

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
 Data File : BF104900.D
 Acq On : 27 Apr 2018 23:46
 Operator : JU/SJ
 Sample : J2549-05
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

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-BF040618.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

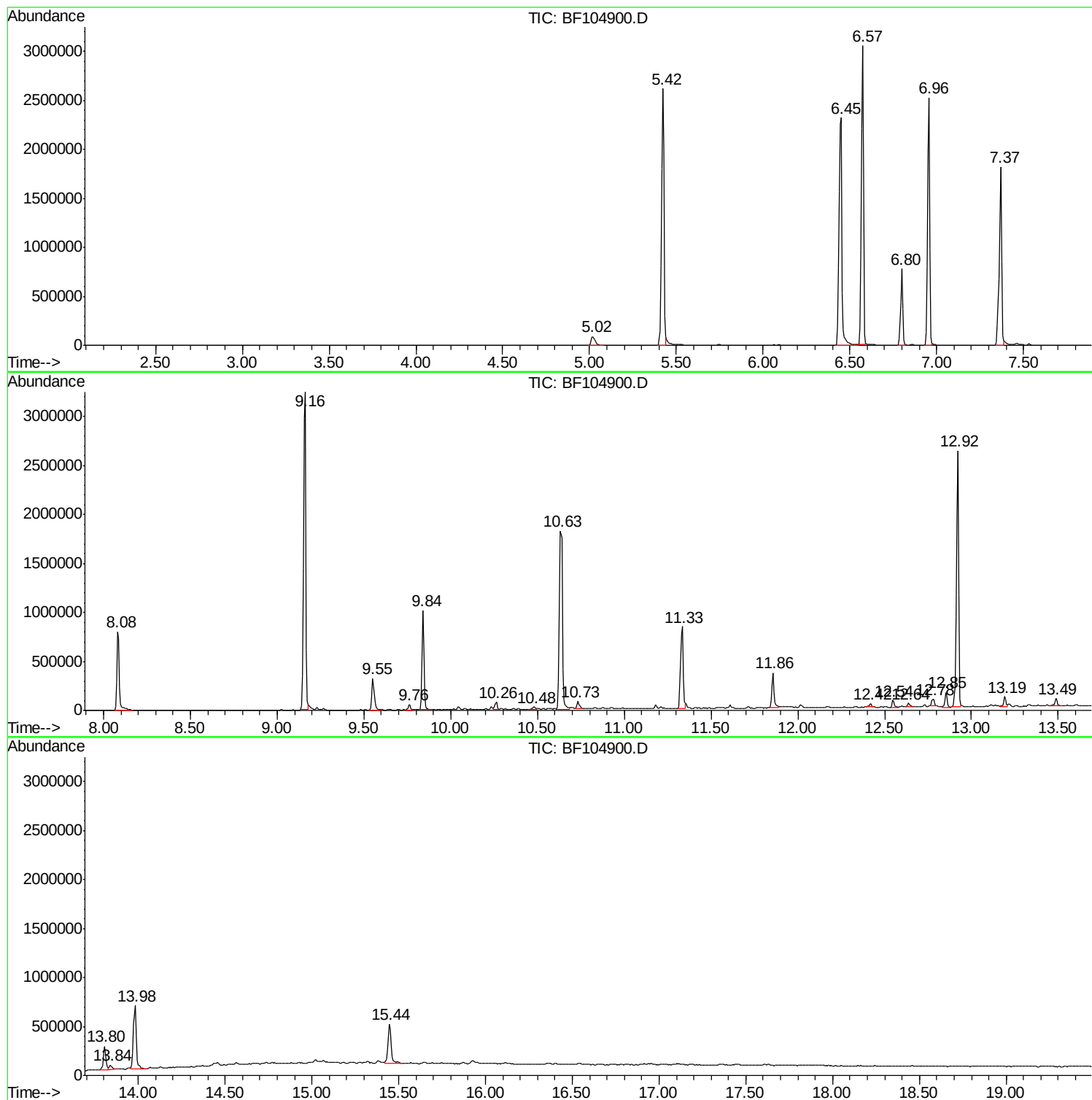
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	494	498	509	rBV	88420	132136	4.25%	0.504%
2	5.422	562	567	570	rBV	2619155	2744152	88.34%	10.471%
3	6.451	736	742	758	rBV	2318872	2870732	92.41%	10.954%
4	6.575	758	763	766	rBV	3052592	2895702	93.21%	11.049%
5	6.798	797	801	805	rBV	775179	605057	19.48%	2.309%
6	6.957	823	828	831	rBV	2527835	2291459	73.76%	8.743%
7	7.369	893	898	901	rBV	1823123	1768103	56.92%	6.746%
8	8.080	1016	1019	1034	rBV	801519	820839	26.42%	3.132%
