

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040518\
 Data File : BF104288.D
 Acq On : 5 Apr 2018 23:38
 Operator : JU/SJ
 Sample : J2226-06
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 040318-DBRI-E-U-S

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-BF032818.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	2.257	24	29	41	rVB	391491	520907	11.57%	2.184%
2	5.169	521	524	535	rBV	54126	77998	1.73%	0.327%
3	5.593	591	596	614	rBV2	97395	463110	10.29%	1.941%
4	6.610	763	769	784	rBV2	79154	402362	8.94%	1.687%
5	6.716	784	787	812	rVV	977076	1850037	41.11%	7.756%
6	6.951	823	827	848	rBV	173320	517604	11.50%	2.170%
7	7.098	848	852	889	rVB	2051340	2893204	64.29%	12.129%
8	7.516	919	923	945	rBV	1006455	2125624	47.23%	8.911%
9	7.657	945	947	957	rVB3	56121	86472	1.92%	0.363%
10	8.228	1040	1044	1076	rBV	404061	878687	19.52%	3.684%
11	9.298	1222	1226	1260	rBV	3218491	4500553	100.00%	18.868%
12	9.622	1277	1281	1285	rVB	57960	55972	1.24%	0.235%
13	9.686	1286	1292	1299	rBV	153275	221033	4.91%	0.927%
14	9.886	1322	1326	1330	rBV	88569	76723	1.70%	0.322%
15	9.980	1339	1342	1354	rBV	783026	943266	20.96%	3.954%
16	10.386	1408	1411	1414	rBV	121311	90884	2.02%	0.381%
17	10.775	1474	1477	1489	rBV	1054482	1679753	37.32%	7.042%
18	10.863	1489	1492	1503	rVB	107270	179711	3.99%	0.753%
19	11.480	1593	1597	1619	rBV	557143	987342	21.94%	4.139%
20	13.063	1861	1866	1894	rBV	2731088	3561870	79.14%	14.932%
21	13.927	2010	2013	2026	rBV	289905	378611	8.41%	1.587%
