

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112217\
 Data File : BF100865.D
 Acq On : 23 Nov 2017 10:40
 Operator : SJ/JU
 Sample : I6541-07
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 111717-SIDI-F-D-S

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-BF110817.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	2.134	6	8	18	rVB2	47174	81222	3.50%	0.645%
2	5.069	504	507	517	rBB	113174	125311	5.41%	0.995%
3	5.475	572	576	579	rBV	674439	630872	27.22%	5.009%
4	6.481	743	747	756	rBB	501531	444324	19.17%	3.528%
5	6.628	767	772	775	rBV	1272125	1116340	48.17%	8.863%
6	6.857	807	811	814	rBV	481691	376163	16.23%	2.986%
7	7.016	833	838	841	rBV	1763760	1525830	65.84%	12.114%
8	7.422	902	907	910	rBV	1195143	1247165	53.82%	9.902%
9	8.139	1025	1029	1032	rBV	635549	494361	21.33%	3.925%
10	9.216	1207	1212	1215	rBV	2462492	2317374	100.00%	18.398%
11	9.604	1275	1278	1281	rBV	39031	30557	1.32%	0.243%
12	9.898	1321	1328	1331	rBV	573361	553026	23.86%	4.391%
13	10.680	1458	1461	1465	rBV	867319	803899	34.69%	6.382%
14	10.792	1477	1480	1488	rVB	22623	24276	1.05%	0.193%
15	11.380	1576	1580	1584	rBV	583378	474615	20.48%	3.768%
16	12.968	1845	1850	1853	rBV	1799864	1608111	69.39%	12.767%
17	13.851	1996	2000	2005	rBV	43949	47986	2.07%	0.381%
18	14.021	2025	2029	2033	rVB	389395	329096	14.20%	2.613%
19	15.492	2274	2279	2286	rVB	299192	364935	15.75%	2.897%

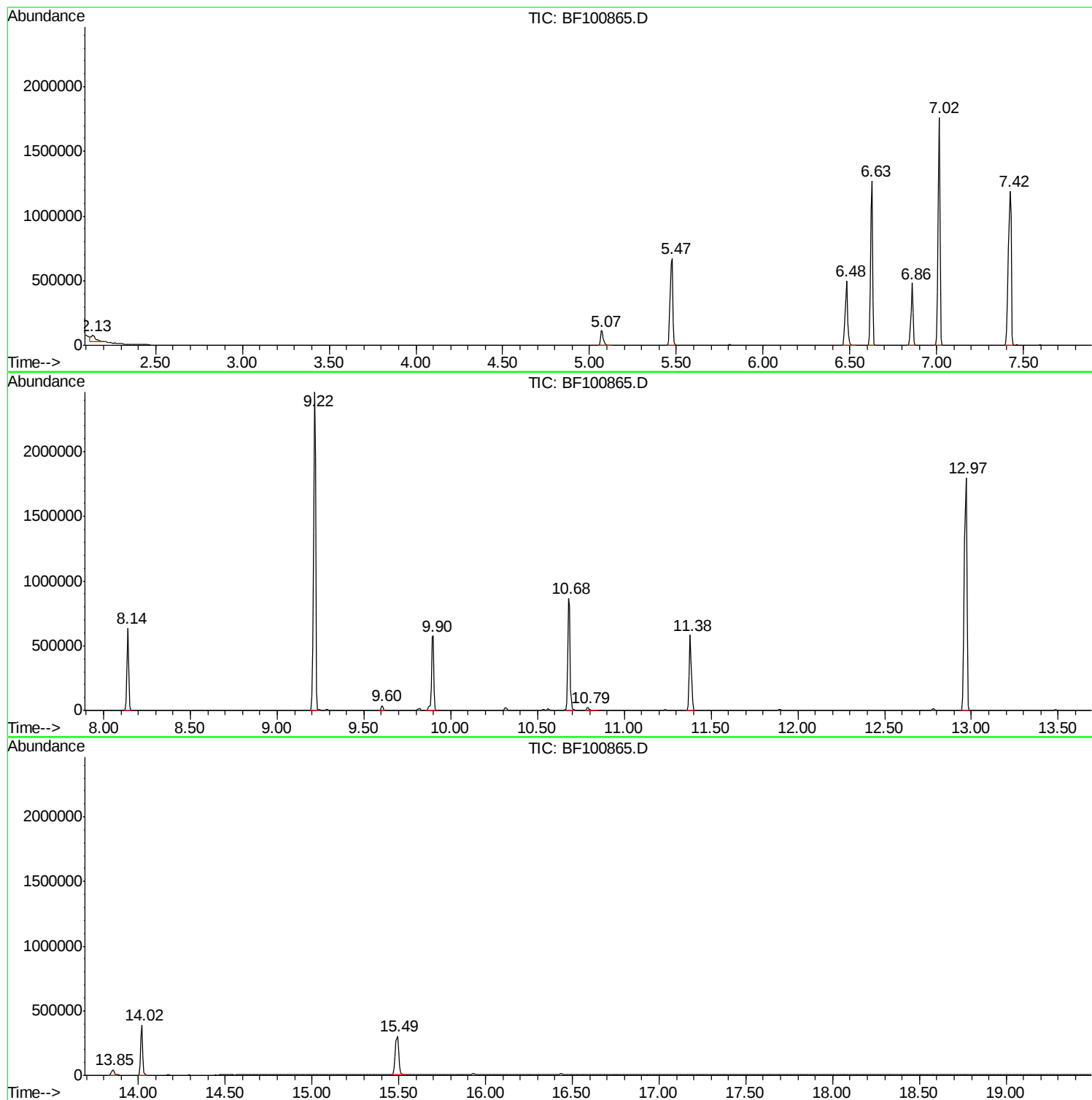
Sum of corrected areas: 12595463

