

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110816\
 Data File : BF091078.D
 Acq On : 8 Nov 2016 12:22
 Operator : UM/SJ
 Sample : H5536-04
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RMAB-MW11-GW

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-BF110316.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	1.755	4	6	51	rVB	3777379	10545398	100.00%	19.329%
2	4.796	270	272	279	rBV	321769	412977	3.92%	0.757%
3	5.253	309	312	314	rBV	1700239	2474557	23.47%	4.536%
4	6.304	402	404	411	rBV	978012	1628029	15.44%	2.984%
5	6.430	412	415	417	rBV	4548017	4515920	42.82%	8.277%
6	6.659	433	435	439	rBV	1206313	1145695	10.86%	2.100%
7	6.819	446	449	451	rVV	4586592	4818127	45.69%	8.831%
8	7.230	482	485	488	rBV	3174688	3524582	33.42%	6.460%
9	7.950	545	548	550	rBV	1406975	1575111	14.94%	2.887%
10	9.025	639	642	645	rBV	5264651	6581454	62.41%	12.063%
11	9.425	674	677	679	rBV	128113	116365	1.10%	0.213%
12	9.699	698	701	703	rBV	1784496	1867907	17.71%	3.424%
13	10.488	767	770	772	rBV	3848274	4099355	38.87%	7.514%
14	11.173	828	830	833	rBV	2057842	1784912	16.93%	3.272%
15	12.762	966	969	972	rBV	5187036	6281355	59.56%	11.513%
16	13.665	1046	1048	1055	rVB	123066	151296	1.43%	0.277%
17	13.802	1058	1060	1063	rBV	1576915	1540469	14.61%	2.824%
18	14.580	1125	1128	1132	rBV2	86962	217382	2.06%	0.398%
19	14.660	1132	1135	1137	rVV2	81855	139341	1.32%	0.255%
20	15.174	1178	1180	1183	rBV	785369	1137493	10.79%	2.085%

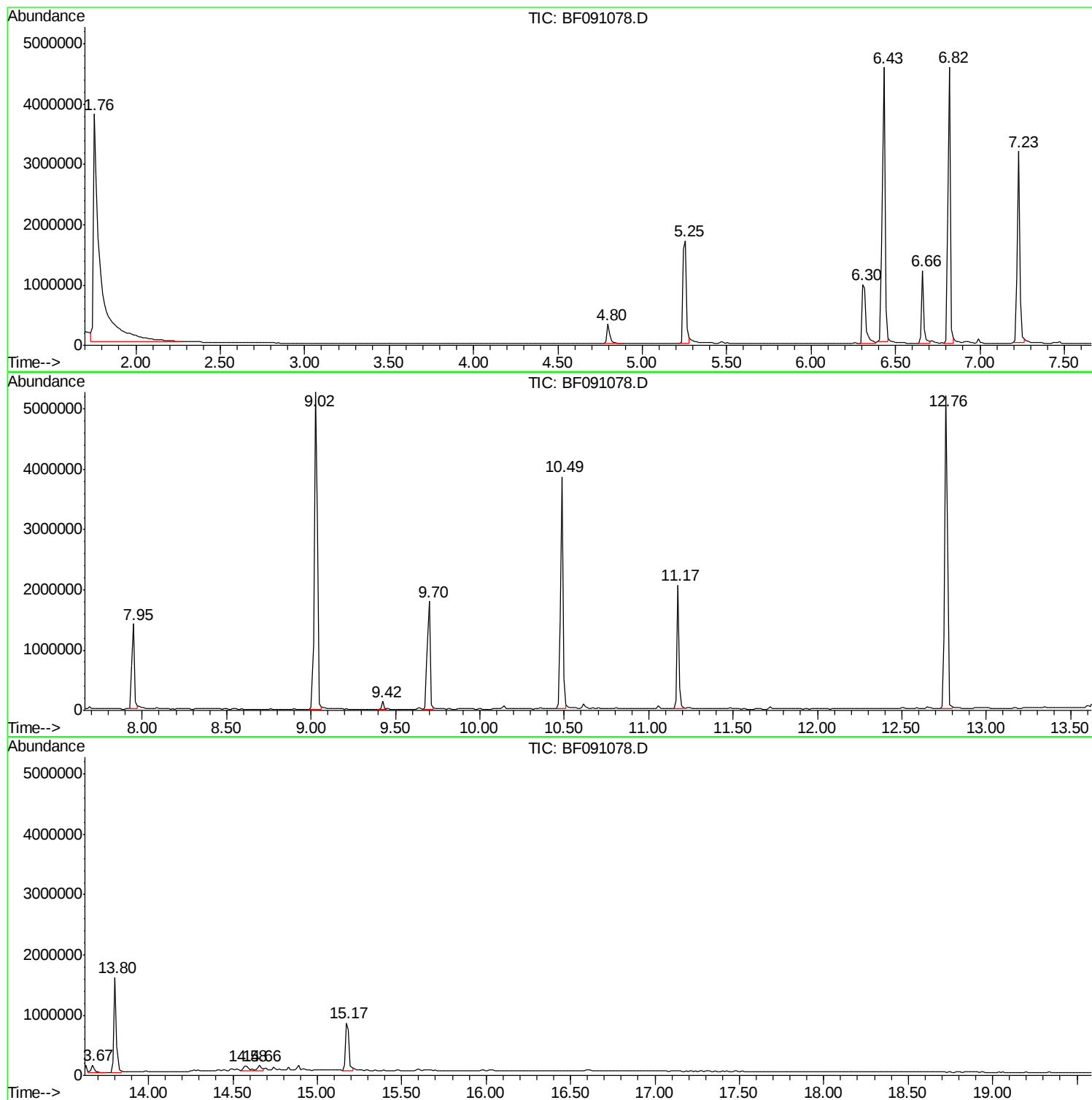
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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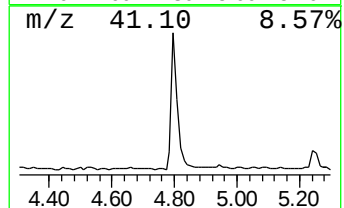
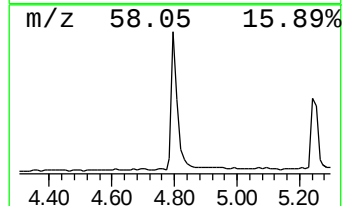
