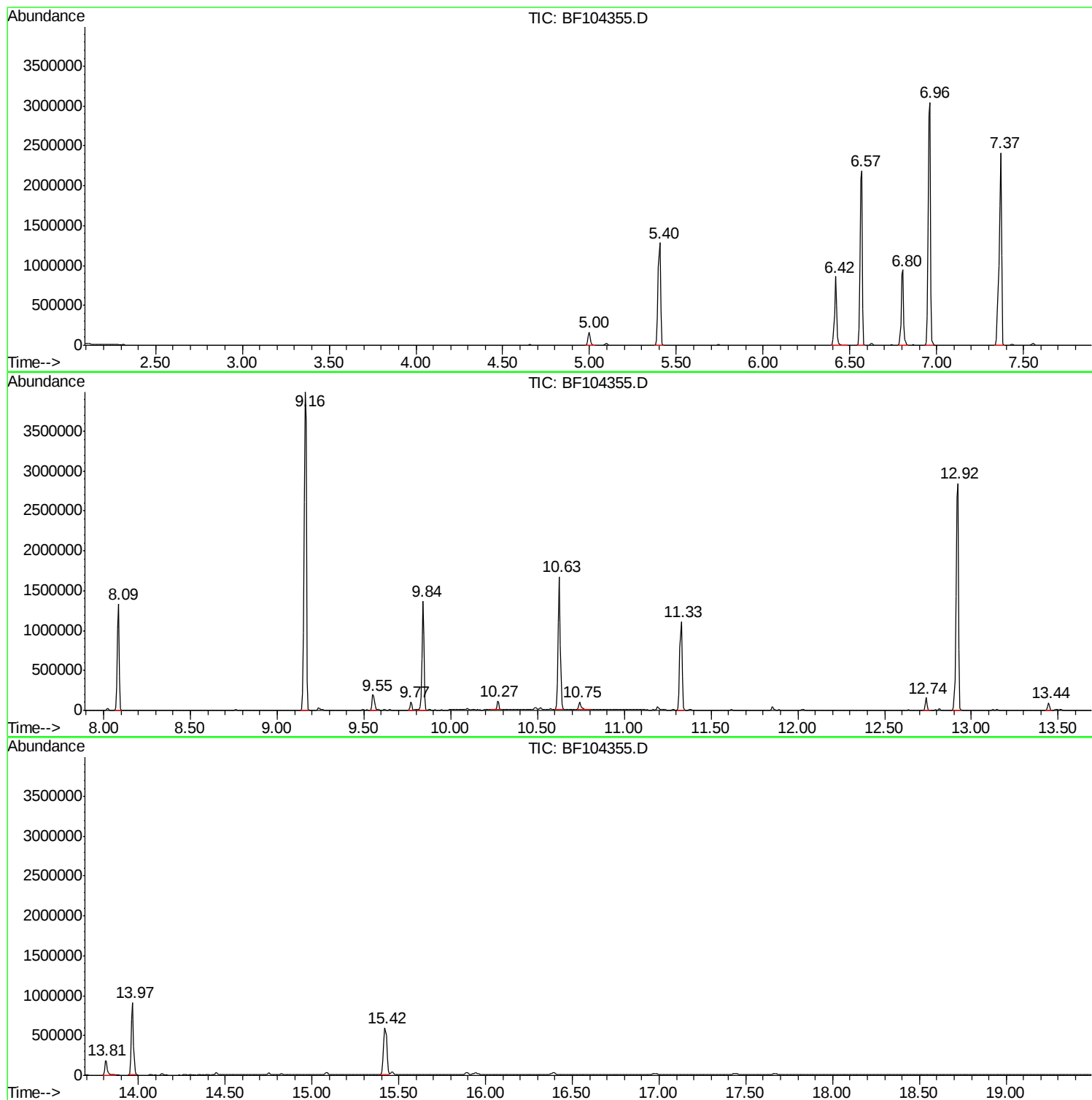
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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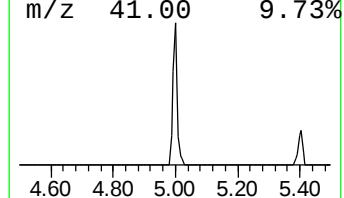
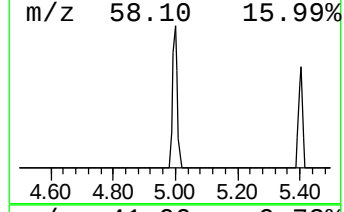
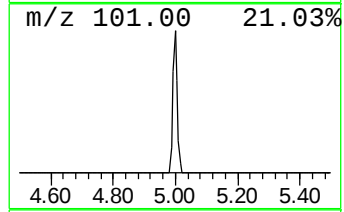
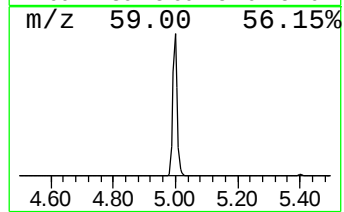
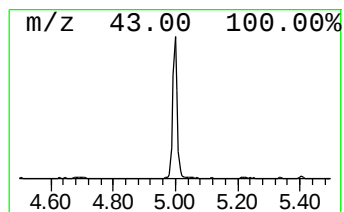
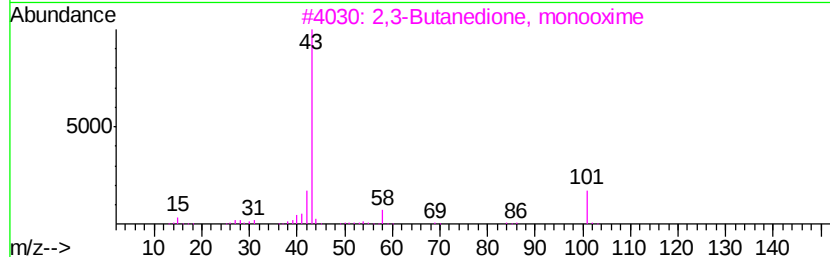
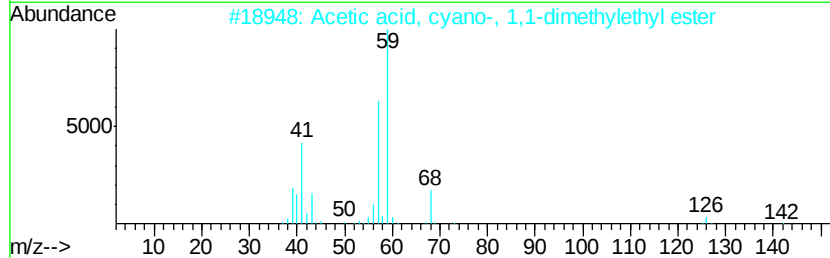
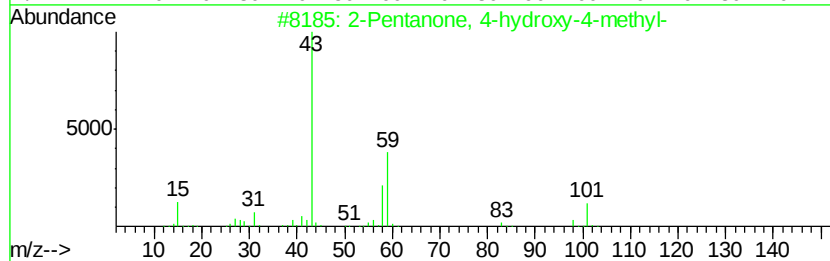
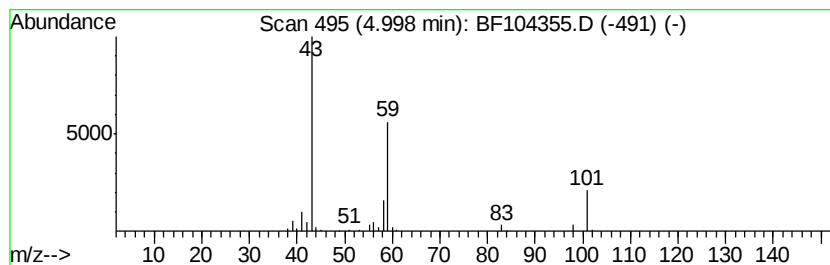