9	9.163	1198	1203	1206	rBV	3244448	3106508	100.00%	11.853%
10	9.551	1265	1269	1277	rBV	322562	302548	9.74%	1.154%
11	9.763	1301	1305	1309	rBV	54730	49850	1.60%	0.190%
12	9.839	1314	1318	1326	rVB	1016038	892950	28.74%	3.407%
13	10.263	1387	1390	1392	rVB	70377	59633	1.92%	0.228%
14	10.480	1421	1427	1430	rBV	25247	32499	1.05%	0.124%
15	10.633	1449	1453	1462	rBV	1815287	1934619	62.28%	7.382%
16	10.733	1467	1470	1474	rVV	73656	69506	2.24%	0.265%
17	11.333	1568	1572	1575	rBV	836559	807899	26.01%	3.083%
18	11.857	1657	1661	1667	rBV	355003	339072	10.91%	1.294%
19	12.421	1752	1757	1760	rBV2	37132	41426	1.33%	0.158%
20	12.545	1776	1778	1784	rBV	70985	71406	2.30%	0.272%
21	12.639	1791	1794	1798	rBV3	39489	37748	1.22%	0.144%
22	12.780	1815	1818	1821	rVB	66885	58175	1.87%	0.222%
23	12.851	1827	1830	1835	rVB	152697	140971	4.54%	0.538%
