

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032318\
 Data File : BF103878.D
 Acq On : 23 Mar 2018 14:20
 Operator : JU/SJ
 Sample : J1998-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-109(15-16)

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-BF031518.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	2.316	34	39	46	rVB	112808	152650	4.43%	0.512%
2	5.222	528	533	540	rBV	121519	166021	4.82%	0.557%
3	5.598	592	597	601	rBV	2901857	3131495	90.90%	10.502%
4	6.598	761	767	770	rBV	2998371	2977708	86.44%	9.987%
5	6.745	787	792	795	rBV	3358000	3149181	91.41%	10.562%
6	6.975	827	831	834	rBV	1046825	886803	25.74%	2.974%
7	7.128	853	857	861	rBV	2616719	2507533	72.79%	8.410%
8	7.533	921	926	929	rBV	1927503	1947901	56.54%	6.533%
9	7.598	933	937	940	rVV	38670	35766	1.04%	0.120%
10	8.257	1045	1049	1052	rBV	1399836	1184094	34.37%	3.971%
11	8.745	1128	1132	1135	rBV	95545	76155	2.21%	0.255%
12	9.327	1227	1231	1235	rBV	3486536	3444961	100.00%	11.554%
13	9.669	1279	1289	1292	rBV	72806	66315	1.92%	0.222%
14	9.716	1294	1297	1305	rVB	323561	296444	8.61%	0.994%
15	9.927	1330	1333	1336	rBV	106222	77010	2.24%	0.258%
16	10.016	1344	1348	1354	rVB	1482299	1299971	37.74%	4.360%
17	10.404	1410	1414	1416	rBV	50675	40939	1.19%	0.137%
18	10.427	1416	1418	1421	rVB	123709	89338	2.59%	0.300%
19	10.651	1451	1456	1458	rBV	30764	36847	1.07%	0.124%
20	10.810	1478	1483	1486	rBV	1970042	1942403	56.38%	6.514%
21	10.904	1496	1499	1510	rVB	103740	111550	3.24%	0.374%
22	11.351	1572	1575	1578	rBV	77589	61804	1.79%	0.207%
23	11.510	1598	1602	1605	rBV	1298805	1134778	32.94%	3.806%
24	12.016	1685	1688	1691	rBV	39936	35621	1.03%	0.119%
25	13.092	1867	1871	1875	rBV	2560988	2513142	72.95%	8.429%
