

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052217\
 Data File : BF095313.D
 Acq On : 22 May 2017 14:42
 Operator : SJ/MA
 Sample : I3278-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT-3873

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-BF050217.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	5.131	539	543	569	rBV	69112	182012	8.42%	1.061%
2	5.731	641	645	675	rBV	606902	1620739	74.95%	9.451%
3	7.295	908	911	928	rBV	727345	1567838	72.50%	9.143%
4	7.425	928	933	954	rVB	1154064	1953522	90.34%	11.392%
5	7.760	986	990	1003	rBV	318043	407642	18.85%	2.377%
6	7.995	1025	1030	1045	rBV	1046762	1346351	62.26%	7.851%
7	8.660	1139	1143	1162	rBV	467684	936466	43.30%	5.461%
8	9.784	1330	1334	1357	rBV	297179	614713	28.43%	3.585%
9	11.548	1629	1634	1658	rBV	1319910	2162514	100.00%	12.611%
10	12.254	1750	1754	1768	rBV	103627	187673	8.68%	1.094%
11	12.613	1810	1815	1831	rBV2	428404	752382	34.79%	4.388%
12	13.442	1952	1956	1961	rVB	23725	27128	1.25%	0.158%
13	13.907	2030	2035	2055	rBV	636450	1201218	55.55%	7.005%
14	14.213	2083	2087	2091	rBV2	21140	28398	1.31%	0.166%
15	15.013	2219	2223	2245	rBV	377350	708315	32.75%	4.131%
16	15.965	2381	2385	2395	rBV3	31078	67655	3.13%	0.395%
17	17.118	2578	2581	2589	rVB2	16310	27712	1.28%	0.162%
18	17.330	2612	2617	2636	rBV	1604218	2017328	93.29%	11.764%
19	18.106	2744	2749	2753	rBV	26472	28646	1.32%	0.167%
20	18.577	2823	2829	2843	rBV2	23389	80216	3.71%	0.468%
21	18.683	2843	2847	2864	rVV	387752	637451	29.48%	3.717%
22	19.795	3033	3036	3041	rVB	100287	105088	4.86%	0.613%
23	20.077	3080	3084	3088	rBV	38405	44827	2.07%	0.261%
24	20.359	3128	3132	3151	rBV	237513	442405	20.46%	2.580%