24	12.921	1837	1842	1845	rBV	2609804	2444067	78.68%	9.326%
25	13.192	1883	1888	1891	rBV	101934	103235	3.32%	0.394%
26	13.486	1933	1938	1944	rVB3	76198	81130	2.61%	0.310%
27	13.804	1988	1992	1996	rBV	239079	251012	8.08%	0.958%
28	13.839	1996	1998	2004	rVB	43208	47786	1.54%	0.182%
29	13.980	2018	2022	2034	rVB	643747	661433	21.29%	2.524%
30	15.445	2267	2271	2284	rVB	403800	546324	17.59%	2.085%

Sum of corrected areas: 26207977

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



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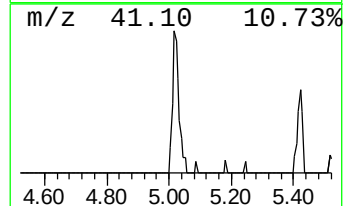
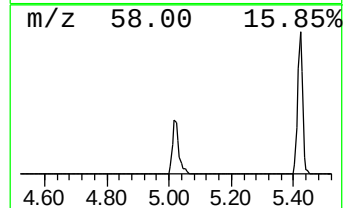
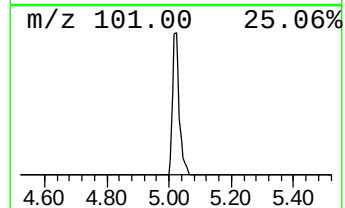
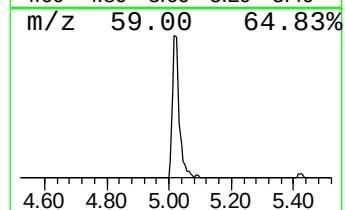
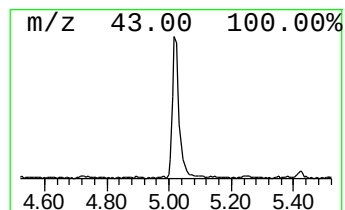
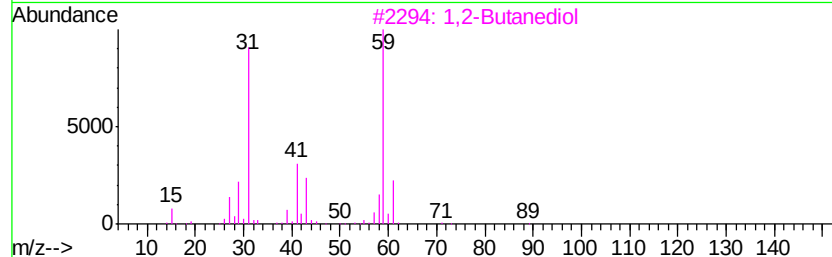
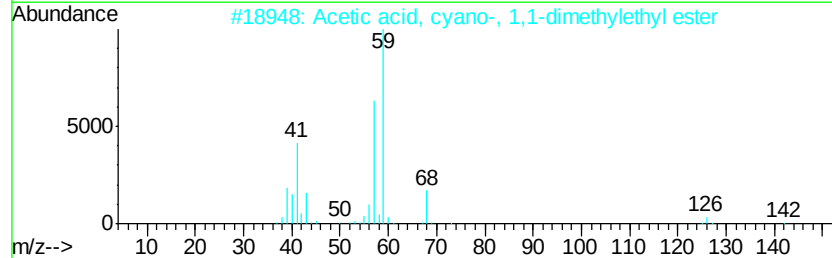
