

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020618\
 Data File : BF102791.D
 Acq On : 6 Feb 2018 18:29
 Operator : SJ/JU
 Sample : J1460-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B1

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-BF020318.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	2.193	11	18	25	rVB	466360	625107	12.30%	1.533%
2	5.122	513	516	525	rVB	120341	164062	3.23%	0.402%
3	5.504	576	581	584	rBV	4703209	5046751	99.30%	12.378%
4	6.510	746	752	755	rBV	4264835	5082467	100.00%	12.465%
5	6.651	771	776	780	rBV	4603376	4856516	95.55%	11.911%
6	6.880	811	815	819	rBV	1509542	1248721	24.57%	3.063%
7	7.039	838	842	845	rBV	4050508	3650135	71.82%	8.952%
8	7.445	905	911	914	rBV	2968465	2906000	57.18%	7.127%
9	8.163	1029	1033	1037	rBV	1836709	1596939	31.42%	3.917%
10	9.239	1211	1216	1219	rBV	4795094	4531566	89.16%	11.114%
11	9.627	1278	1282	1285	rBV	467368	417011	8.20%	1.023%
12	9.845	1316	1319	1323	rVB	181833	144191	2.84%	0.354%
13	9.921	1328	1332	1336	rVV	1704079	1507557	29.66%	3.697%
14	10.345	1401	1404	1407	rVB	195909	150996	2.97%	0.370%
15	10.563	1436	1441	1444	rBV	52769	66246	1.30%	0.162%
16	10.710	1459	1466	1469	rBV	2180493	2065602	40.64%	5.066%
17	10.816	1481	1484	1493	rVB	154728	155237	3.05%	0.381%
18	11.263	1558	1560	1563	rBV	60283	53346	1.05%	0.131%
19	11.410	1581	1585	1588	rBV	1226125	1151020	22.65%	2.823%
20	11.927	1670	1673	1678	rBV	71122	80141	1.58%	0.197%
21	12.992	1849	1854	1857	rBV	3150042	2877506	56.62%	7.057%
22	13.874	2001	2004	2008	rBV	409314	373846	7.36%	0.917%