26	13.974	2018	2021	2031	rVB	486303	452298	13.13%	1.517%
27	14.157	2048	2052	2056	rBV	908893	899457	26.11%	3.017%
28	14.621	2128	2131	2136	rBV7	41945	47756	1.39%	0.160%
29	15.704	2309	2315	2325	rVB	704594	952099	27.64%	3.193%
30	16.221	2399	2403	2410	rVB2	58235	98689	2.86%	0.331%

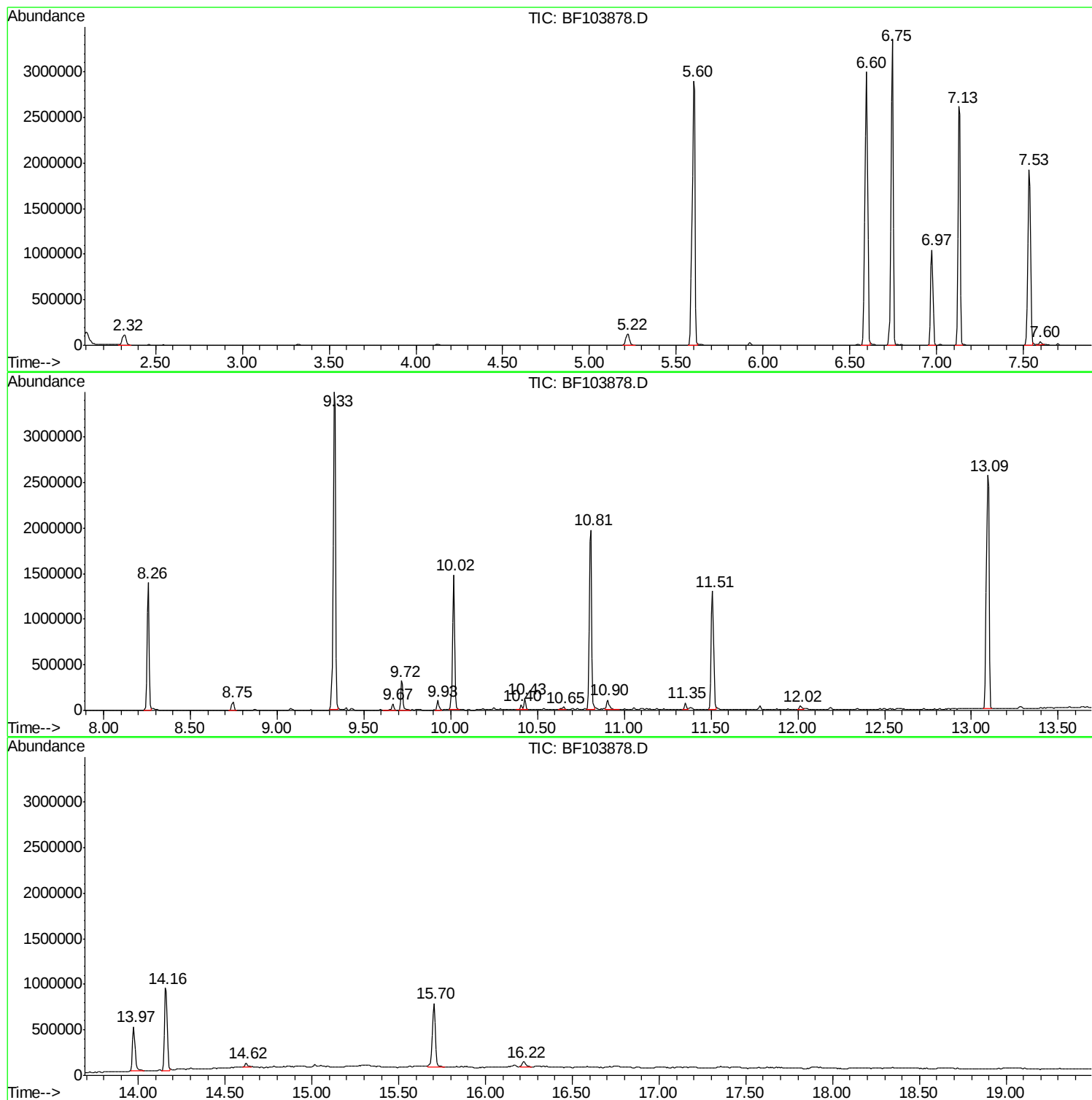
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Instrument :
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ClientSampleId :
SB-109(15-16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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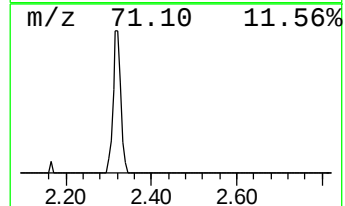
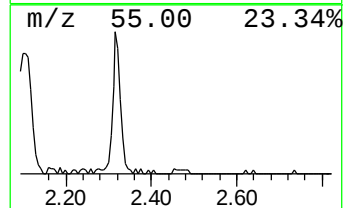
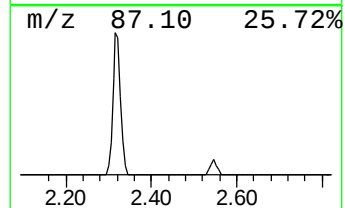
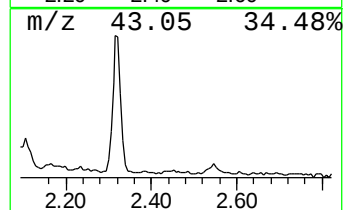
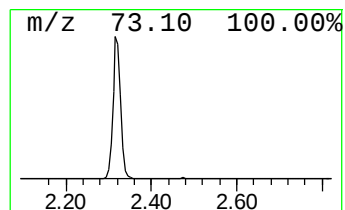
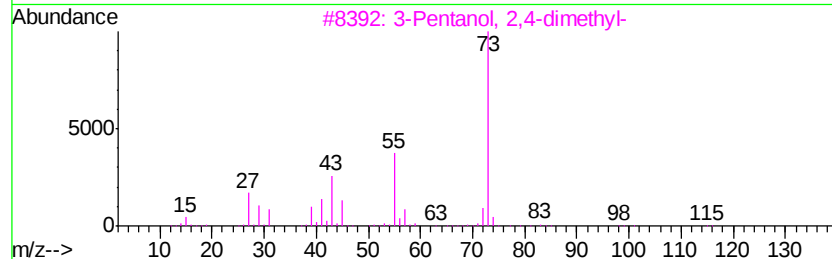
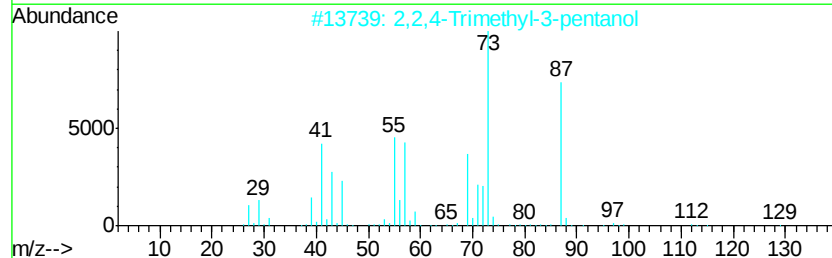
