

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF070518\
 Data File : BF107155.D
 Acq On : 6 Jul 2018 6:25
 Operator : JU/SJ
 Sample : J3851-02
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 070218-DBRI-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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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	5.172	479	482	493	rBV	35218	40249	2.27%	0.375%
2	5.584	549	552	567	rBV	532029	531002	29.89%	4.947%
3	6.589	720	723	733	rBV	351160	363842	20.48%	3.390%
4	6.725	742	746	749	rBV	987178	918761	51.71%	8.560%
5	6.942	780	783	787	rBV	410585	357295	20.11%	3.329%
6	7.101	806	810	814	rBV	1318635	1260830	70.96%	11.746%
7	7.513	875	880	883	rBV	973397	1007352	56.70%	9.385%
8	8.230	998	1002	1017	rVB	462854	439750	24.75%	4.097%
9	9.301	1179	1184	1188	rBV	1751061	1776699	100.00%	16.552%
10	9.695	1247	1251	1258	rBV	67267	63404	3.57%	0.591%
11	9.989	1298	1301	1310	rVB	477798	443398	24.96%	4.131%
12	10.648	1409	1413	1416	rBV	187695	165053	9.29%	1.538%
13	10.783	1432	1436	1447	rBV	718064	657619	37.01%	6.127%
14	10.866	1447	1450	1454	rVB	19170	18088	1.02%	0.169%
15	11.483	1551	1555	1562	rBV	389982	374783	21.09%	3.492%
16	13.065	1819	1824	1827	rBV	1635986	1533724	86.32%	14.289%
17	13.883	1951	1963	1966	rBV8	9639	28583	1.61%	0.266%
18	13.954	1971	1975	1983	rVB6	10816	22263	1.25%	0.207%
19	14.130	2002	2005	2016	rVB	398036	406769	22.89%	3.790%
20	14.512	2063	2070	2074	rBV5	9620	21435	1.21%	0.200%
21	15.030	2154	2158	2170	rVB2	19470	45401	2.56%	0.423%
22	15.630	2257	2260	2261	rBV	16391	19242	1.08%	0.179%
23	15.665	2262	2266	2270	rVB	183842	238274	13.41%	2.220%

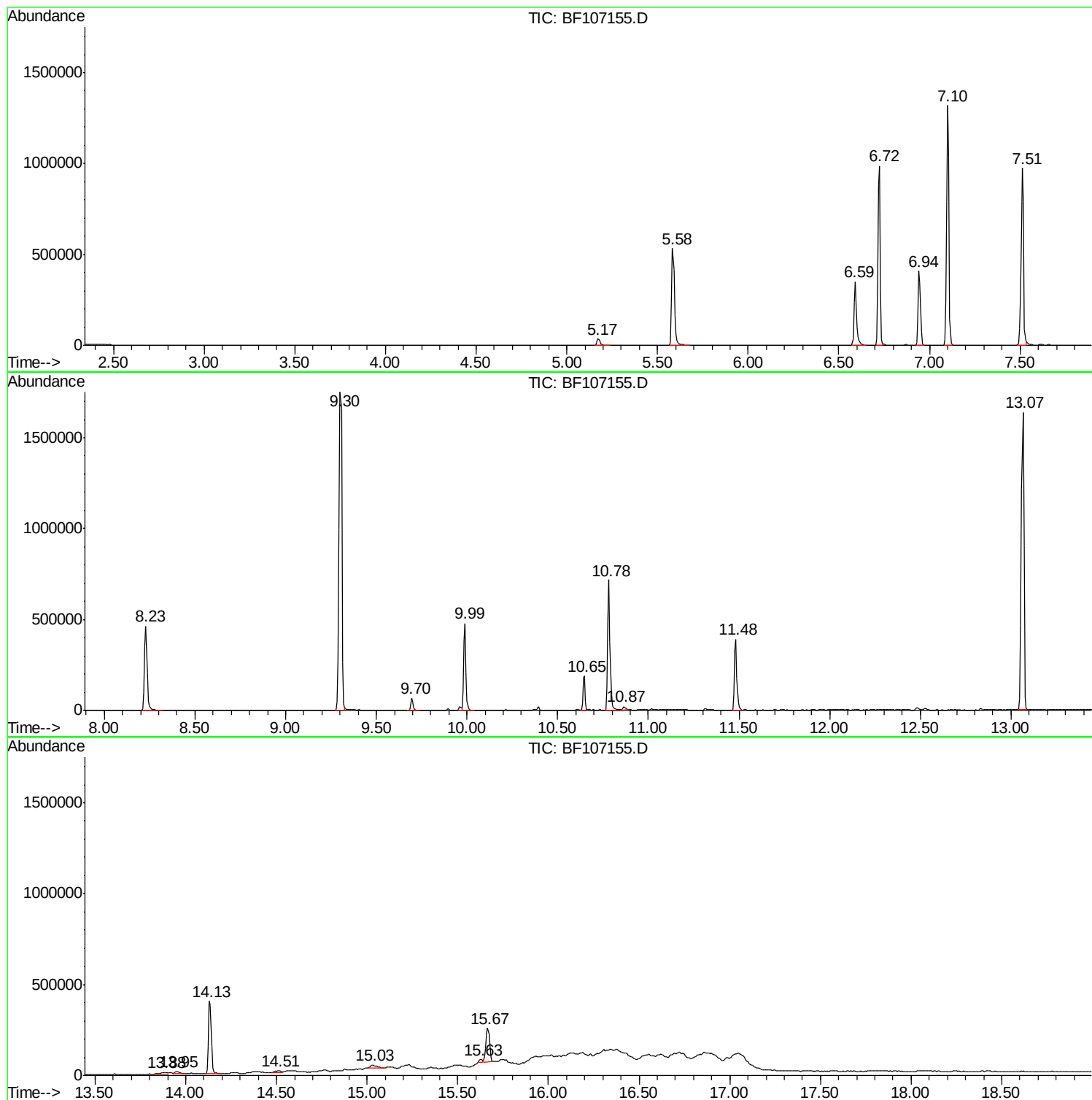
Sum of corrected areas: 10733816

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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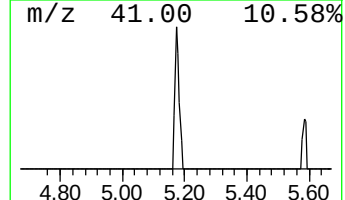