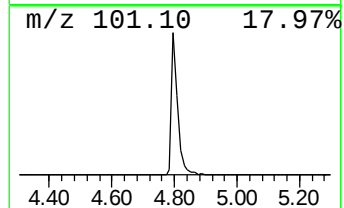
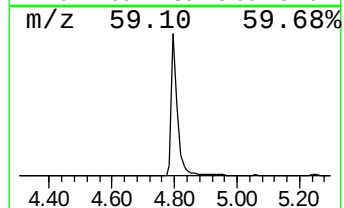
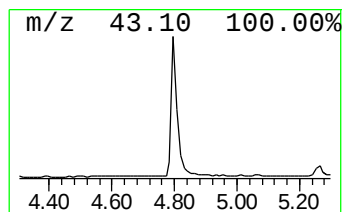
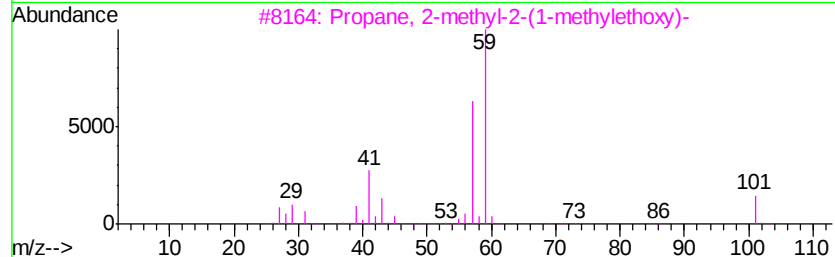
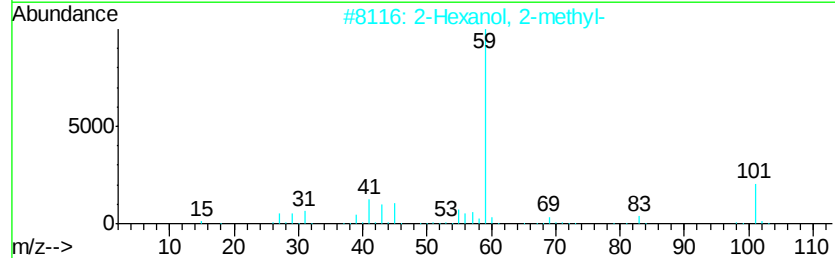
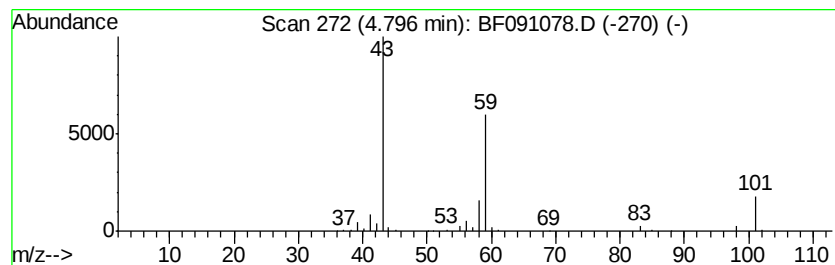
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	7.21 ng	412977	1,4-Dichlorobenzene-d4	6.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3			Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25



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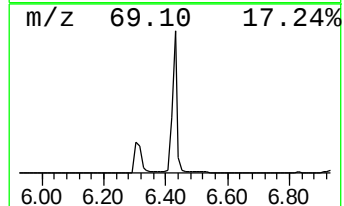
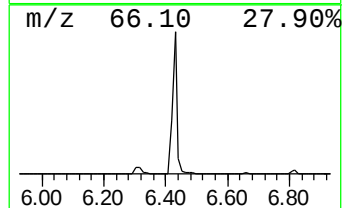
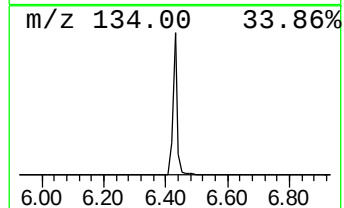
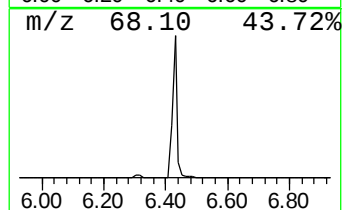
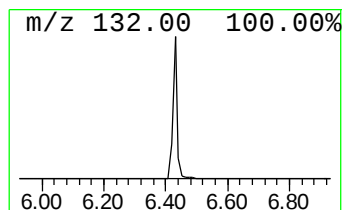
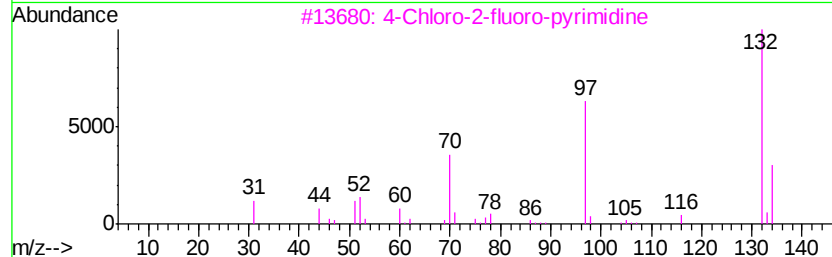
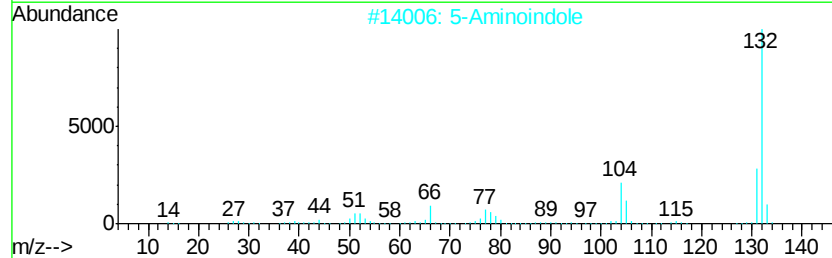
