

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021315\
 Data File : BF077318.D
 Acq On : 13 Feb 2015 20:49
 Operator : TP/IZ
 Sample : G1294-07
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 118-00(0-2)

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-BF021215.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	1.275	33	34	38	rBV	4980	8466	1.15%	0.131%
2	1.333	38	39	54	rVB3	34211	73527	10.00%	1.140%
3	3.481	224	227	240	rBV	69605	190873	25.96%	2.960%
4	4.499	313	316	333	rBV	243586	569115	77.40%	8.826%
5	5.367	390	392	397	rBB	3500	8456	1.15%	0.131%
6	6.922	526	528	532	rBV	272433	537756	73.13%	8.340%
7	6.990	532	534	547	rVB	390852	695118	94.54%	10.780%
8	7.493	576	578	587	rBB	77648	146559	19.93%	2.273%
9	7.813	603	606	615	rBB	275405	472659	64.28%	7.330%
10	8.808	690	693	706	rBV	222850	371268	50.49%	5.758%
11	10.408	830	833	842	rBB	126438	206789	28.12%	3.207%
12	13.059	1062	1065	1069	rBV	396667	701410	95.39%	10.878%
13	14.145	1157	1160	1164	rBB	8473	12839	1.75%	0.199%
14	14.522	1190	1193	1198	rBB2	135361	224158	30.49%	3.476%
15	16.248	1342	1344	1346	rBV	11621	15573	2.12%	0.242%
16	16.294	1346	1348	1357	rVB	270533	375765	51.10%	5.828%
17	17.437	1445	1448	1451	rBV	173160	227686	30.97%	3.531%
18	19.129	1594	1596	1600	rBB	8696	9641	1.31%	0.150%
19	19.689	1643	1645	1648	rBV	506833	735296	100.00%	11.403%
20	19.837	1655	1658	1665	rBV3	1549	7396	1.01%	0.115%
21	20.557	1719	1721	1725	rBV3	4641	9299	1.26%	0.144%
22	20.957	1753	1756	1764	rBV	253877	421333	57.30%	6.534%
23	21.369	1789	1792	1798	rBV4	11589	21672	2.95%	0.336%
24	21.746	1823	1825	1827	rBV2	19071	27473	3.74%	0.426%
25	22.123	1856	1858	1860	rBV2	11194	12319	1.68%	0.191%
26	22.180	1860	1863	1865	rVV	29405	45490	6.19%	0.705%
27	22.489	1888	1890	1894	rBV5	11558	25427	3.46%	0.394%
28	22.603	1898	1900	1903	rBV	198295	249933	33.99%	3.876%
