

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF083118\
 Data File : BF108727.D
 Acq On : 1 Sep 2018 9:11
 Operator : JU/SJ
 Sample : J4729-13
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 082918-SIDI-F-U-B

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:\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	5.231	489	492	501	rBV	26140	37470	1.47%	0.285%
2	5.684	560	569	571	rBV4	31804	91954	3.60%	0.698%
3	6.660	730	735	739	rBV	54984	106651	4.18%	0.810%
4	6.772	751	754	790	rVV	416494	1008135	39.47%	7.658%
5	7.007	790	794	815	rVB	124942	363374	14.23%	2.760%
6	7.154	815	819	851	rVB	1263692	1877971	73.52%	14.265%
7	7.566	885	889	911	rBV	481124	1247615	48.84%	9.477%
8	8.284	1007	1011	1044	rBV	141288	431435	16.89%	3.277%
9	9.348	1189	1192	1238	rBV	1549061	2499385	97.85%	18.985%
10	9.742	1257	1259	1273	rVB	28079	44346	1.74%	0.337%
11	10.042	1306	1310	1321	rBV	266427	402243	15.75%	3.055%
12	10.695	1417	1421	1426	rBV	33665	32541	1.27%	0.247%
13	10.836	1441	1445	1473	rBV	373568	831816	32.56%	6.318%
14	11.542	1561	1565	1586	rBV	236990	479489	18.77%	3.642%
15	13.119	1829	1833	1857	rBV	2136800	2554373	100.00%	19.403%
16	14.095	1989	1999	2011	rBV9	21737	92228	3.61%	0.701%
17	14.195	2012	2016	2026	rBV	381521	539000	21.10%	4.094%
18	15.019	2152	2156	2161	rBV	38036	42648	1.67%	0.324%
19	15.295	2200	2203	2210	rVB2	28514	32106	1.26%	0.244%
20	15.707	2268	2273	2276	rBV	26883	35493	1.39%	0.270%
21	15.754	2276	2281	2297	rVB	166967	343849	13.46%	2.612%
22	16.171	2348	2352	2359	rVB2	24381	35955	1.41%	0.273%
23	16.724	2439	2446	2450	rBV3	17763	34747	1.36%	0.264%

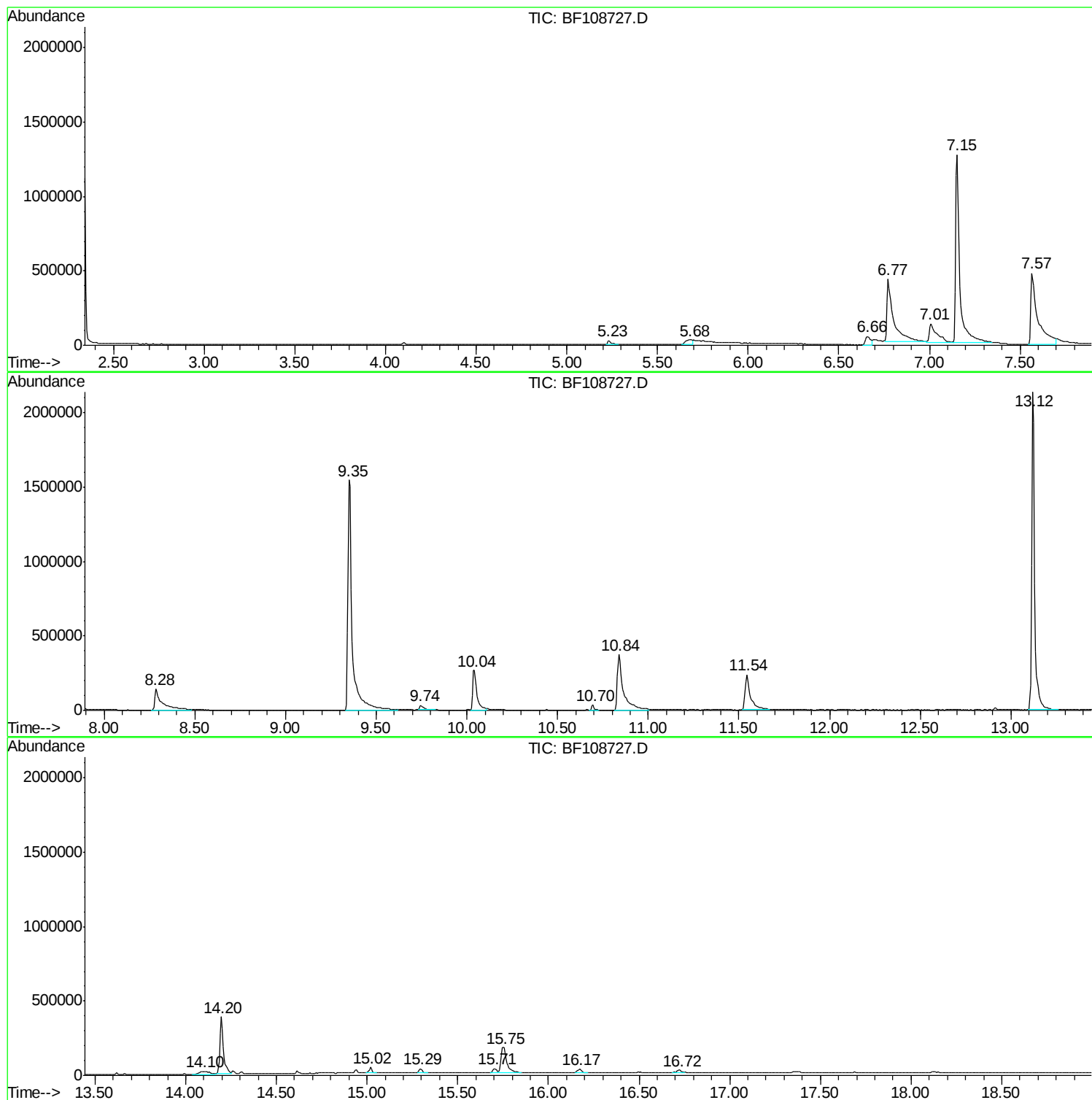
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ClientSampled :
