

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112017\
 Data File : BF100739.D
 Acq On : 20 Nov 2017 19:26
 Operator : SJ/JU
 Sample : I6521-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-(0-12)

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-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	5.110	511	514	525	rBV	121235	178966	6.36%	0.717%
2	5.492	574	579	582	rBV	2197993	2480151	88.18%	9.930%
3	6.504	744	751	754	rBV	2024590	2552313	90.75%	10.219%
4	6.645	769	775	778	rBV	2284535	2518346	89.54%	10.083%
5	6.869	810	813	817	rVB	692952	563276	20.03%	2.255%
6	7.028	835	840	843	rBV	2177637	1927450	68.53%	7.717%
7	7.433	903	909	912	rBV	1522476	1596472	56.76%	6.392%
8	8.151	1026	1031	1034	rBV	897739	758299	26.96%	3.036%
9	9.227	1208	1214	1217	rBV	2855385	2812513	100.00%	11.261%
10	9.616	1276	1280	1283	rBV	267709	206402	7.34%	0.826%
11	9.827	1313	1316	1320	rVB	80497	68486	2.44%	0.274%
12	9.910	1325	1330	1333	rBV	906201	857554	30.49%	3.434%
13	10.327	1399	1401	1404	rVB	93376	72344	2.57%	0.290%
14	10.451	1419	1422	1426	rVB	39637	34412	1.22%	0.138%
15	10.698	1459	1464	1467	rBV	1841667	1805297	64.19%	7.228%
16	10.804	1478	1482	1491	rBV	73960	84636	3.01%	0.339%
17	11.392	1578	1582	1585	rBV	1092375	940491	33.44%	3.766%
18	11.416	1585	1586	1589	rVV	104435	52521	1.87%	0.210%
19	11.468	1592	1595	1597	rVB	56198	51612	1.84%	0.207%
20	11.910	1668	1670	1677	rVB3	81573	77205	2.75%	0.309%
21	12.004	1683	1686	1689	rBV2	51818	54787	1.95%	0.219%
22	12.604	1784	1788	1791	rBV	279656	230541	8.20%	0.923%
23	12.833	1821	1827	1830	rBV	219195	217333	7.73%	0.870%
24	12.980	1847	1852	1855	rVB	2627292	2573349	91.50%	10.303%
25	13.157	1879	1882	1891	rVB	44505	53171	1.89%	0.213%
26	13.227	1891	1894	1896	rBV	45486	36939	1.31%	0.148%
27	13.410	1922	1925	1929	rVB	35670	34804	1.24%	0.139%
28	13.757	1980	1984	1987	rBV	122297	115694	4.11%	0.463%
29	13.857	1999	2001	2012	rVB2	175232	213174	7.58%	0.854%
30	14.027	2022	2030	2033	rBV	851570	906379	32.23%	3.629%
