

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091817\
 Data File : BF098629.D
 Acq On : 19 Sep 2017 4:33
 Operator : SJ/JU
 Sample : I5262-04
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 091417-SIDI-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-BF091117.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	4.804	459	462	475	rBV	127923	168524	4.93%	0.806%
2	5.240	533	536	552	rBV	862794	1037347	30.33%	4.964%
3	6.287	711	714	728	rBV	656809	723849	21.16%	3.464%
4	6.404	731	734	747	rVB	2179730	1913925	55.95%	9.159%
5	6.634	769	773	783	rVB	844497	707684	20.69%	3.386%
6	6.792	795	800	803	rBV	2694582	2587451	75.64%	12.382%
7	7.204	866	870	873	rBV	2011230	2056699	60.13%	9.842%
8	7.916	988	991	1005	rVB	1074984	918572	26.85%	4.396%
9	8.998	1170	1175	1178	rBV	3686252	3420664	100.00%	16.369%
10	9.392	1239	1242	1252	rVB	86225	69482	2.03%	0.332%
11	9.669	1285	1289	1295	rBV	940135	838835	24.52%	4.014%
12	10.457	1419	1423	1436	rVB	1176681	1010040	29.53%	4.833%
13	11.151	1537	1541	1547	rBV	876314	782609	22.88%	3.745%
14	12.733	1806	1810	1813	rBV	2966889	2509919	73.38%	12.011%
15	13.633	1960	1963	1973	rBV3	33278	47809	1.40%	0.229%
16	13.780	1985	1988	1995	rVB	619849	585364	17.11%	2.801%
17	15.180	2221	2226	2234	rBV	643503	771730	22.56%	3.693%
18	15.574	2289	2293	2299	rVB2	66865	95769	2.80%	0.458%
19	16.021	2363	2369	2376	rBV	88950	150326	4.39%	0.719%