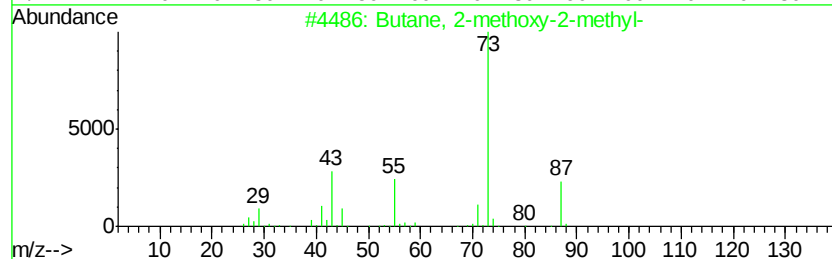
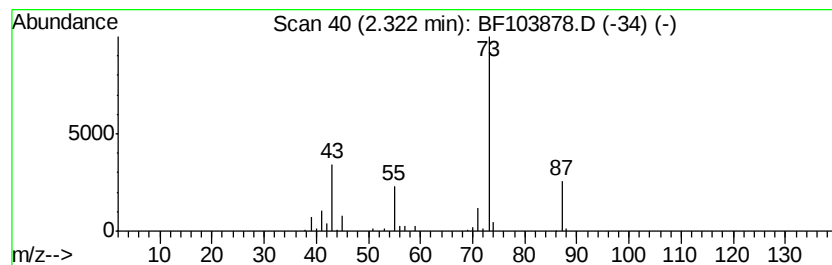
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	3.44 ng	152650	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17



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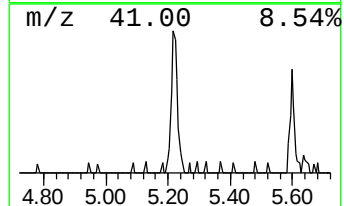
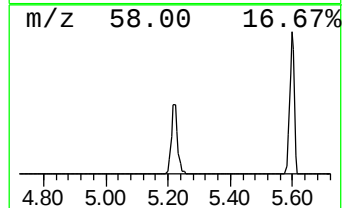
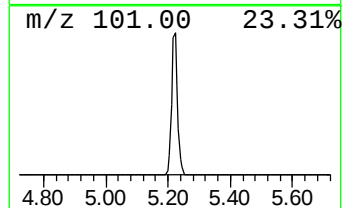
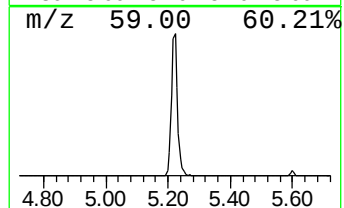
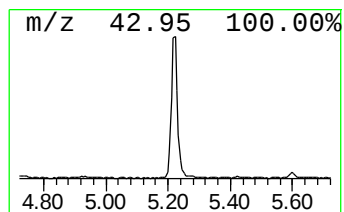
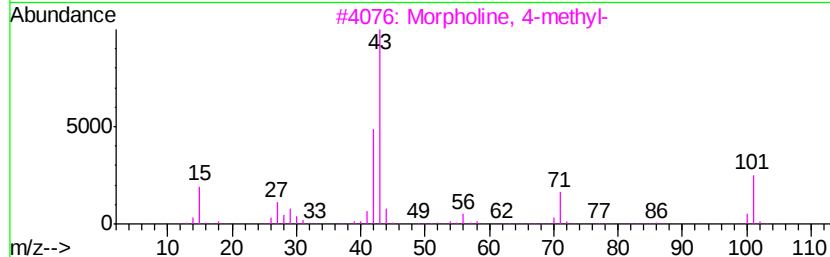
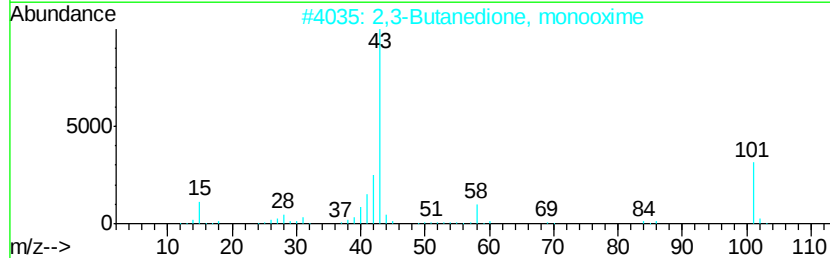
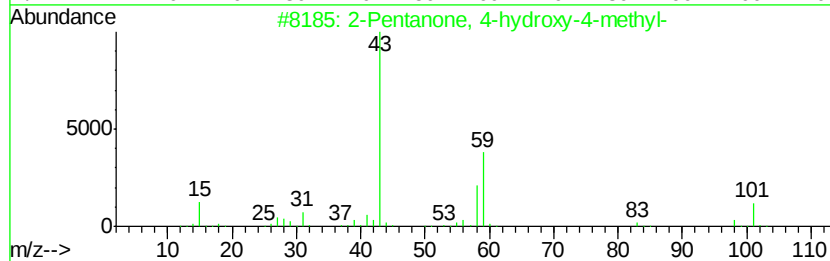
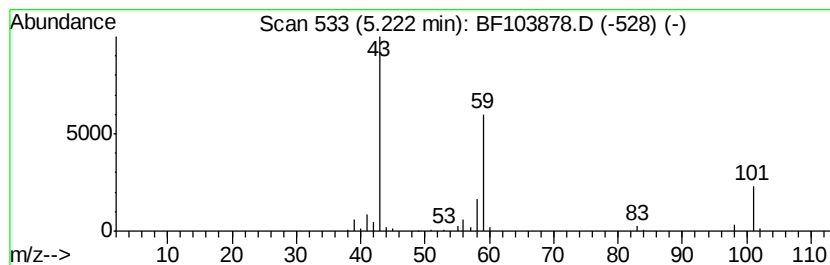
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	3.74 ng	166021	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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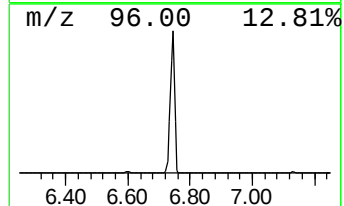