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	3.71 ng	162494	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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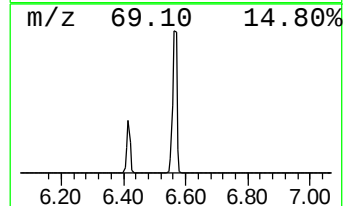
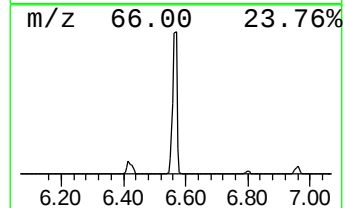
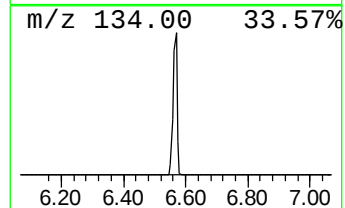
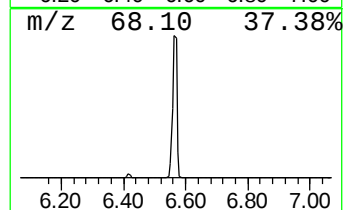
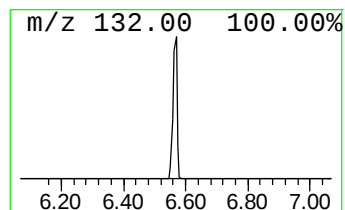
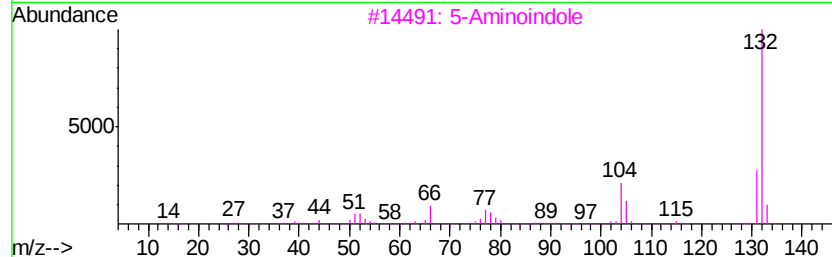
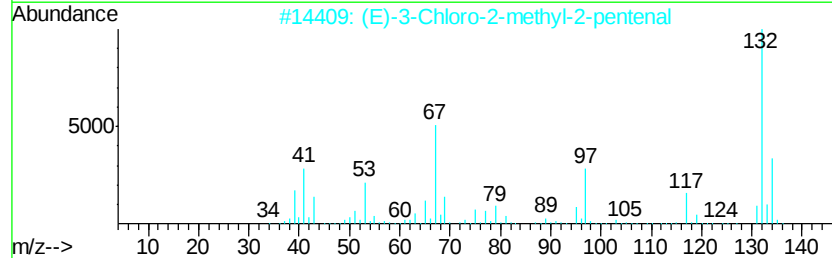
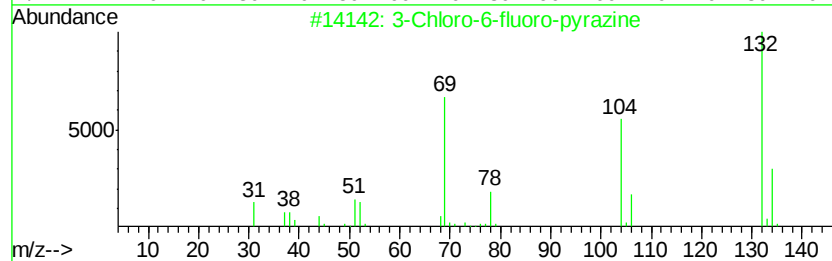
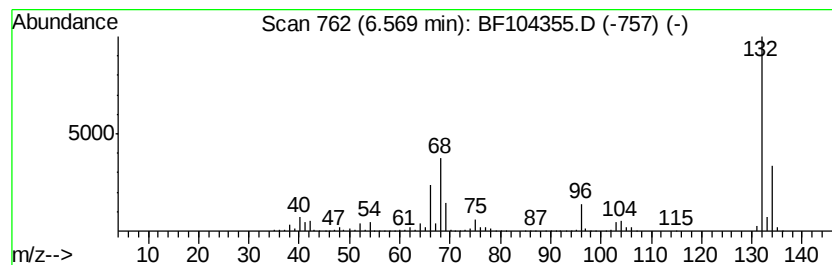