20	16.539	2452	2457	2464	rVB2	73281	136595	3.99%	0.654%
21	17.151	2555	2561	2570	rVB2	64821	147351	4.31%	0.705%
22	17.880	2678	2685	2692	rVB3	40225	100876	2.95%	0.483%
23	18.739	2823	2831	2842	rVB4	36487	116253	3.40%	0.556%

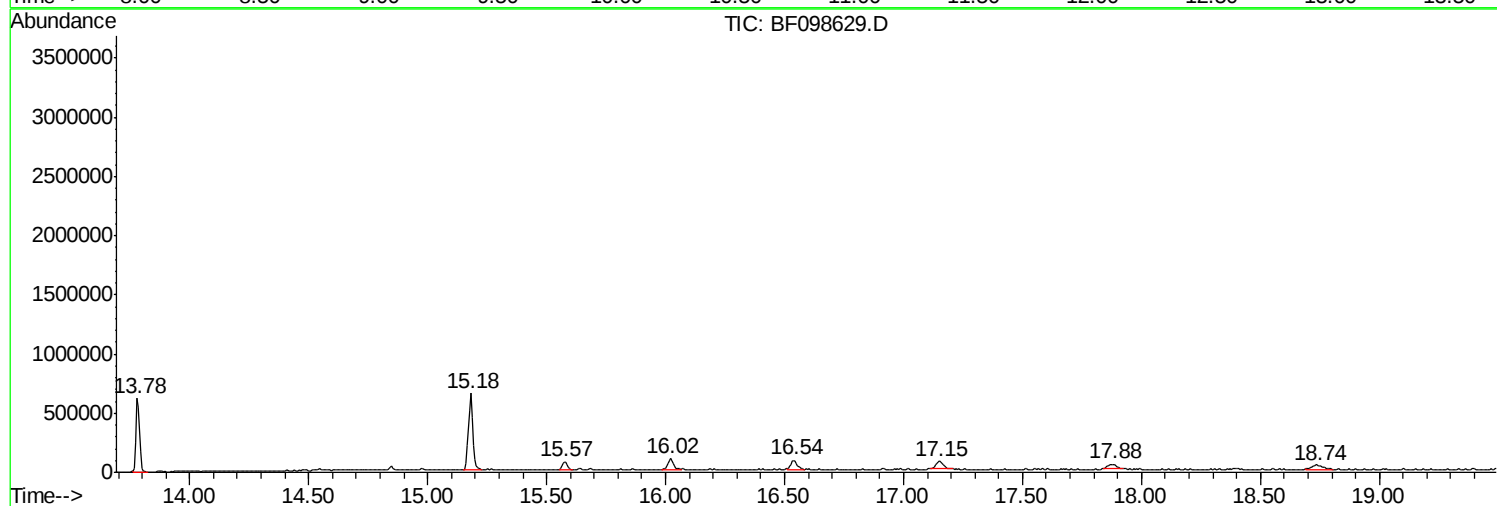
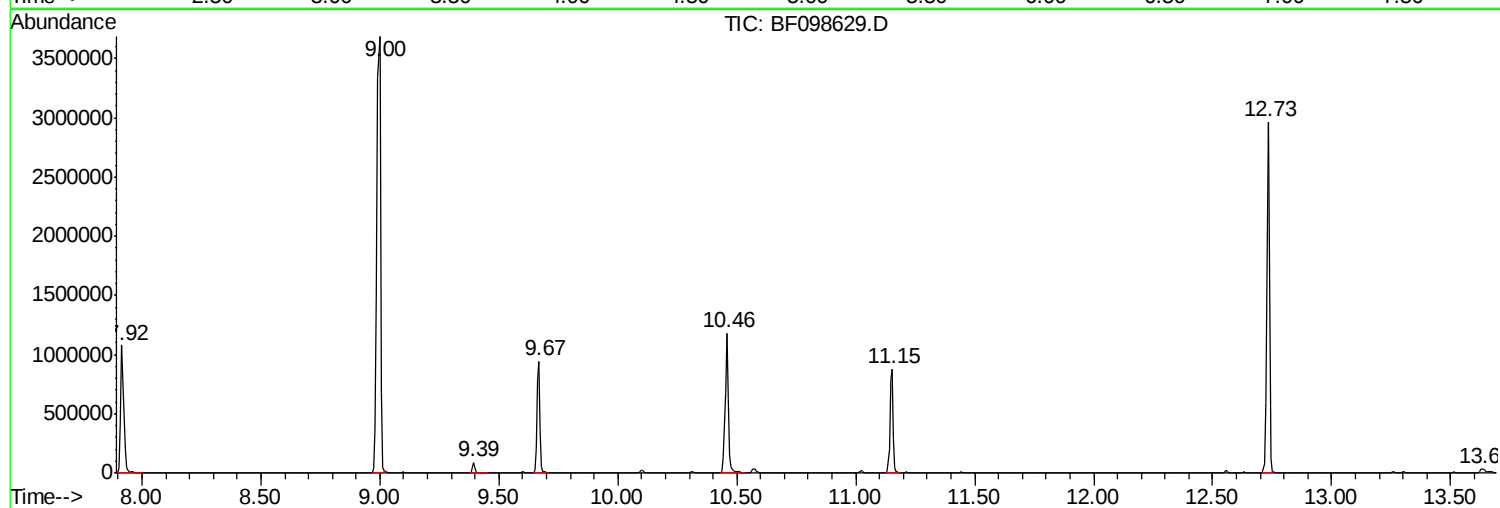
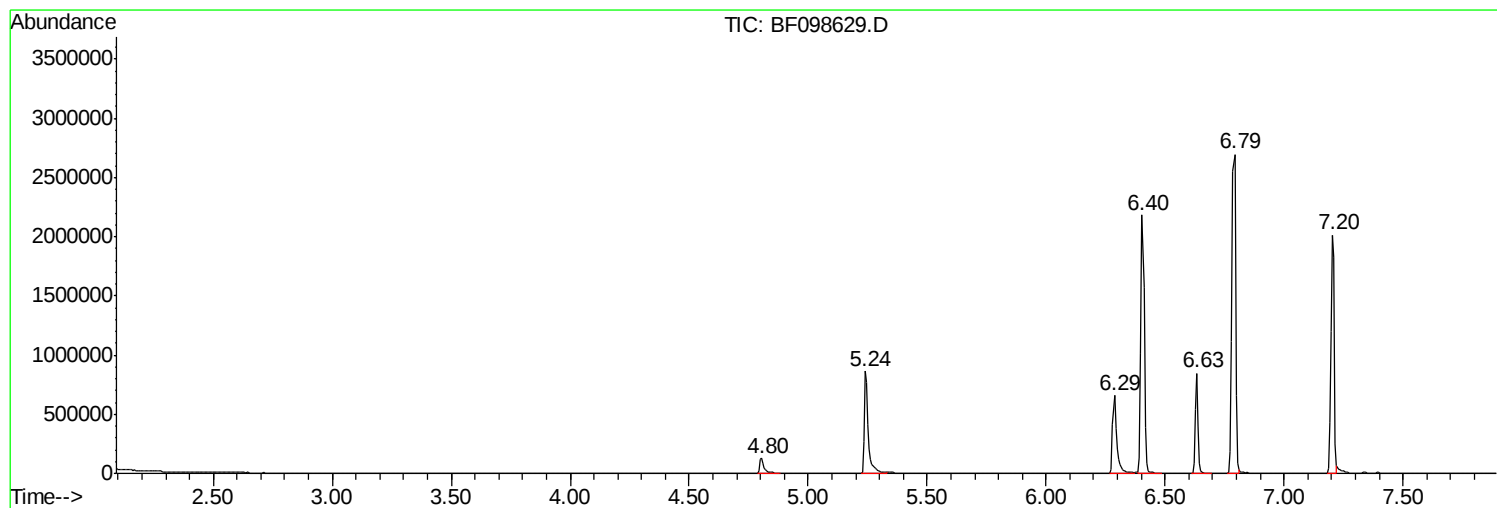
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ALS Vial : 33 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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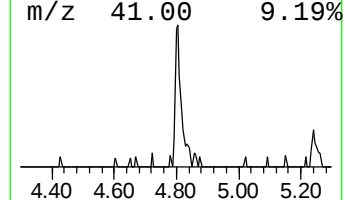
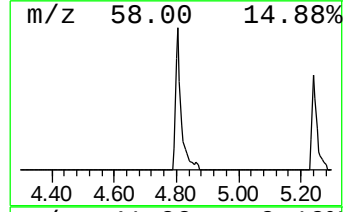
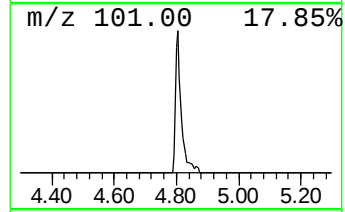
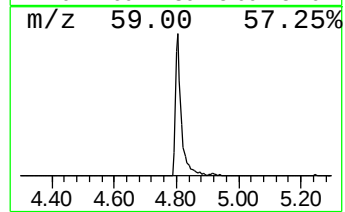
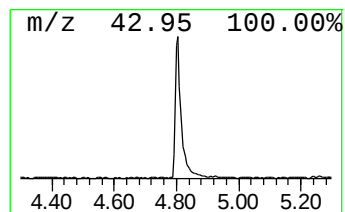