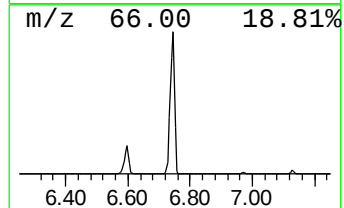
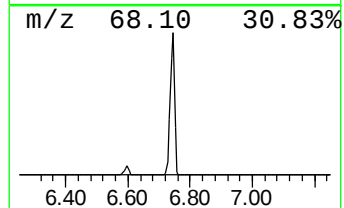
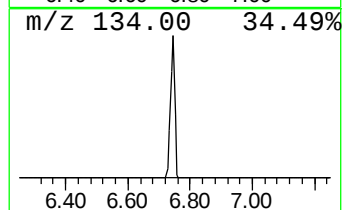
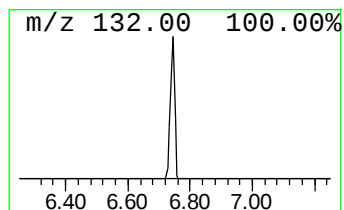
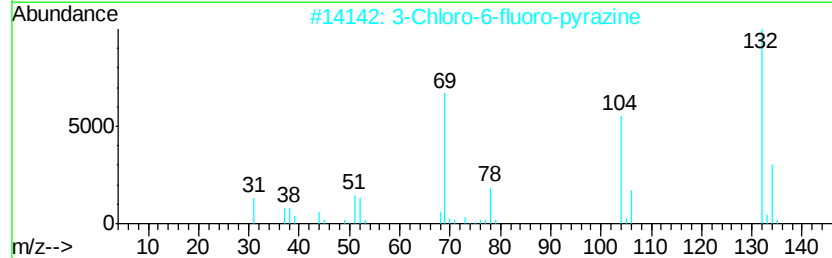
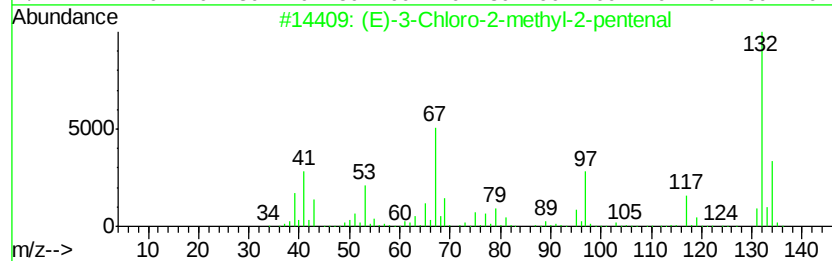
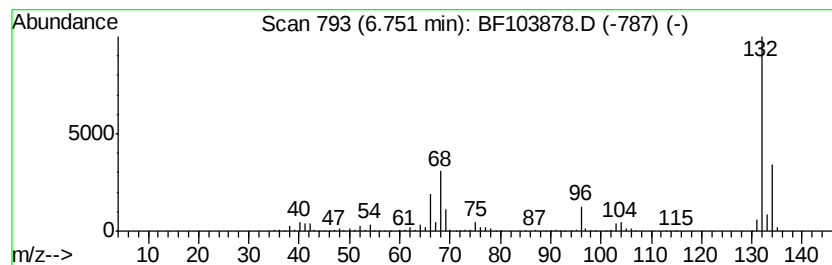
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Peak Number 3 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	71.02 ng	3149180	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	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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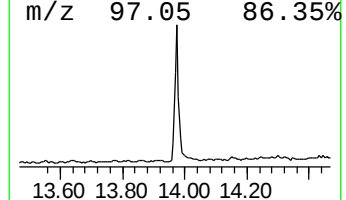
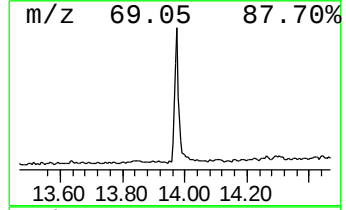
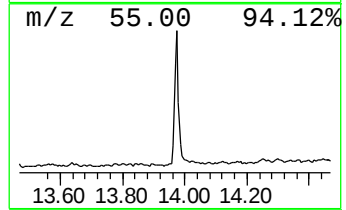
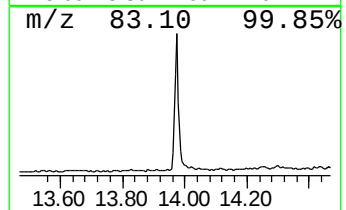
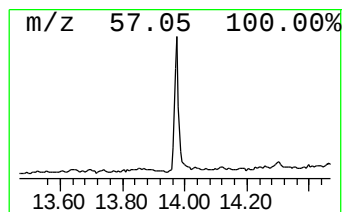
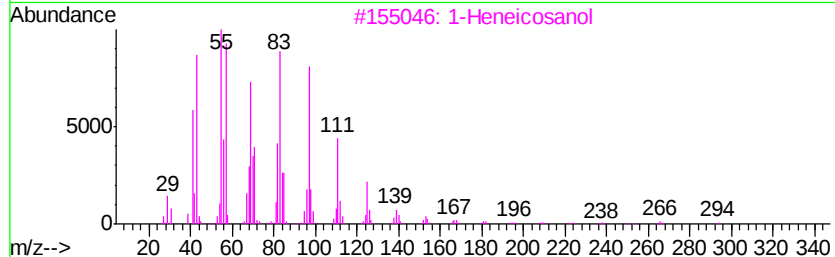
