

Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
 Data File : BF096568.D
 Acq On : 7 Jul 2017 19:28
 Operator : SJ/MA
 Sample : I4069-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-1

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:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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	3.657	261	267	274	rBV	109600	169211	7.66%	0.836%
2	4.881	470	475	484	rVB	344465	445685	20.17%	2.202%
3	5.310	543	548	551	rBV	2074366	2155940	97.56%	10.653%
4	6.333	717	722	733	rVB	2245106	2209928	100.00%	10.920%
5	6.463	740	744	747	rBV	2344447	2148675	97.23%	10.617%
6	6.692	780	783	787	rBV	775877	662786	29.99%	3.275%
7	6.851	806	810	813	rBV	1814381	1528043	69.14%	7.550%
8	7.251	873	878	882	rBV	1348830	1369182	61.96%	6.765%
9	7.974	997	1001	1005	rBV	967508	818565	37.04%	4.045%
10	9.051	1179	1184	1188	rBV	2072231	2006313	90.79%	9.914%
11	9.445	1247	1251	1254	rBV	232830	176697	8.00%	0.873%
12	9.627	1277	1282	1288	rBV2	13089	22326	1.01%	0.110%
13	9.727	1294	1299	1303	rVB	1127087	946013	42.81%	4.674%
14	10.139	1364	1369	1372	rBV	59013	84759	3.84%	0.419%
15	10.174	1372	1375	1378	rVB	40658	33369	1.51%	0.165%
16	10.510	1428	1432	1436	rBV	1305036	1223352	55.36%	6.045%
17	10.645	1452	1455	1462	rBV	47279	51727	2.34%	0.256%
18	11.204	1546	1550	1554	rVB	969848	823352	37.26%	4.068%
19	11.745	1635	1642	1645	rBV	62685	61646	2.79%	0.305%
20	12.527	1772	1775	1781	rBV2	23876	26072	1.18%	0.129%
21	12.792	1815	1820	1823	rBV	1771052	1727623	78.18%	8.537%
22	13.692	1969	1973	1982	rBV	106705	118596	5.37%	0.586%
23	13.833	1993	1997	2000	rBV	848968	760754	34.42%	3.759%
24	14.686	2138	2142	2146	rVB	76985	68051	3.08%	0.336%