29	24.101	2029	2031	2035	rVB4	19094	44727	6.08%	0.694%

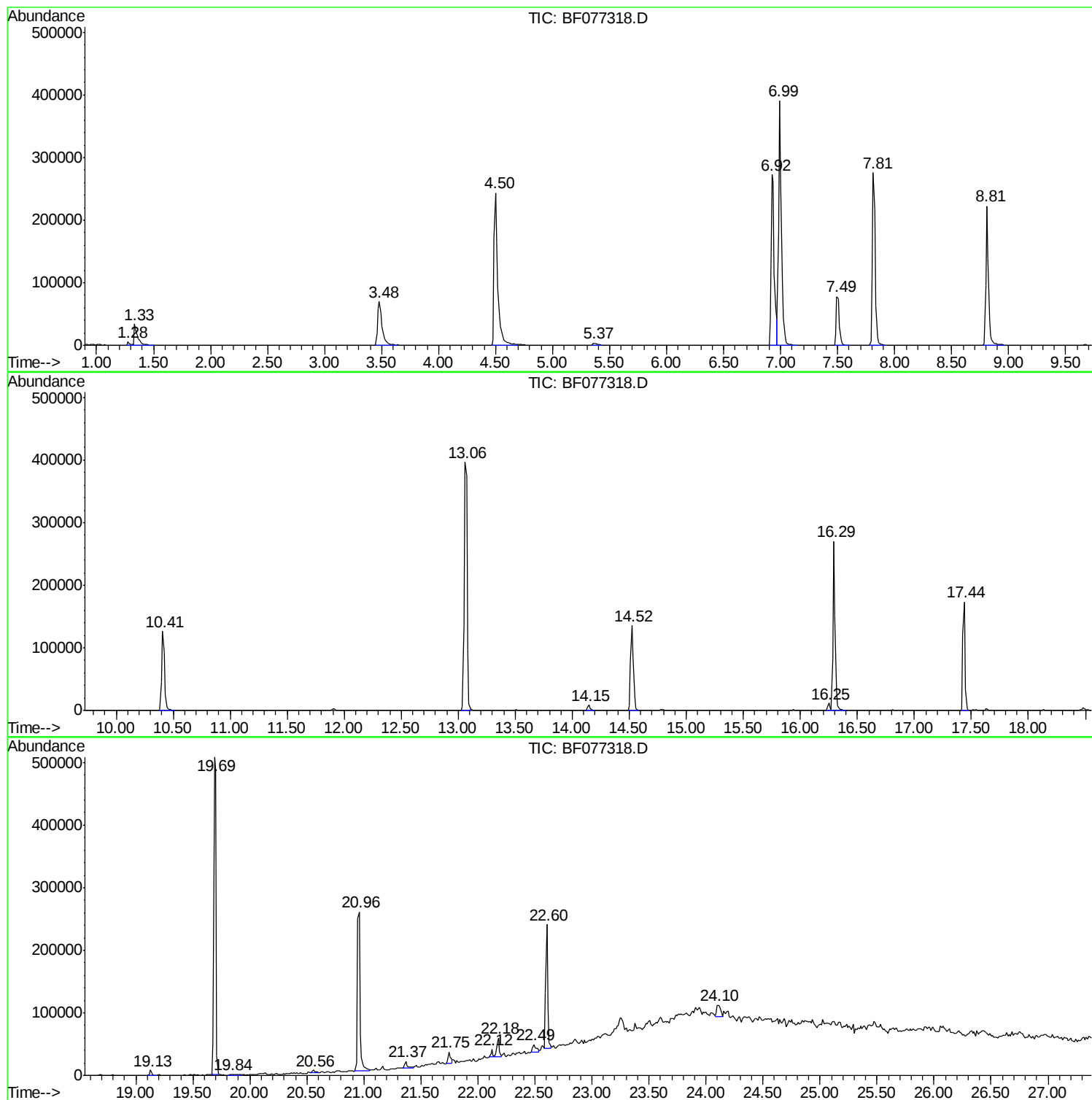
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF021215.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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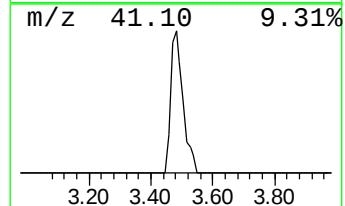
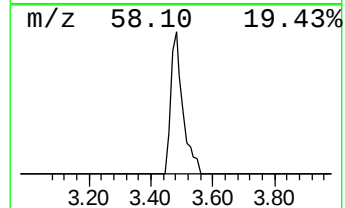
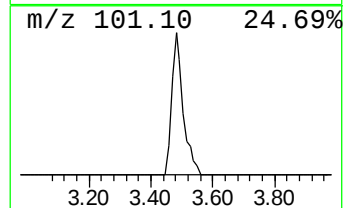
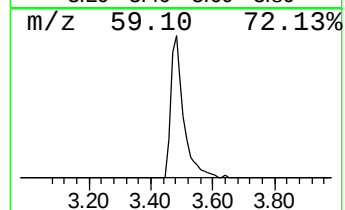
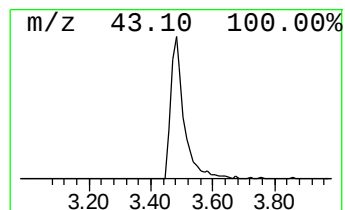
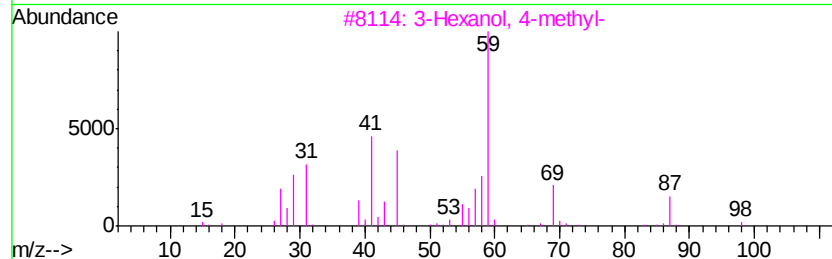
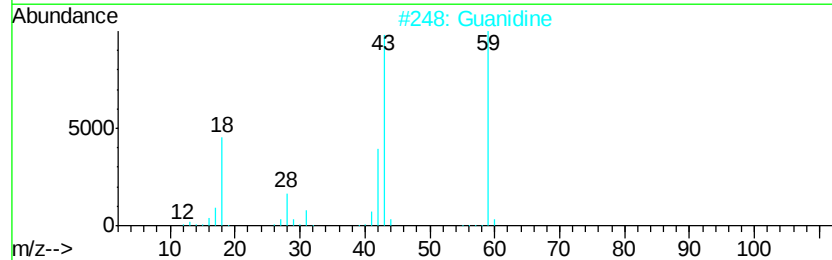
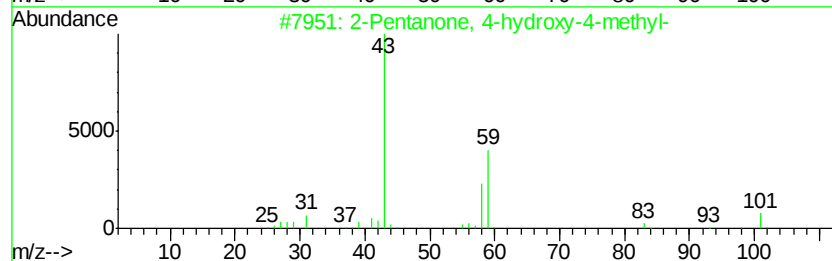
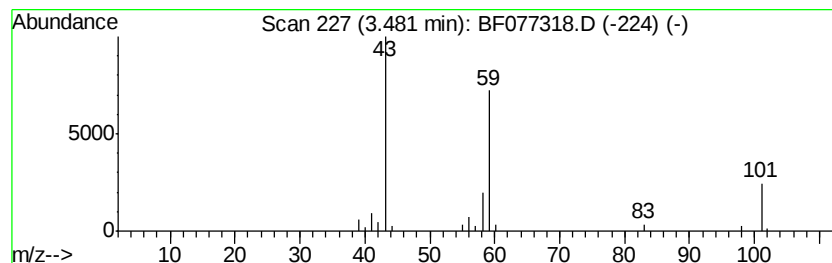
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
3.48	26.05 ng	190873	1,4-Dichlorobenzene-d4	7.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Guanidine	59	CH5N3	000113-00-8	38