31	14.051	2033	2034	2041	rVB	87232	75867	2.70%	0.304%
32	14.127	2041	2047	2052	rBV2	36000	50868	1.81%	0.204%
33	14.509	2104	2112	2114	rBV4	15364	28657	1.02%	0.115%
34	15.068	2203	2207	2210	rBV	47812	74641	2.65%	0.299%

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35	15.368	2255	2258	2264	rVB	26376	32187	1.14%	0.129%
36	15.433	2264	2269	2275	rBV	44587	54371	1.93%	0.218%
37	15.498	2275	2280	2292	rVV	424391	547228	19.46%	2.191%
38	16.962	2524	2529	2539	rBV3	17974	37228	1.32%	0.149%

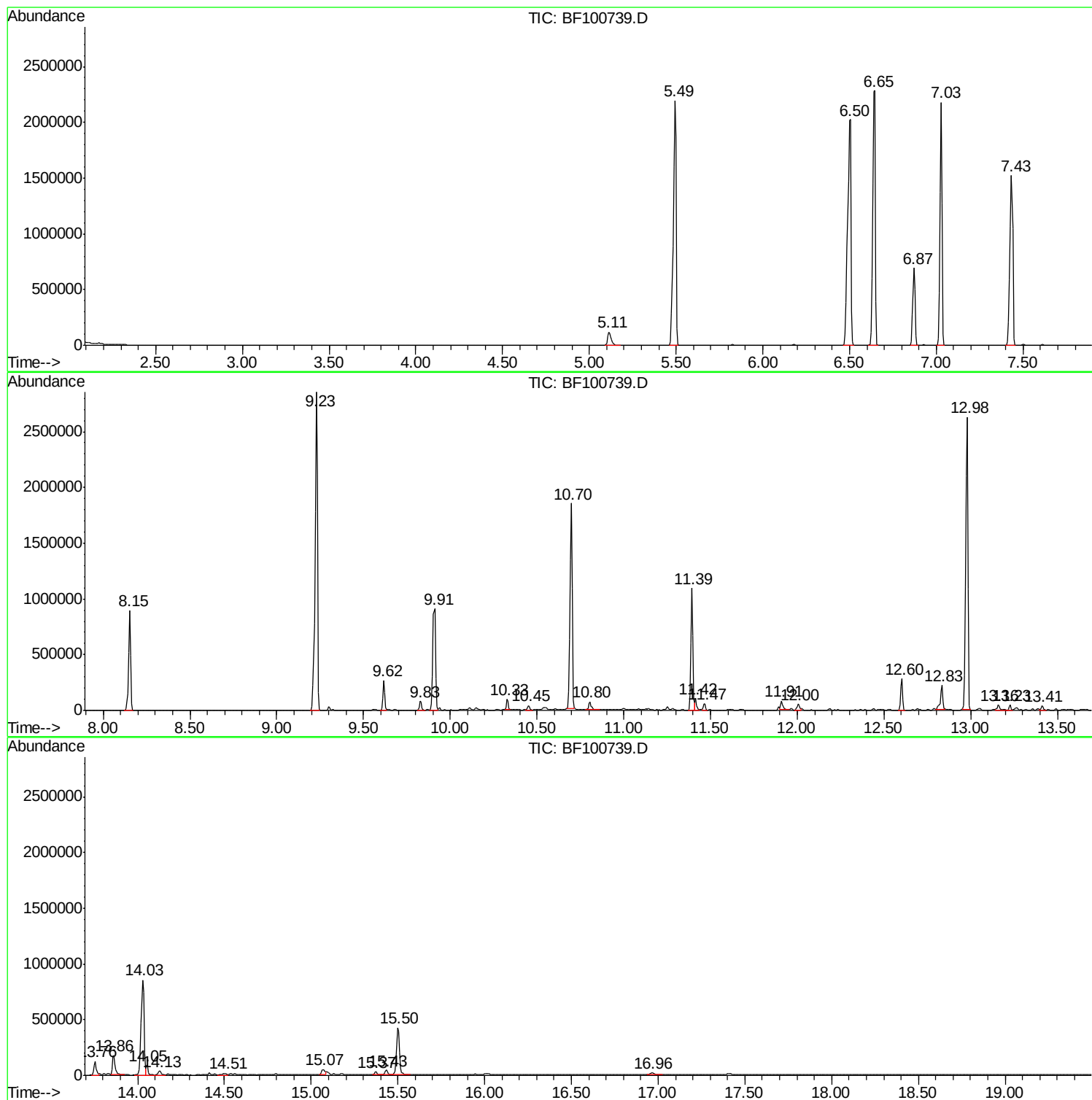
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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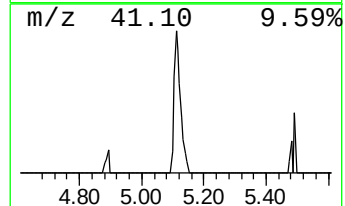
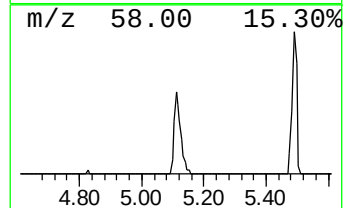
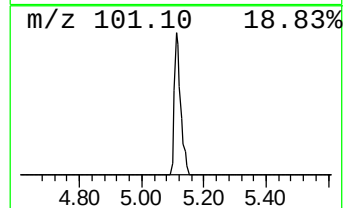
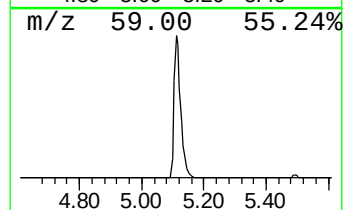
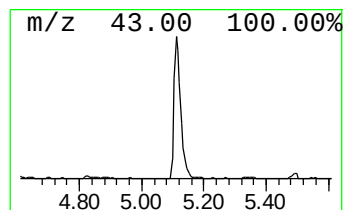
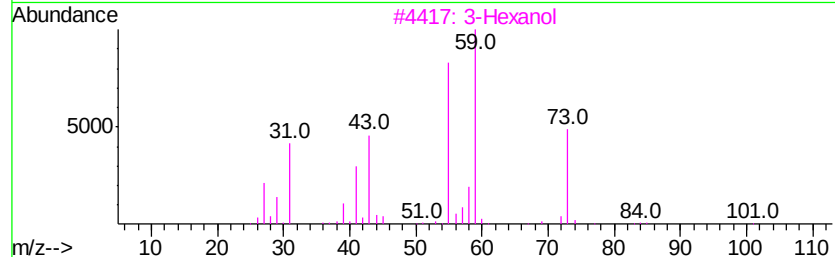
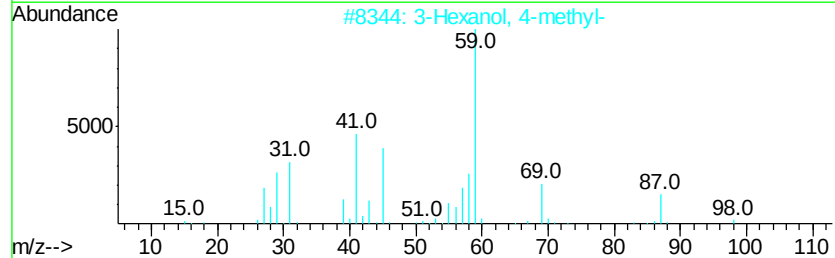
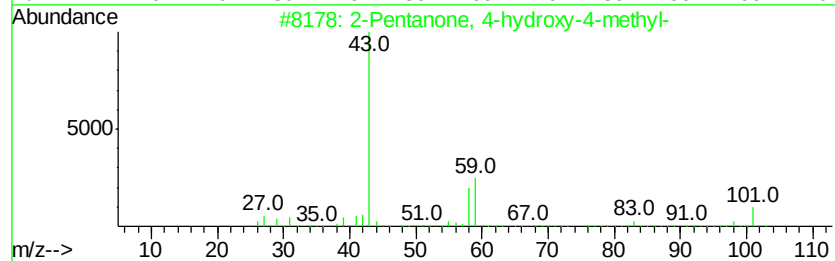