25	15.233	2230	2235	2240	rBV	475331	535544	24.23%	2.646%
26	16.150	2386	2391	2397	rVB7	18363	37174	1.68%	0.184%
27	16.692	2478	2483	2489	rVB9	12834	26541	1.20%	0.131%

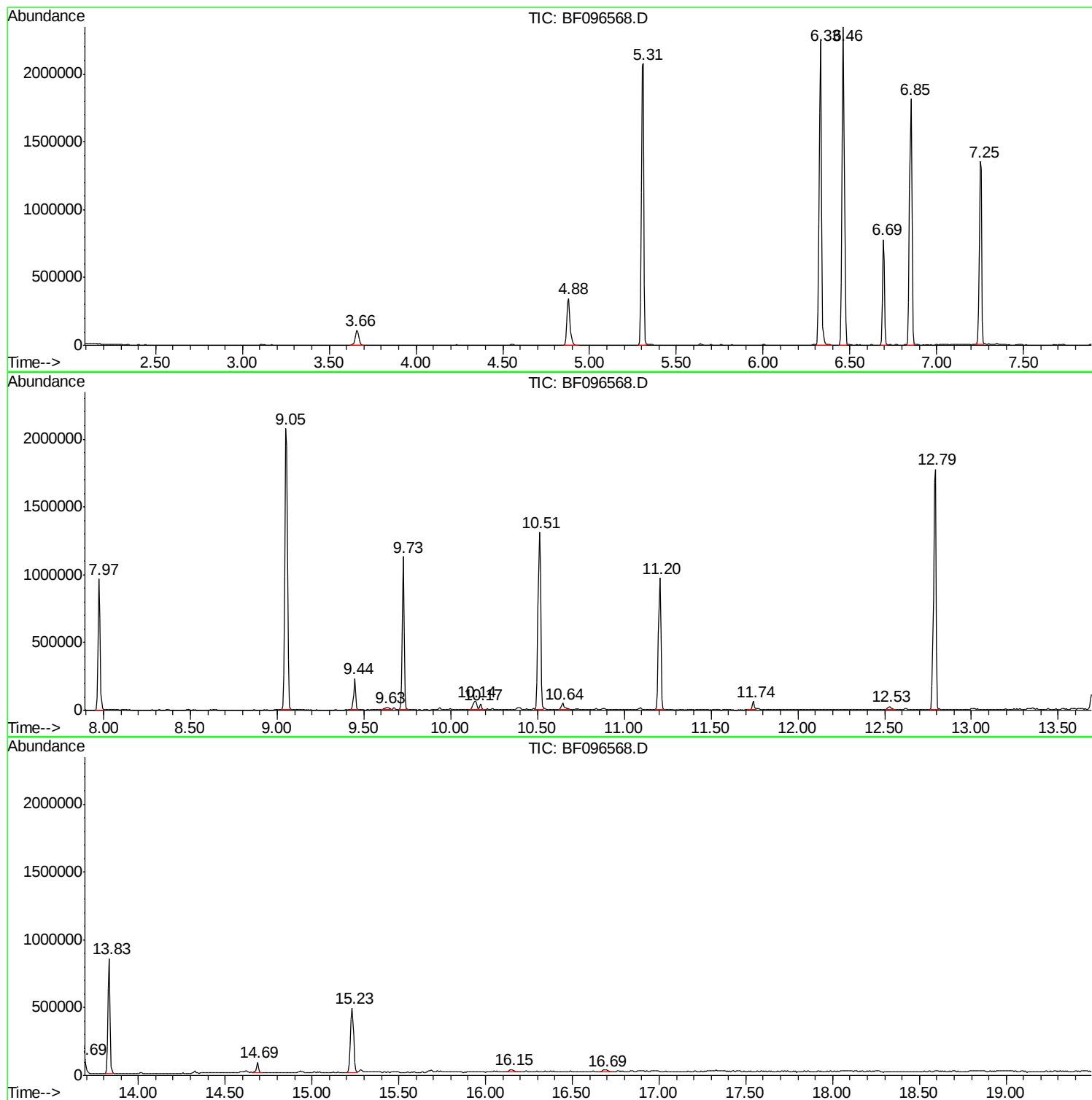
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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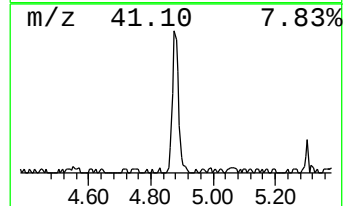
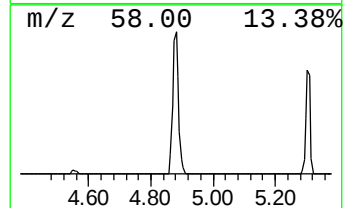
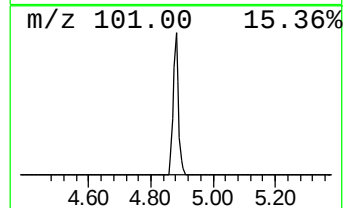
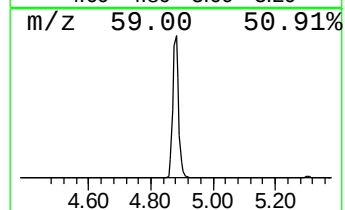
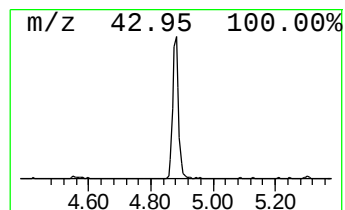
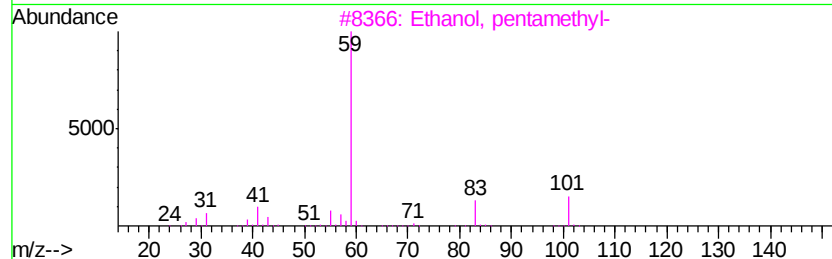
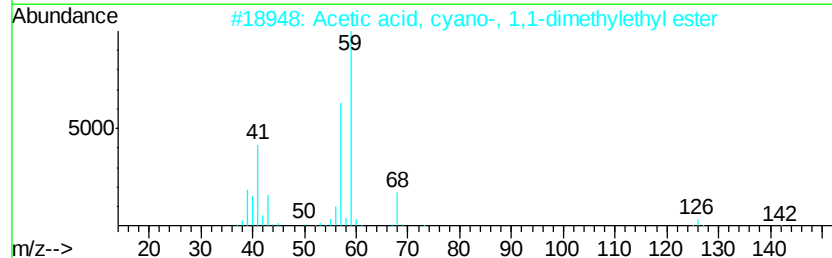
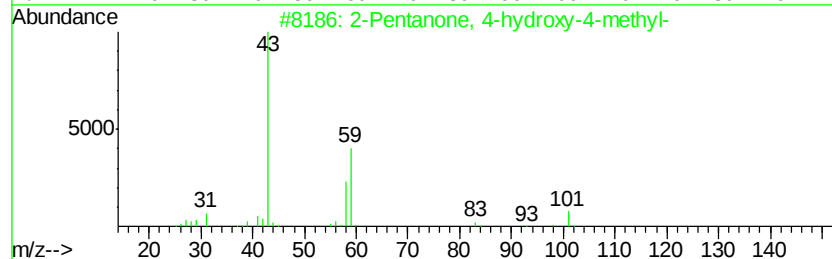
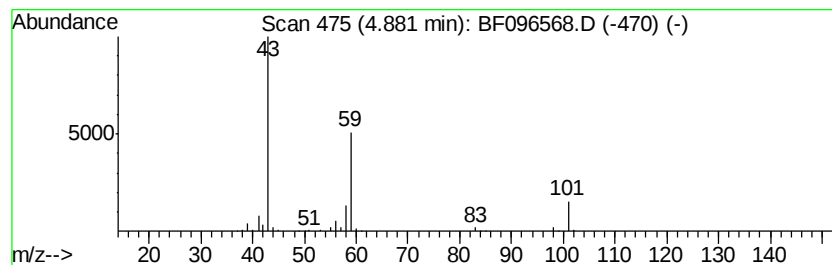
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	13.45 ng	445685	1,4-Dichlorobenzene-d4	6.69

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9