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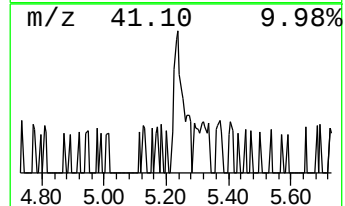
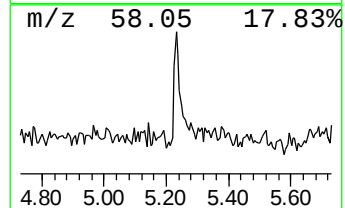
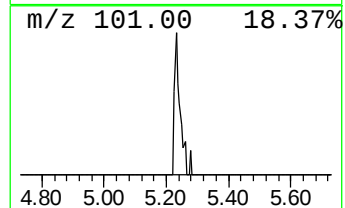
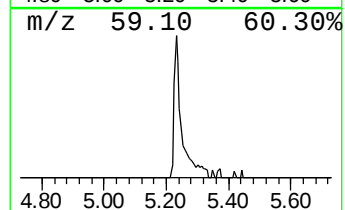
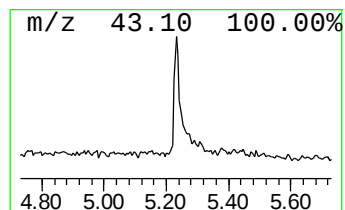
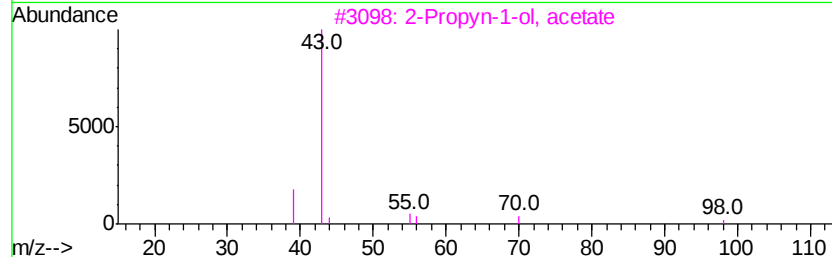
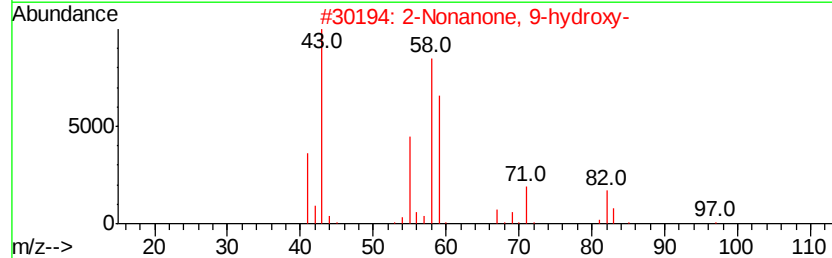
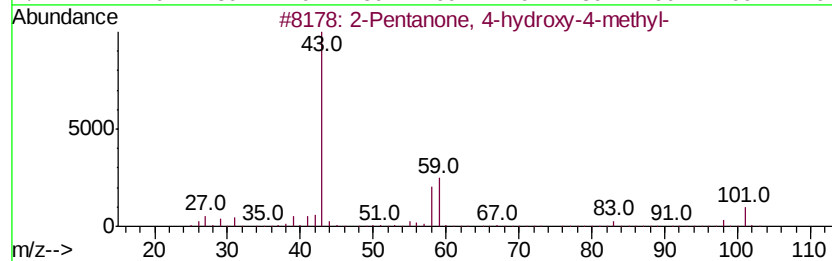
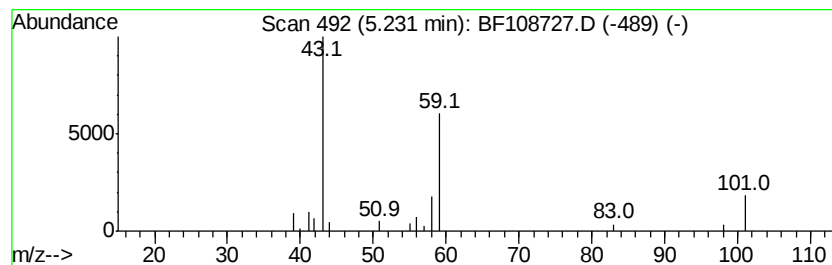
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF083018.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	2.06 ng	37470	1,4-Dichlorobenzene-d4	7.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	33
3			2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9



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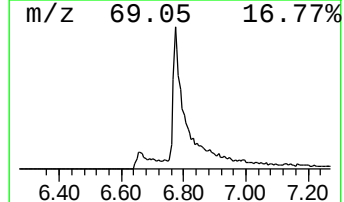