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	47.80 ng	2090930	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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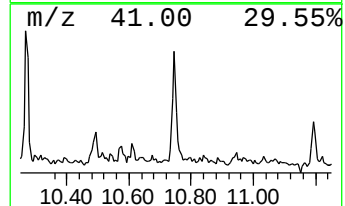
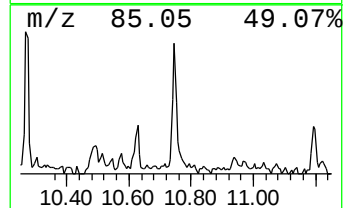
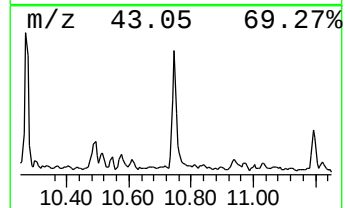
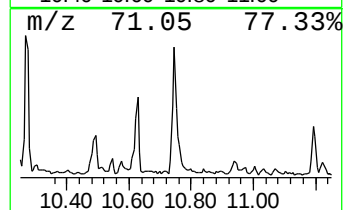
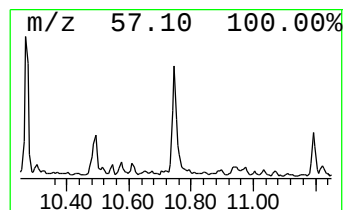
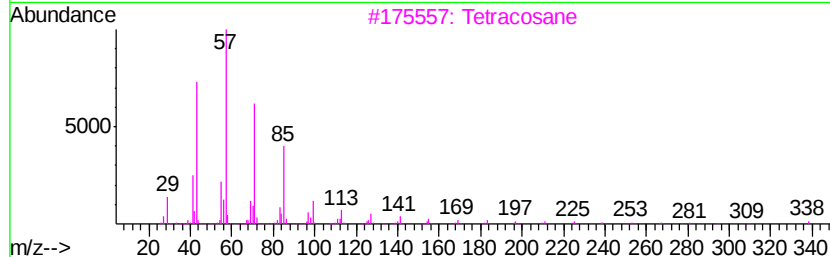
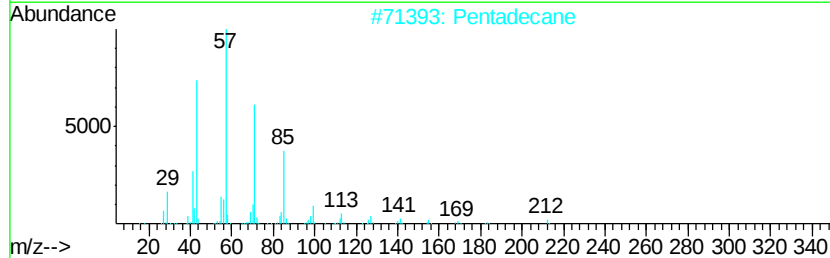
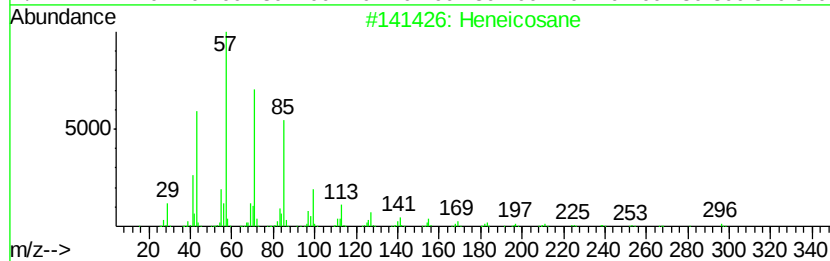
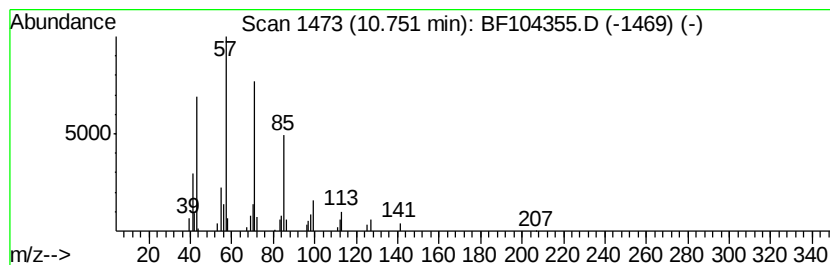