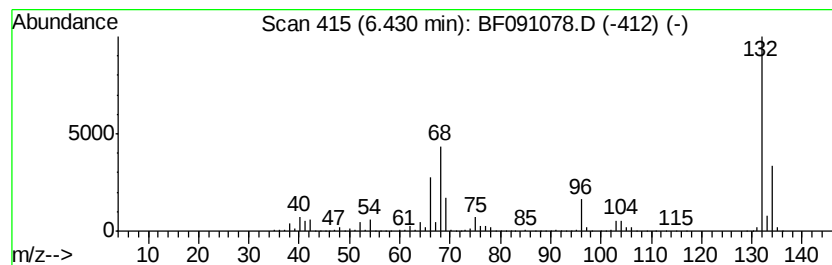
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Peak Number 3 unknown6.43 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	78.83 ng	4515920	1,4-Dichlorobenzene-d4	6.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5			4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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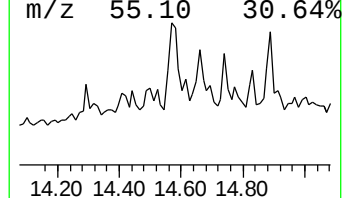
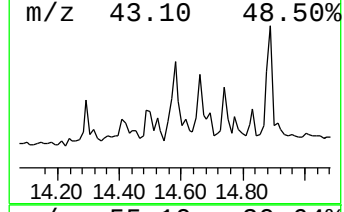
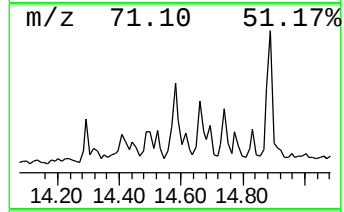
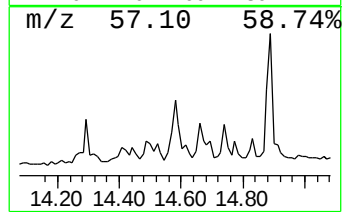
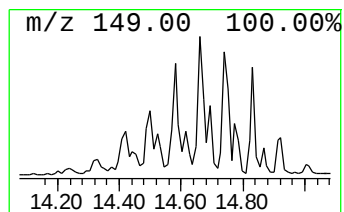
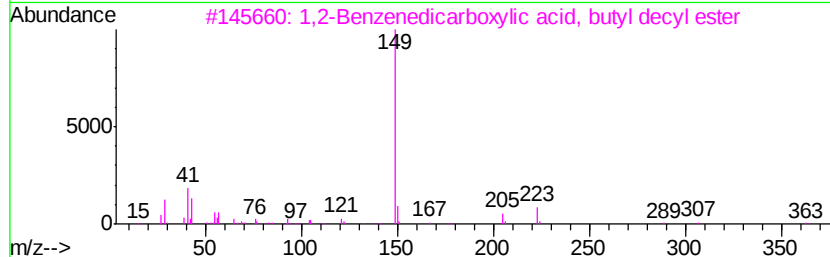
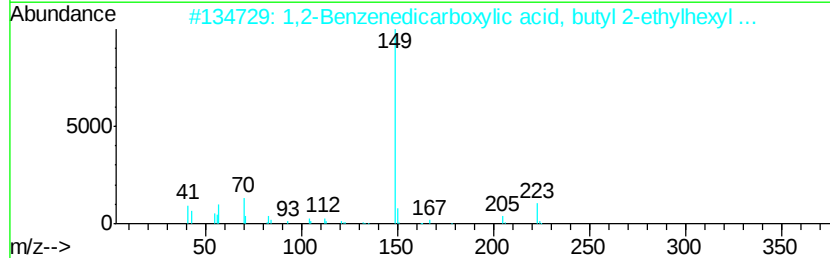
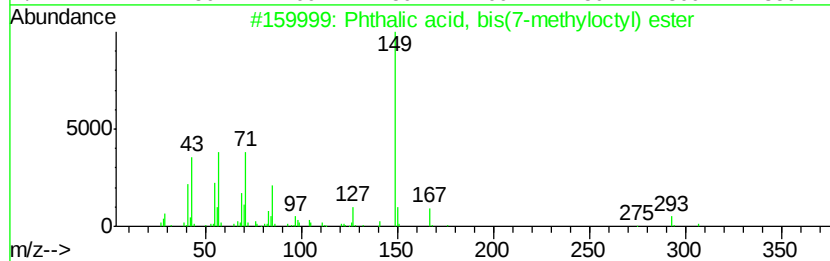
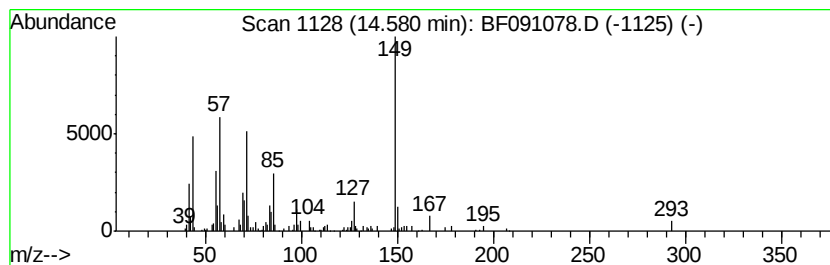