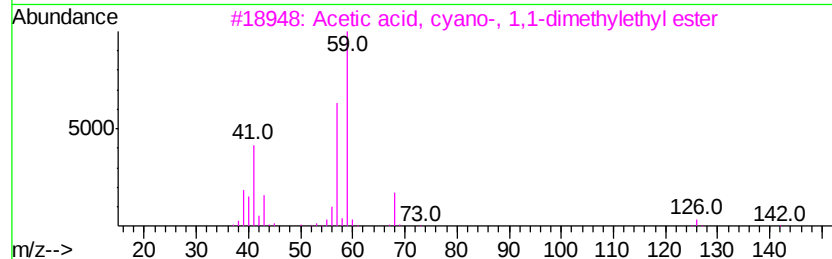
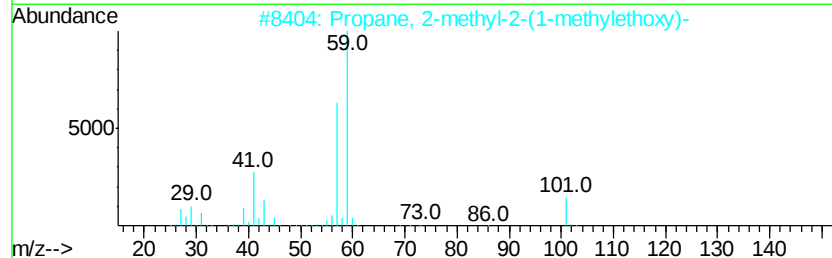
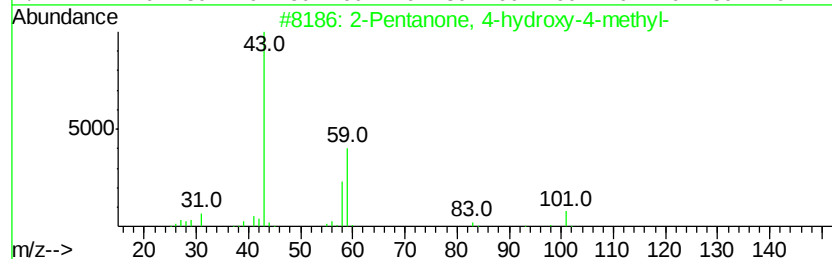
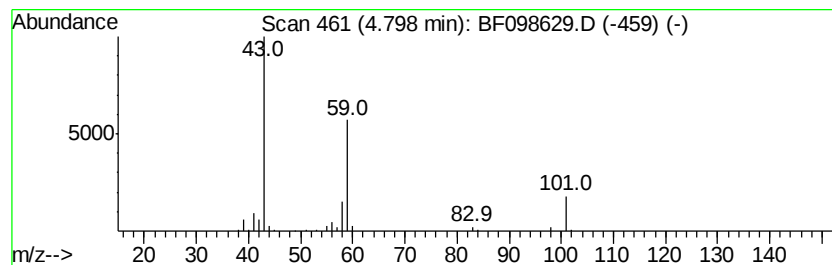
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	4.76 ng	168524	1,4-Dichlorobenzene-d4	6.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	53
3			Acetic acid, cyano-, 1,1-dimethyl-	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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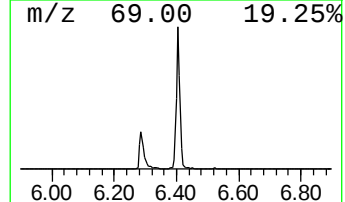
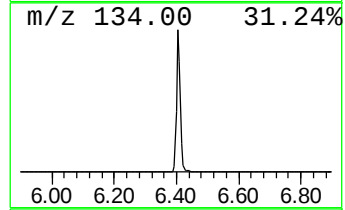
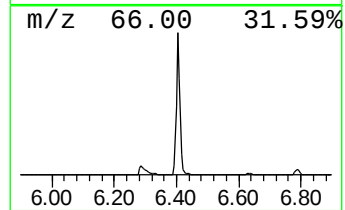
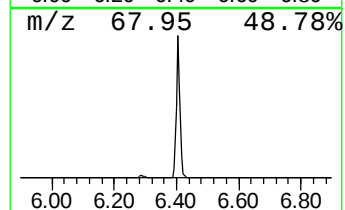
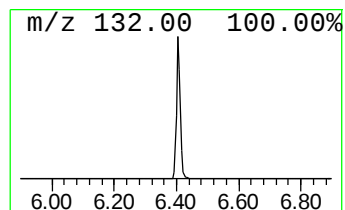
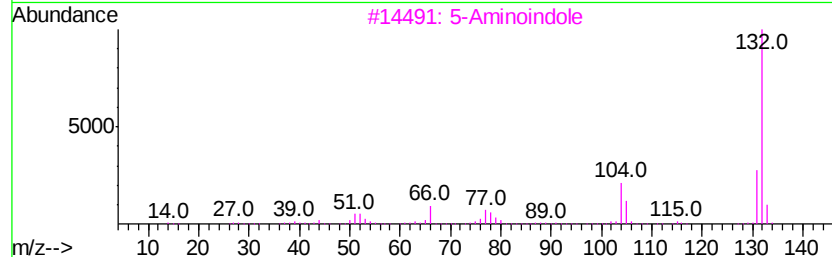
