

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052516\
 Data File : BF087399.D
 Acq On : 26 May 2016 7:01
 Operator : UM/SJ
 Sample : H3220-10
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-38-COMP

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-BF052316.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	1.644	4	5	50	rVB	2227129	4251991	100.00%	12.137%
2	4.787	277	280	293	rBV	157539	441709	10.39%	1.261%
3	5.450	335	338	359	rBV	2274489	3750244	88.20%	10.705%
4	7.096	478	482	484	rBV	2115499	3756518	88.35%	10.723%
5	7.187	487	490	502	rVB	2694749	3933303	92.50%	11.228%
6	7.519	516	519	524	rBV	541415	673442	15.84%	1.922%
7	7.759	537	540	543	rBV	2240296	2776308	65.29%	7.925%
8	8.433	596	599	602	rBV	1490277	2341719	55.07%	6.684%
9	9.553	694	697	709	rBV	596335	817593	19.23%	2.334%
10	11.336	849	853	855	rBV	2742277	3799143	89.35%	10.845%
11	12.022	910	913	916	rBV	622345	717651	16.88%	2.049%
12	12.376	941	944	950	rBV	621768	796364	18.73%	2.273%
13	13.211	1015	1017	1020	rVB	38684	57436	1.35%	0.164%
14	13.668	1054	1057	1060	rBV	1190055	1899231	44.67%	5.421%
15	13.988	1082	1085	1090	rBV	68134	108212	2.54%	0.309%
16	14.777	1151	1154	1162	rVB	535090	682086	16.04%	1.947%
17	17.131	1357	1360	1363	rBV	2559328	2887960	67.92%	8.244%
18	18.388	1468	1470	1474	rBV	34363	65054	1.53%	0.186%
19	18.468	1474	1477	1480	rVV	543339	635720	14.95%	1.815%
20	18.537	1480	1483	1489	rVB	40941	89497	2.10%	0.255%
21	19.600	1574	1576	1579	rBV	50997	75743	1.78%	0.216%
22	20.137	1620	1623	1630	rBV	350171	475580	11.18%	1.358%

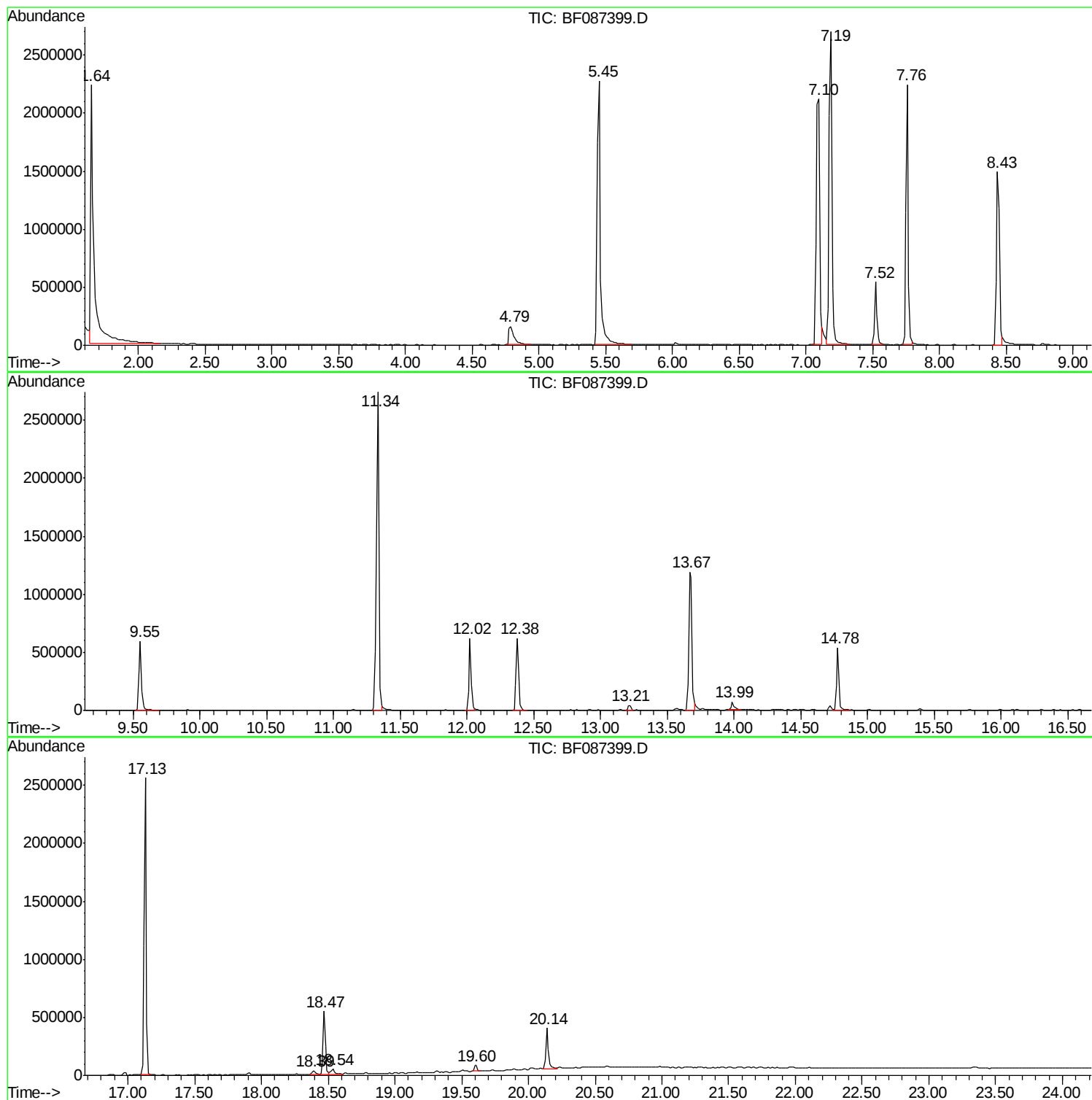