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Peak Number 4 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.20 ng	99409	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Pentadecane		212	C15H32	000629-62-9	91
3	Tetracosane		338	C24H50	000646-31-1	91
4	Octadecane		254	C18H38	000593-45-3	90
5	Hexadecane		226	C16H34	000544-76-3	90



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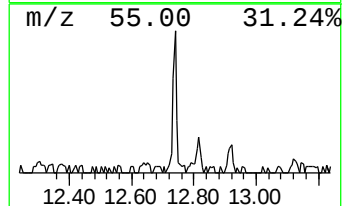
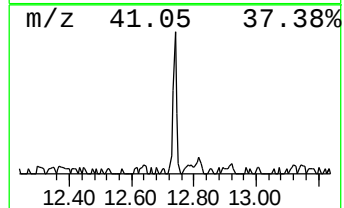
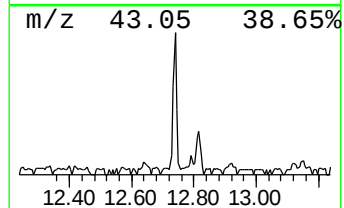
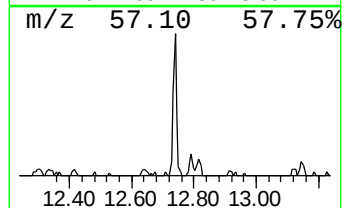
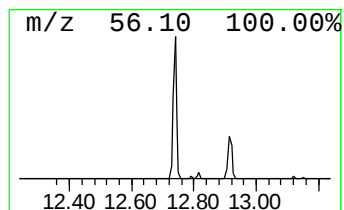
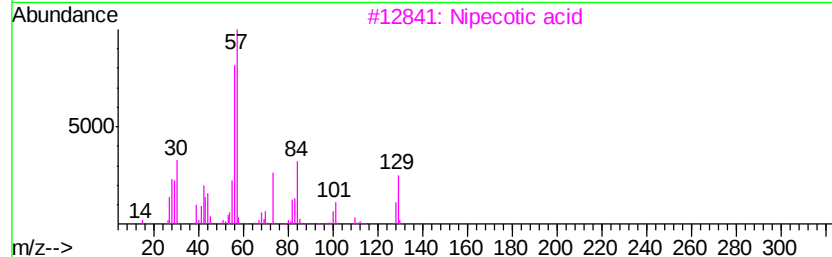
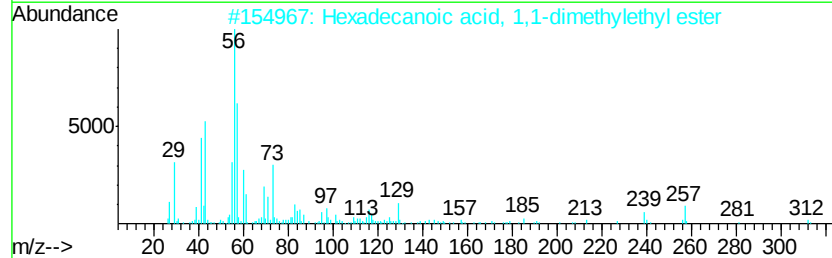
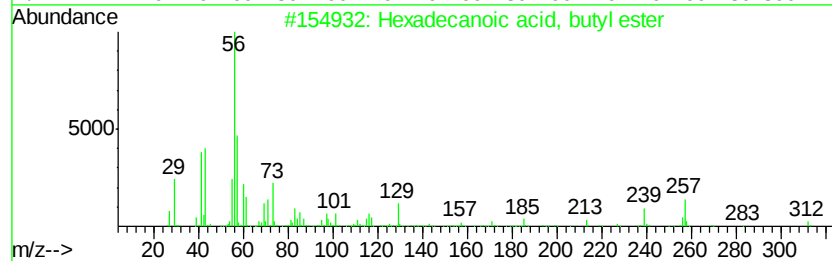
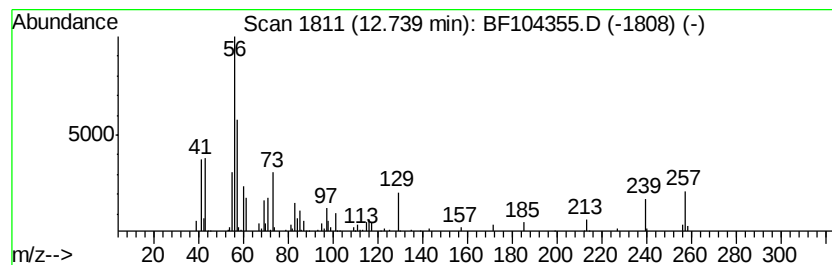
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.99 ng	117419	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3		Nipecotic acid	129	C6H11NO2	000498-95-3	47
4		Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	32
5		Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	27