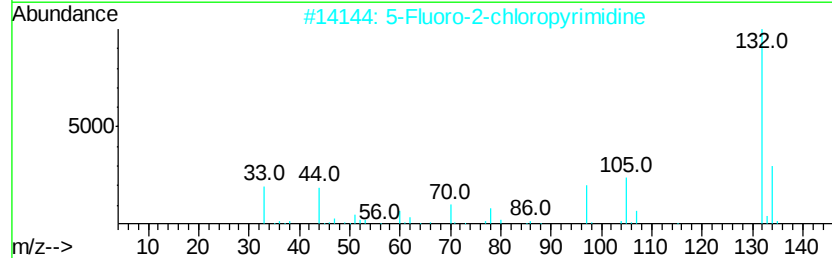
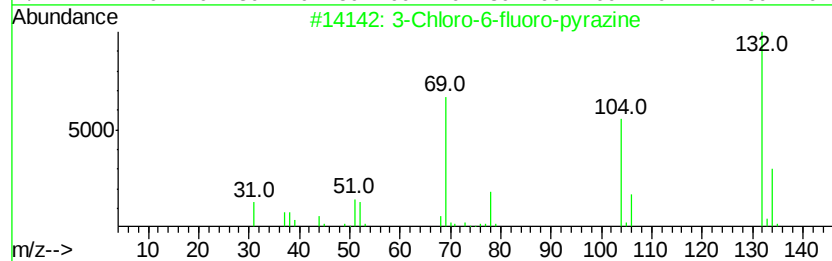
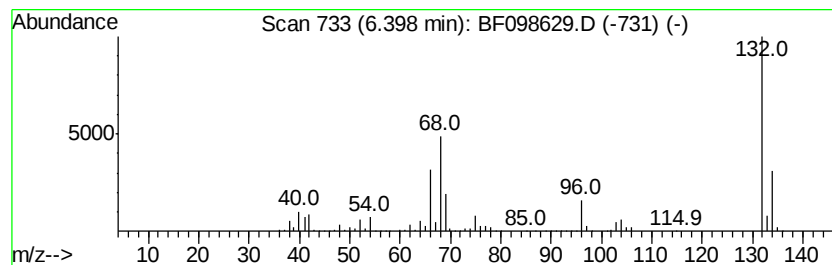
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Peak Number 2 unknown6.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	54.09 ng	1913930	1,4-Dichlorobenzene-d4	6.63

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	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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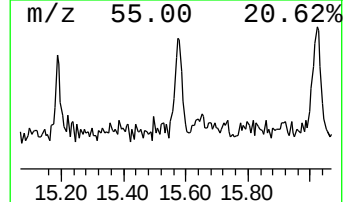
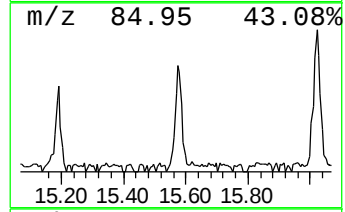
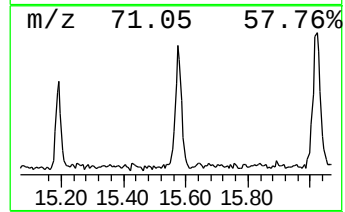
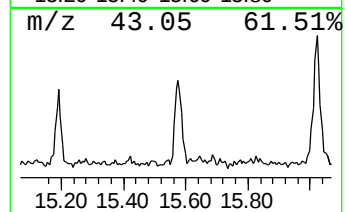
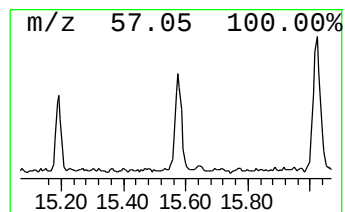
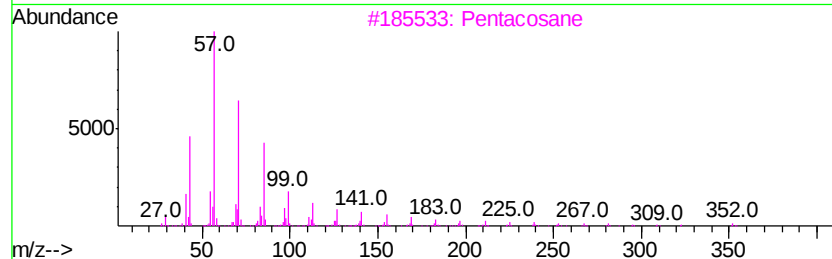