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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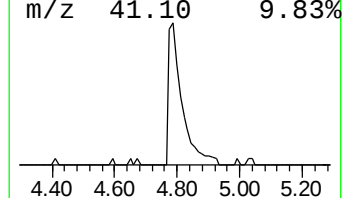
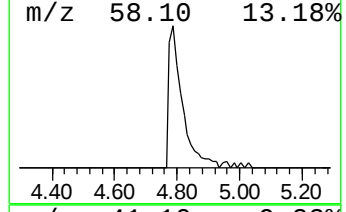
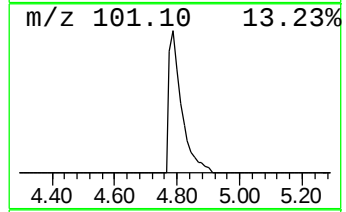
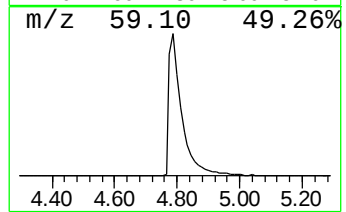
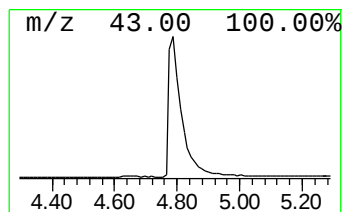
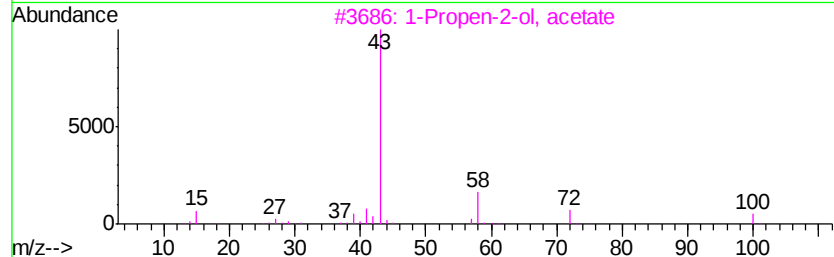
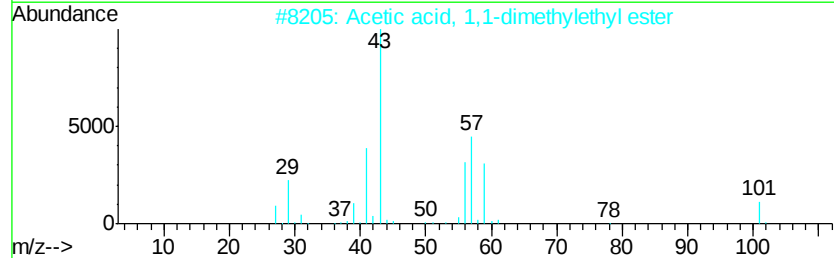
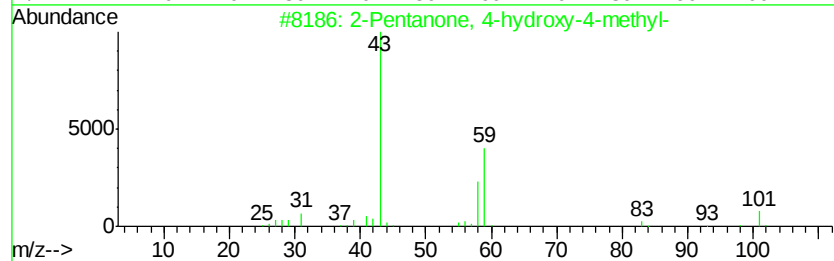
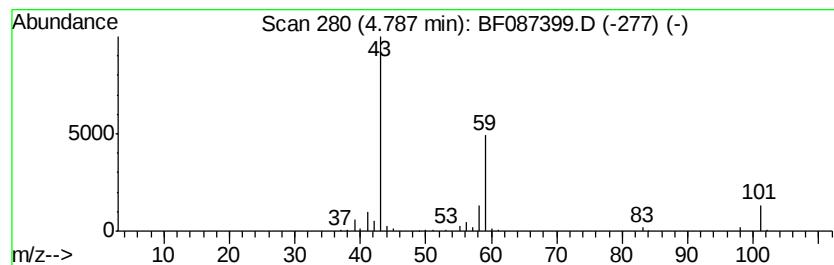
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	13.12 ng	441709	1,4-Dichlorobenzene-d4	7.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Diacetamide	101	C4H7NO2	000625-77-4	9



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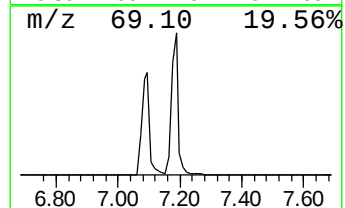