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Peak Number 5 Phthalic acid, bis(7-methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	3.82 ng	217382	Perylene-d12	15.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, bis(7-methyloctyl...	418	C26H42O4	020548-62-3	87
2		1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	43
3		1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-19-0	35
4		1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	35
5		1,2-Benzenedicarboxylic acid, bu...	304	C18H24O4	000084-64-0	35



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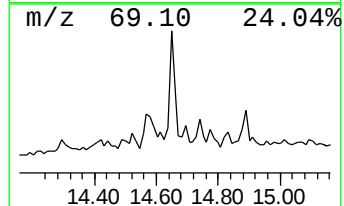
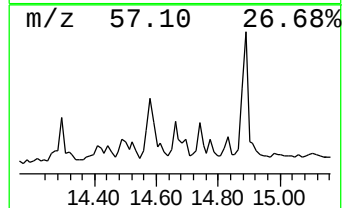
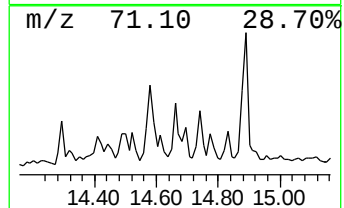
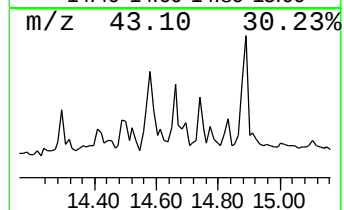
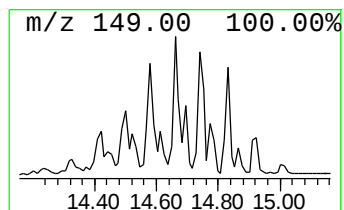
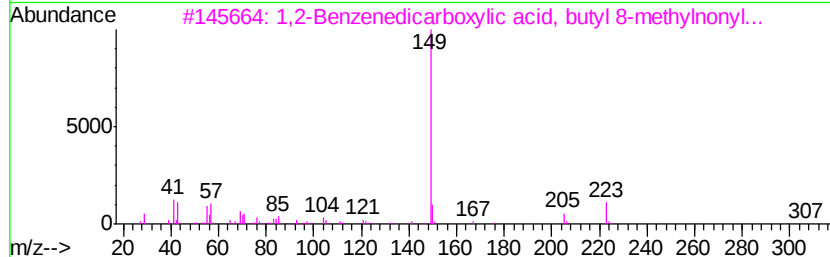
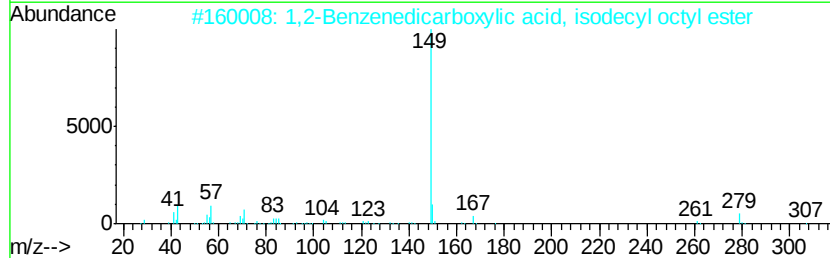
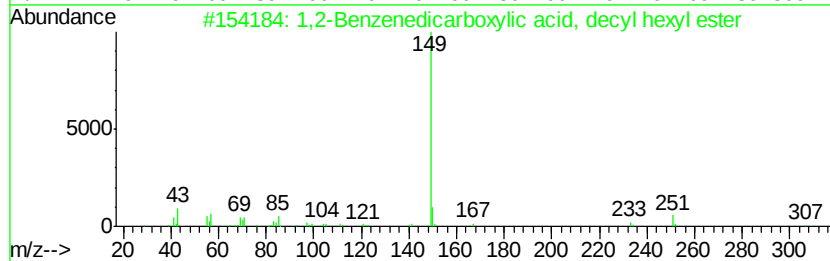