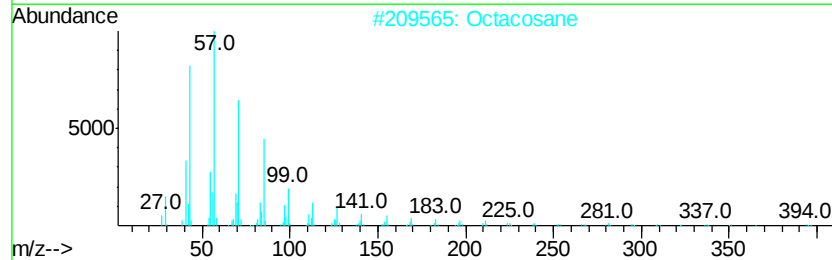
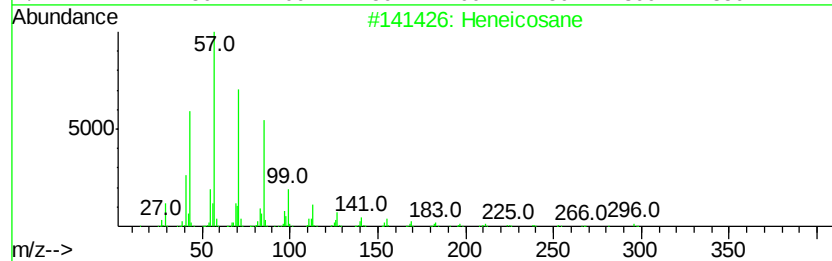
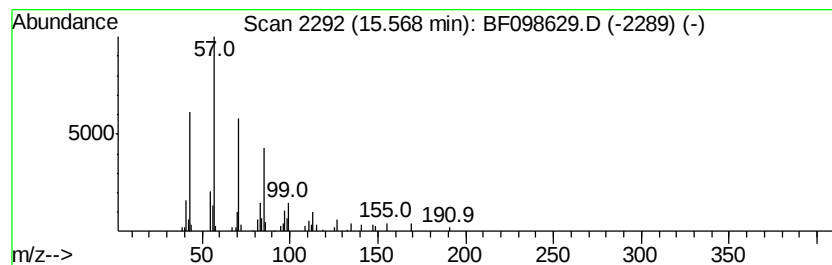
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	2.48 ng	95769	Perylene-d12	15.18

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octacosane		394	C28H58	000630-02-4	91
3	Pentacosane		352	C25H52	000629-99-2	91
4	Heptacosane		380	C27H56	000593-49-7	91
5	Hexacosane		366	C26H54	000630-01-3	90



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ALS Vial : 33 Sample Multiplier: 1

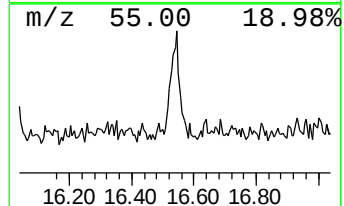
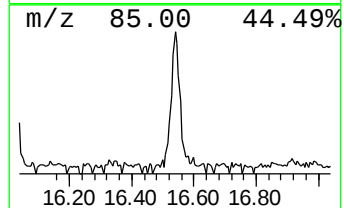
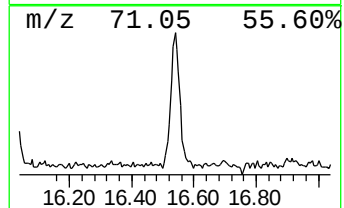
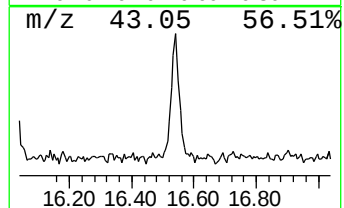