4		5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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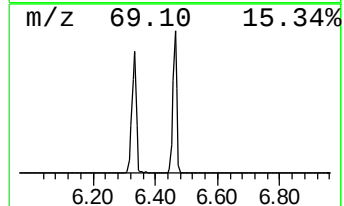
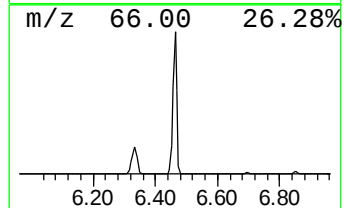
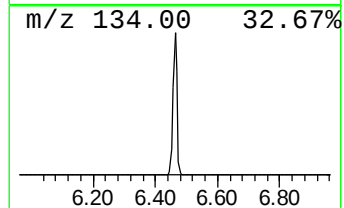
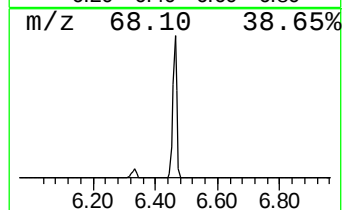
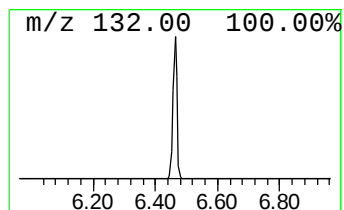
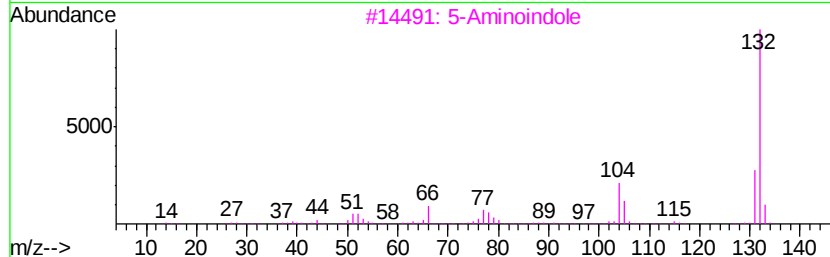
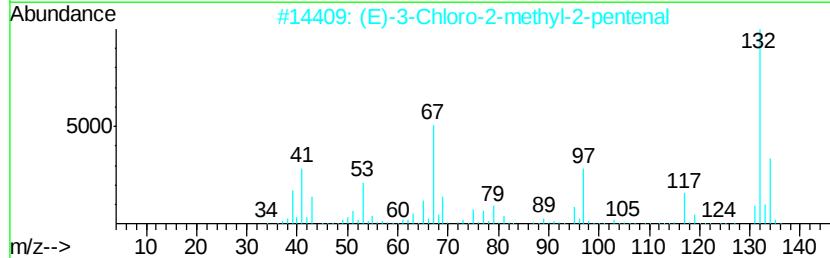
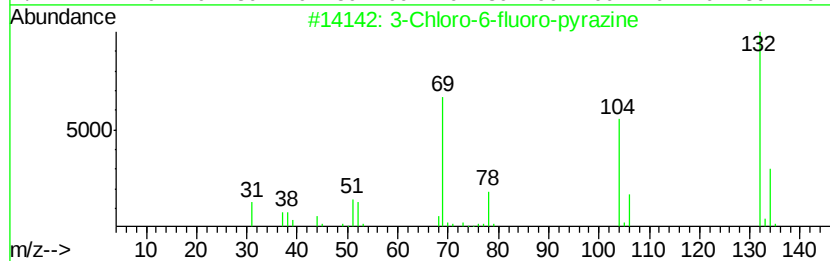
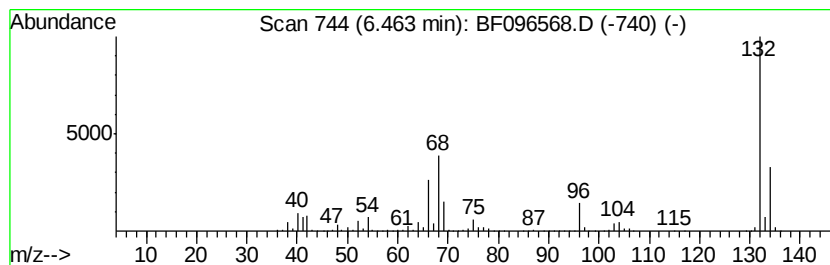
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	64.84 ng	2148680	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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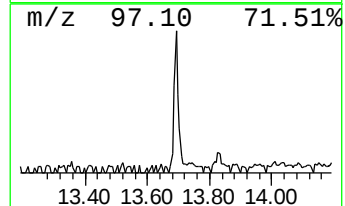
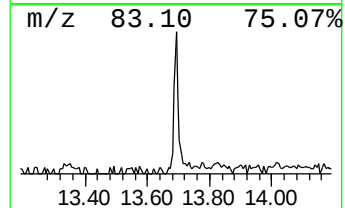
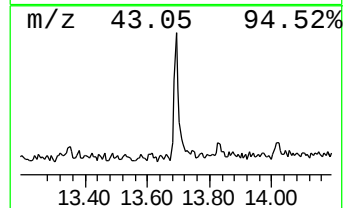
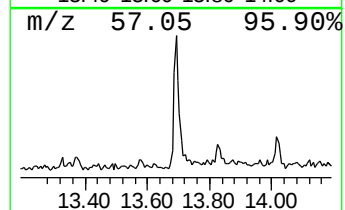