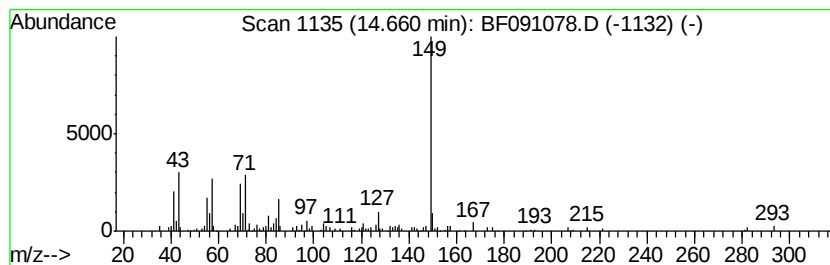
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Peak Number 6 1,2-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.45 ng	139341	Perylene-d12	15.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid, de...	390	C24H38O4	025724-58-7	59
2		1,2-Benzenedicarboxylic acid, is...	418	C26H42O4	001330-96-7	59
3		1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-18-9	53
4		1,2-Benzenedicarboxylic acid, bi...	334	C20H30O4	000146-50-9	53
5		1,2-Benzenedicarboxylic acid, di...	362	C22H34O4	003648-21-3	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.80	7.2	ng	412977	1	6.66	1145700	20.0
unknown6.43	6.43	78.8	ng	4515920	1	6.66	1145700	20.0
Phthalic acid, bi...	14.58	3.8	ng	217382	6	15.19	1137490	20.0
1,2-Benzenedicarb...	14.66	2.5	ng	139341	6	15.19	1137490	20.0