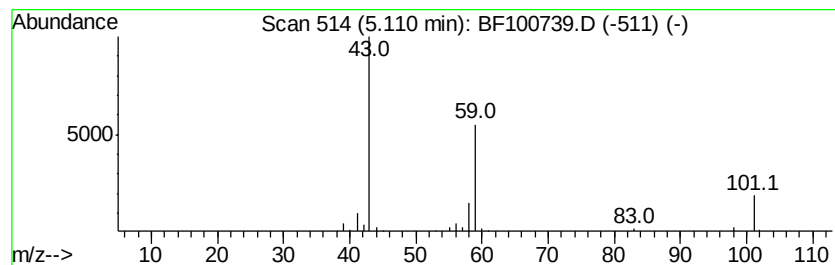
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	6.35 ng	178966	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			3-Hexanol	102	C6H14O	000623-37-0	33
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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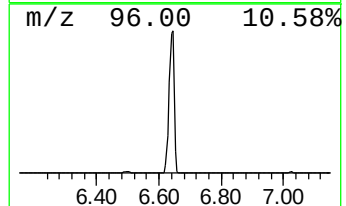
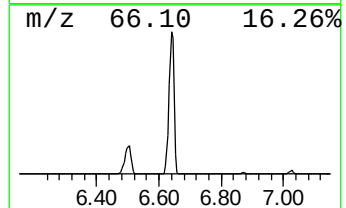
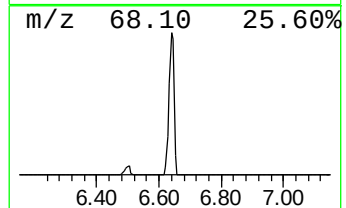
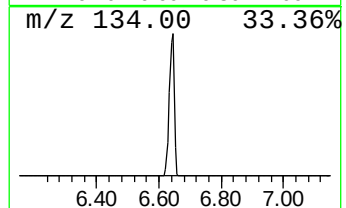
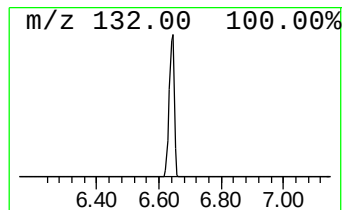
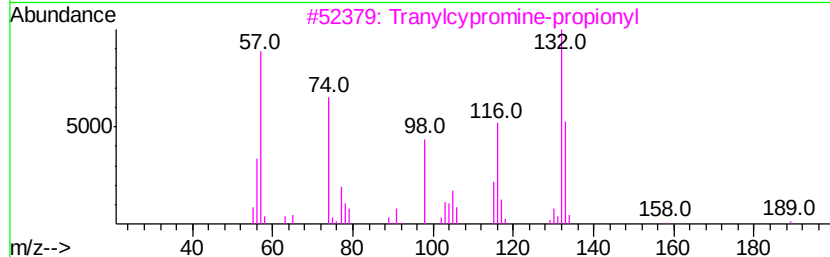
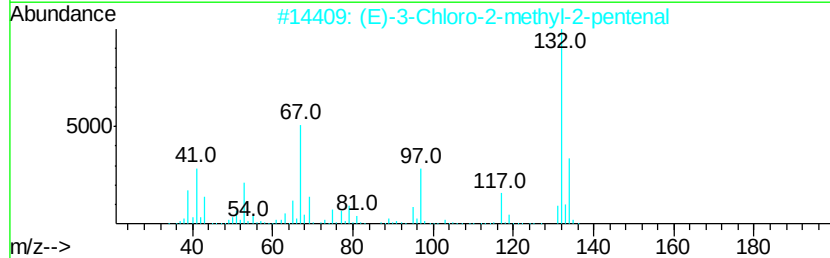
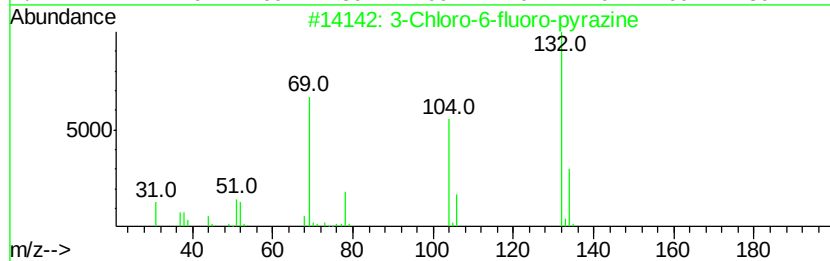
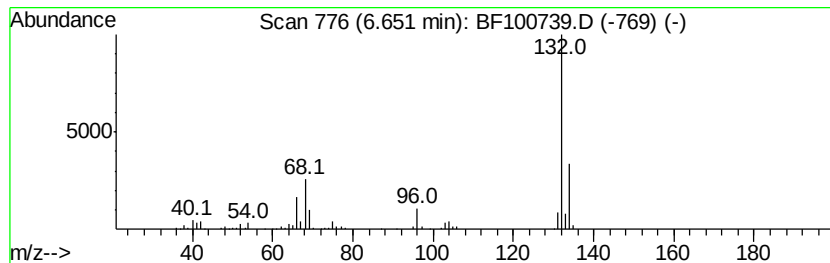
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Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	89.42 ng	2518350	1,4-Dichlorobenzene-d4	6.87

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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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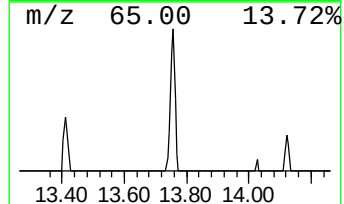