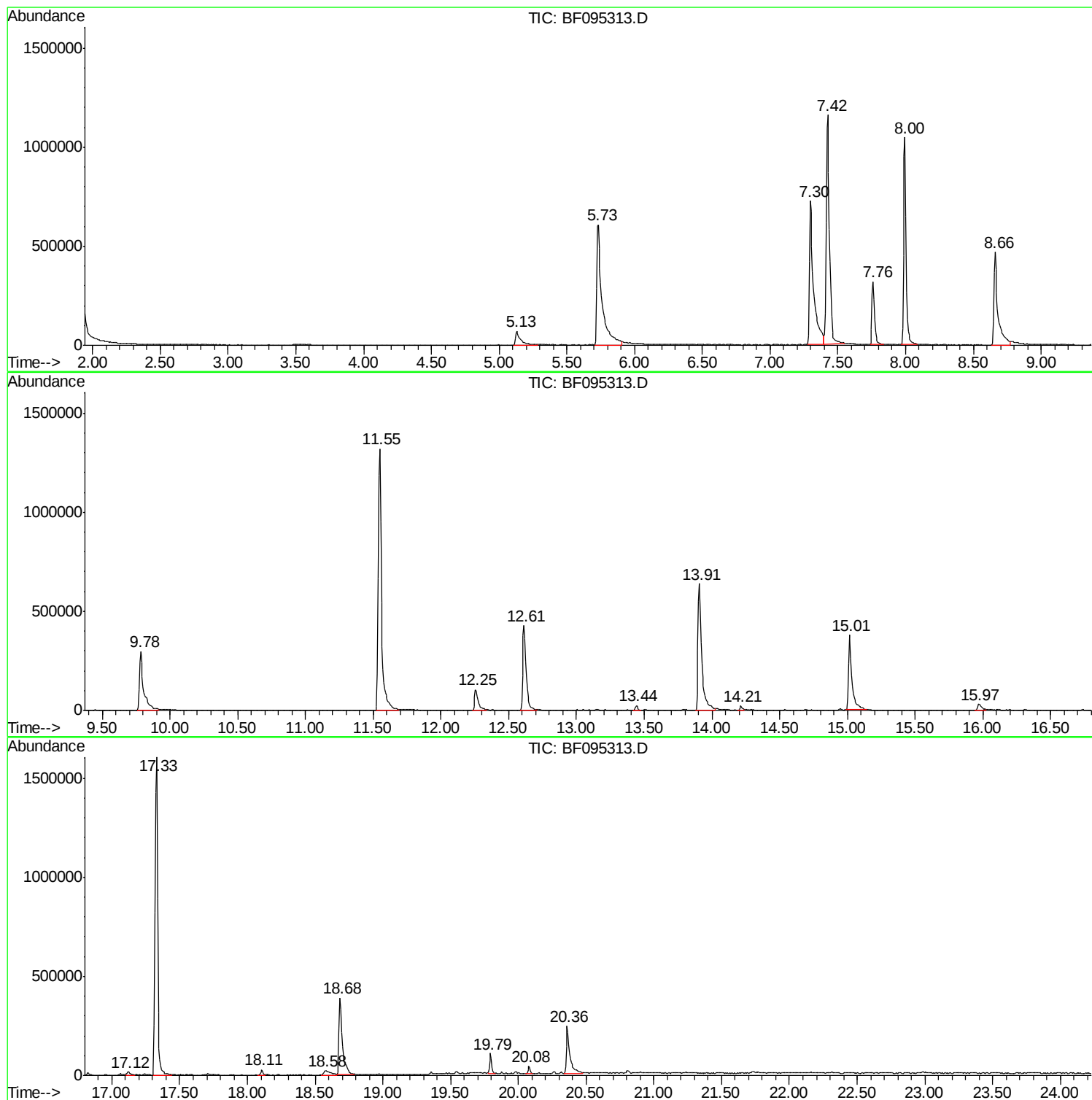
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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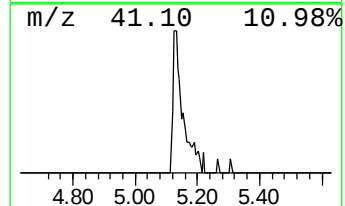
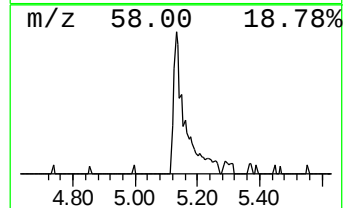
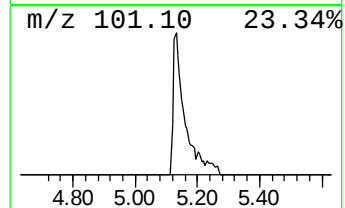
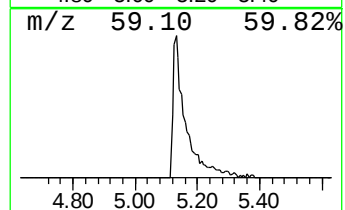
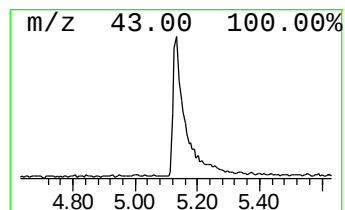
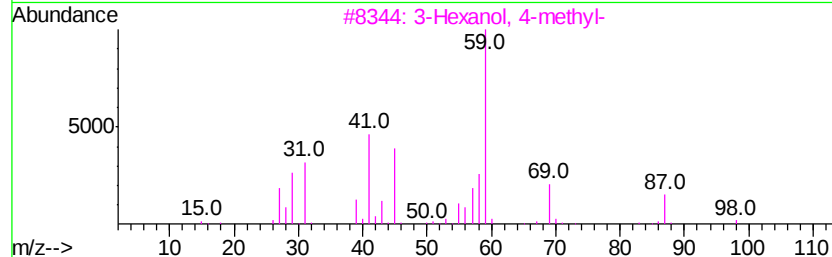
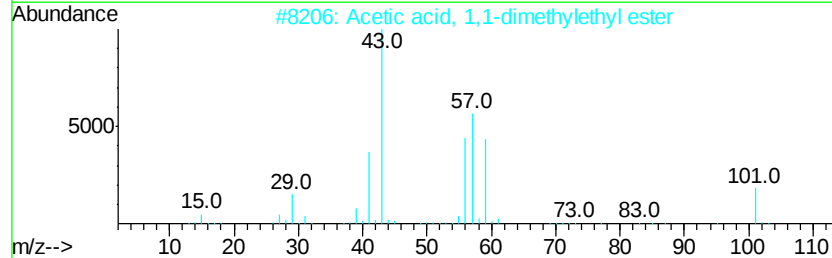
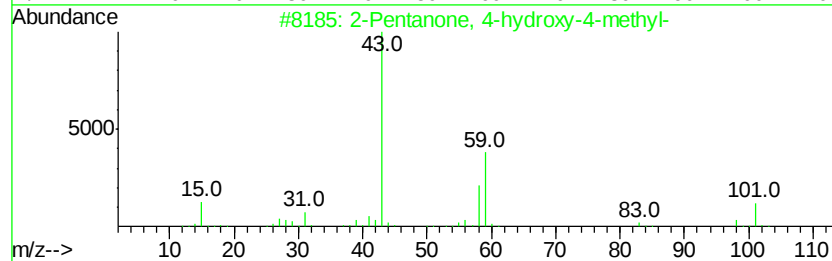
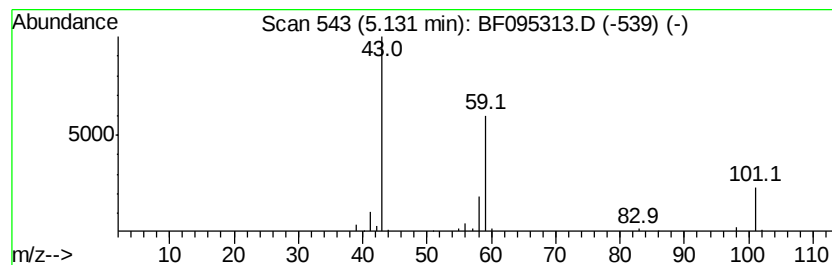
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.13	8.93 ng	182012	1,4-Dichlorobenzene-d4	7.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Acetone	58	C3H6O	000067-64-1	9



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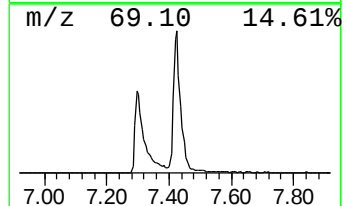
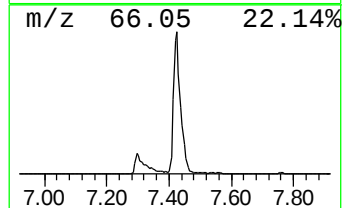