22	14.133	2044	2048	2066	rBV	493996	792158	17.60%	3.321%
23	15.668	2304	2309	2325	rVB	290450	569507	12.65%	2.388%

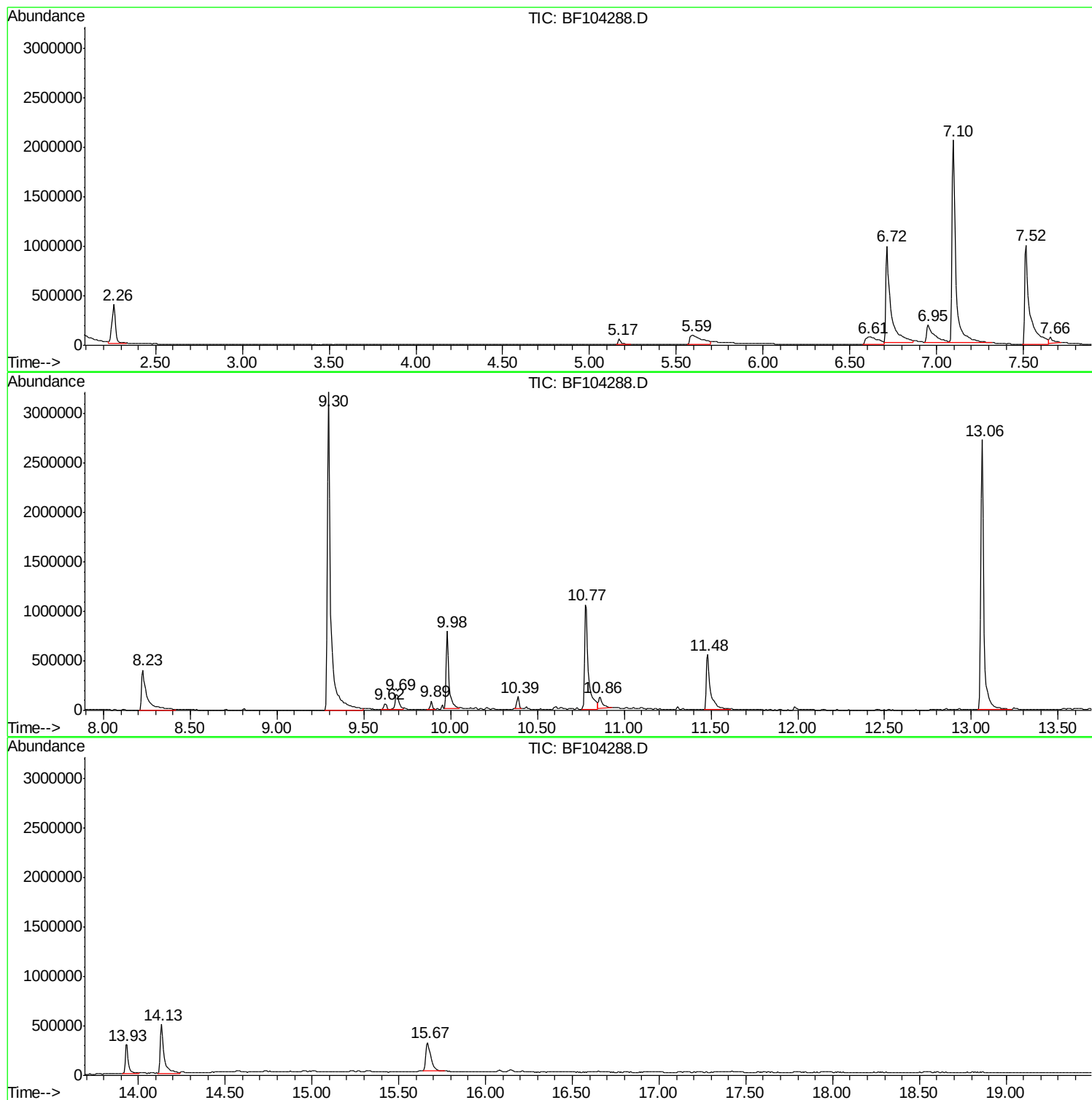
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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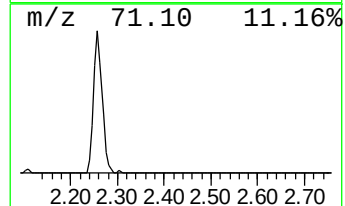
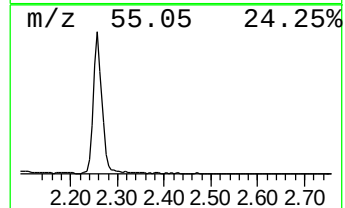
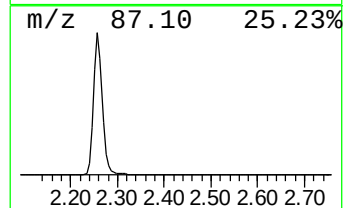
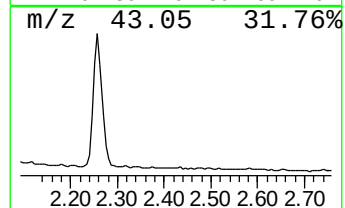
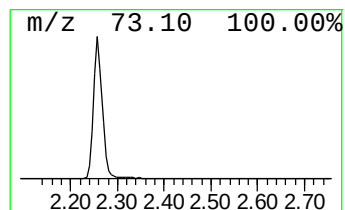
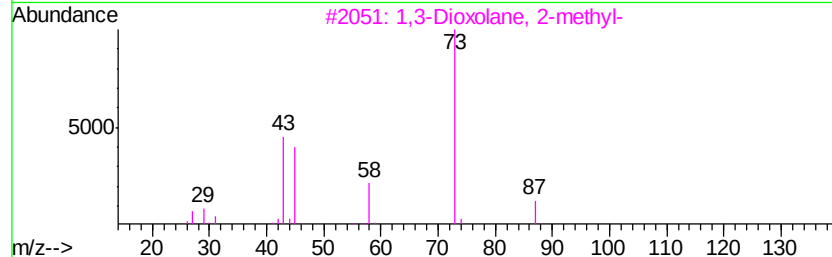
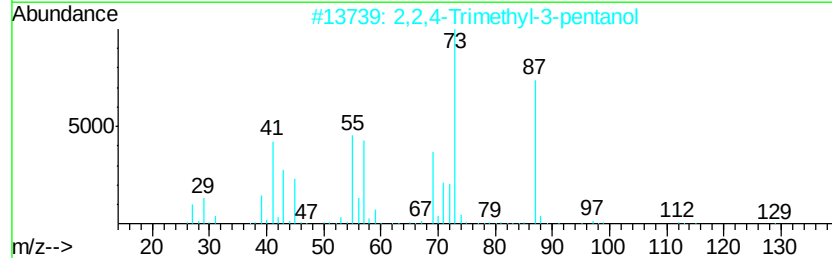
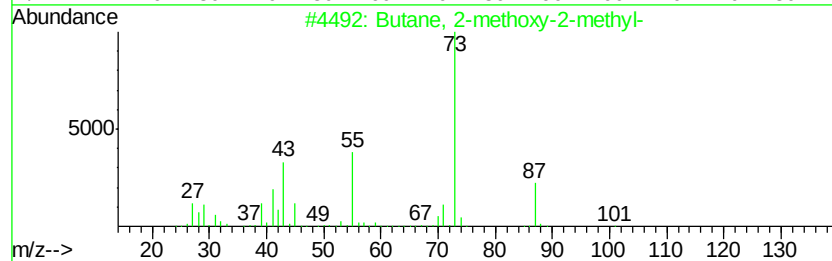
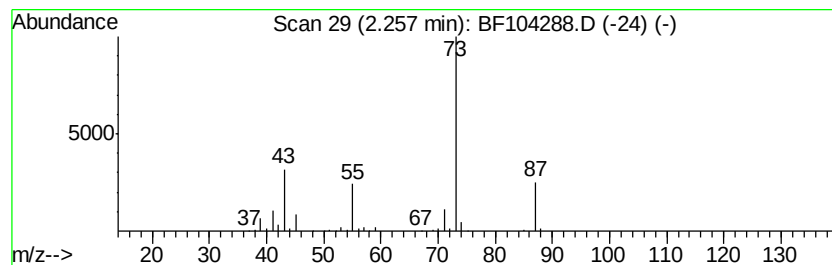