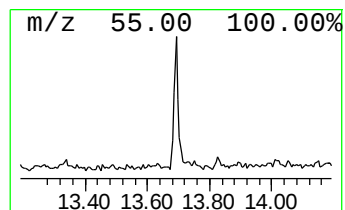
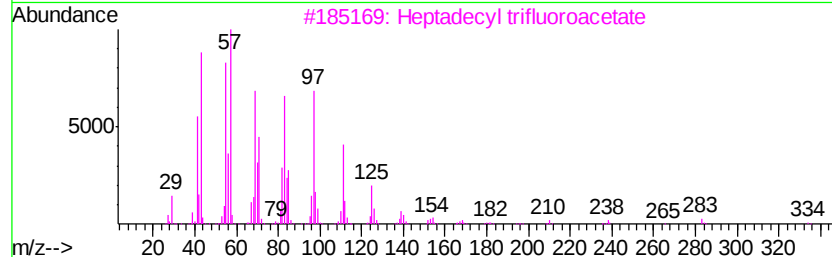
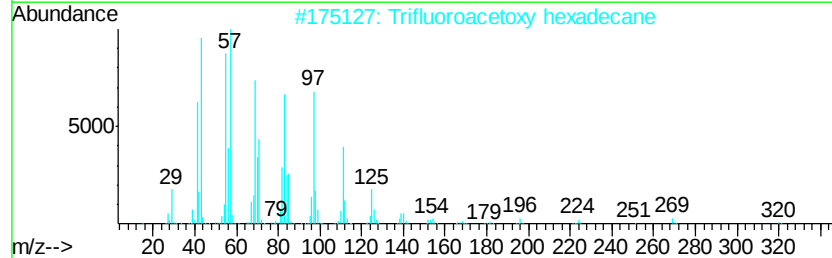
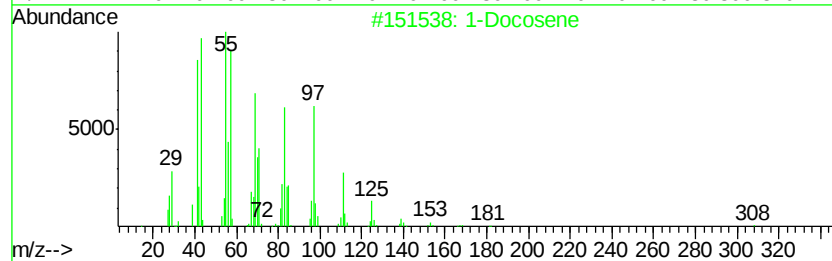
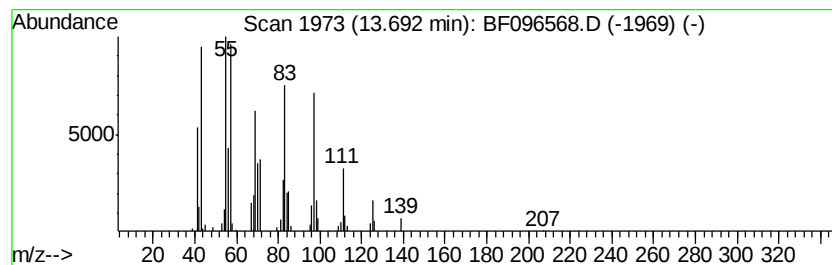
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Peak Number 5 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	3.12 ng	118596	Chrysene-d12	13.83
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosene		308 C22H44	001599-67-3 94
2	Trifluoroacetoxy hexadecane		338 C18H33F3O2	006222-03-3 91
3	Heptadecyl trifluoroacetate		352 C19H35F3O2	1000351-87-0 91
4	1-Nonadecene		266 C19H38	018435-45-5 91
5	3-Chloropropionic acid, heptadec...		346 C20H39ClO2	1000283-05-1 91



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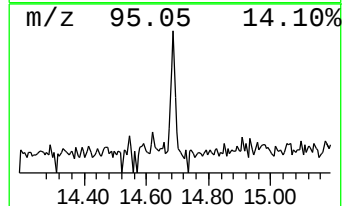
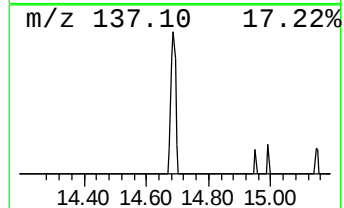