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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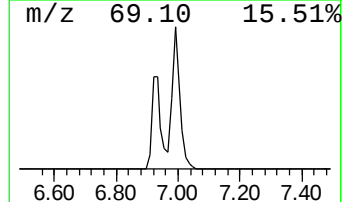
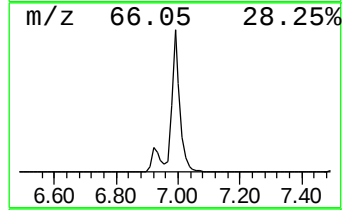
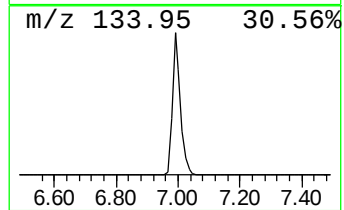
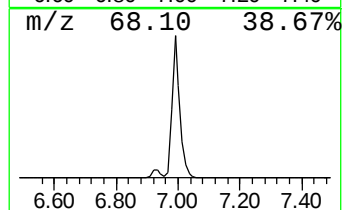
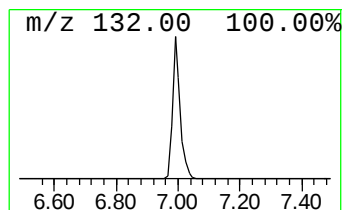
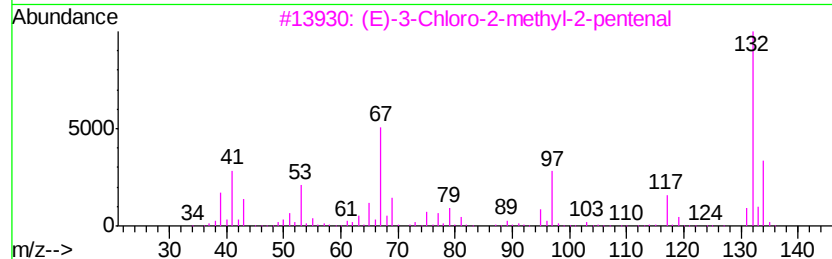
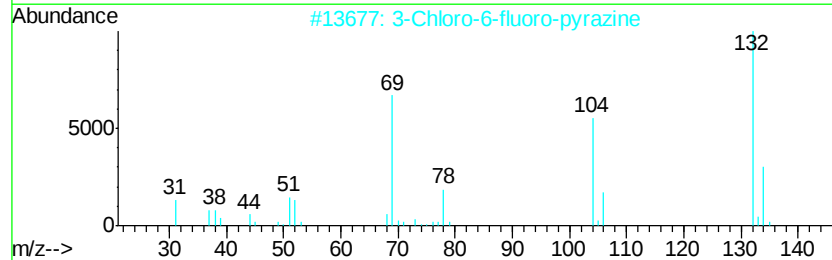
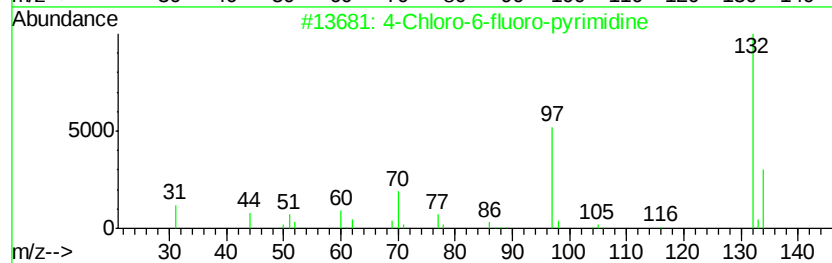
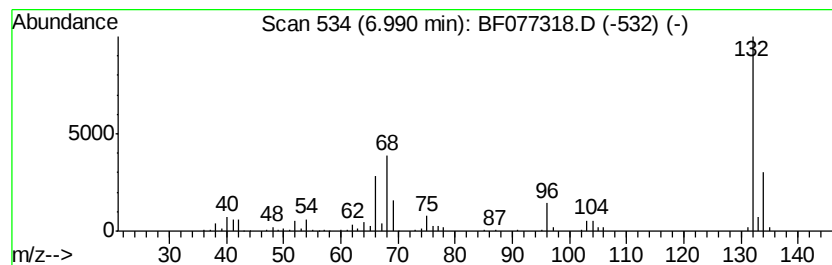
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Peak Number 3 unknown6.99 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.99	94.86 ng	695118	1,4-Dichlorobenzene-d4	7.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
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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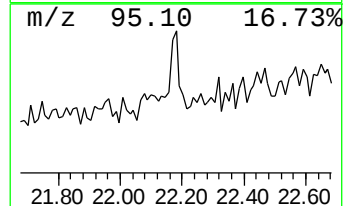
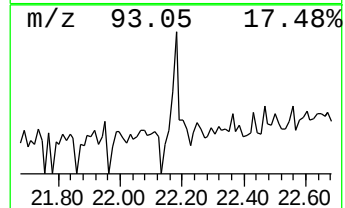
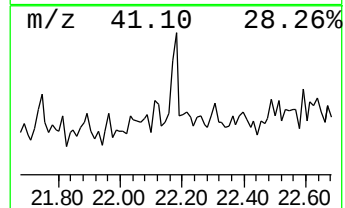
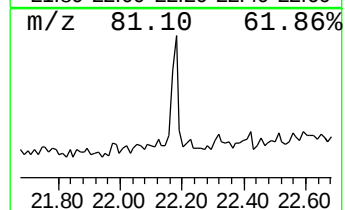
