

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF083118\
 Data File : BF108724.D
 Acq On : 1 Sep 2018 7:49
 Operator : JU/SJ
 Sample : J4729-10
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 082918-DBRI-F-U-S

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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	5.237	490	493	501	rBV	19141	29495	1.04%	0.216%
2	5.678	561	568	572	rBV3	30602	91824	3.25%	0.672%
3	6.660	730	735	740	rBV	53647	114336	4.04%	0.837%
4	6.772	751	754	767	rBV	371988	817580	28.92%	5.984%
5	7.007	790	794	815	rVB	121487	358364	12.67%	2.623%
6	7.154	815	819	848	rBV	1202814	1772785	62.70%	12.976%
7	7.566	886	889	911	rBV	448971	1191440	42.14%	8.721%
8	8.283	1007	1011	1033	rBV	151475	401232	14.19%	2.937%
9	9.354	1189	1193	1232	rBV	1656020	2556735	90.43%	18.714%
10	9.748	1256	1260	1273	rVB	32721	53316	1.89%	0.390%
11	10.042	1306	1310	1331	rBV	332687	484288	17.13%	3.545%
12	10.695	1418	1421	1426	rBV	35316	33922	1.20%	0.248%
13	10.836	1441	1445	1464	rBV	458202	922691	32.63%	6.754%
14	11.542	1560	1565	1587	rBV	304450	602489	21.31%	4.410%
15	13.118	1829	1833	1852	rBV	2300175	2827414	100.00%	20.695%
16	14.089	1990	1998	2012	rBV10	22388	93937	3.32%	0.688%
17	14.195	2012	2016	2026	rBV	462574	635682	22.48%	4.653%
18	14.936	2139	2142	2145	rBV	36899	36065	1.28%	0.264%
19	15.018	2152	2156	2161	rBV	44767	49255	1.74%	0.361%
20	15.295	2199	2203	2208	rBV	42522	50830	1.80%	0.372%
21	15.707	2268	2273	2276	rBV	40058	53671	1.90%	0.393%
22	15.754	2276	2281	2295	rVB	201729	396649	14.03%	2.903%
23	16.171	2348	2352	2359	rVB2	34054	56643	2.00%	0.415%
24	16.718	2440	2445	2450	rBV4	17424	31393	1.11%	0.230%

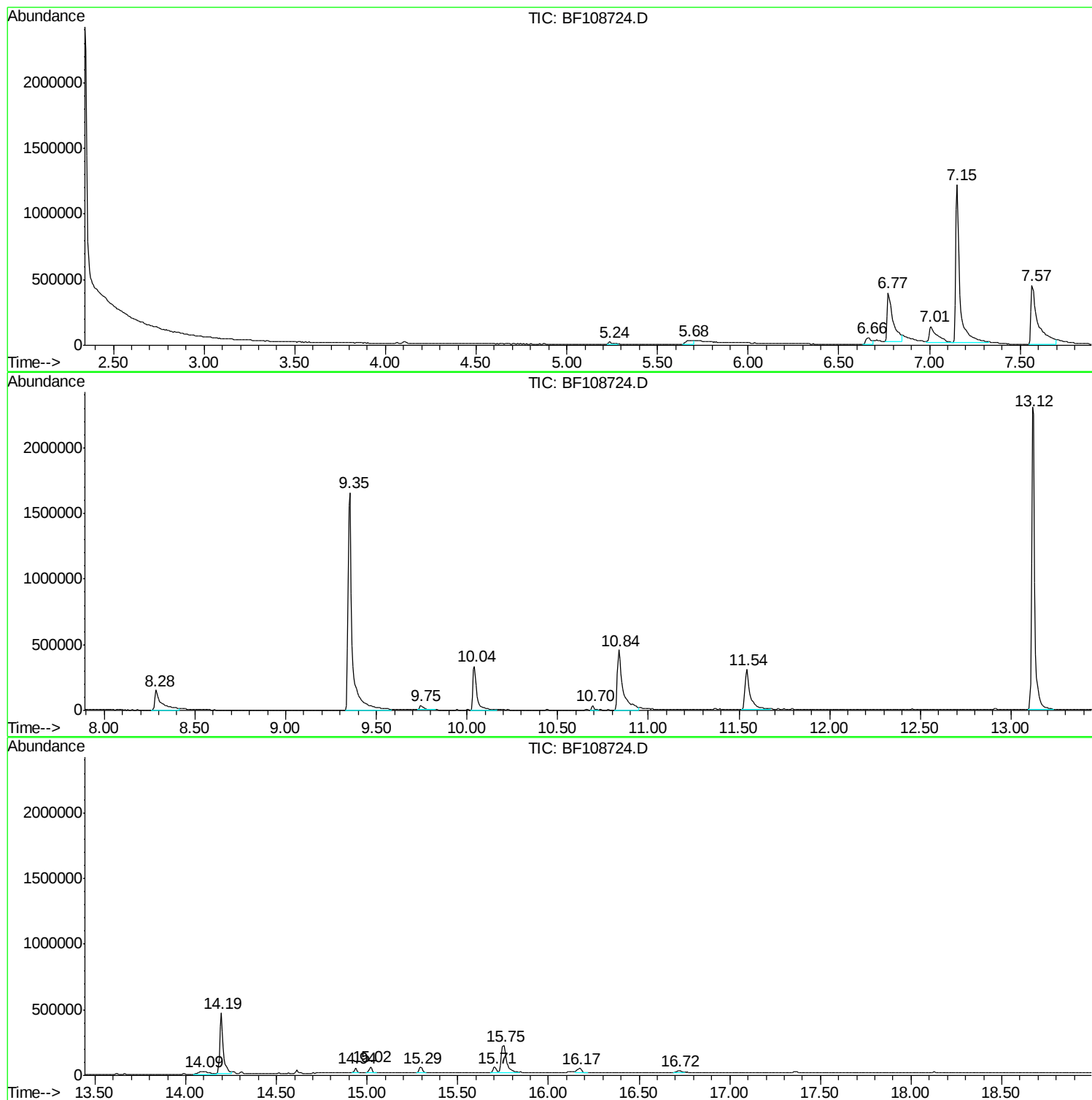