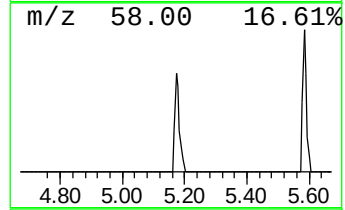
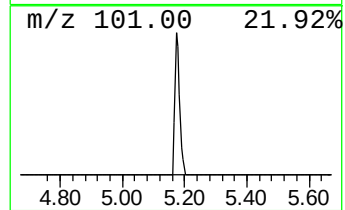
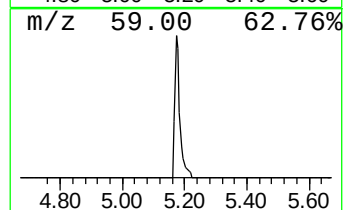
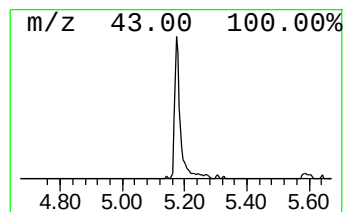
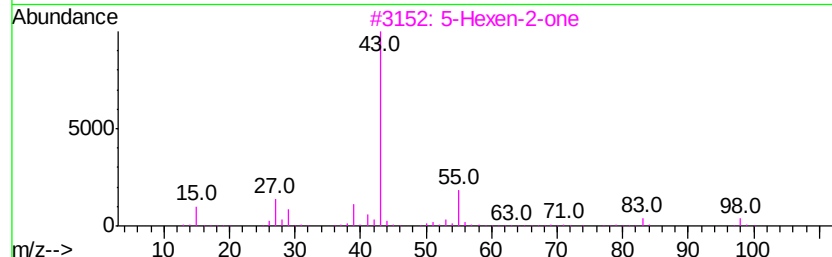
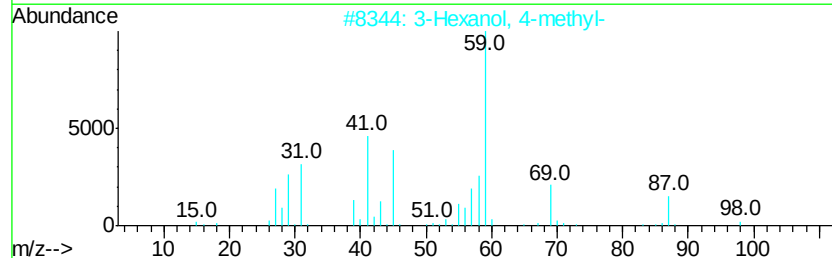
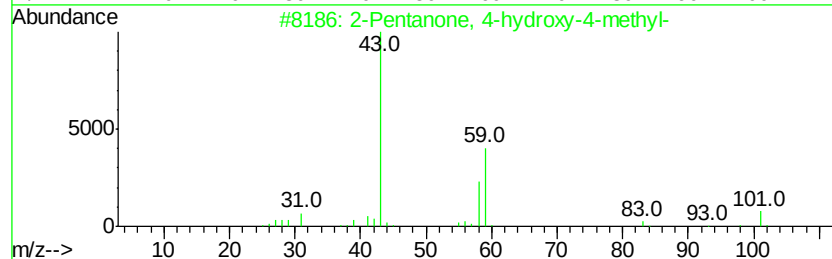
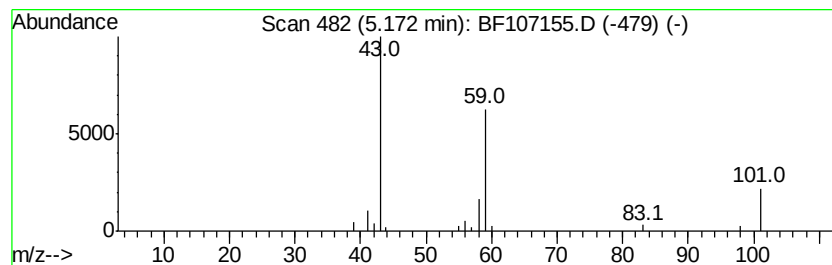
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	2.25 ng	40249	1,4-Dichlorobenzene-d4	6.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
5		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9



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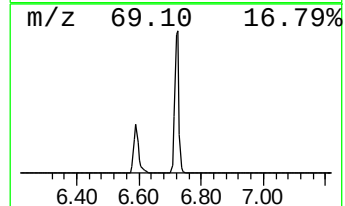
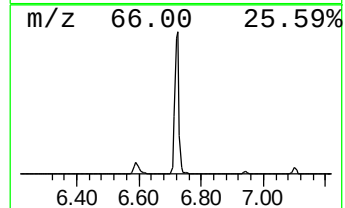
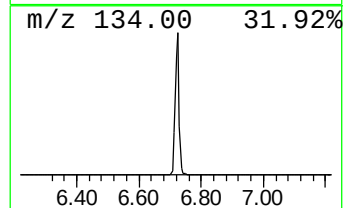
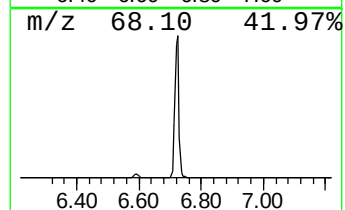
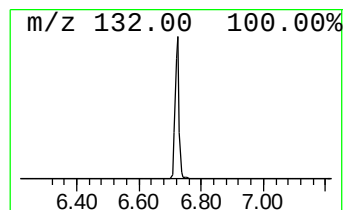
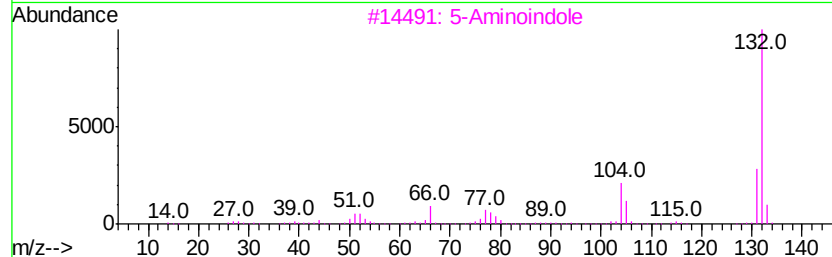