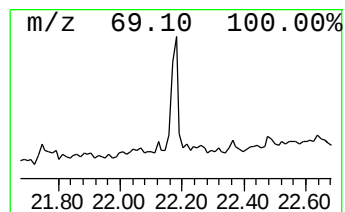
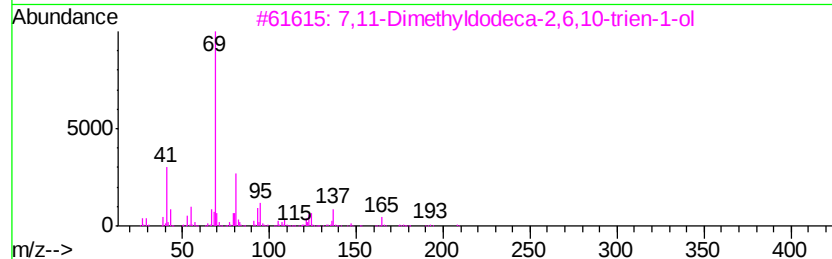
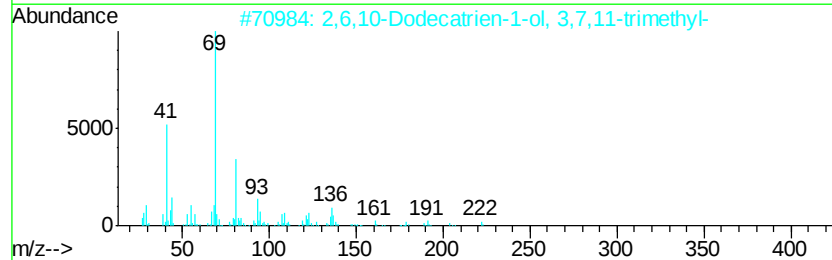
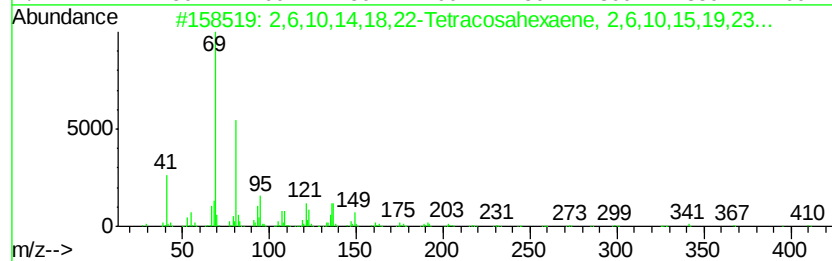
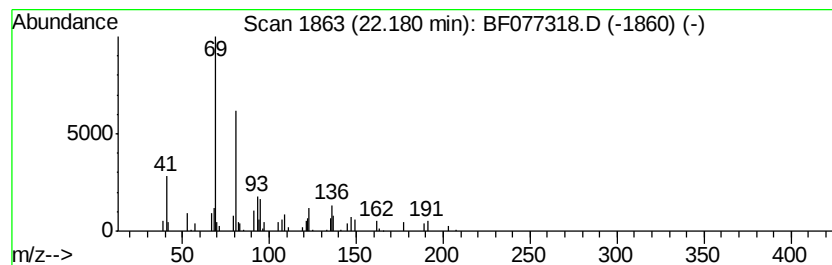
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Peak Number 5 2,6,10,14,18,22-Tetracosahexaene... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.18	3.64 ng	45490	Perylene-d12	22.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	80		
2	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64		
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59		
4	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	59		
5	Farnesol isomer a	222	C15H26O	1000108-92-4	53		



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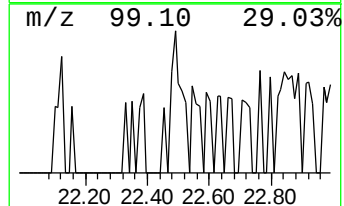
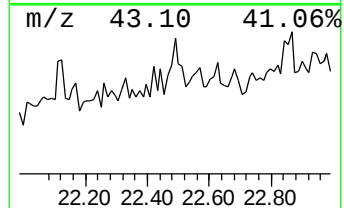
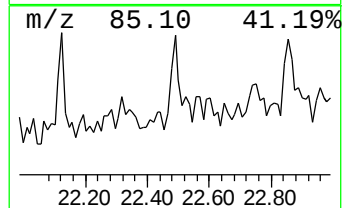
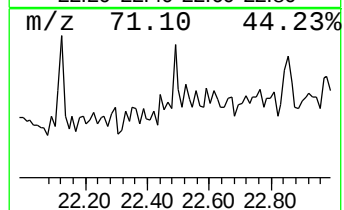