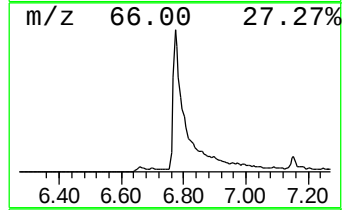
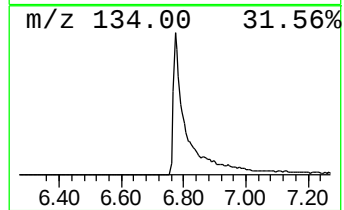
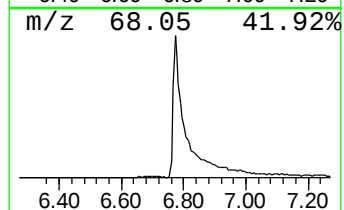
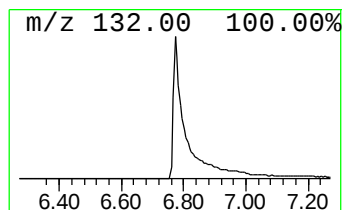
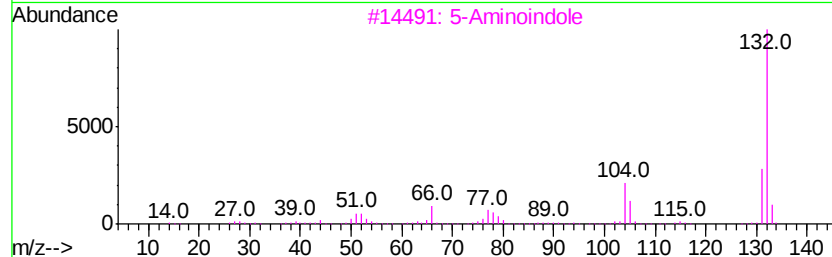
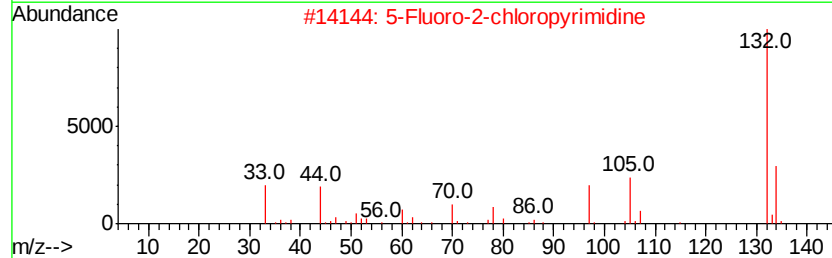
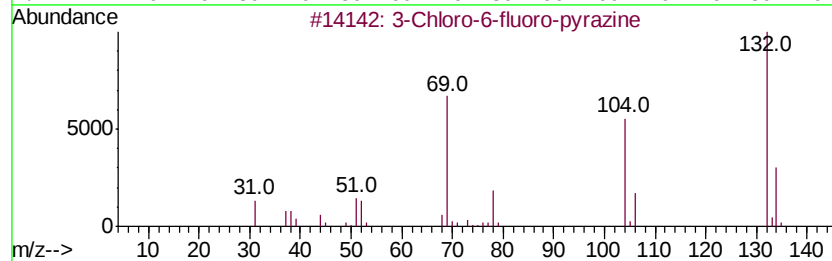
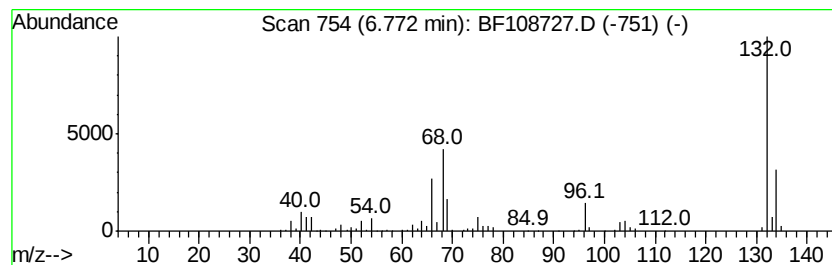
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Peak Number 2 unknown6.77 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	55.49 ng	1008140	1,4-Dichlorobenzene-d4	7.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			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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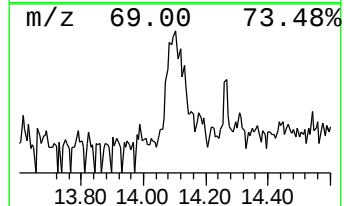
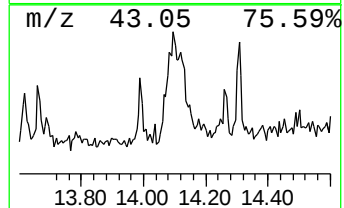
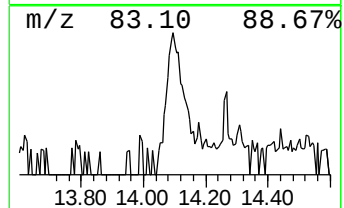
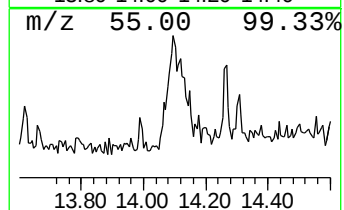