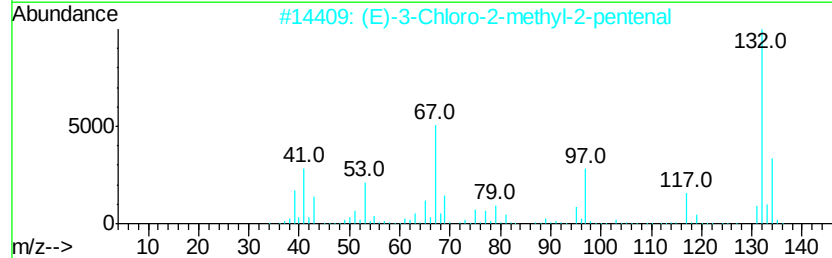
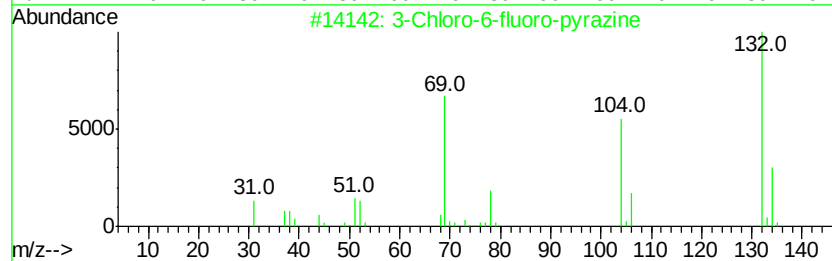
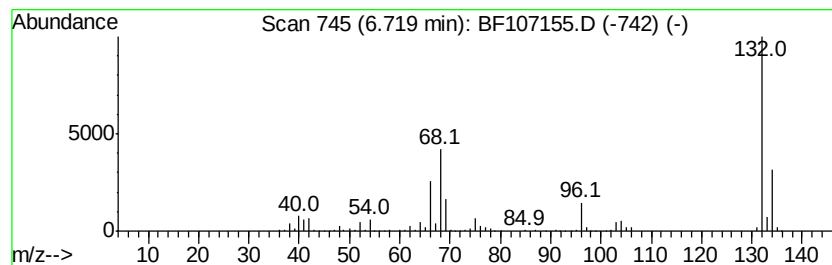
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.72 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	51.43 ng	918761	1,4-Dichlorobenzene-d4	6.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25		
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17		
3	5-Aminoindole	132	C8H8N2	005192-03-0	12		
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9		
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9		



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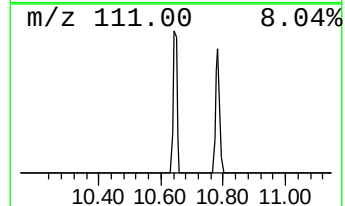
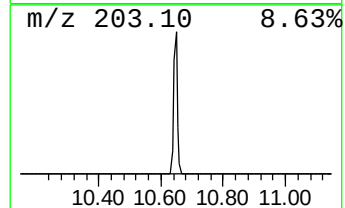
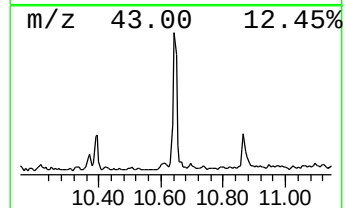
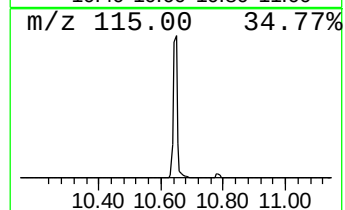
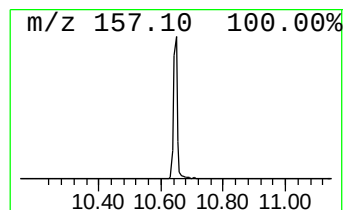
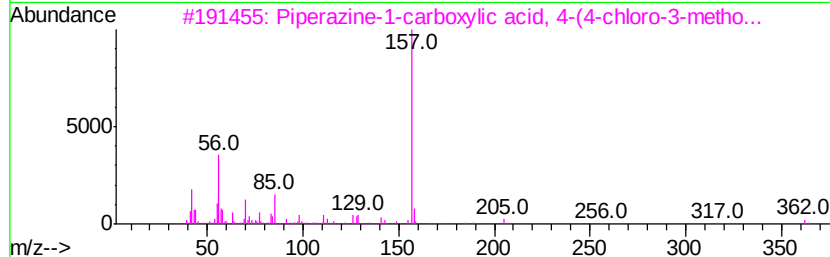
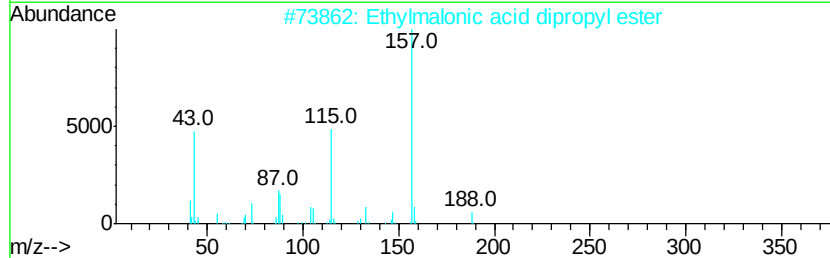