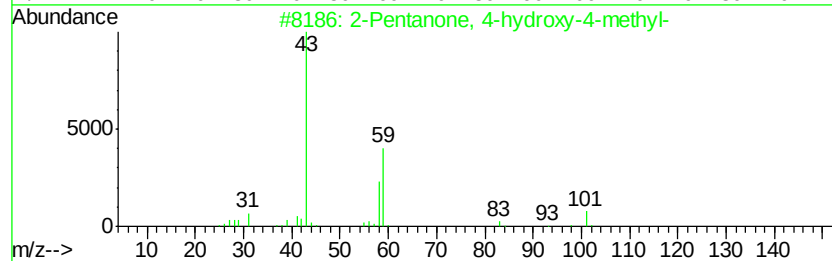
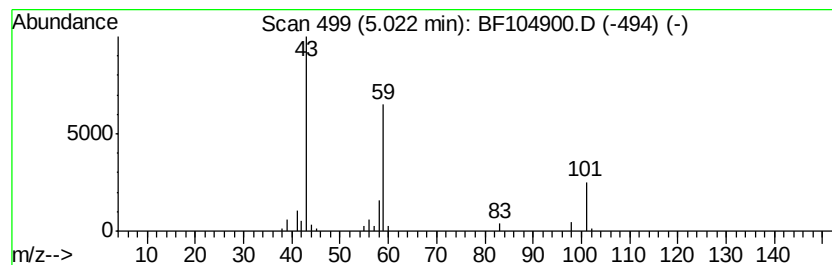
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	4.37 ng	132136	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		1,2-Butanediol	90	C4H10O2	000584-03-2	23
4		Acetone	58	C3H6O	000067-64-1	10
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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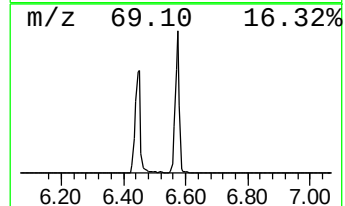
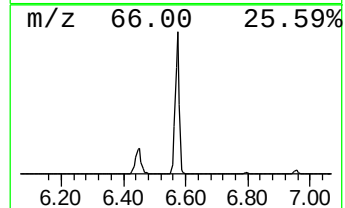
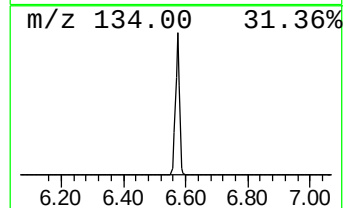
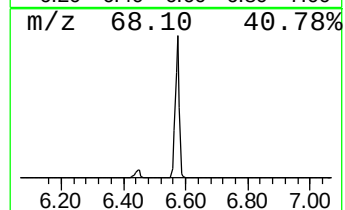
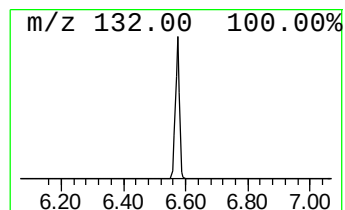
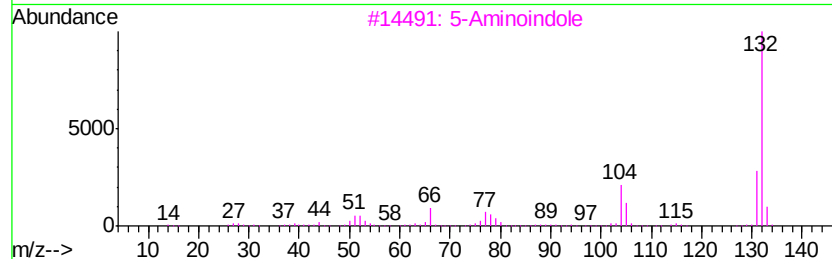
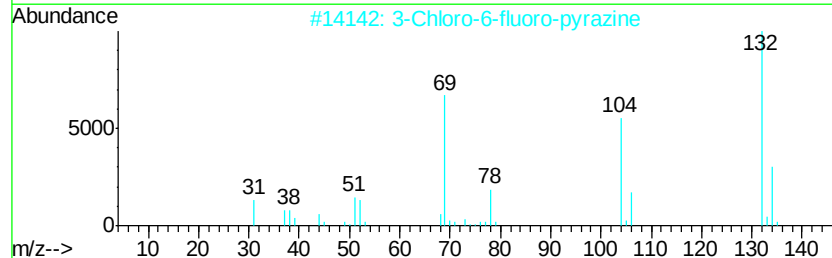
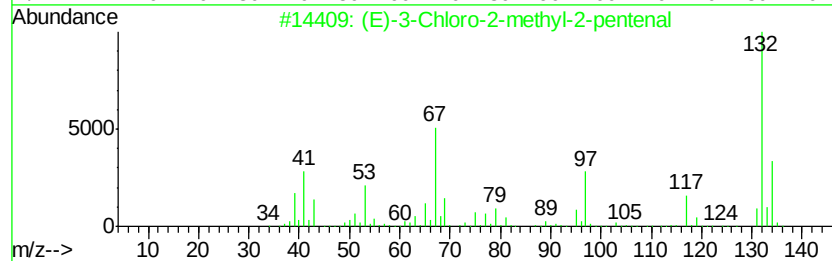
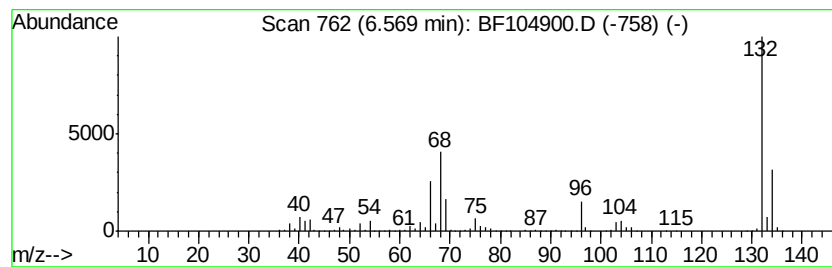