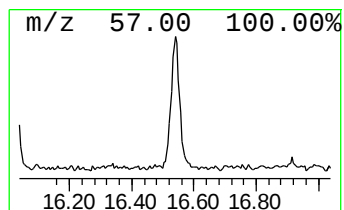
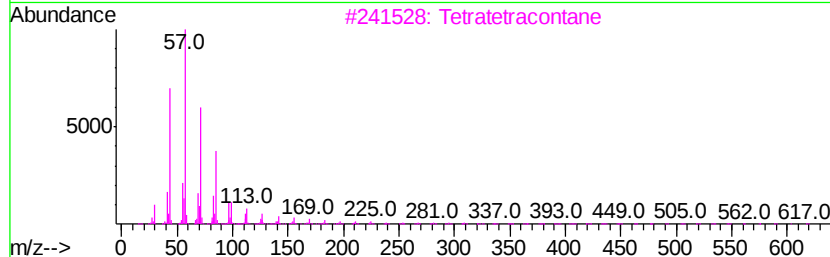
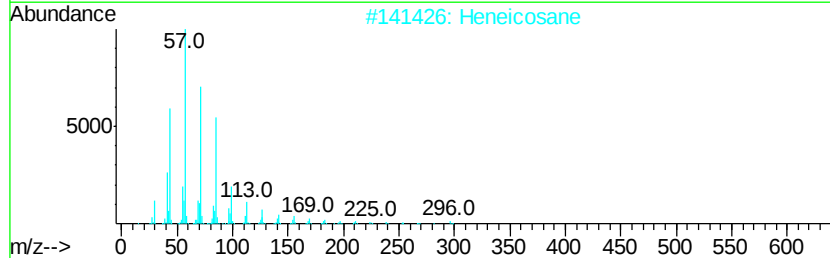
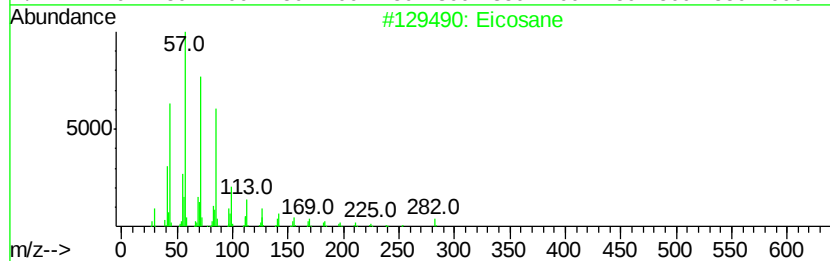
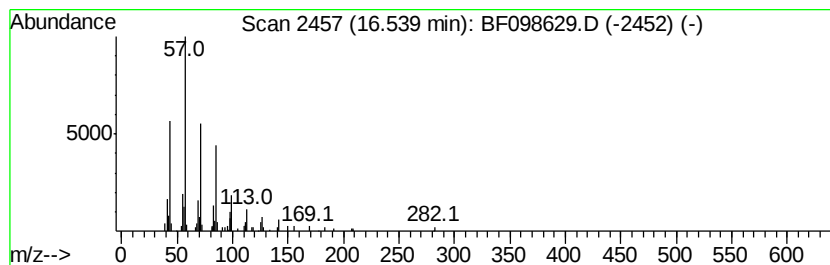
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.54	3.54 ng	136595	Perylene-d12	15.18	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Octacosane	394	C28H58	000630-02-4	91



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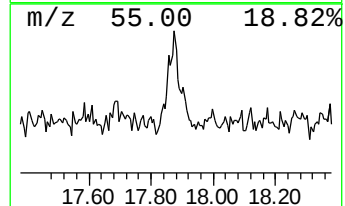
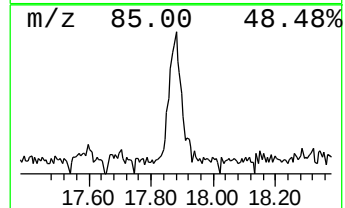
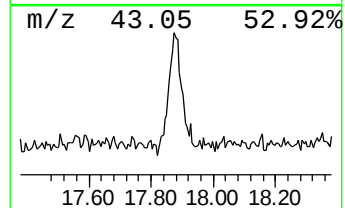
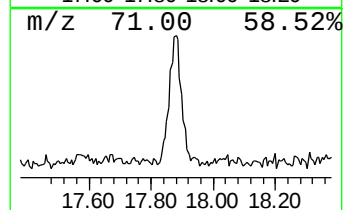
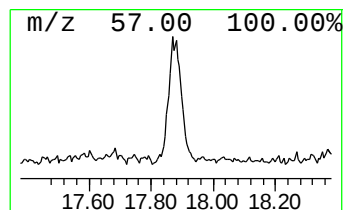
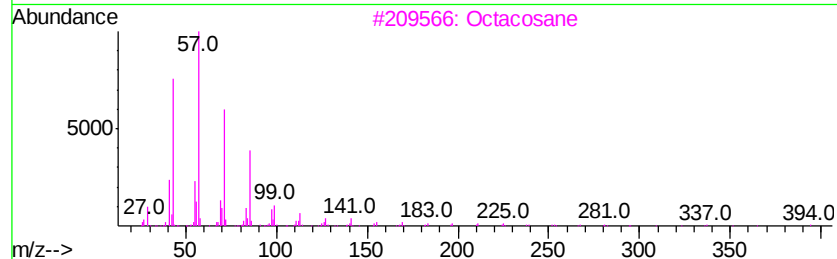
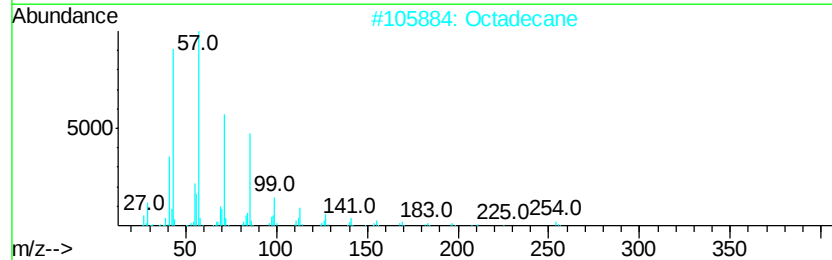