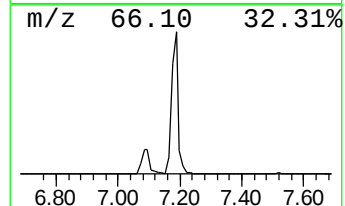
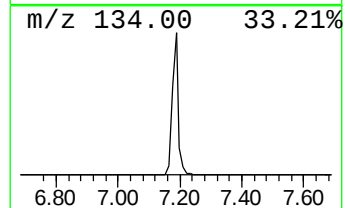
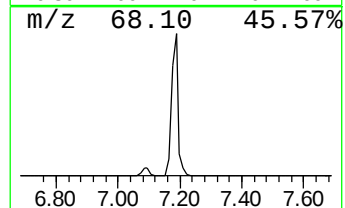
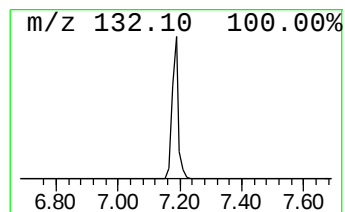
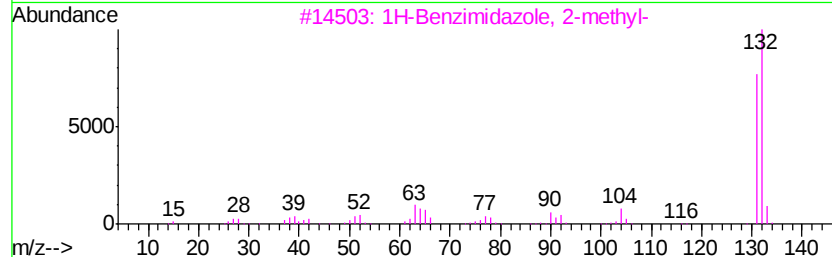
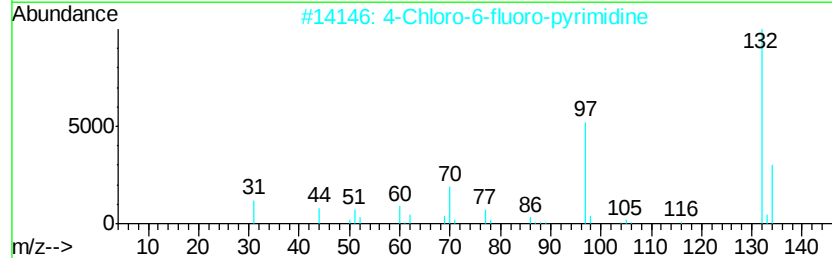
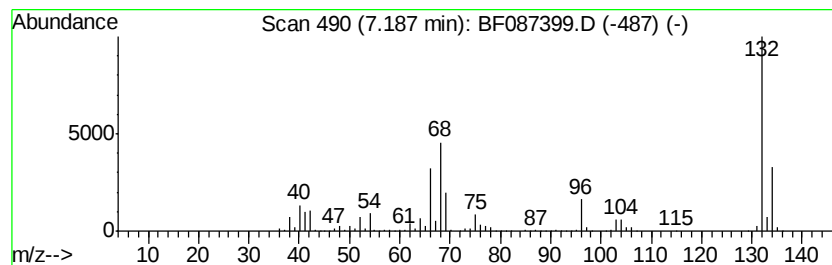
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.19 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	116.81 ng	3933300	1,4-Dichlorobenzene-d4	7.52

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5			(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10



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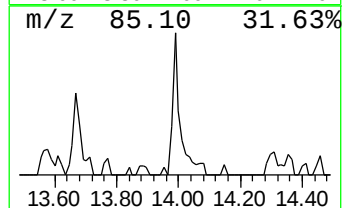
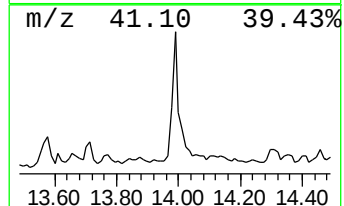
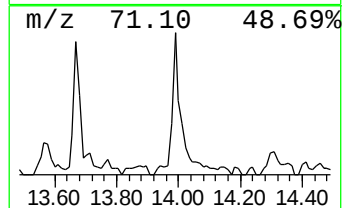
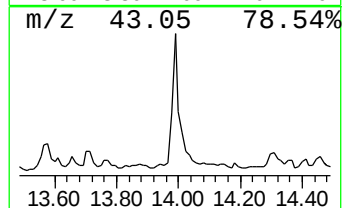