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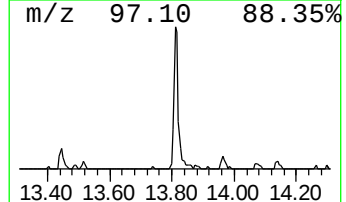
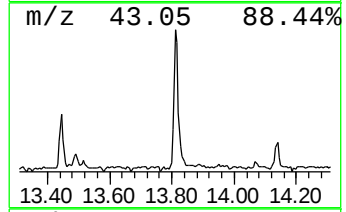
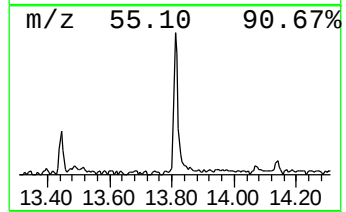
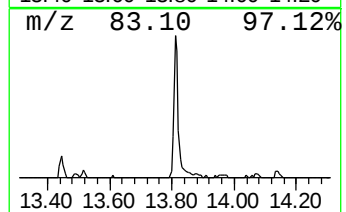
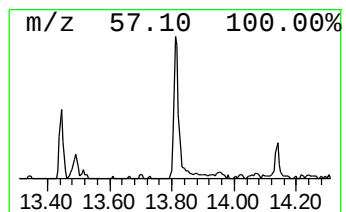
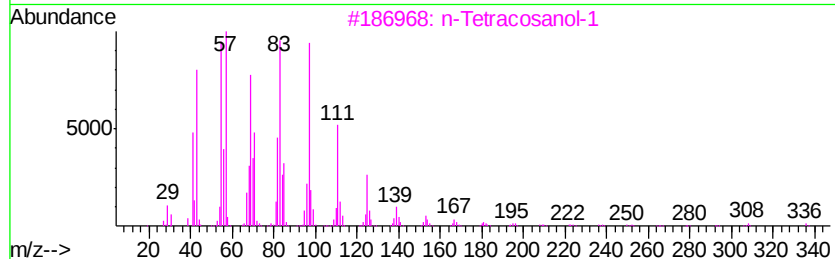
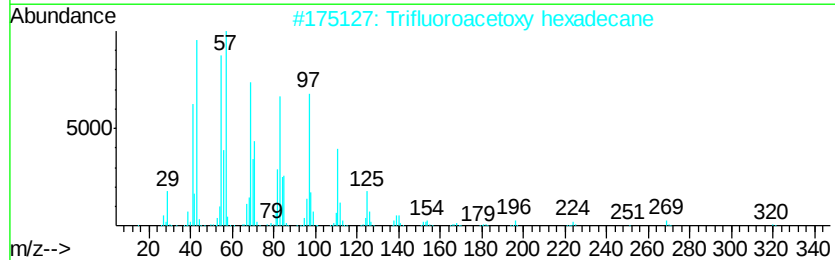
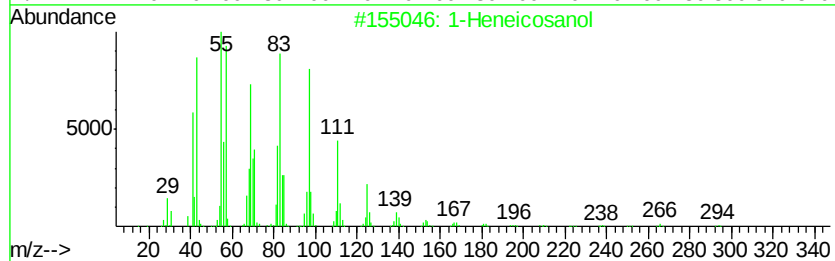
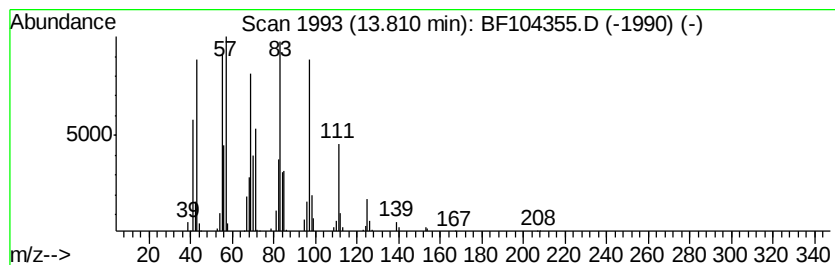
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Peak Number 6 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.81	5.20 ng	204140	Chrysene-d12	13.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetox y hexadecane	338	C18H33F3O2	006222-03-3	93
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	1-Nonadecene	266	C19H38	018435-45-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	3.7	ng	162494	1	6.80	874887	20.0
unknown6.57	6.57	47.8	ng	2090930	1	6.80	874887	20.0
Heneicosane	10.75	2.2	ng	99409	4	11.33	902045	20.0
Hexadecanoic acid...	12.74	3.0	ng	117419	5	13.97	784489	20.0
1-Heneicosanol	13.81	5.2	ng	204140	5	13.97	784489	20.0