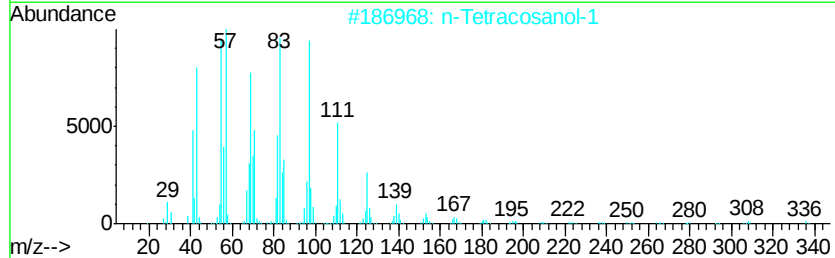
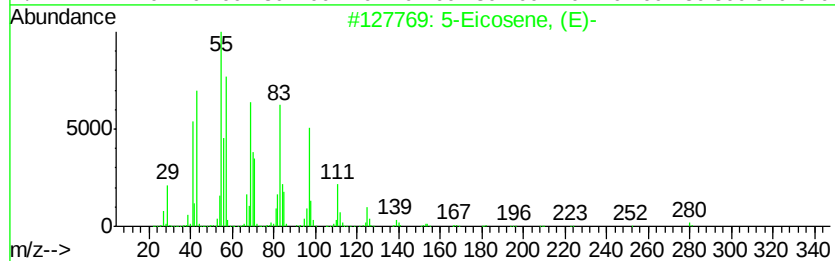
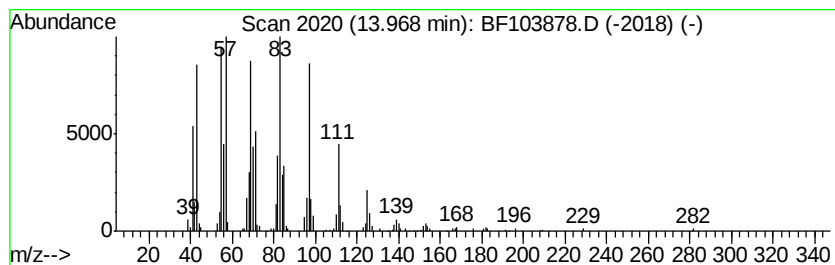
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Peak Number 5 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	10.06 ng	452298	Chrysene-d12	14.16

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	99
2	n-Tetracosanol-1		354	C24H50O	000506-51-4	95
3	1-Heneicosanol		312	C21H44O	015594-90-8	95
4	n-Nonadecanol-1		284	C19H40O	001454-84-8	95
5	1-Nonadecene		266	C19H38	018435-45-5	94



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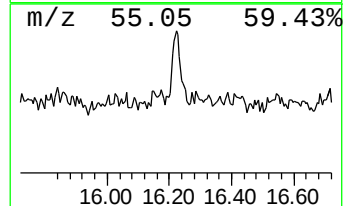
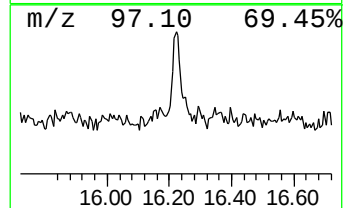
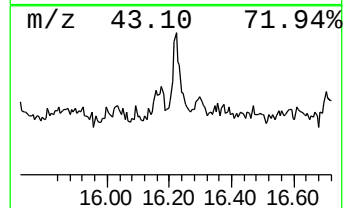
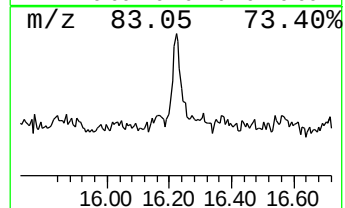
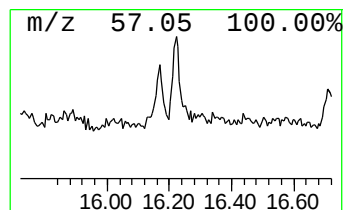
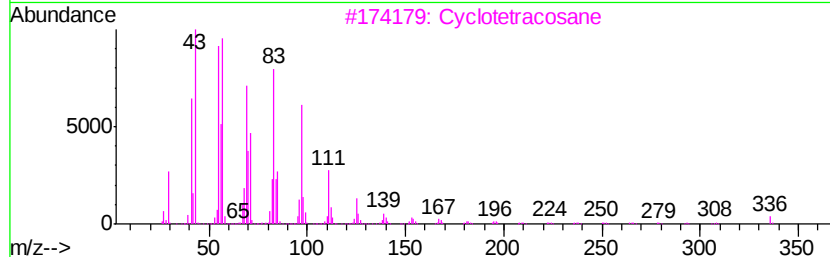
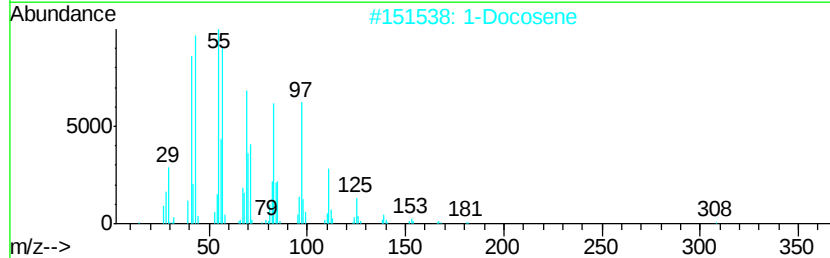