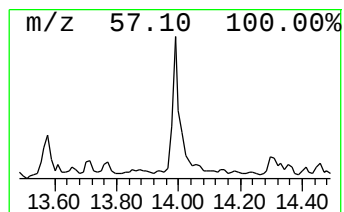
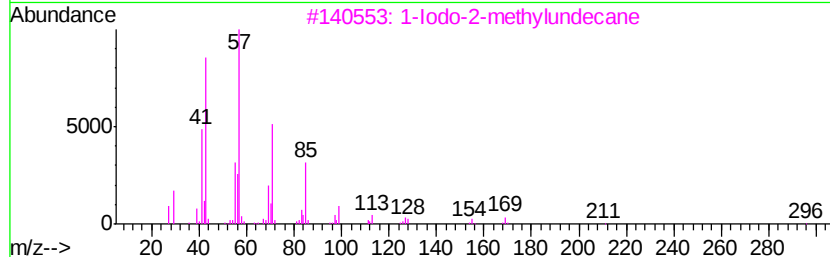
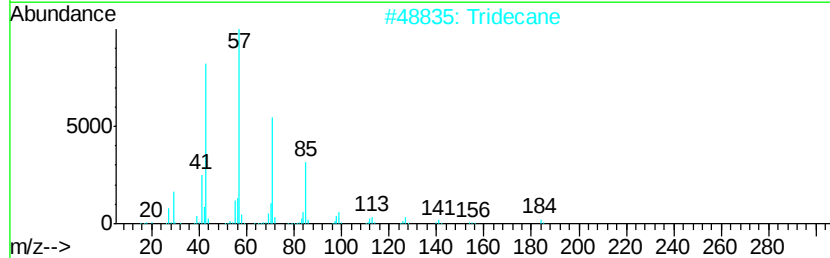
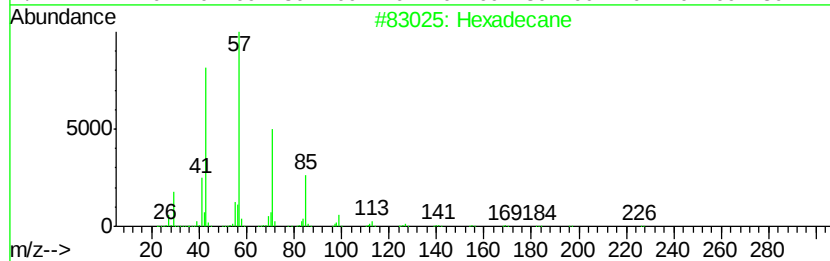
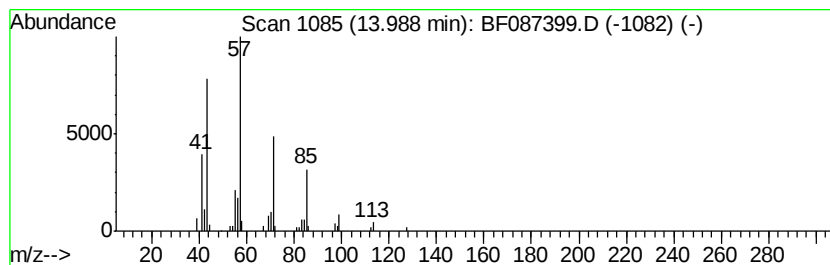
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Peak Number 5 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	3.17 ng	108212	Phenanthrene-d10	14.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tridecane	184	C13H28	000629-50-5	83
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	83
4	Tetradecane	198	C14H30	000629-59-4	72
5	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	64



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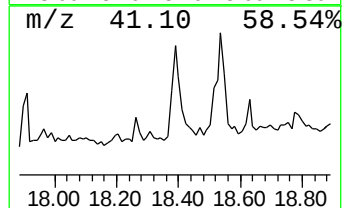
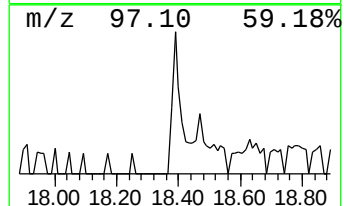
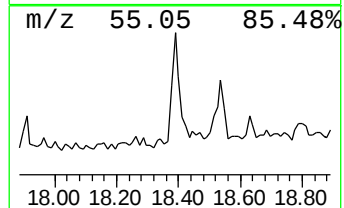