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.26	20.13 ng	520907	1,4-Dichlorobenzene-d4	6.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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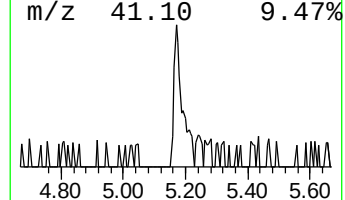
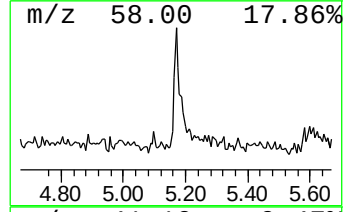
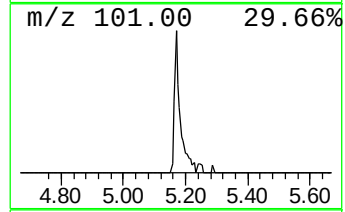
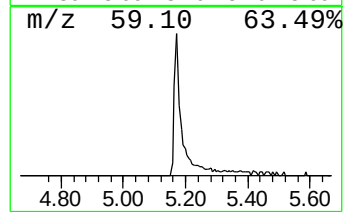
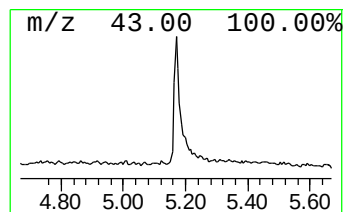
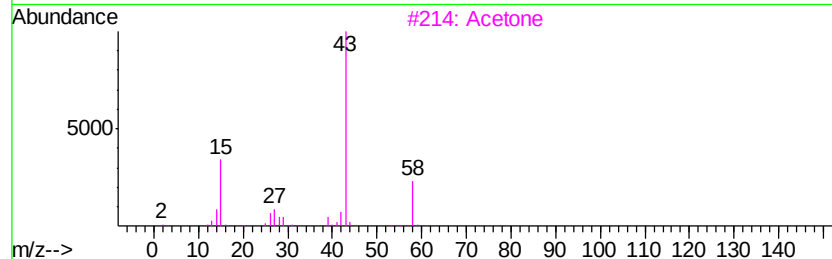
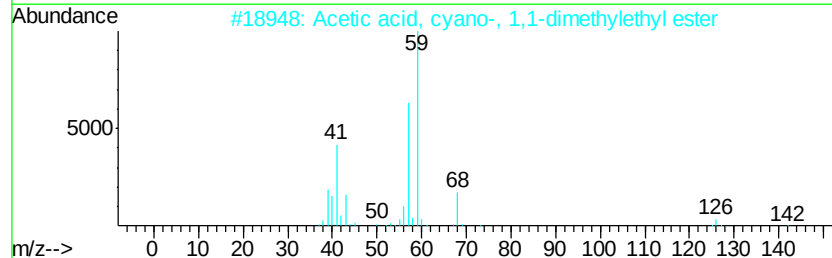
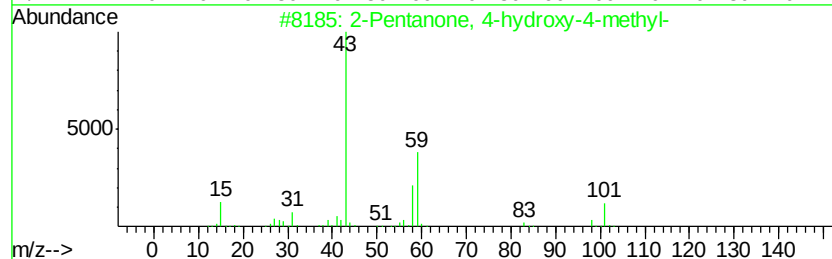
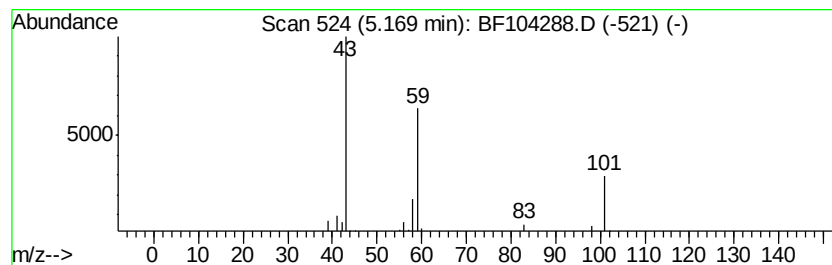
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	3.01 ng	77998	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			Acetone	58	C3H6O	000067-64-1	9
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9