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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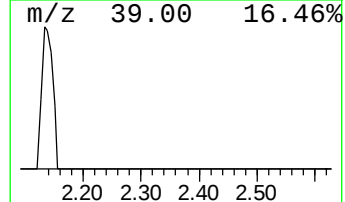
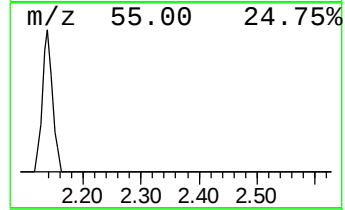
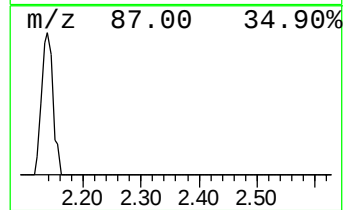
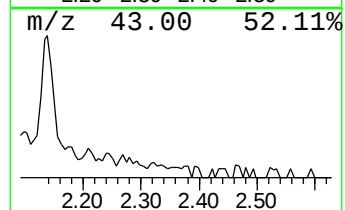
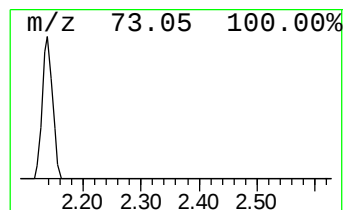
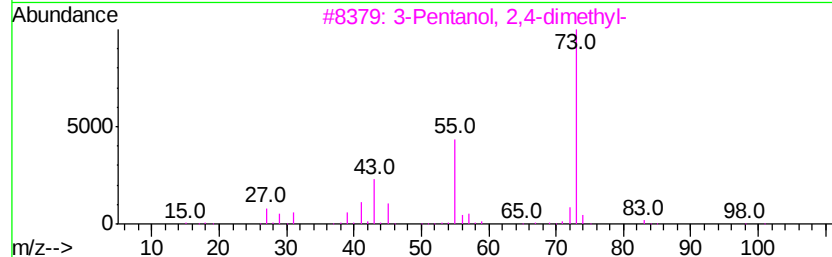
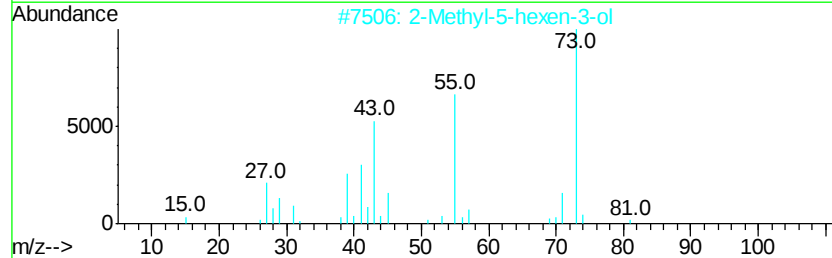
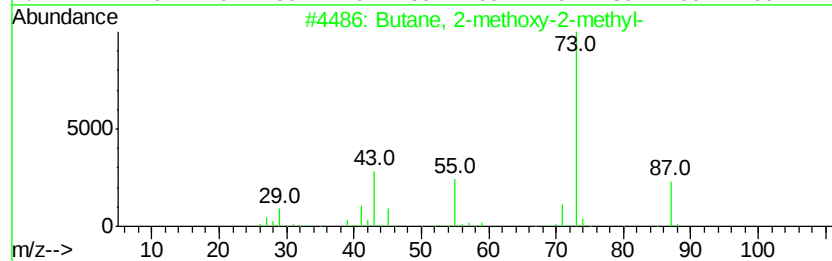
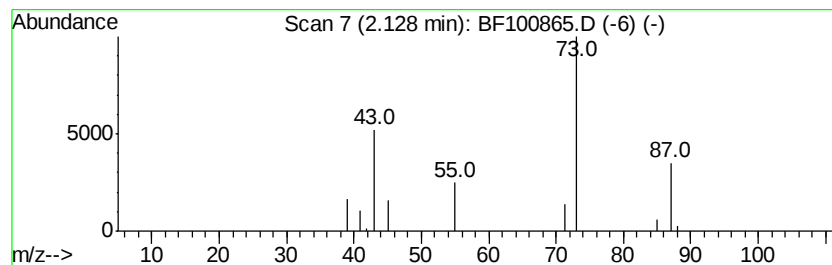
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	4.32 ng	81222	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
4		Formamide, N,N-dimethyl-	73	C3H7NO	000068-12-2	5
5		N-Ethylformamide	73	C3H7NO	000627-45-2	5



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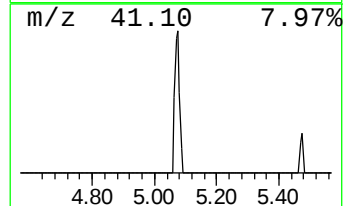