23	14.045	2029	2033	2039	rVB	1214186	1060400	20.86%	2.601%
24	15.527	2280	2285	2291	rBV	718386	961585	18.92%	2.358%

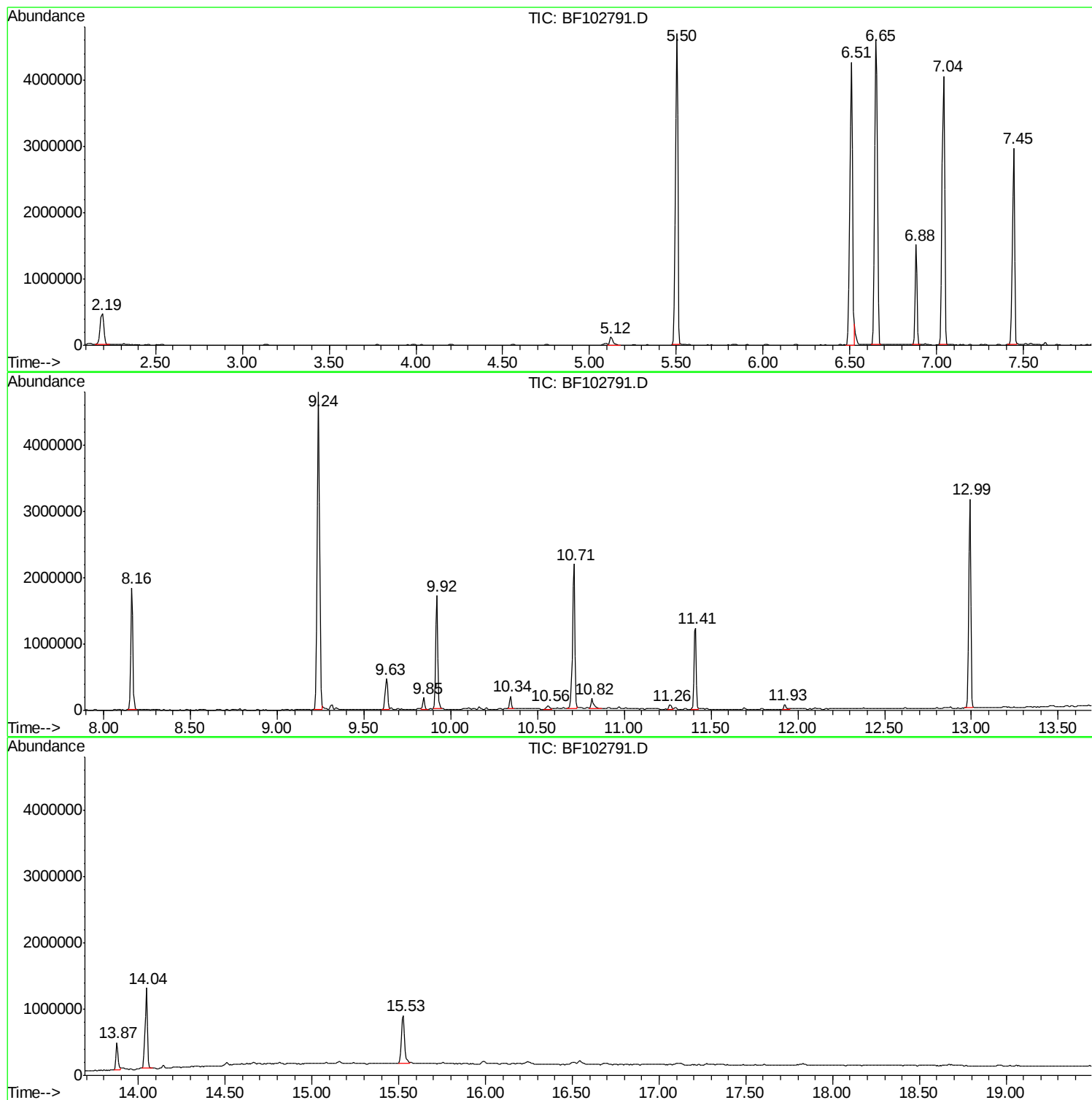
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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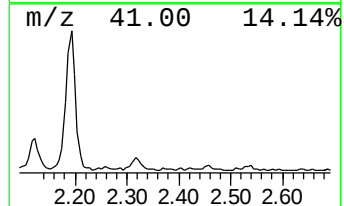
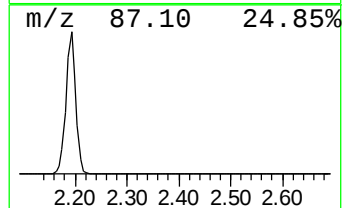
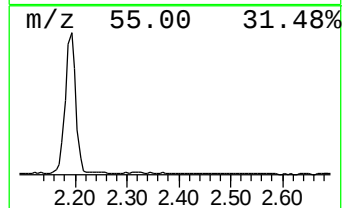
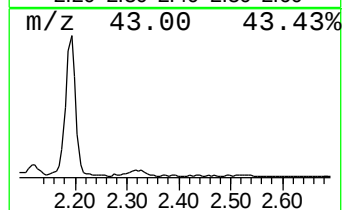
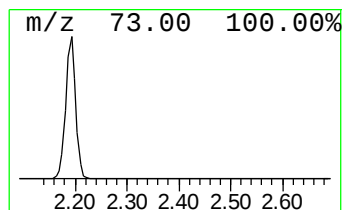
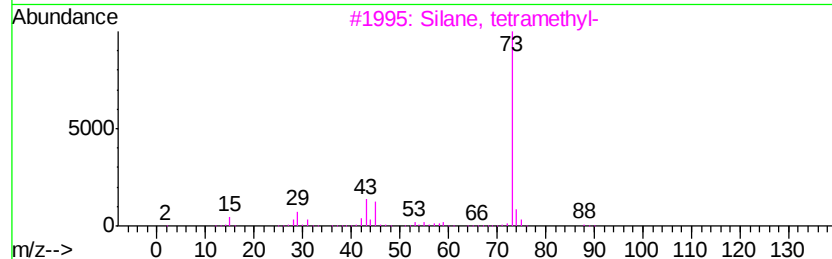
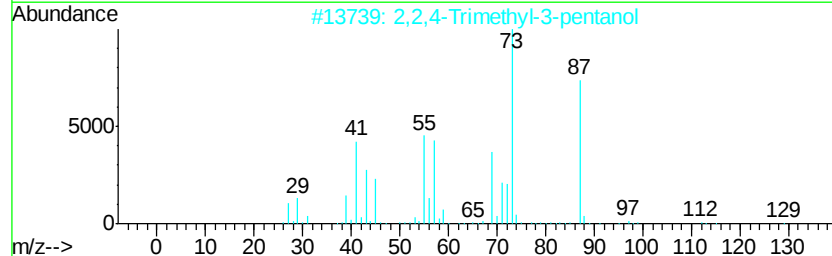
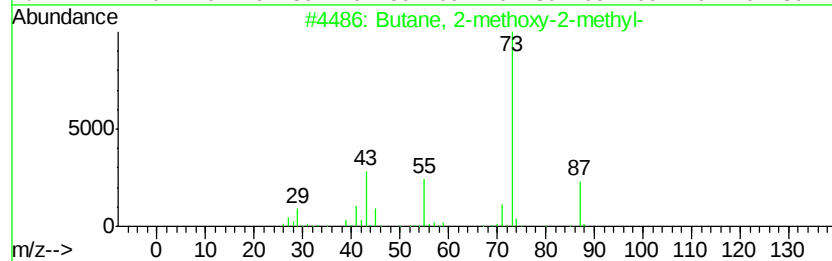
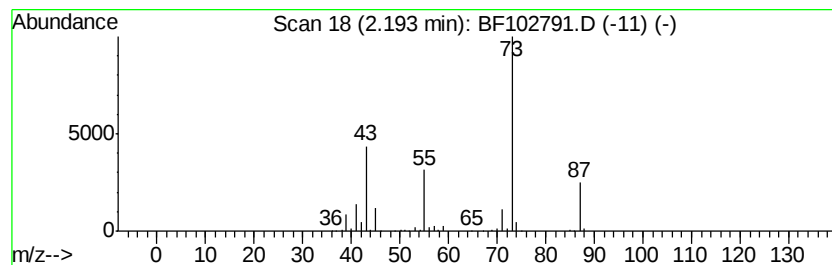
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.19	10.01 ng	625107	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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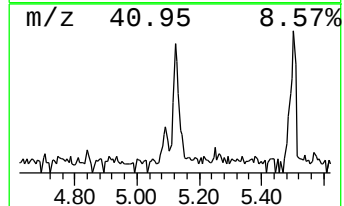