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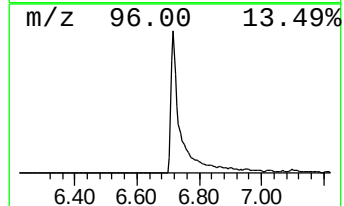
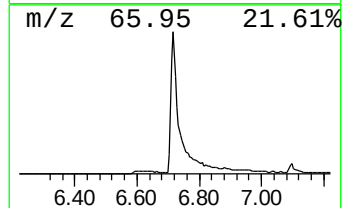
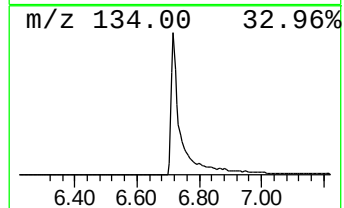
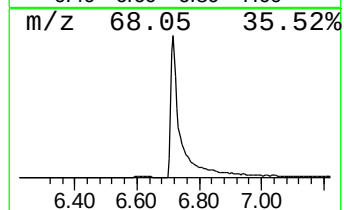
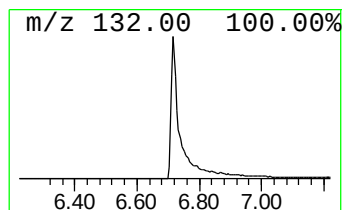
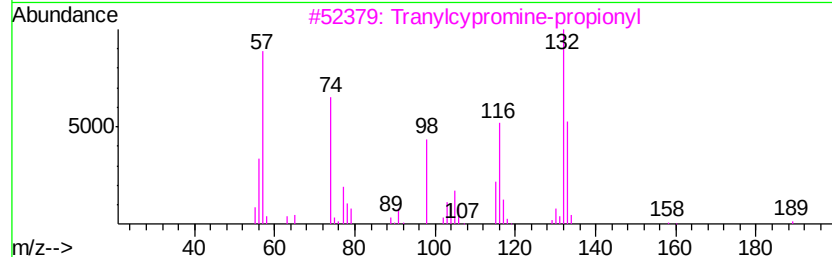
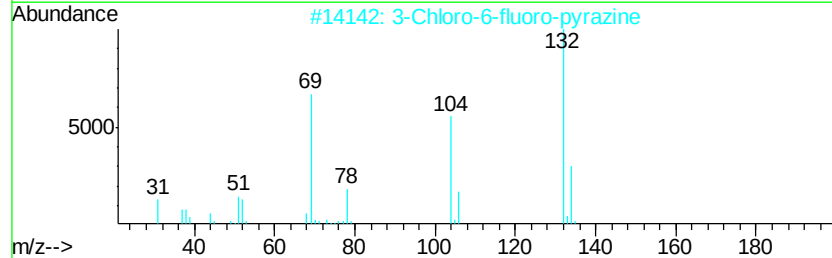
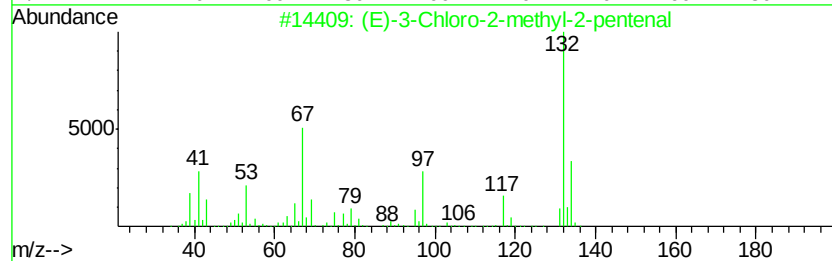
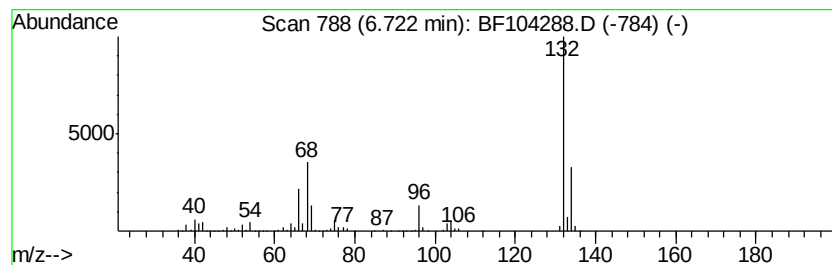
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Peak Number 3 unknown6.72 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	71.48 ng	1850040	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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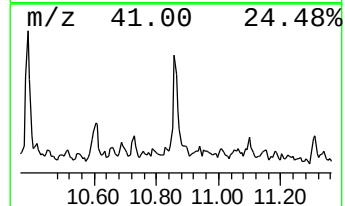
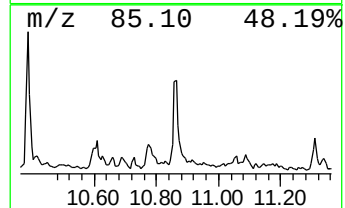