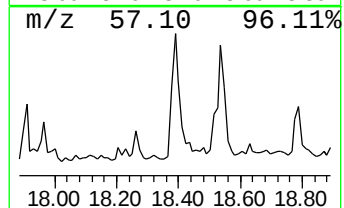
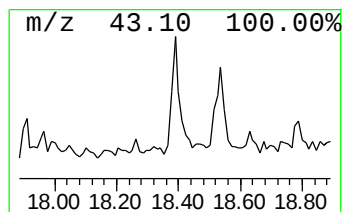
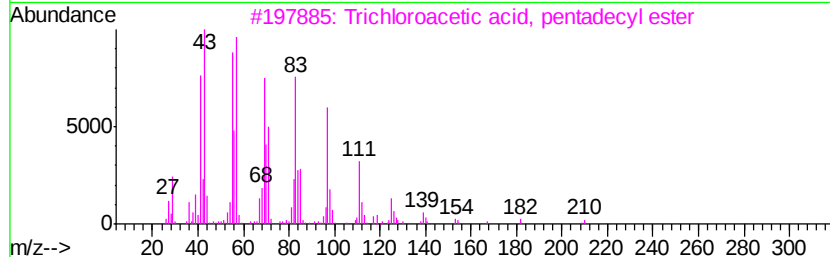
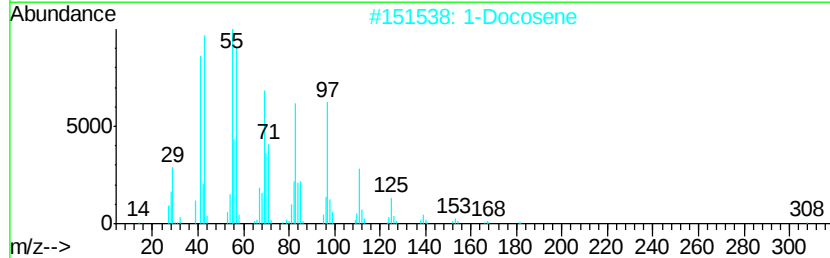
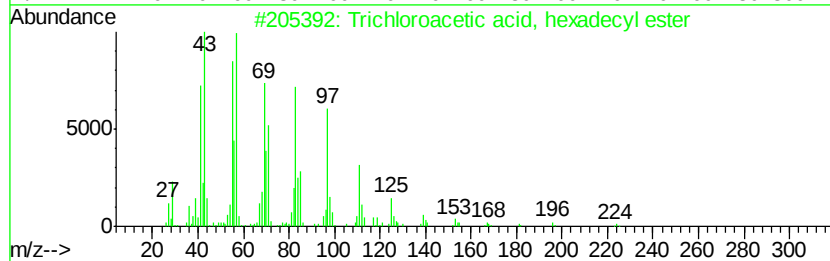
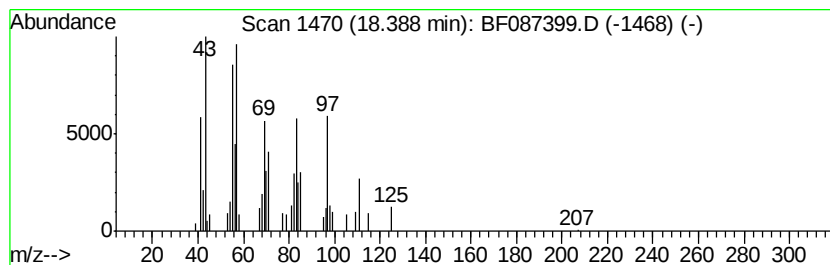
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Peak Number 6 Trichloroacetic acid, hexadecyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	2.05 ng	65054	Chrysene-d12	18.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2		1-Docosene	308	C22H44	001599-67-3	90
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87



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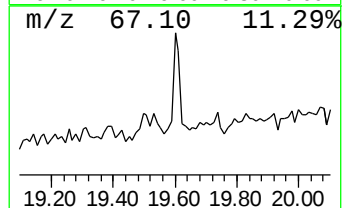
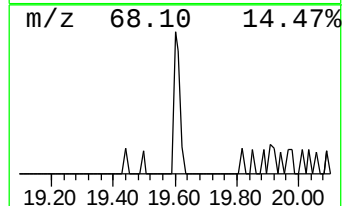
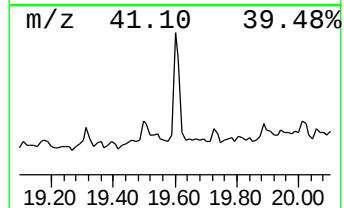
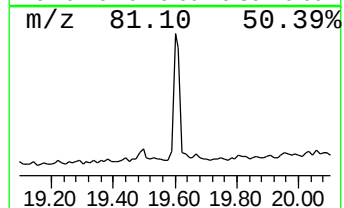