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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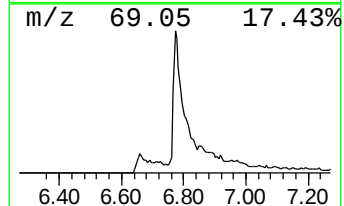
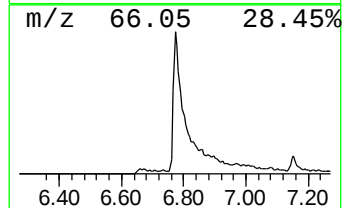
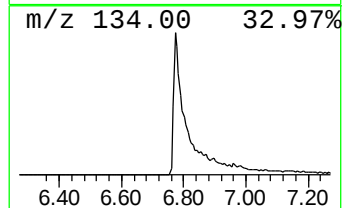
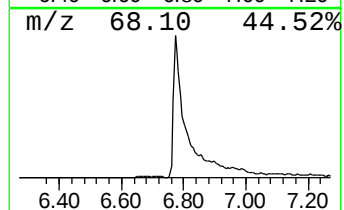
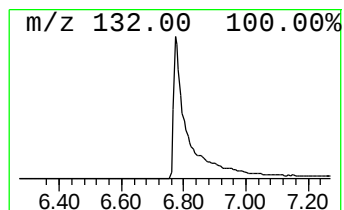
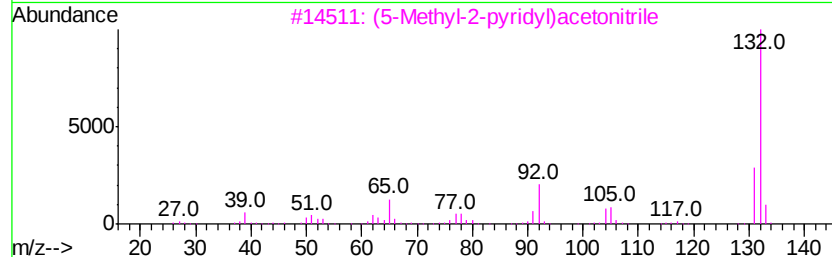
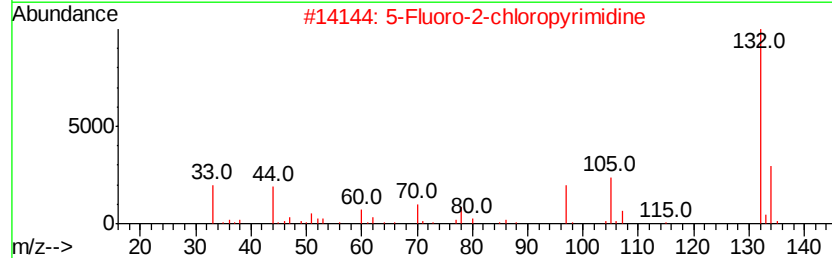
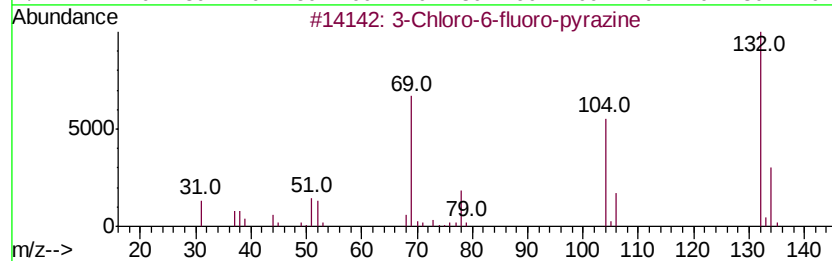
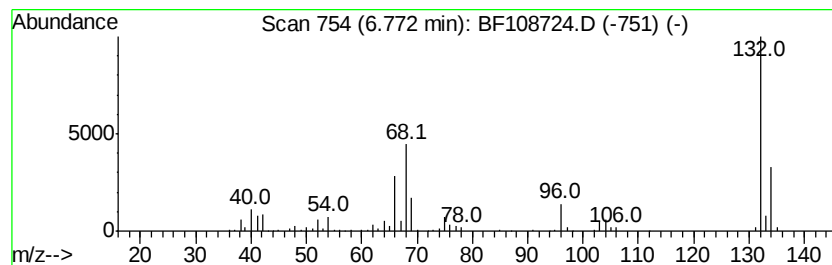
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.77 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	45.63 ng	817580	1,4-Dichlorobenzene-d4	7.01

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	16
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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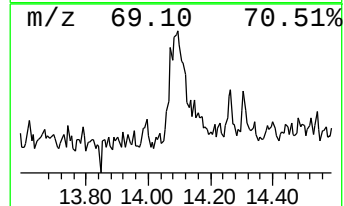