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	95.72 ng	2895700	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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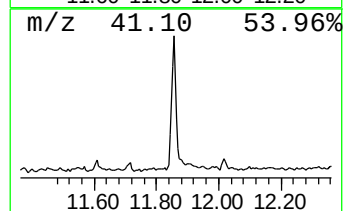
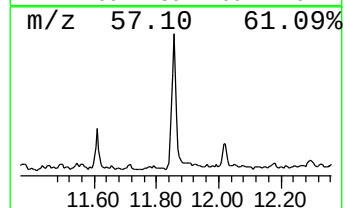
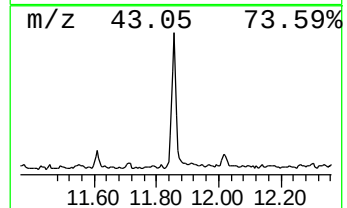
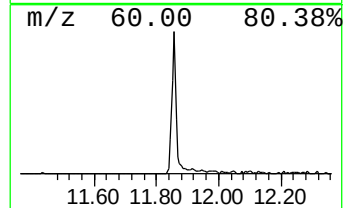
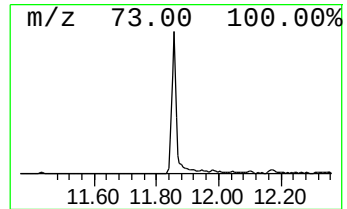
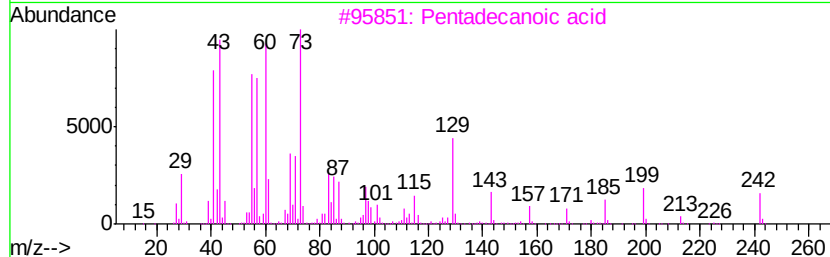
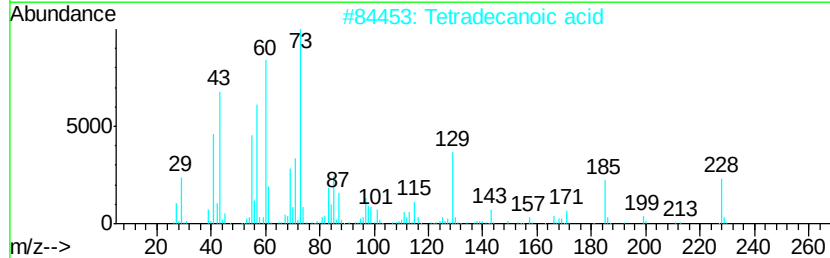
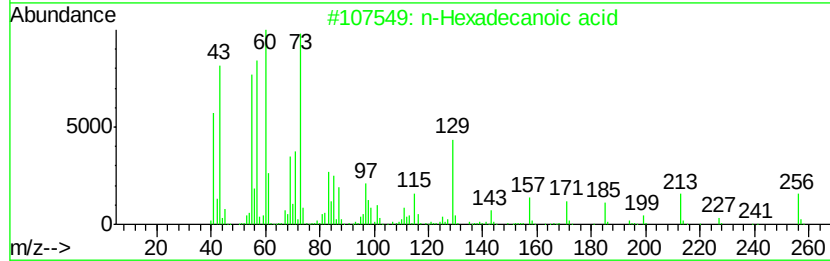
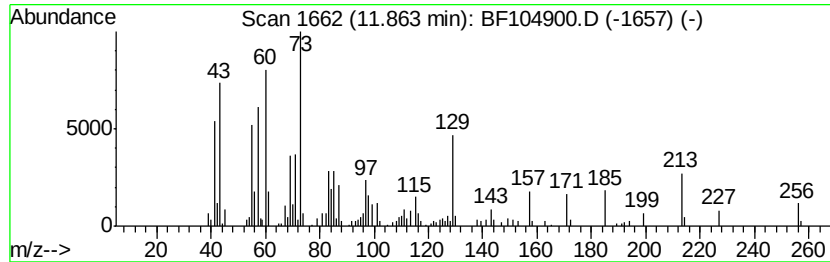
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	8.39 ng	339072	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tridecanoic acid	214	C13H26O2	000638-53-9	86
5		Undecanoic acid	186	C11H22O2	000112-37-8	80



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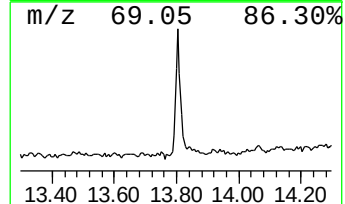
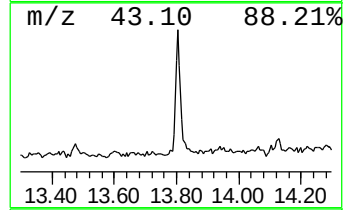