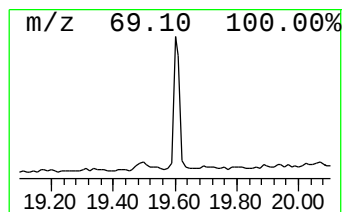
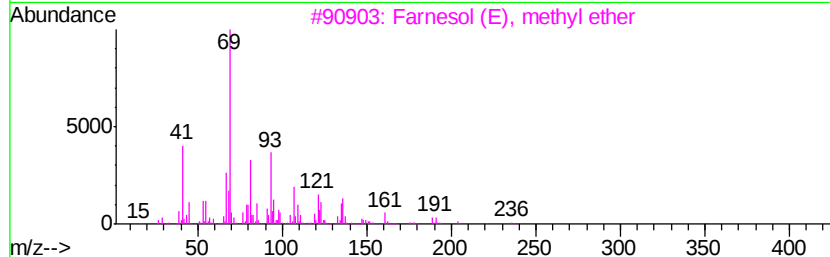
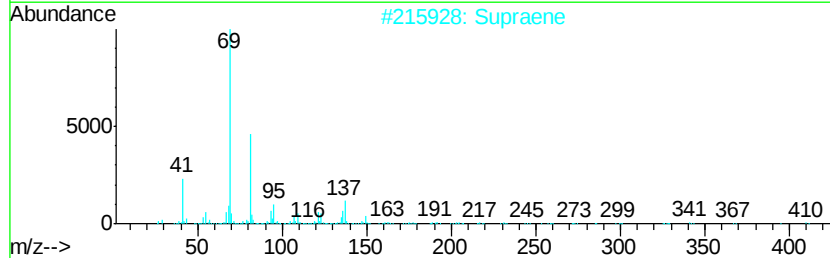
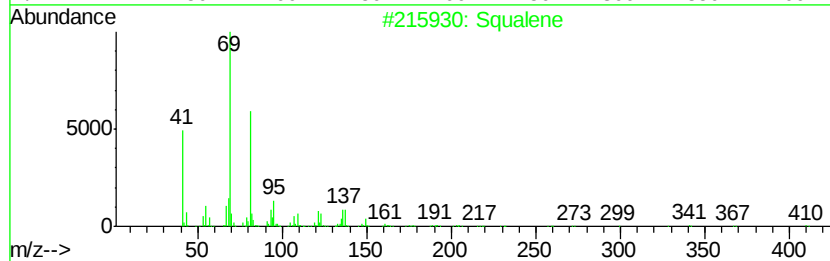
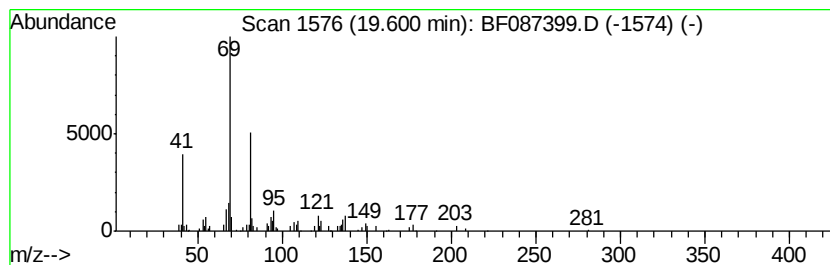
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Peak Number 7 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.60	3.19 ng	75743	Perylene-d12	20.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	78
4		trans-Geranylgeraniol	290	C20H34O	024034-73-9	78
5		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.79	13.1	ng	441709	1	7.52	673442	20.0
unknown7.19	7.19	116.8	ng	3933300	1	7.52	673442	20.0
Hexadecane	13.99	3.2	ng	108212	4	14.78	682086	20.0
Trichloroacetic a...	18.39	2.0	ng	65054	5	18.47	635720	20.0
Squalene	19.60	3.2	ng	75743	6	20.14	475580	20.0