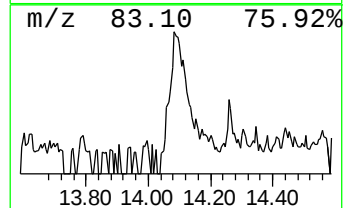
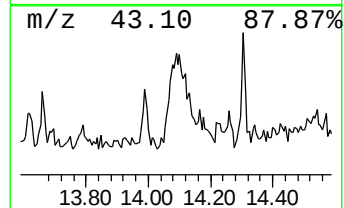
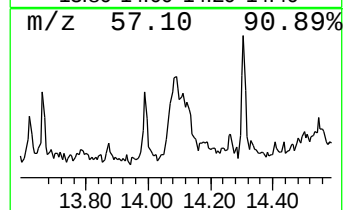
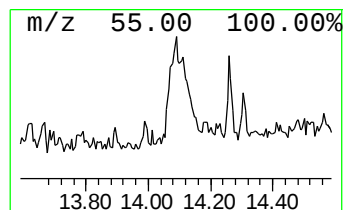
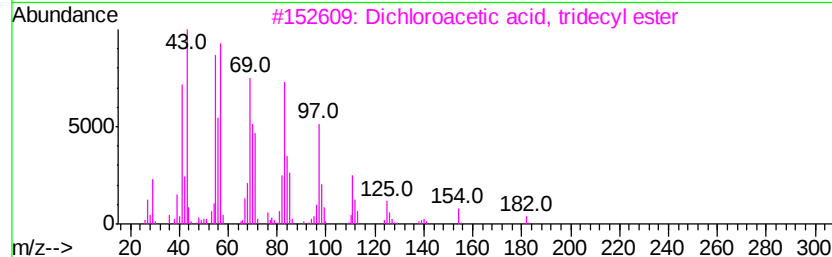
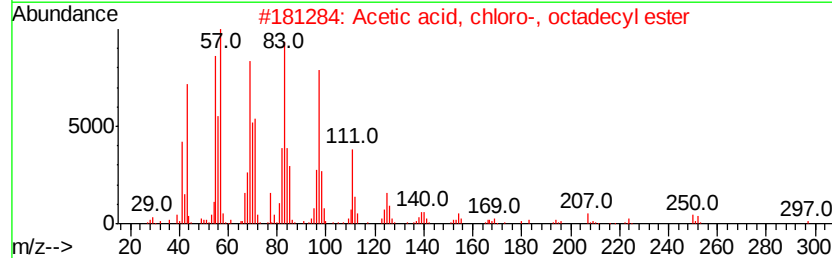
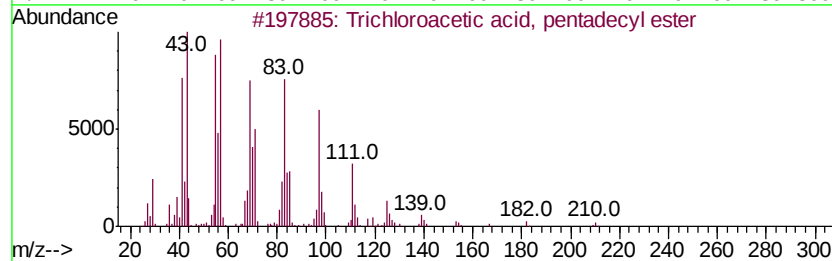
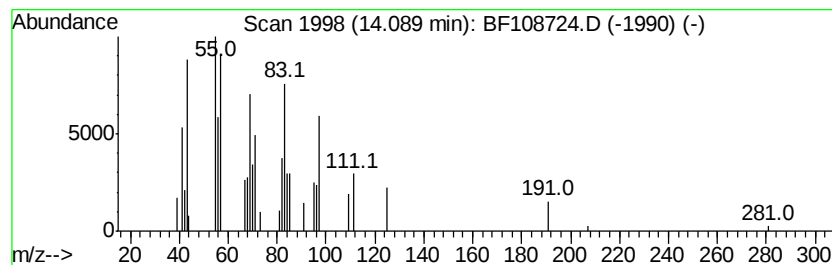
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Peak Number 3 Trichloroacetic acid, penta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.09	2.96 ng	93937	Chrysene-d12	14.19

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
2			Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	86
3			Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	83
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	83
5			1-Heneicosanol	312	C21H44O	015594-90-8	83