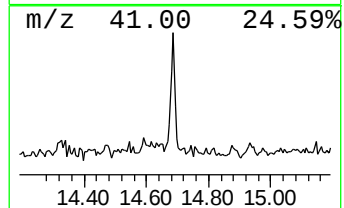
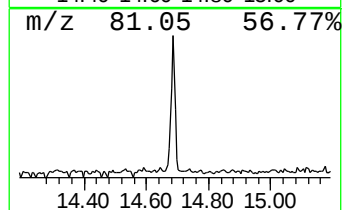
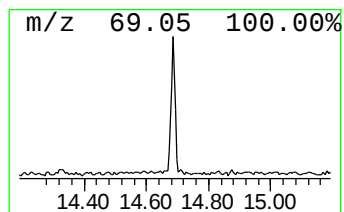
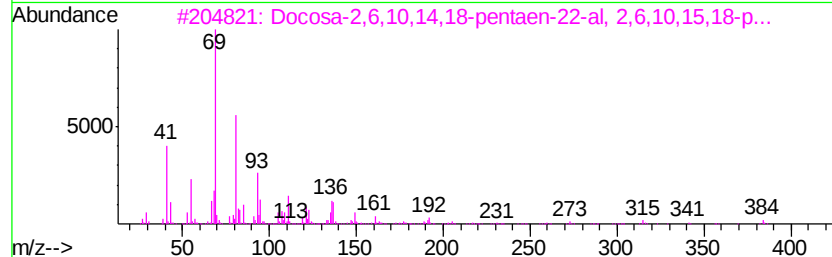
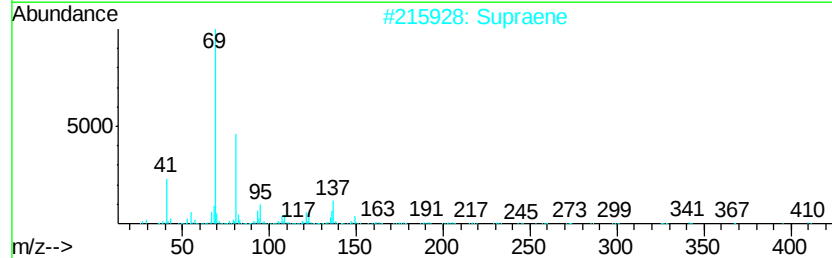
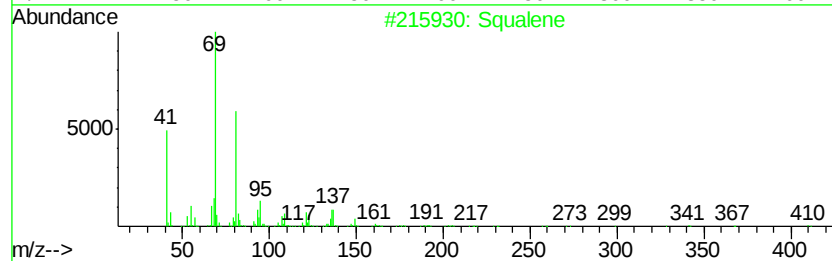
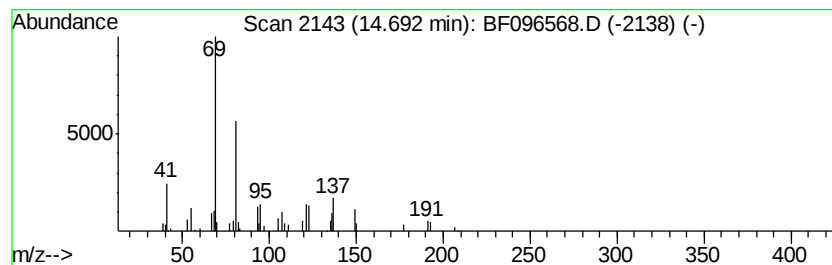
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Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	2.54 ng	68051	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	87
2		Supraene	410	C30H50	007683-64-9	80
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5		trans-Farnesol	222	C15H26O	000106-28-5	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.88	13.4	ng	445685	1	6.69	662786	20.0
unknown6.46	6.46	64.8	ng	2148680	1	6.69	662786	20.0
1-Docosene	13.69	3.1	ng	118596	5	13.83	760754	20.0
Squalene	14.69	2.5	ng	68051	6	15.23	535544	20.0