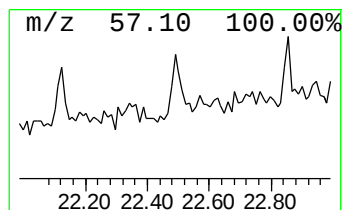
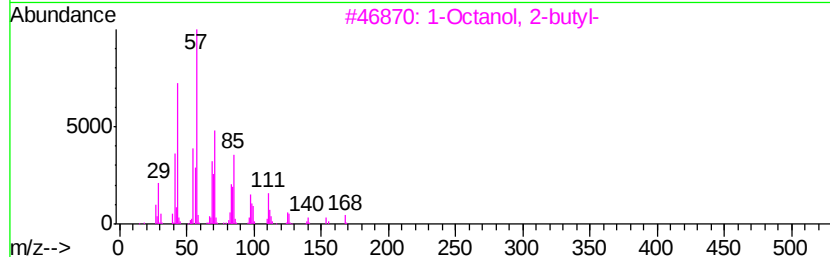
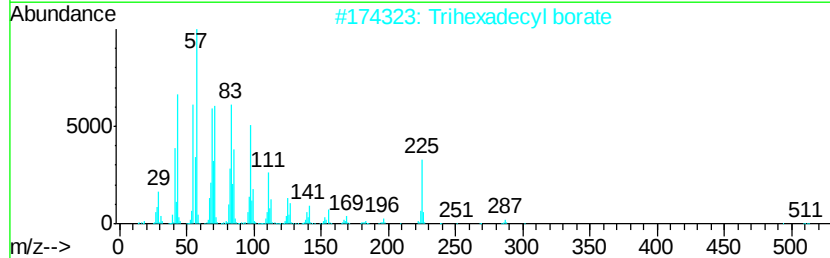
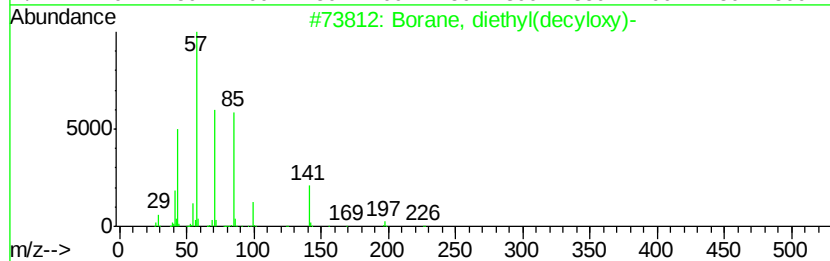
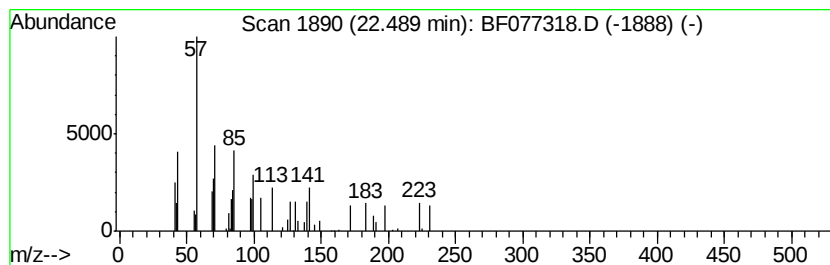
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Peak Number 6 unknown22.49 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.49	2.03 ng	25427	Perylene-d12	22.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Borane, diethyl(decyloxy)-	226	C14H31BO	1000152-34-3	43
2		Trihexadecyl borate	735	C48H99BO3	002665-11-4	38
3		1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	38
4		1-Bromodocosane	388	C22H45Br	006938-66-5	35
5		Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	3.48	26.1	ng	190873	1	7.50	146559	20.0
unknown6.99	6.99	94.9	ng	695118	1	7.50	146559	20.0
2,6,10,14,18,22-T...	22.18	3.6	ng	45490	6	22.60	249933	20.0
unknown22.49	22.49	2.0	ng	25427	6	22.60	249933	20.0