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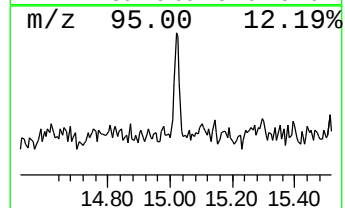
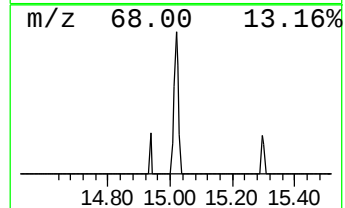
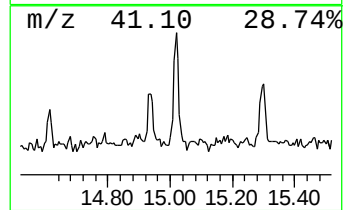
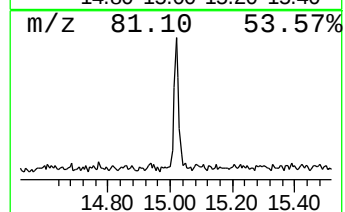
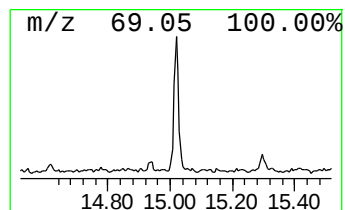
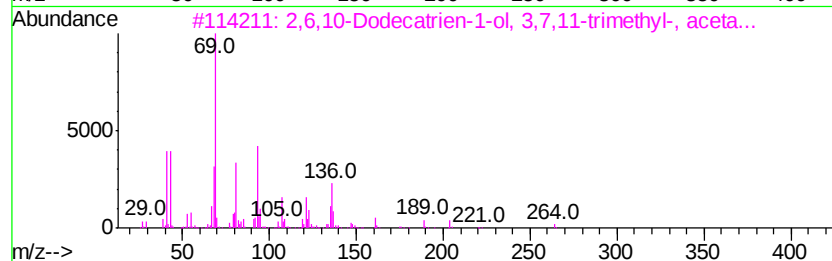
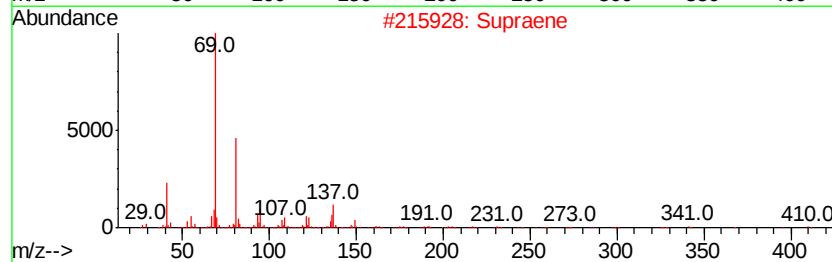
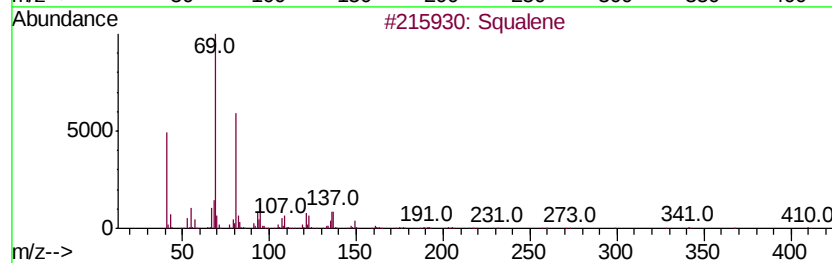
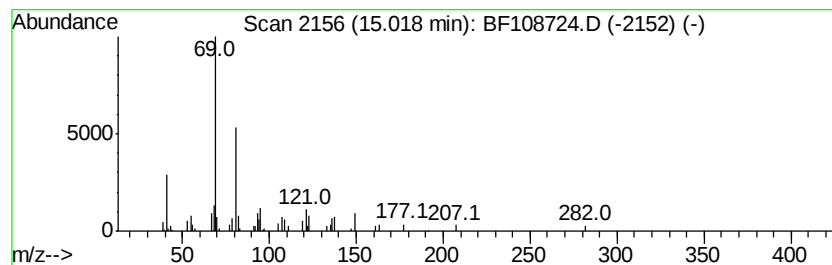
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Peak Number 4 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	2.48 ng	49255	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	87
2		Supraene	410	C30H50	007683-64-9	72
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59
5		1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	53



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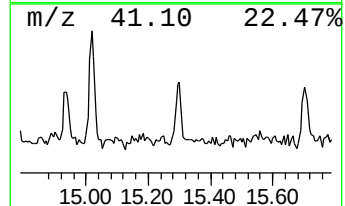