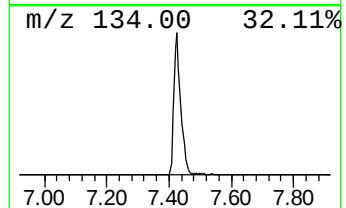
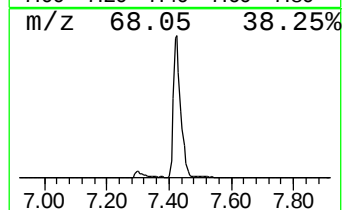
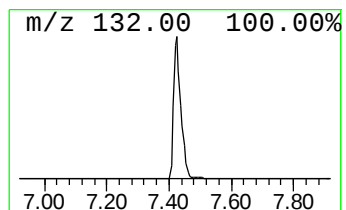
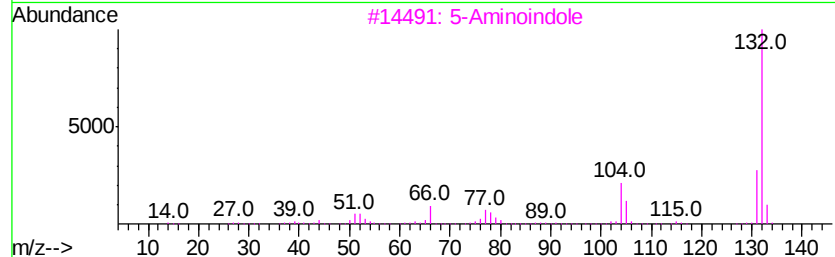
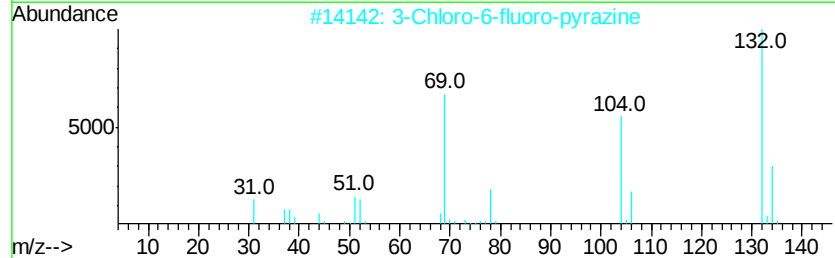
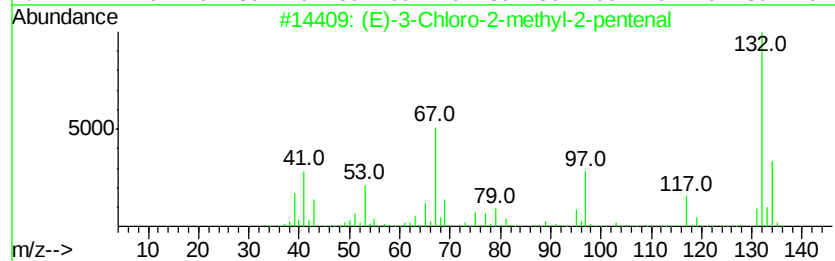
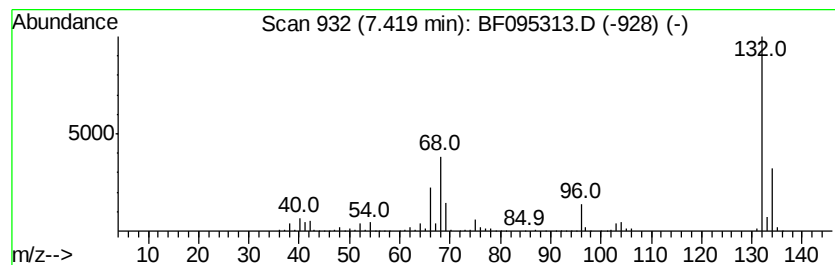
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Peak Number 2 unknown7.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	95.85 ng	1953520	1,4-Dichlorobenzene-d4	7.76

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10



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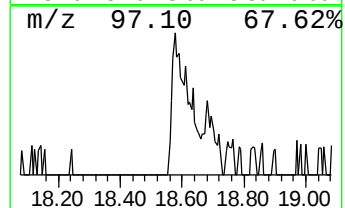
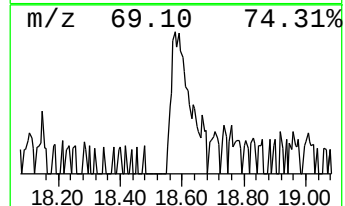
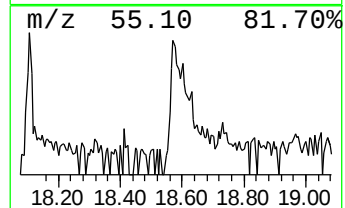
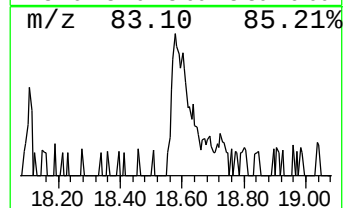
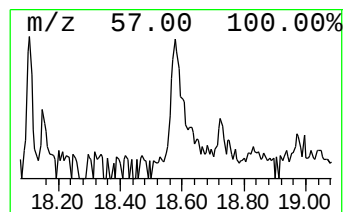
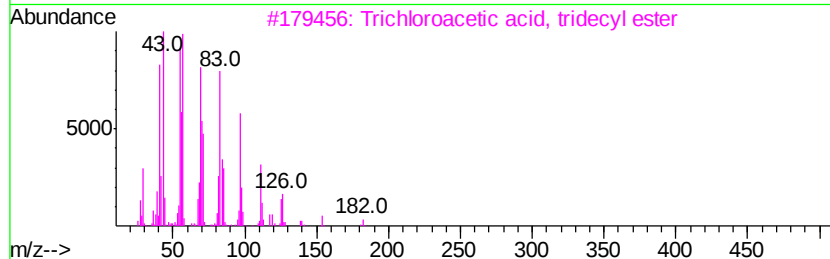