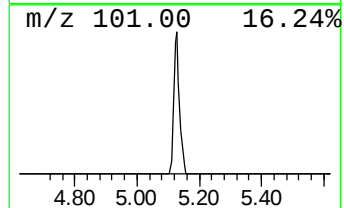
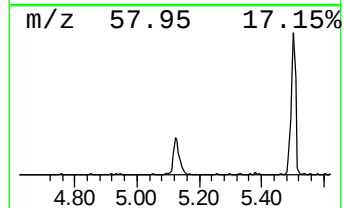
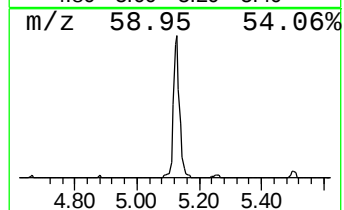
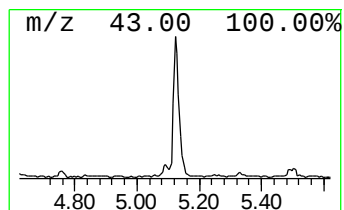
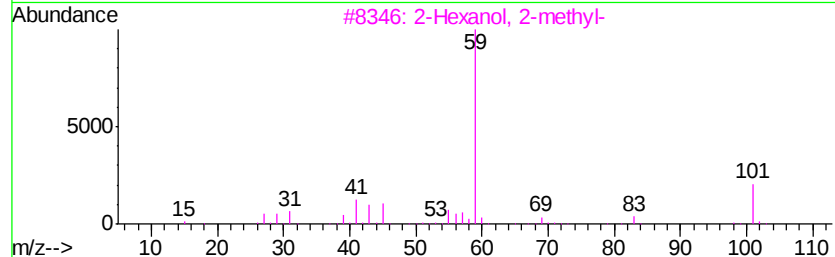
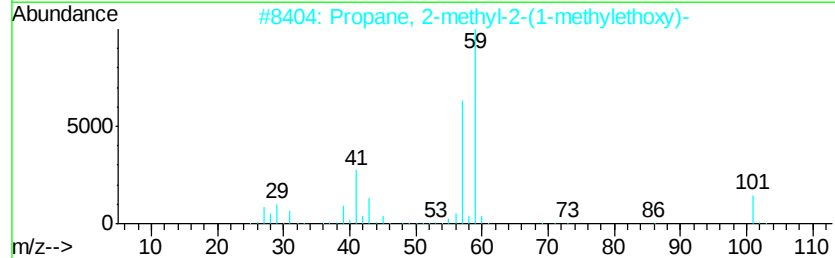
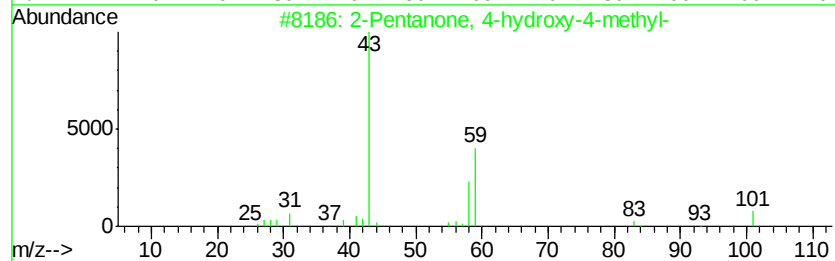
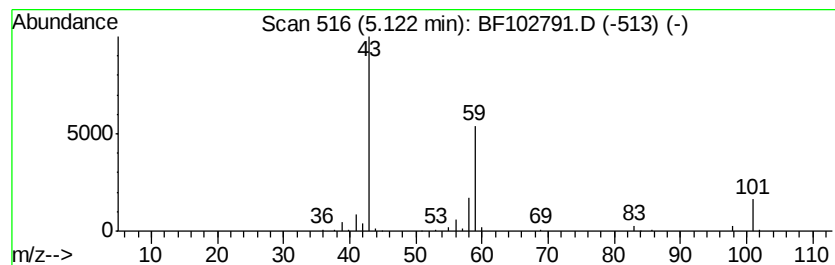
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.63 ng	164062	1,4-Dichlorobenzene-d4	6.88

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28	
4	2,3-Butanediol, 2,3-dimethyl-	118	C6H14O2	000076-09-5	25	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	



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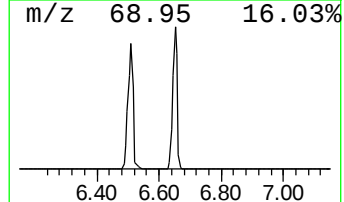