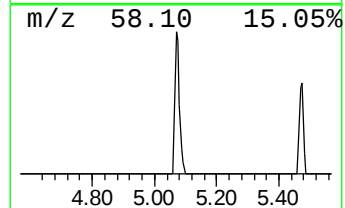
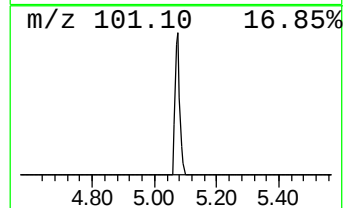
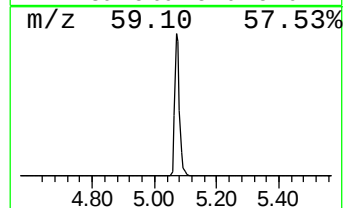
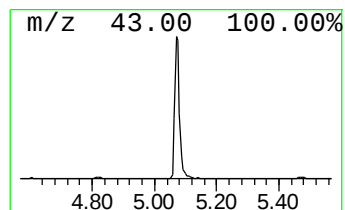
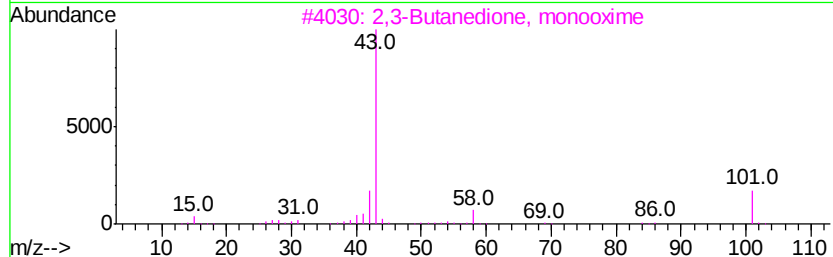
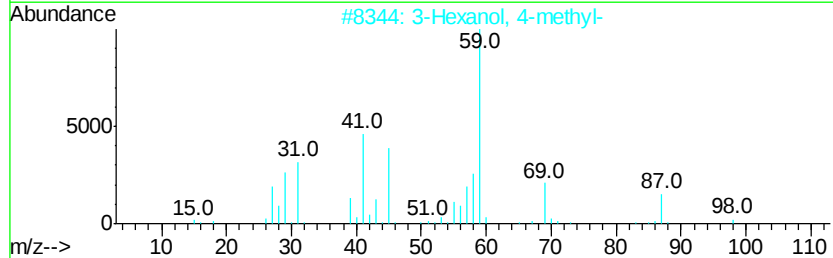
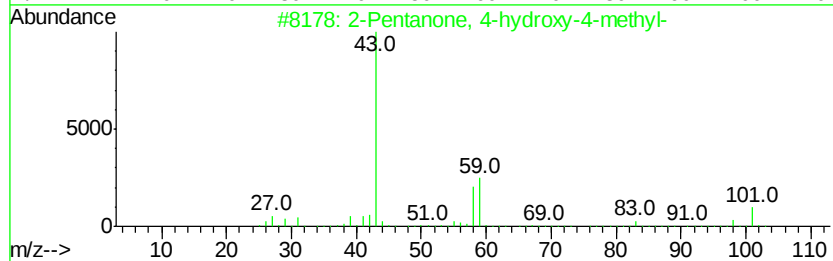
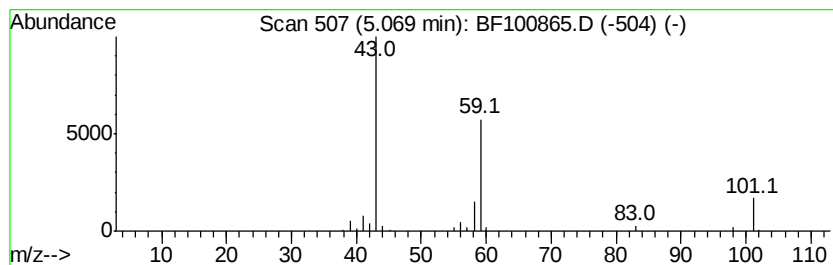
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	6.66 ng	125311	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
5		3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	9



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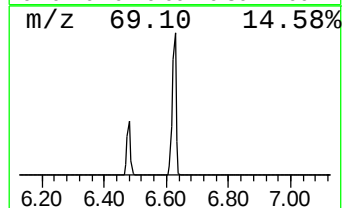
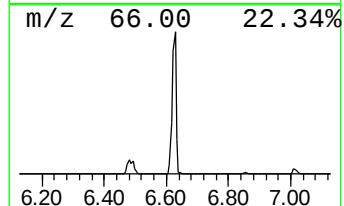
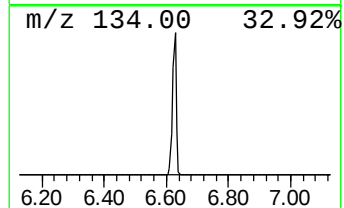