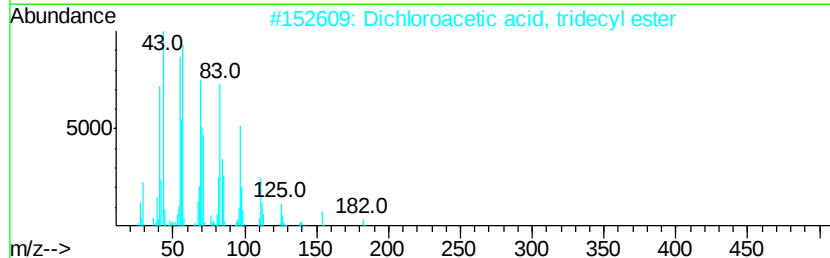
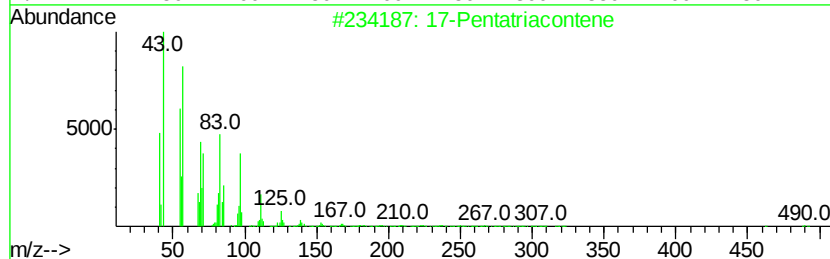
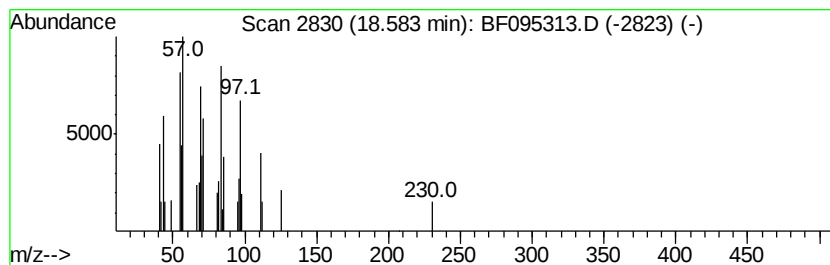
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Peak Number 4 17-Pentatriacontene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.58	2.52 ng	80216	Chrysene-d12	18.68		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-Pentatriacontene	491	C35H70	006971-40-0	87
2		Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	80
3		Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	72
4		1-Heptacosanol	396	C27H56O	002004-39-9	72
5		Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	64



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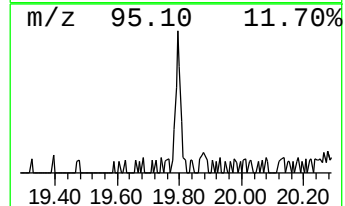
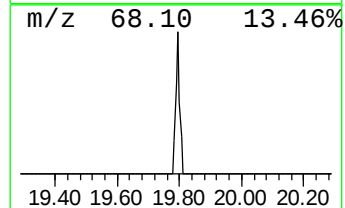
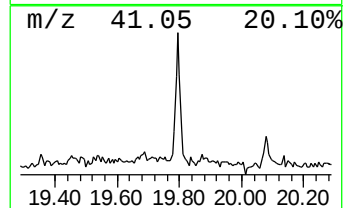