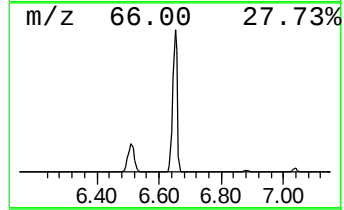
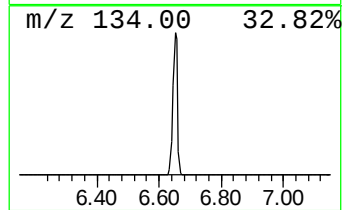
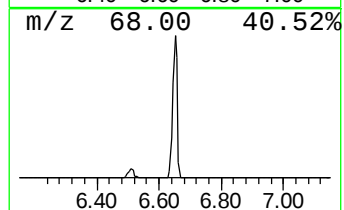
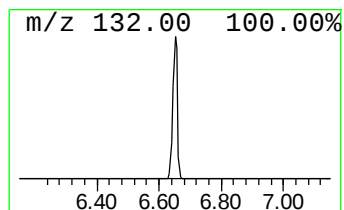
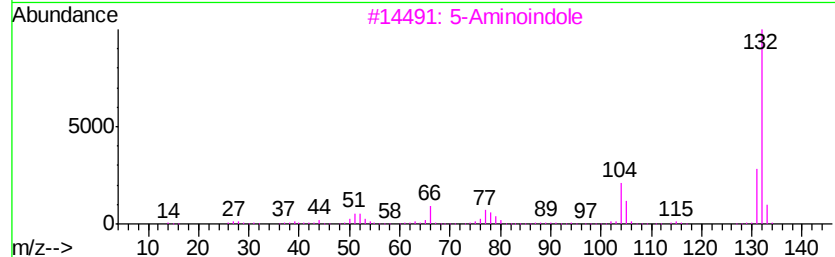
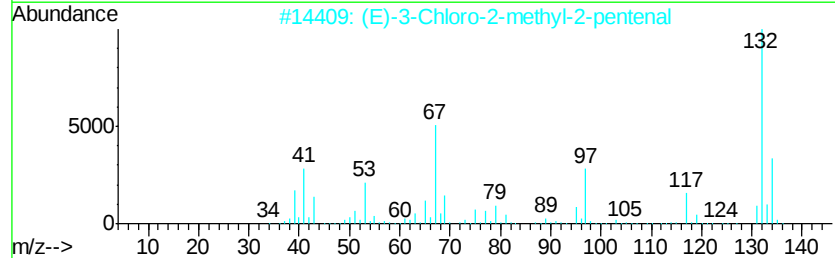
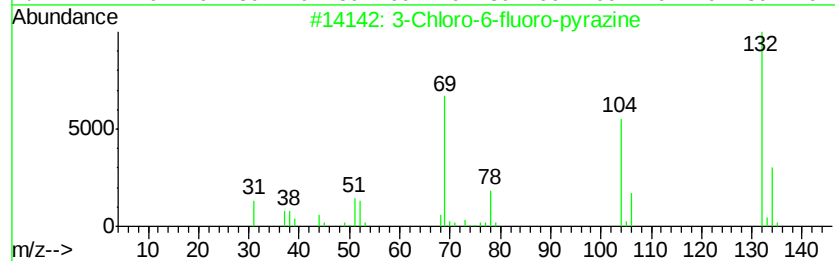
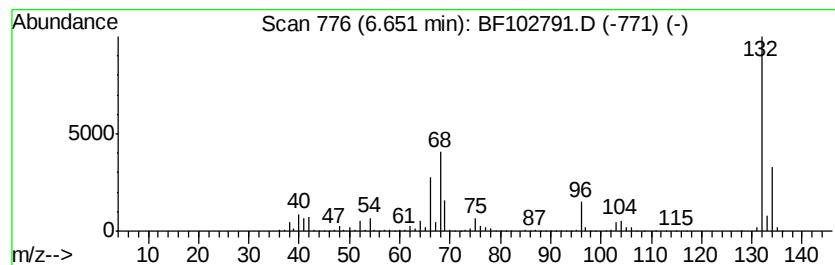
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TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	77.78 ng	4856520	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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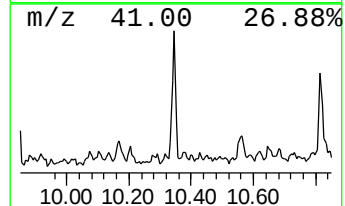
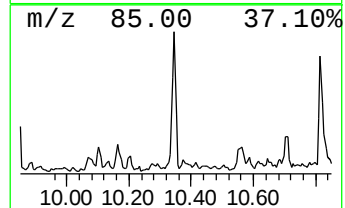
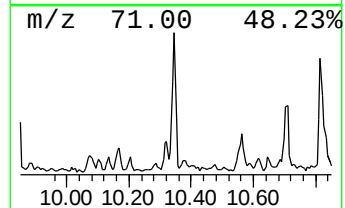
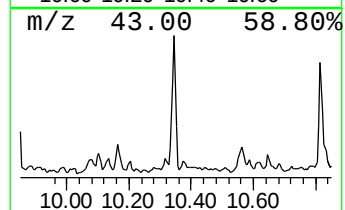