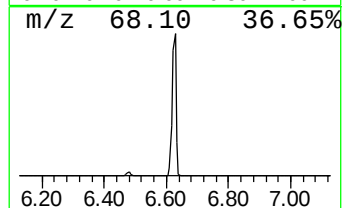
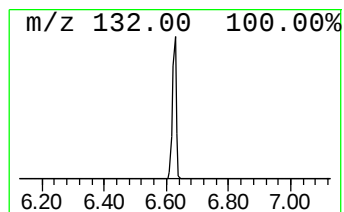
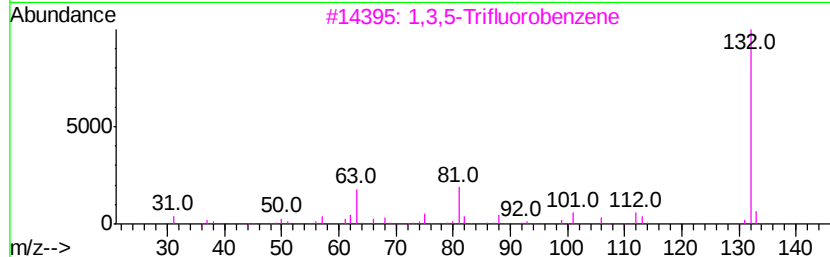
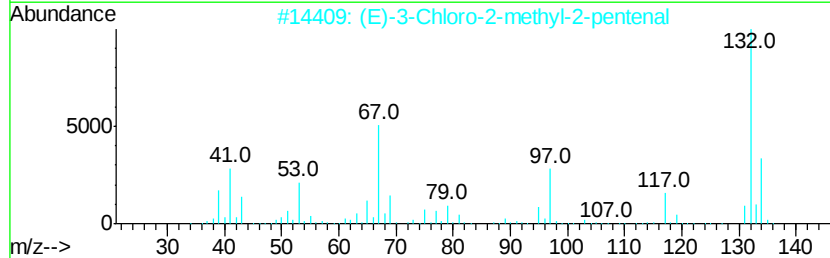
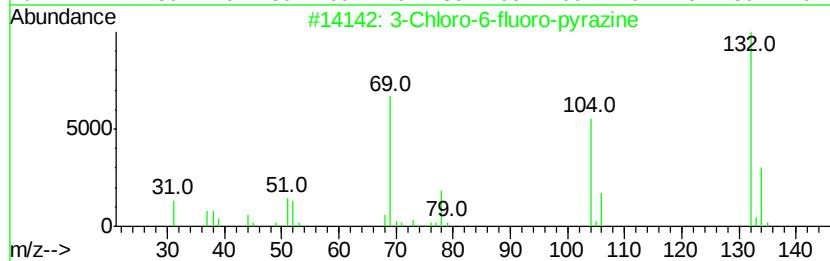
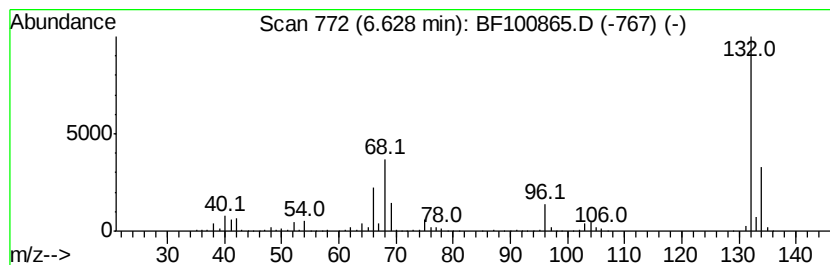
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Peak Number 3 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	59.35 ng	1116340	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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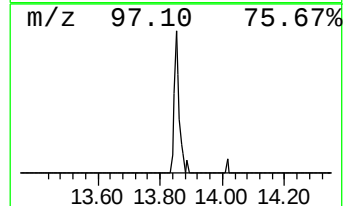
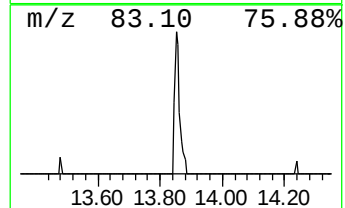
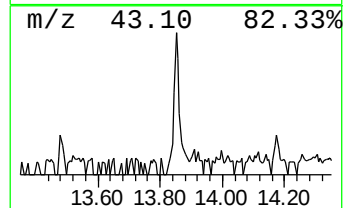
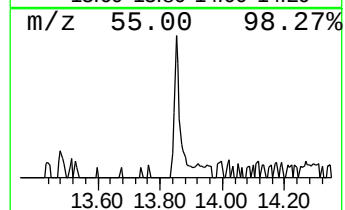
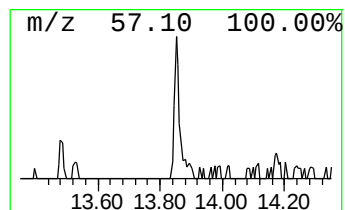
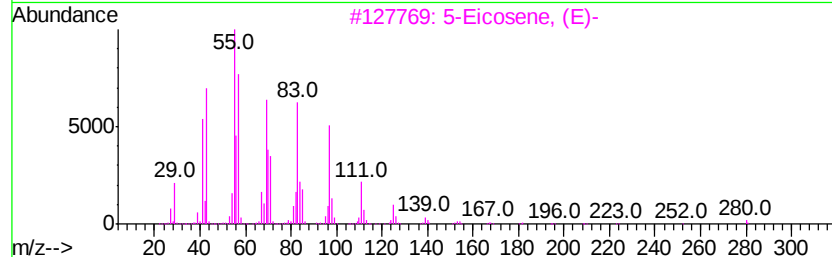
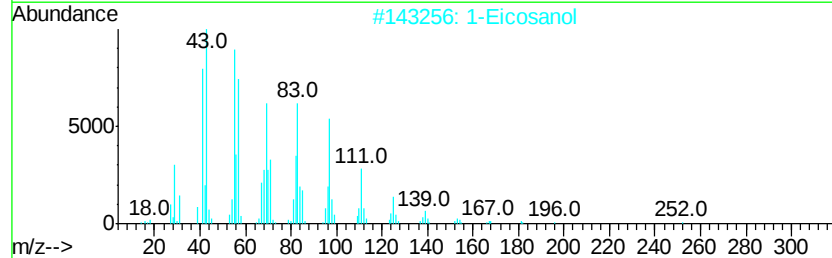