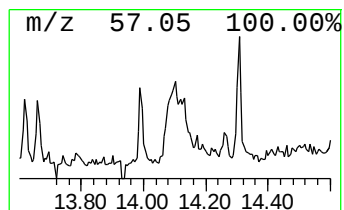
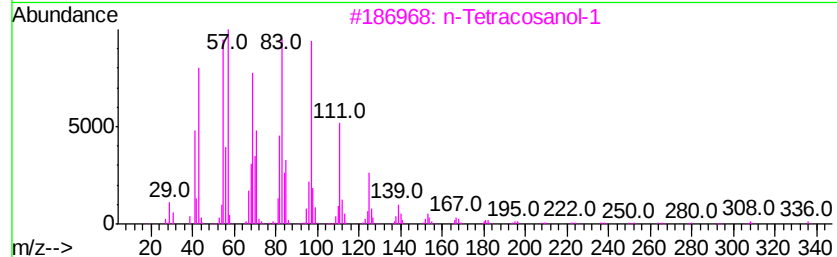
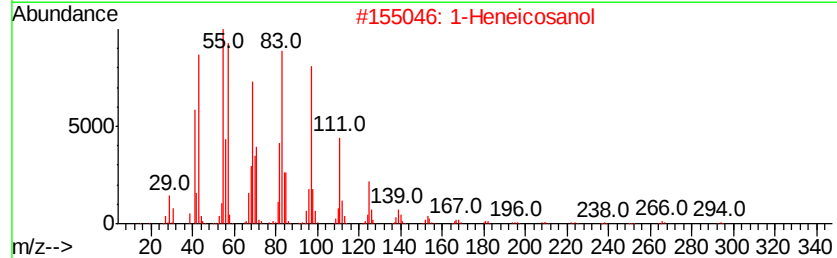
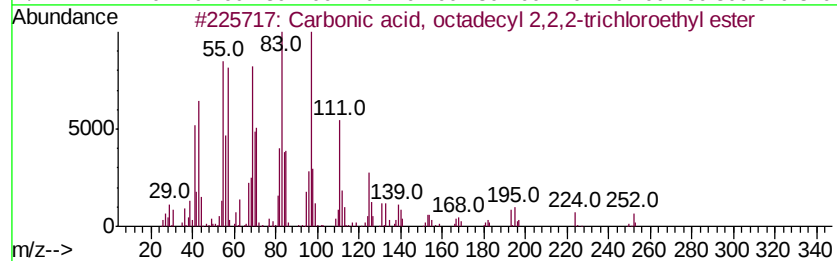
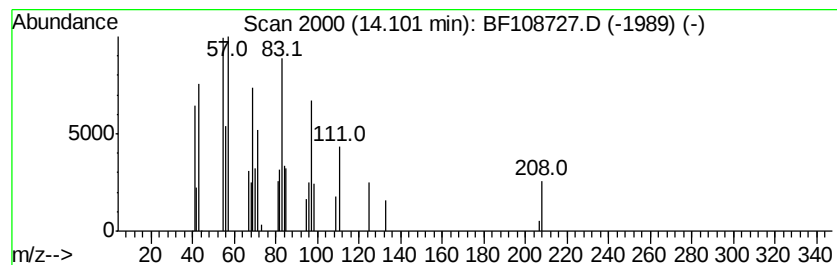
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Peak Number 4 Carbonic acid, octadecyl 2,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.10	3.42 ng	92228	Chrysene-d12	14.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	83
2		1-Heneicosanol	312	C21H44O	015594-90-8	81
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	81
4		Behenic alcohol	326	C22H46O	000661-19-8	81
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	74



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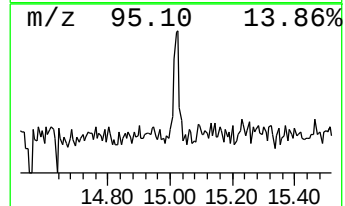
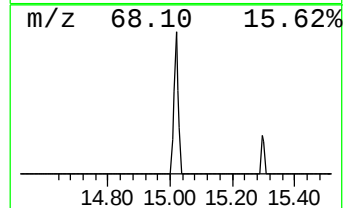
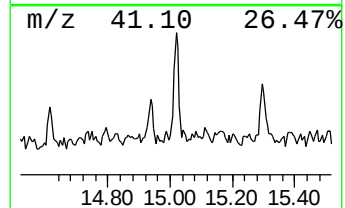
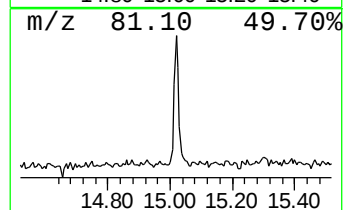