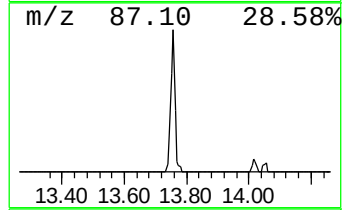
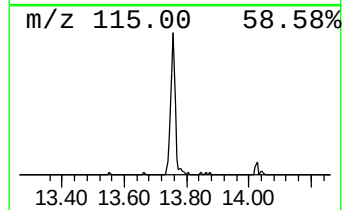
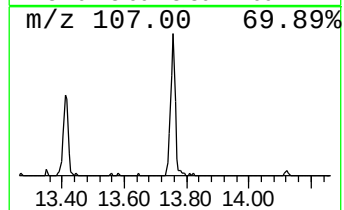
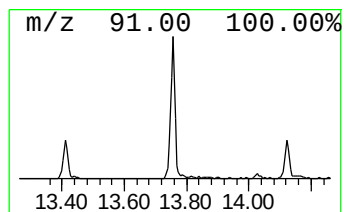
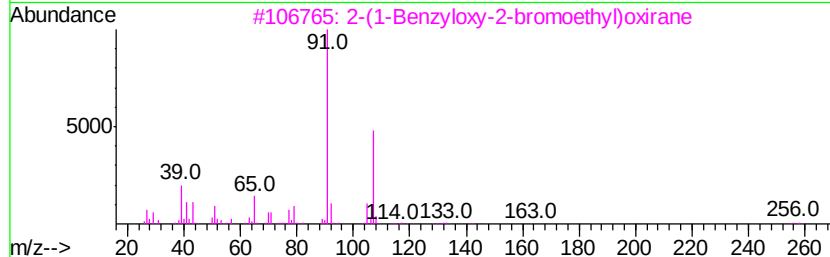
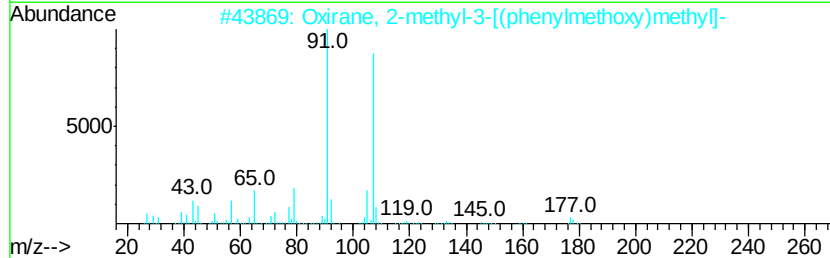
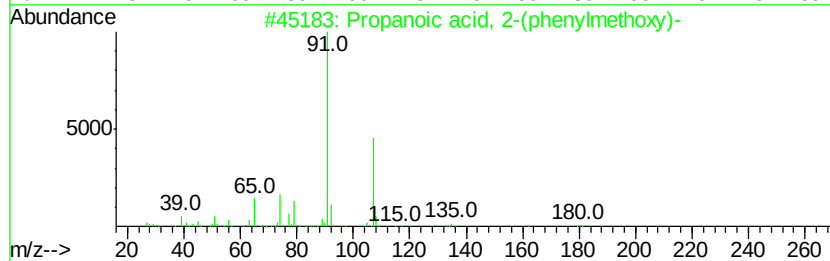
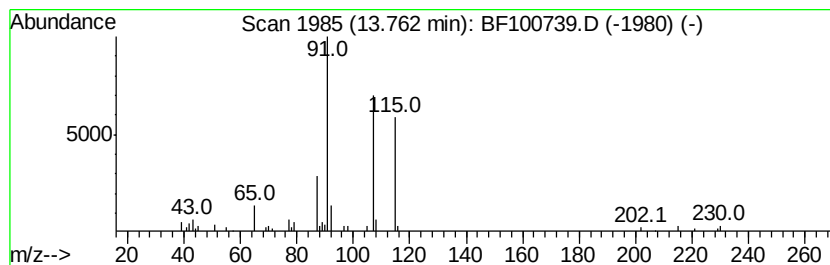
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Peak Number 4 unknown13.76 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	2.55 ng	115694	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-(phenylmethoxy)-	180	C10H12O3	006625-78-1	43
2		Oxirane, 2-methyl-3-[(phenylmethoxy)methyl]-	178	C11H14O2	116296-88-9	43
3		2-(1-Benzyl-2-bromoethyl)oxirane	256	C11H13BrO2	101514-16-3	37
4		Butanoic acid, 2-hydroxy-3-methyl-	224	C12H16O4	111833-00-2	35
5		3-Benzyl-2-bromobutanoic acid, methyl-	208	C12H16O3	116761-24-1	32