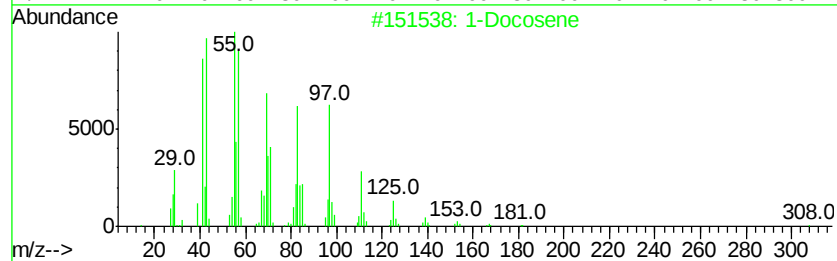
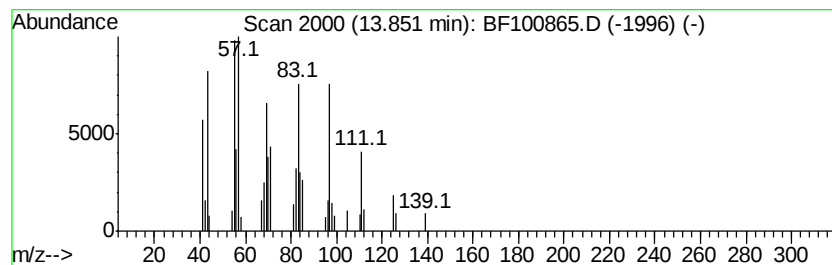
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Peak Number 5 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.92 ng	47986	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	91
2		1-Eicosanol	298	C20H42O	000629-96-9	91
3		5-Eicosene, (E)-	280	C20H40	074685-30-6	91
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	83
5		Hexadecen-1-ol, trans-9-	240	C16H32O	064437-47-4	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.13	4.3	ng	81222	1	6.86	376163	20.0
2-Pentanone, 4-hy...	5.07	6.7	ng	125311	1	6.86	376163	20.0
unknown6.63	6.63	59.4	ng	1116340	1	6.86	376163	20.0
1-Docosene	13.85	2.9	ng	47986	5	14.02	329096	20.0