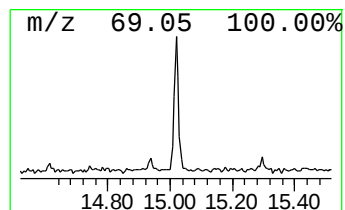
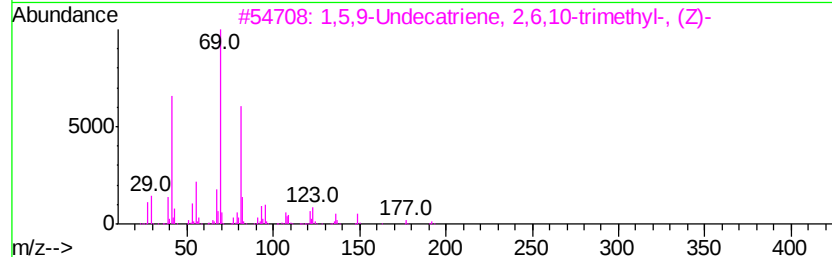
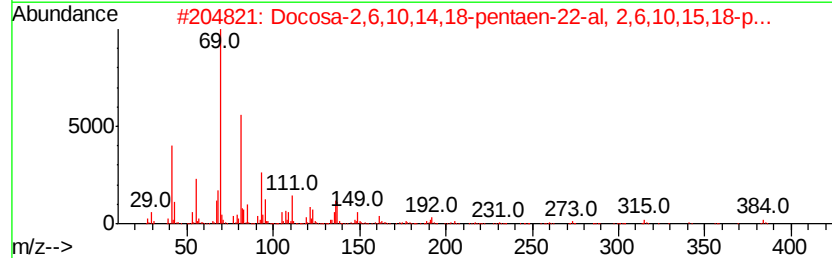
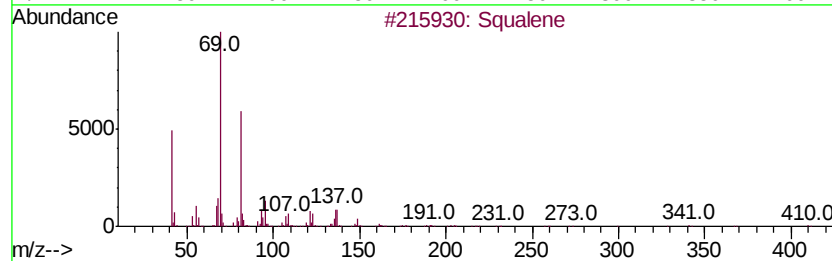
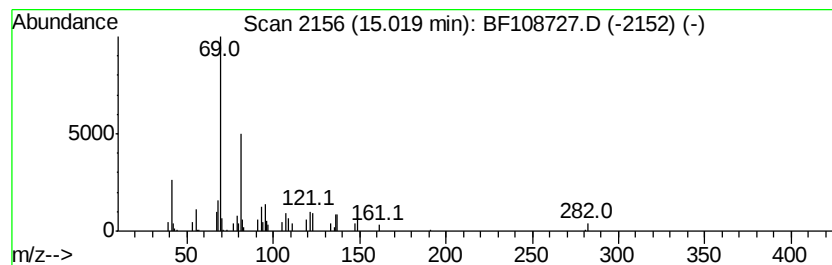
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Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	2.48 ng	42648	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	90
2		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	78
4		trans-Farnesol	222	C15H26O	000106-28-5	78
5		Farnesol isomer a	222	C15H26O	1000108-92-4	64



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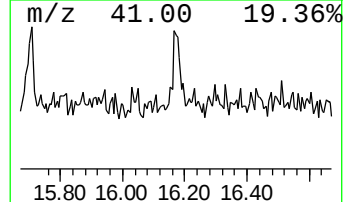
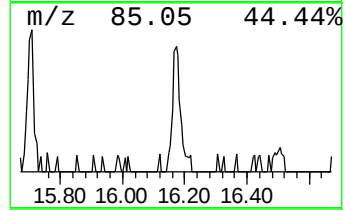
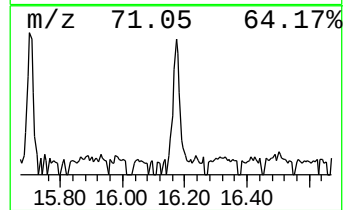
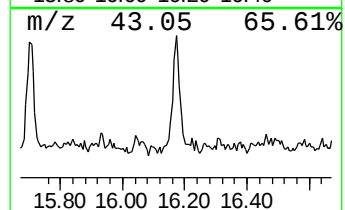
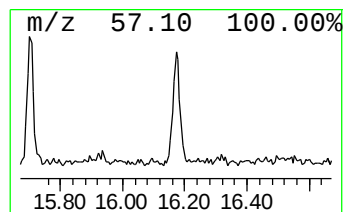
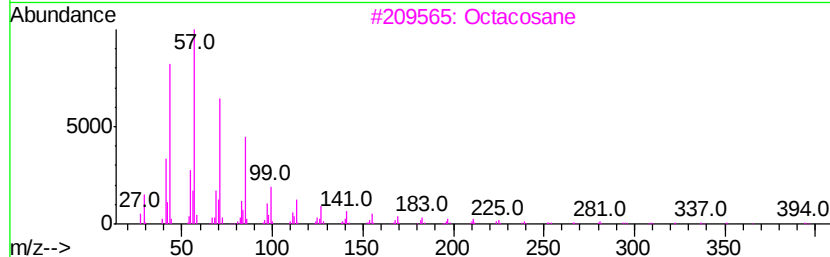