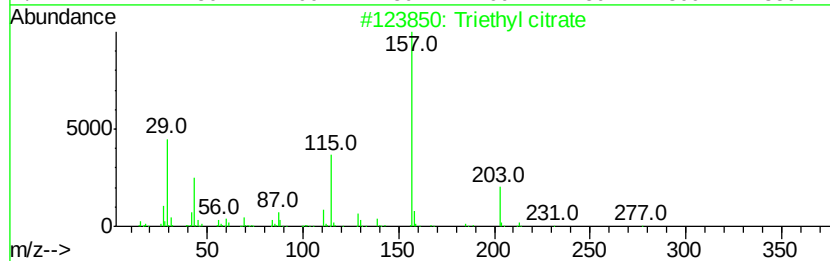
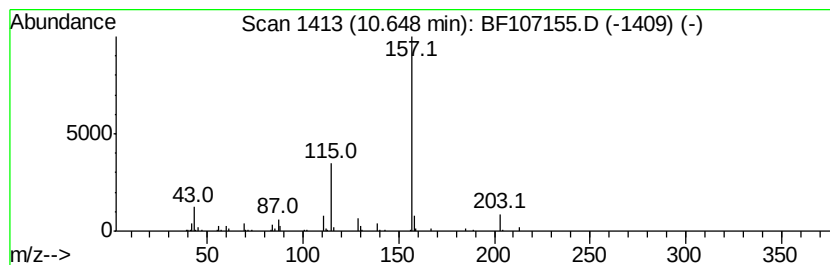
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Peak Number 4 Triethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	7.44 ng	165053	Acenaphthene-d10	9.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triethyl citrate	276	C12H20O7	000077-93-0	90
2		Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3		Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-79-9	42
4		3-Chloro2-fluorobenzoic acid, 3-...	370	C21H32ClFO2	1000338-64-6	36
5		1,4-Dioxaspiro[4.4]nonane, 7,8-b...	188	C9H16O4	1000155-54-9	36



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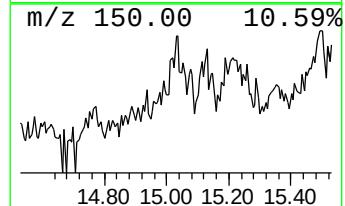
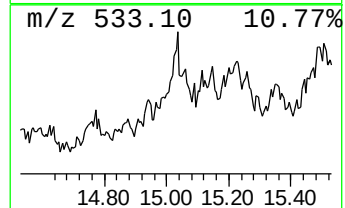
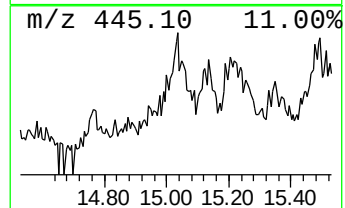
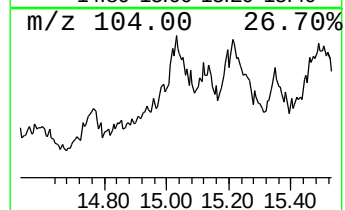
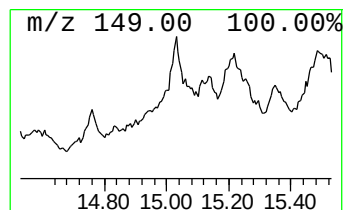
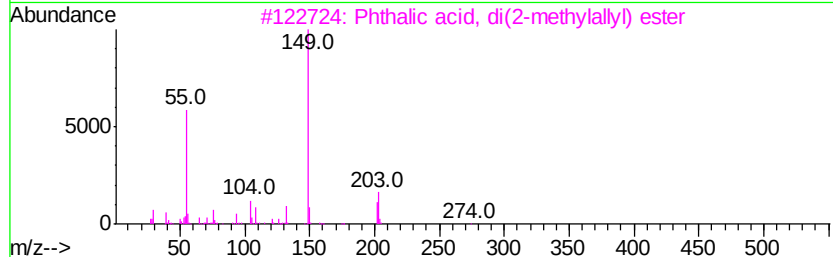