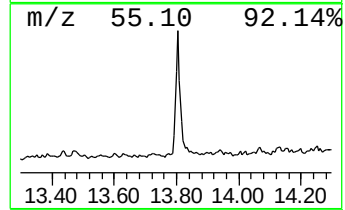
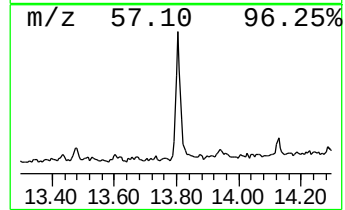
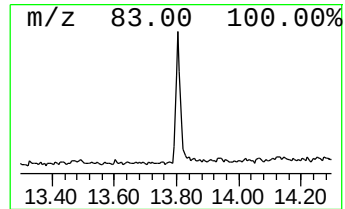
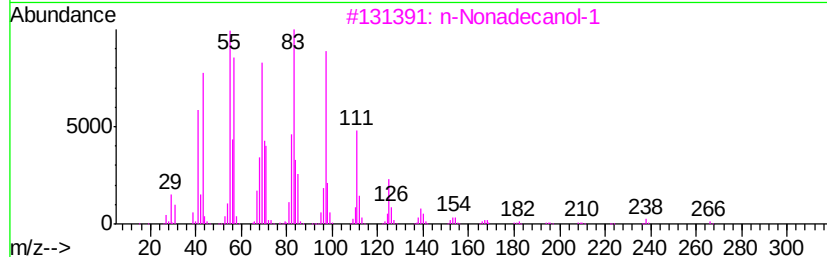
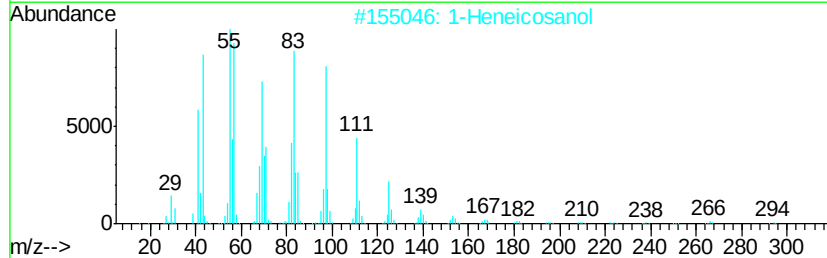
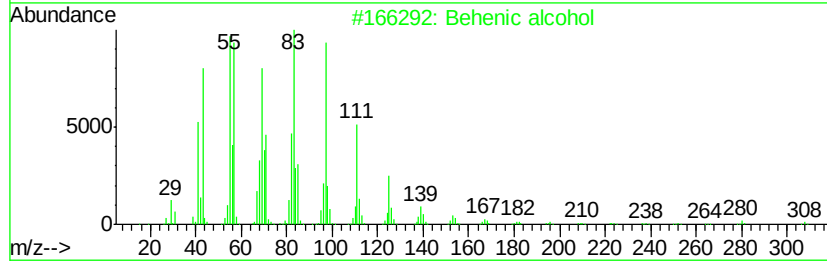
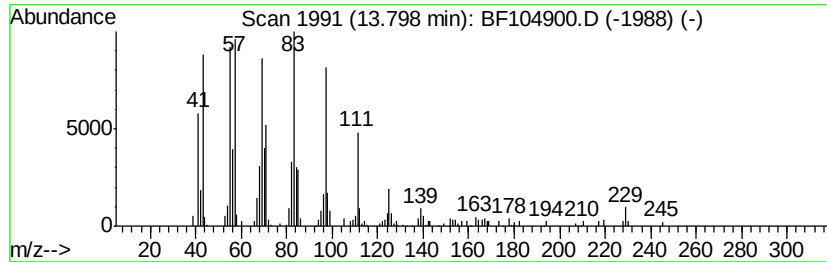
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Peak Number 8 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	7.59 ng	251012	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Behenic alcohol	326	C22H46O	000661-19-8	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
5		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	4.4	ng	132136	1	6.80	605057	20.0
unknown6.57	6.57	95.7	ng	2895700	1	6.80	605057	20.0
n-Hexadecanoic acid	11.86	8.4	ng	339072	4	11.33	807899	20.0
Behenic alcohol	13.80	7.6	ng	251012	5	13.98	661433	20.0