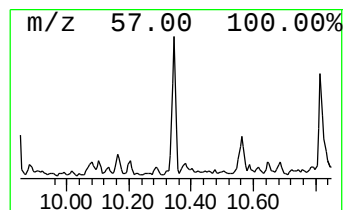
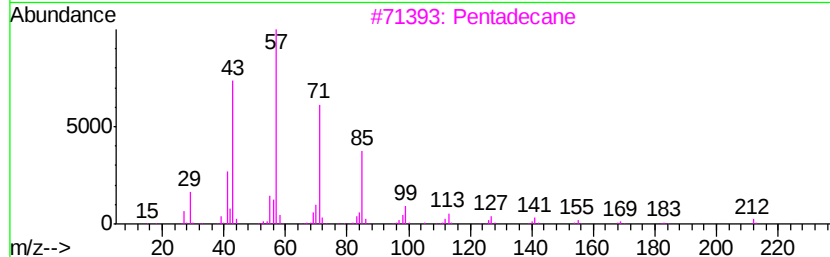
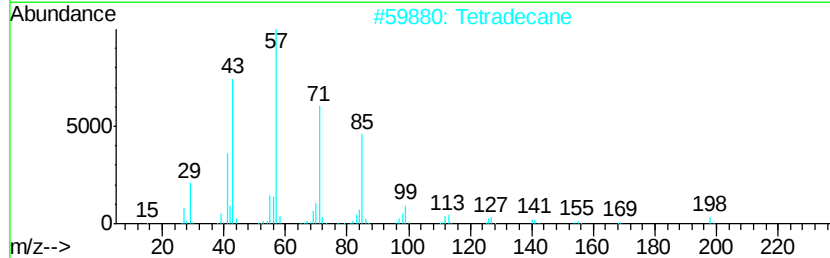
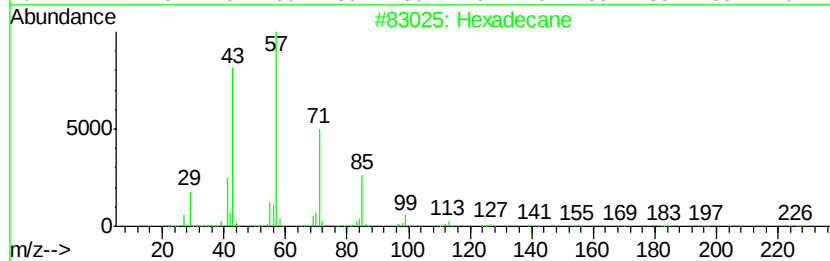
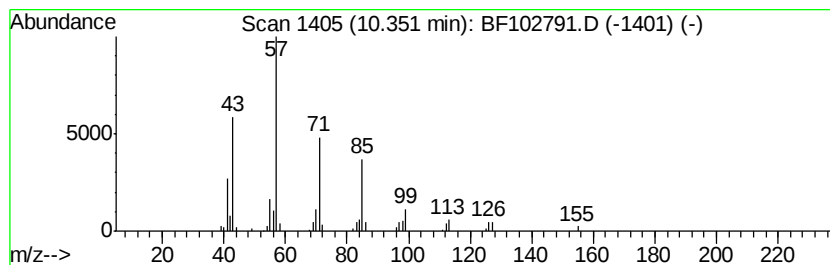
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	2.00 ng	150996	Acenaphthene-d10	9.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	86
2	Tetradecane	198 C14H30	000629-59-4	78
3	Pentadecane	212 C15H32	000629-62-9	78
4	Eicosane	282 C20H42	000112-95-8	72
5	Tetracosane	338 C24H50	000646-31-1	72



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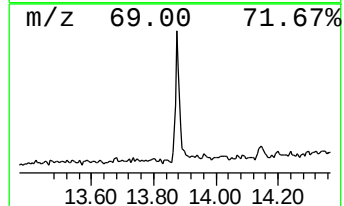
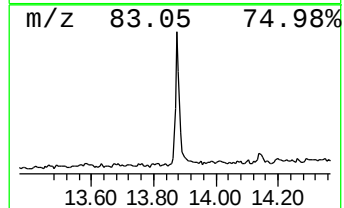
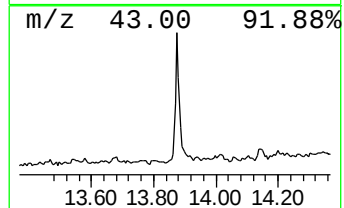
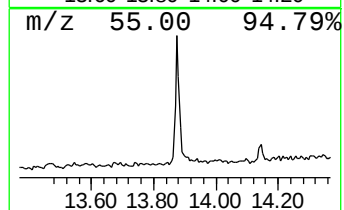
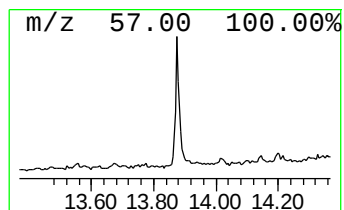