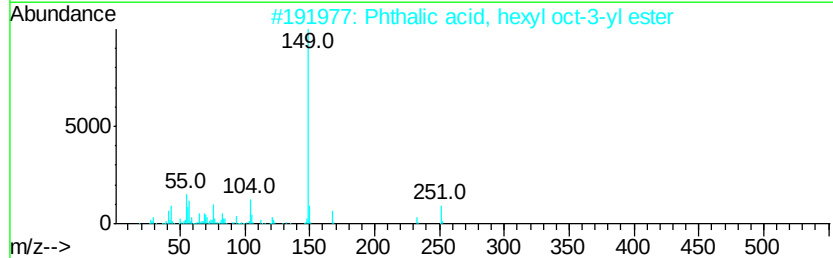
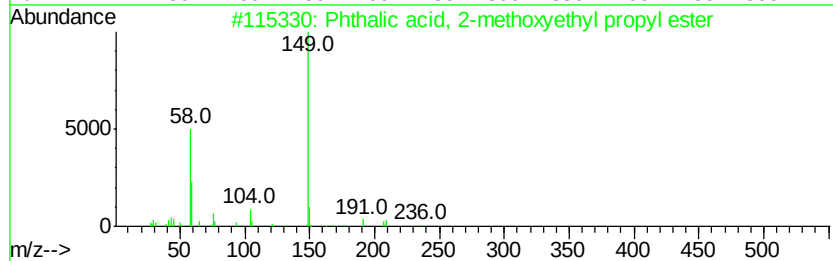
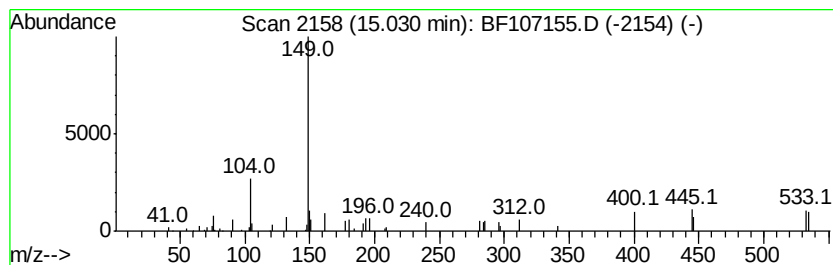
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Peak Number 5 unknown15.03 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	3.81 ng	45401	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, 2-methoxyethyl pr...	266	C14H18O5	1000315-79-8	38
2		Phthalic acid, hexyl oct-3-yl ester	362	C22H34O4	1000377-71-5	37
3		Phthalic acid, di(2-methylallyl)...	274	C16H18O4	1000315-58-3	37
4		Phthalic acid, butyl pent-2-en-4...	286	C17H18O4	1000315-45-3	37
5		Phthalic acid, 5-methylhex-2-yl ...	292	C17H24O4	1000371-09-3	32



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	2.3	ng	40249	1	6.94	357295	20.0
unknown6.72	6.72	51.4	ng	918761	1	6.94	357295	20.0
Triethyl citrate	10.65	7.4	ng	165053	3	9.99	443398	20.0
unknown15.03	15.03	3.8	ng	45401	6	15.67	238274	20.0