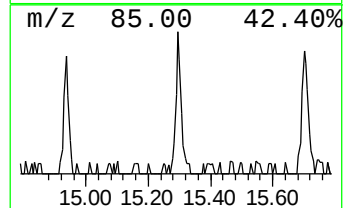
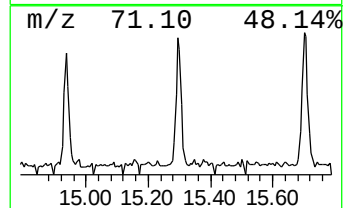
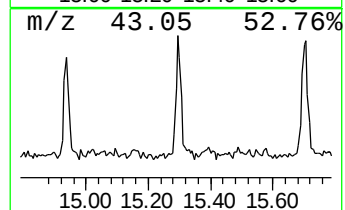
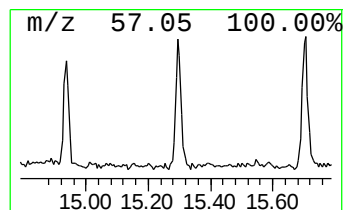
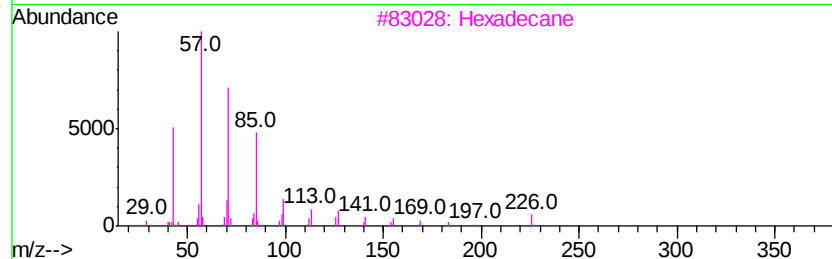
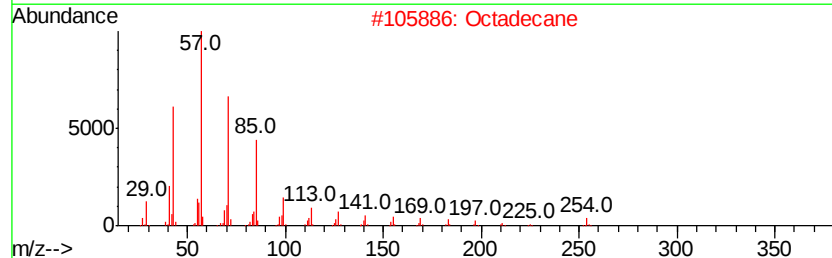
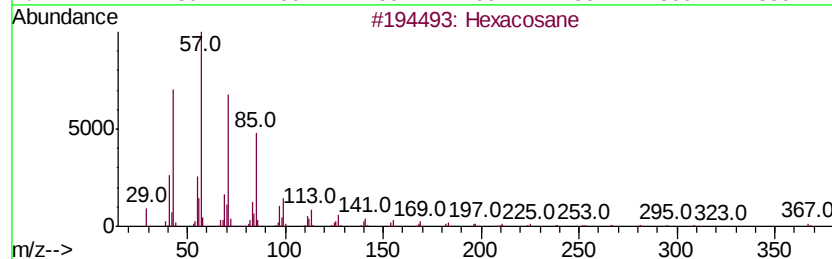
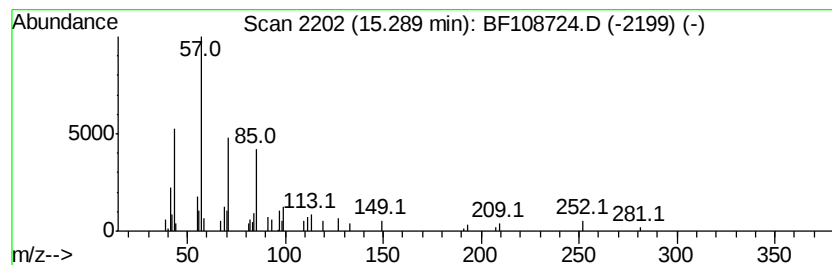
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Peak Number 5 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	2.56 ng	50830	Perylene-d12	15.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Octadecane		254	C18H38	000593-45-3	91
3	Hexadecane		226	C16H34	000544-76-3	90
4	Heptadecane		240	C17H36	000629-78-7	90
5	Heneicosane		296	C21H44	000629-94-7	87



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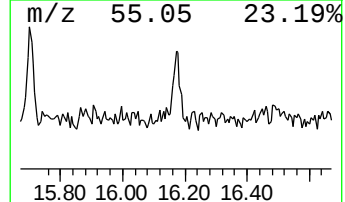
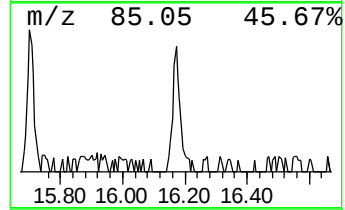