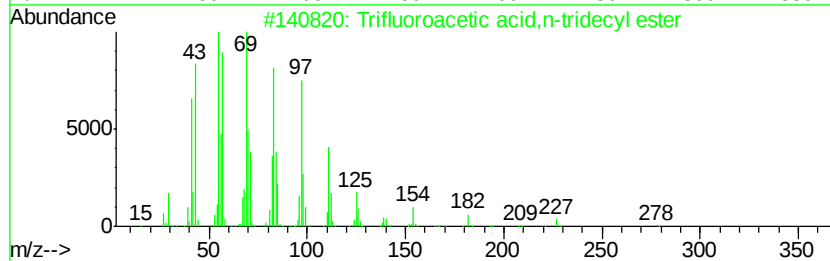
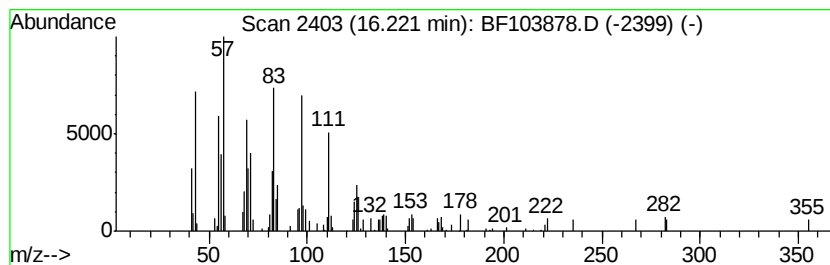
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Trifluoroacetic acid,n-trid... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	2.07 ng	98689	Perylene-d12	15.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	86
2		1-Docosene	308	C22H44	001599-67-3	83
3		Cyclotetracosane	336	C24H48	000297-03-0	72
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	70
5		Dotriacontyl trifluoroacetate	562	C34H65F3O2	1000351-75-4	68



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.32	3.4	ng	152650	1	6.97	886803	20.0
2-Pentanone, 4-hy...	5.22	3.7	ng	166021	1	6.97	886803	20.0
unknown6.75	6.75	71.0	ng	3149180	1	6.97	886803	20.0
5-Eicosene, (E)-	13.97	10.1	ng	452298	5	14.16	899457	20.0
Trifluoroacetic a...	16.22	2.1	ng	98689	6	15.70	952099	20.0