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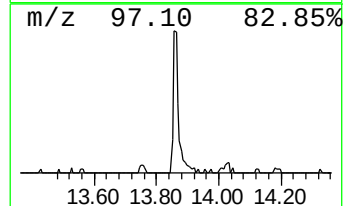
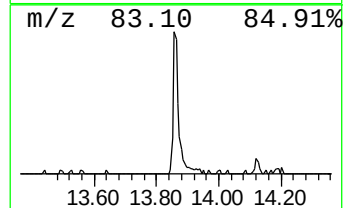
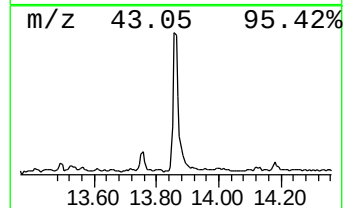
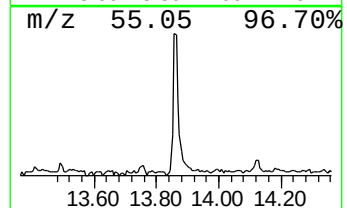
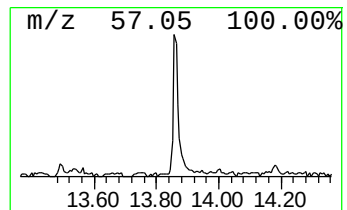
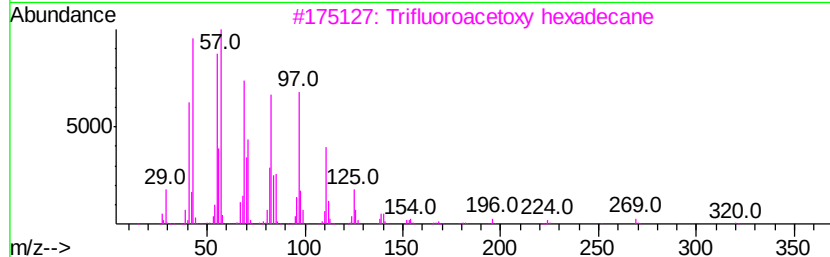
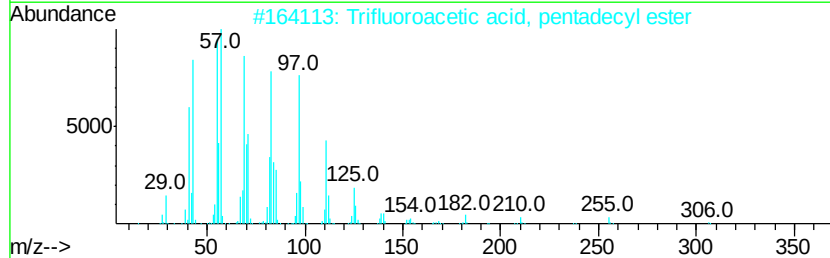
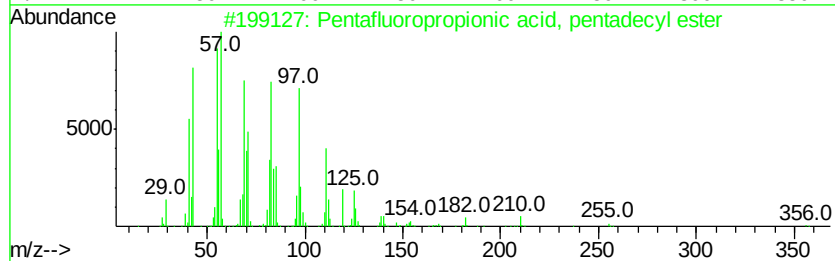
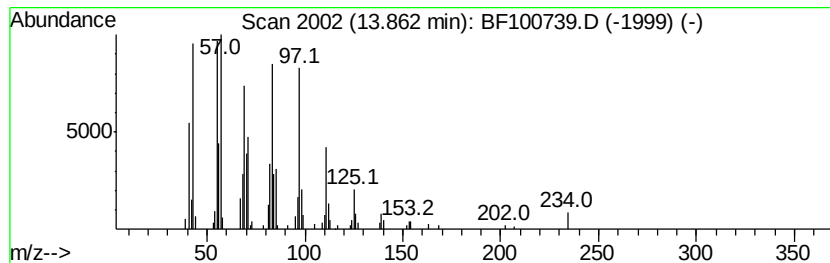
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Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	4.70 ng	213174	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
2		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
3		Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	95
4		Behenic alcohol	326	C22H46O	000661-19-8	94
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.11	6.3	ng	178966	1	6.87	563276	20.0
unknown6.65	6.65	89.4	ng	2518350	1	6.87	563276	20.0
unknown13.76	13.76	2.5	ng	115694	5	14.03	906379	20.0
Pentafluoropropio...	13.86	4.7	ng	213174	5	14.03	906379	20.0