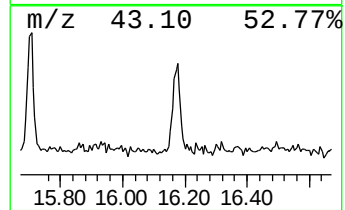
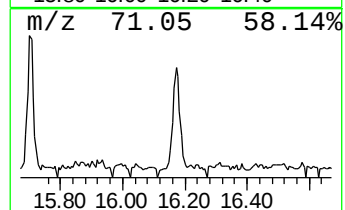
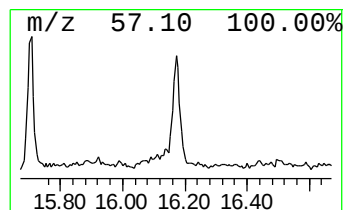
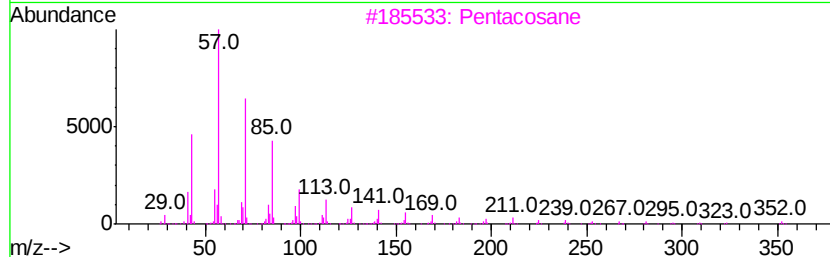
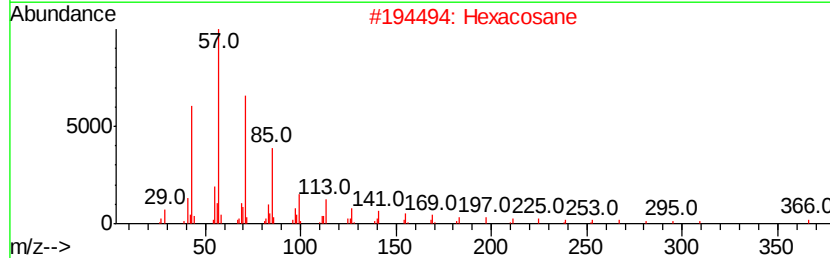
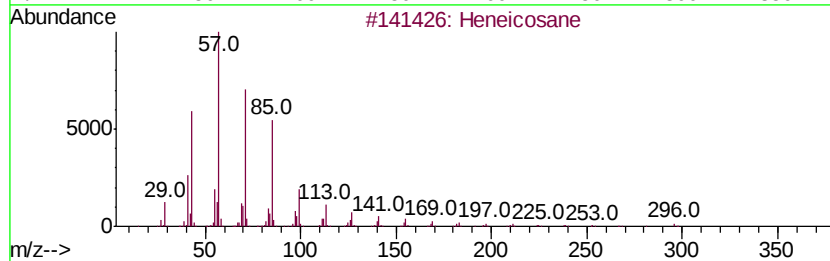
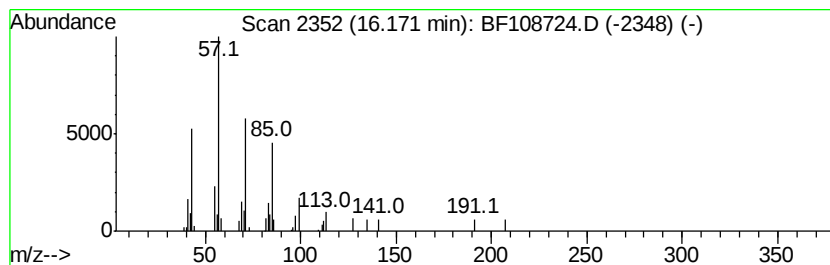
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	2.86 ng	56643	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	87
2		Hexacosane	366	C26H54	000630-01-3	87
3		Pentacosane	352	C25H52	000629-99-2	86
4		10-Methylnonadecane	282	C20H42	056862-62-5	80
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.77	6.77	45.6	ng	817580	1	7.01	358364	20.0
Trichloroacetic a...	14.09	3.0	ng	93937	5	14.19	635682	20.0
Squalene	15.02	2.5	ng	49255	6	15.75	396649	20.0
Hexacosane	15.29	2.6	ng	50830	6	15.75	396649	20.0
Heneicosane	16.17	2.9	ng	56643	6	15.75	396649	20.0