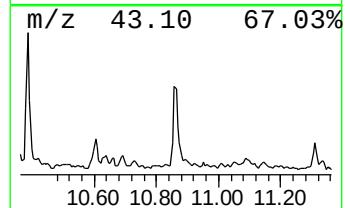
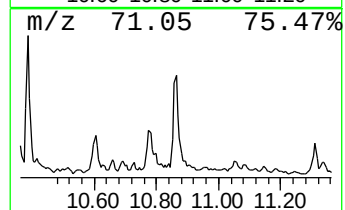
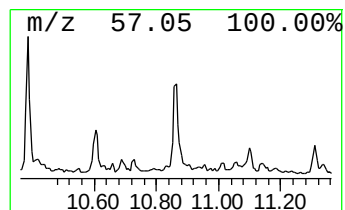
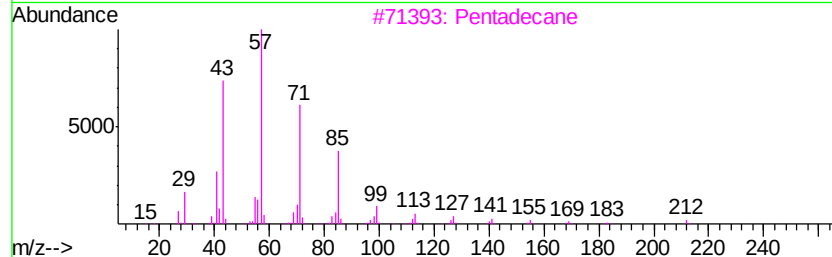
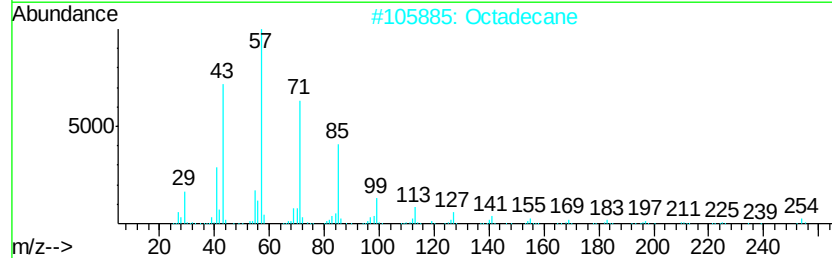
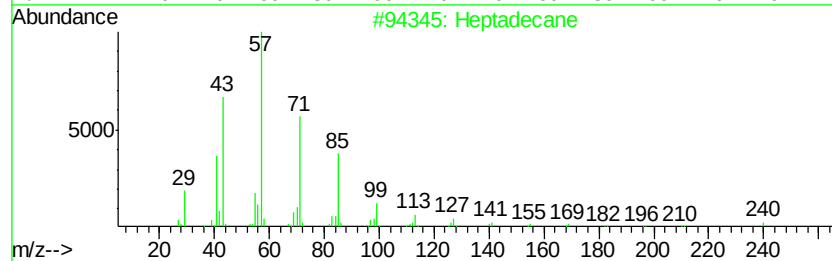
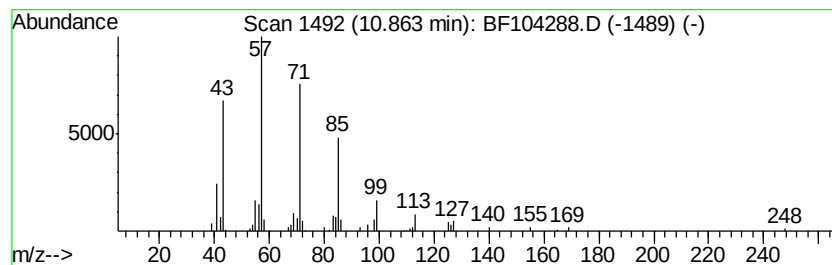
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.86	3.64 ng	179711	Phenanthrene-d10		11.48
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	86
2	Octadecane	254	C18H38	000593-45-3	86
3	Pentadecane	212	C15H32	000629-62-9	86
4	Octacosane	394	C28H58	000630-02-4	86
5	Hexadecane	226	C16H34	000544-76-3	86



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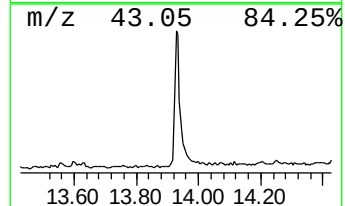
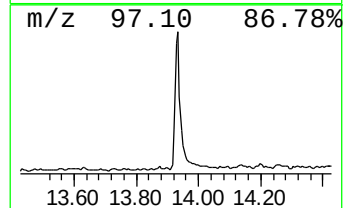