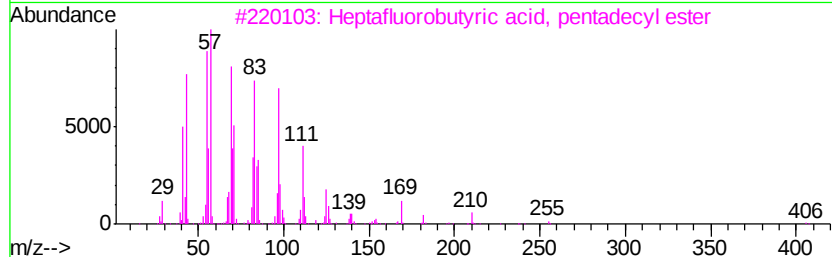
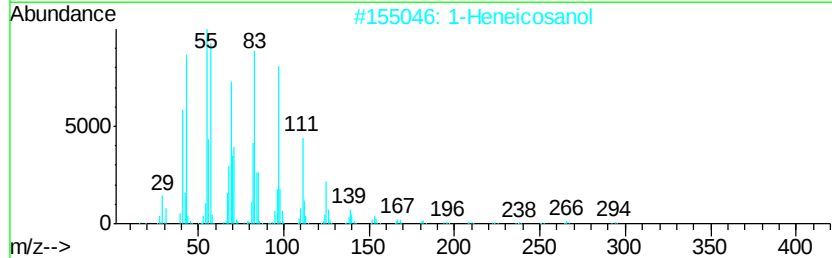
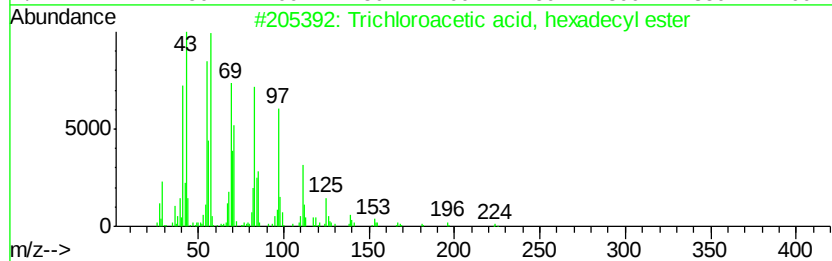
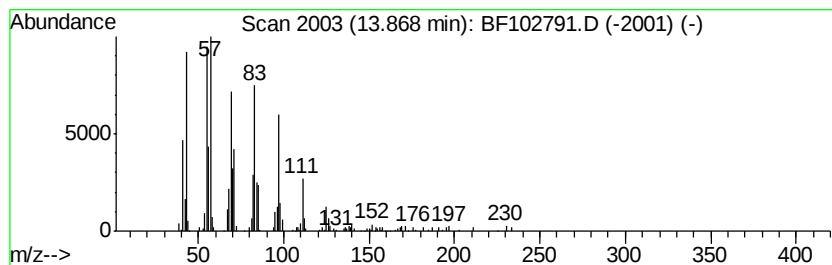
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	7.05 ng	373846	Chrysene-d12	14.04

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2			1-Heneicosanol	312	C21H44O	015594-90-8	94
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5			1-Docosene	308	C22H44	001599-67-3	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.19	10.0	ng	625107	1	6.88	1248720	20.0
2-Pentanone, 4-hy...	5.12	2.6	ng	164062	1	6.88	1248720	20.0
unknown6.65	6.65	77.8	ng	4856520	1	6.88	1248720	20.0
Hexadecane	10.35	2.0	ng	150996	3	9.92	1507560	20.0
Trichloroacetic a...	13.87	7.0	ng	373846	5	14.04	1060400	20.0