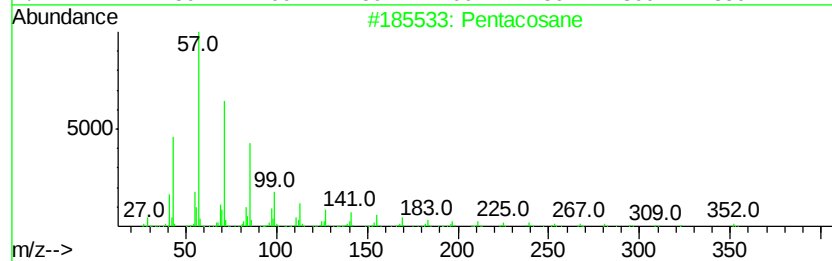
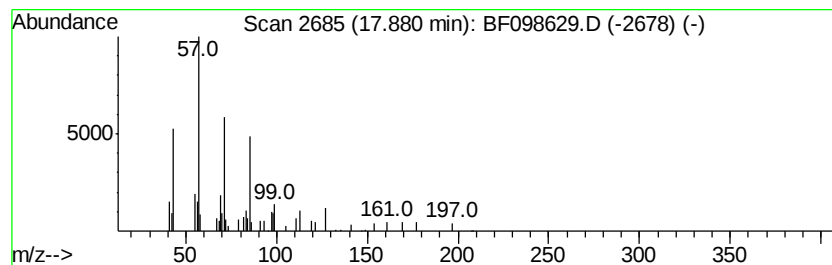
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.88	2.61 ng	100876	Perylene-d12	15.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	87
2		Octadecane	254	C18H38	000593-45-3	86
3		Octacosane	394	C28H58	000630-02-4	86
4		2-Bromotetradecane	276	C14H29Br	074036-95-6	86
5		2-methyloctacosane	408	C29H60	1000376-72-8	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.80	4.8	ng	168524	1	6.63	707684	20.0
unknown6.40	6.40	54.1	ng	1913930	1	6.63	707684	20.0
Heneicosane	15.57	2.5	ng	95769	6	15.18	771730	20.0
Eicosane	16.54	3.5	ng	136595	6	15.18	771730	20.0
Pentacosane	17.88	2.6	ng	100876	6	15.18	771730	20.0