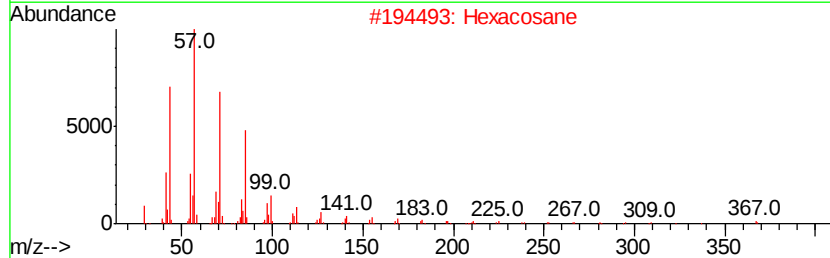
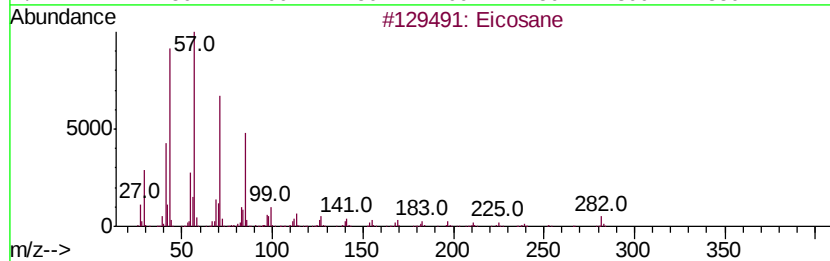
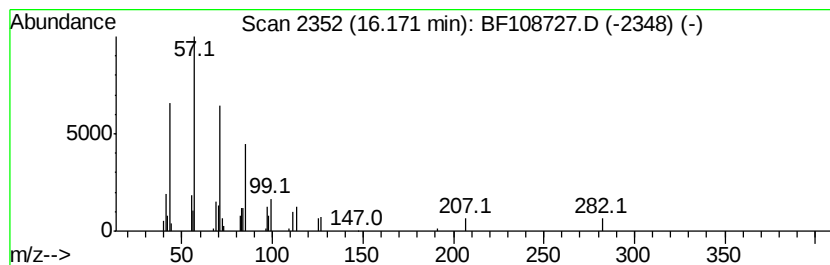
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Peak Number 6 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	2.09 ng	35955	Perylene-d12	15.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	94
2	Hexacosane		366	C26H54	000630-01-3	87
3	Octacosane		394	C28H58	000630-02-4	86
4	Methoxyacetic acid, 2-tetradecyl...		286	C17H34O3	1000282-04-8	86
5	Hentriacontane		437	C31H64	000630-04-6	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.23	2.1	ng	37470	1	7.01	363374	20.0
unknown6.77	6.77	55.5	ng	1008140	1	7.01	363374	20.0
Carbonic acid, oc...	14.10	3.4	ng	92228	5	14.20	539000	20.0
Squalene	15.02	2.5	ng	42648	6	15.75	343849	20.0
Eicosane	16.17	2.1	ng	35955	6	15.75	343849	20.0