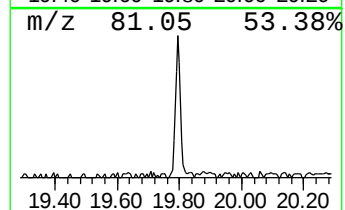
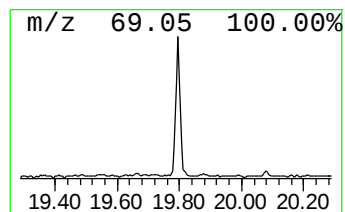
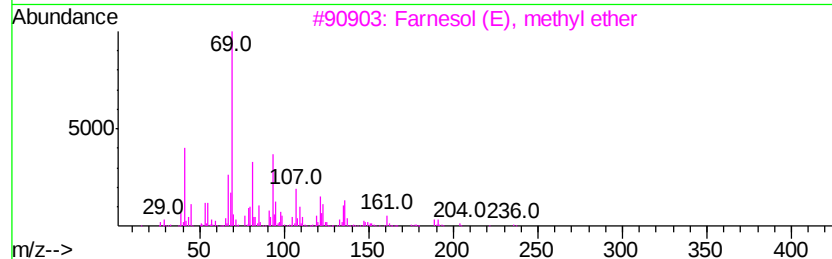
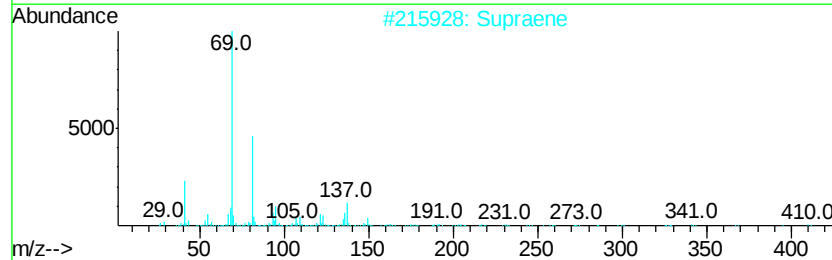
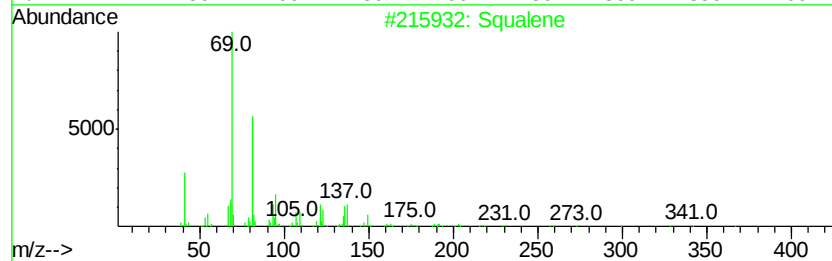
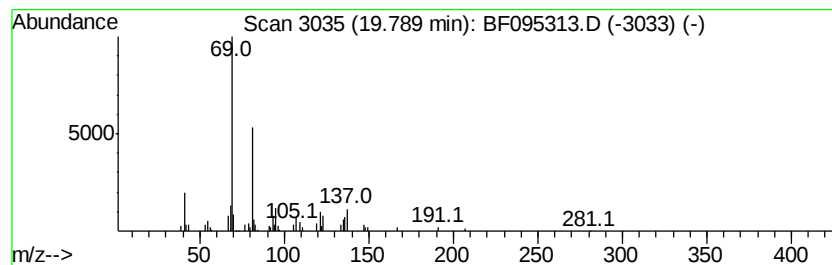
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Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.79	4.75 ng	105088	Perylene-d12	20.36

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	72
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5		3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	72



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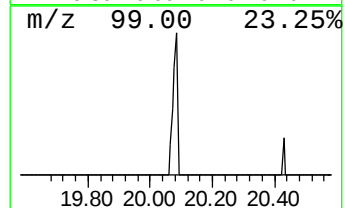
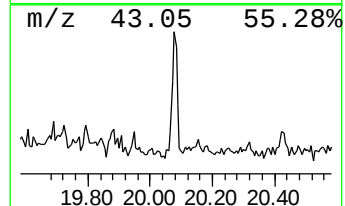
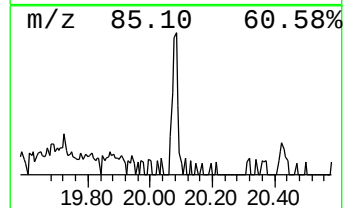
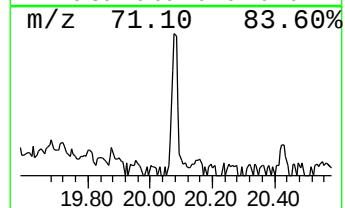
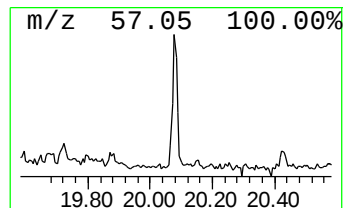