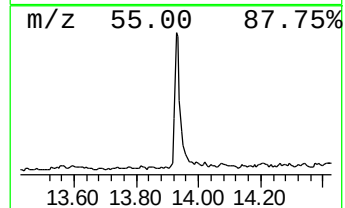
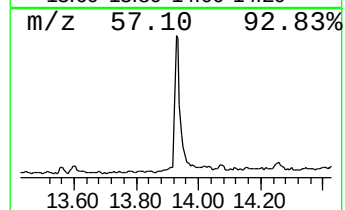
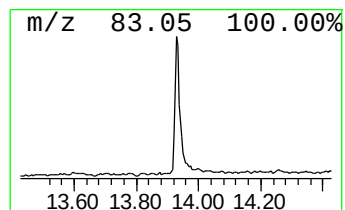
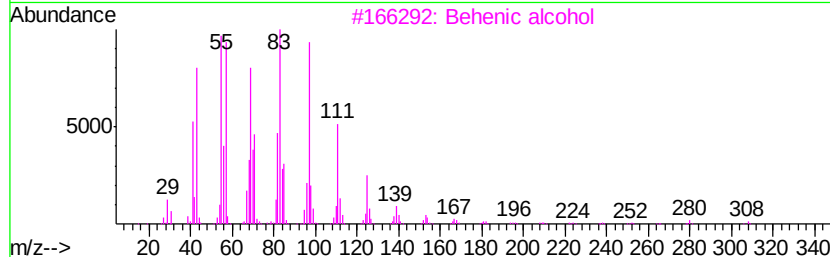
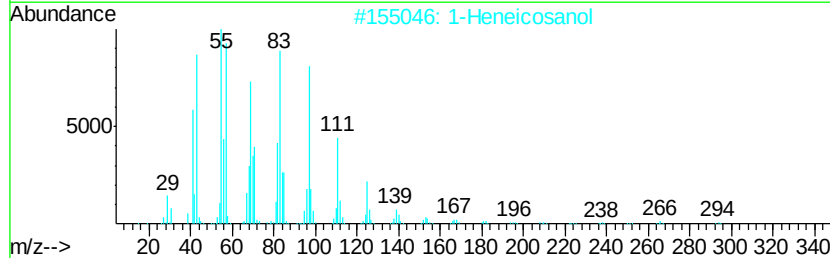
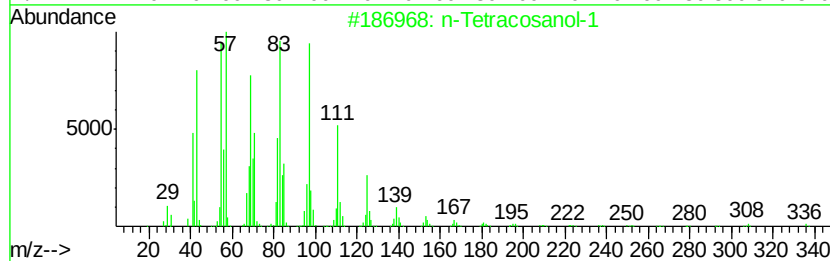
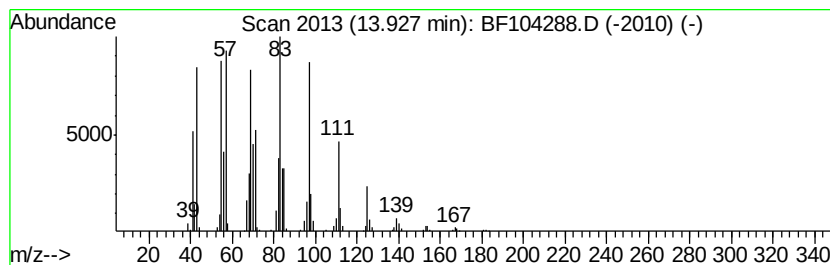
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Peak Number 6 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.93	9.56 ng	378611	Chrysene-d12		14.13
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.26	20.1	ng	520907	1	6.95	517604	20.0
2-Pentanone, 4-hy...	5.17	3.0	ng	77998	1	6.95	517604	20.0
unknown6.72	6.72	71.5	ng	1850040	1	6.95	517604	20.0
Heptadecane	10.86	3.6	ng	179711	4	11.48	987342	20.0
n-Tetracosanol-1	13.93	9.6	ng	378611	5	14.13	792158	20.0