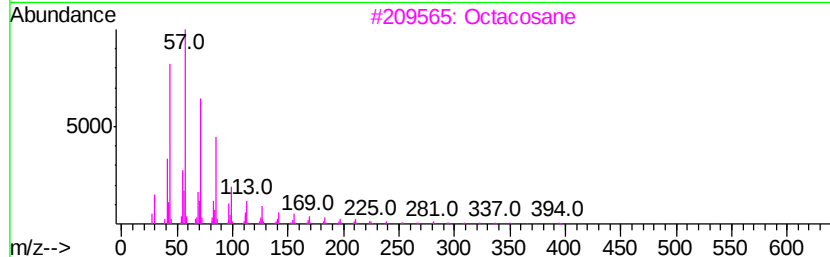
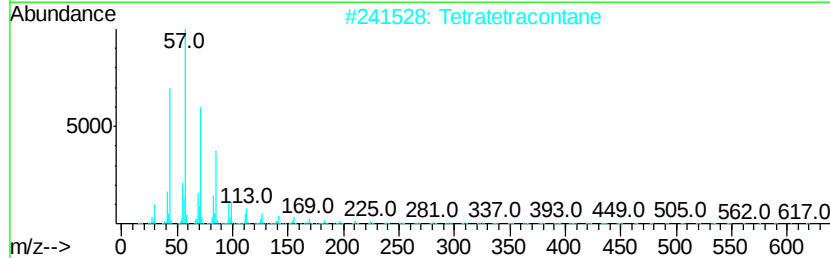
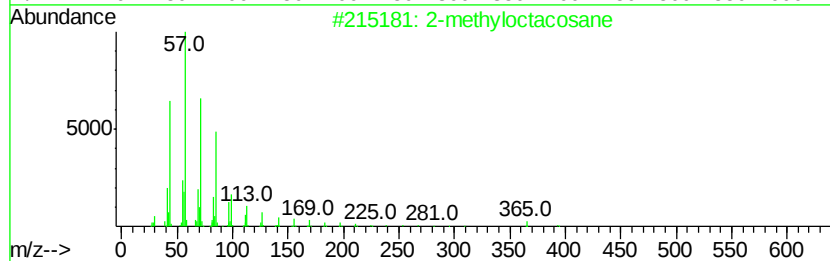
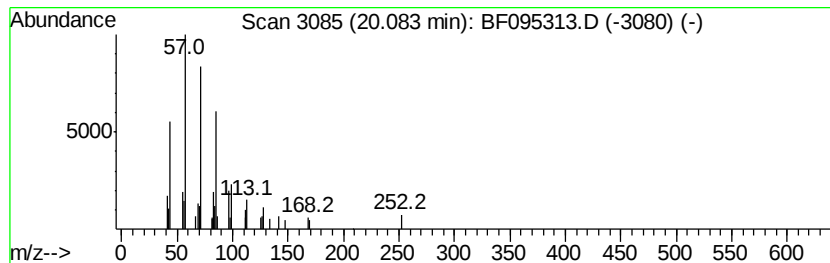
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Peak Number 6 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.08	2.03 ng	44827	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Tetratetracontane	619	C44H90	007098-22-8	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Hentriacontane	437	C31H64	000630-04-6	90
5		triacontane	422	C30H62	000638-68-6	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.13	8.9	ng	182012	1	7.76	407642	20.0
unknown7.42	7.42	95.8	ng	1953520	1	7.76	407642	20.0
17-Pentatriacontene	18.58	2.5	ng	80216	5	18.68	637451	20.0
Squalene	19.79	4.8	ng	105088	6	20.36	442405	20.0
2-methyloctacosane	20.08	2.0	ng	44827	6	20.36	442405	20.0