

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122216\
 Data File : BF091878.D
 Acq On : 22 Dec 2016 11:39
 Operator : UM/SJ
 Sample : H6156-21
 Misc :
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-17

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-BF122116.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	4.910	244	247	261	rVB	1060118	1273001	13.58%	2.063%
2	5.344	283	285	288	rBV	3073360	3974313	42.41%	6.439%
3	6.384	374	376	379	rBV	1870389	2534063	27.04%	4.106%
4	6.522	385	388	390	rBV	5115558	6958101	74.25%	11.274%
5	6.739	405	407	410	rBV	1328105	1682445	17.95%	2.726%
6	6.899	418	421	424	rVB	5019607	6091413	65.00%	9.870%
7	7.310	454	457	460	rBV	3560618	5369784	57.30%	8.700%
8	8.030	517	520	523	rBV	2319304	2228321	23.78%	3.610%
9	9.116	611	615	617	rBV	6884026	9370859	100.00%	15.183%
10	9.779	670	673	676	rBV	2383286	2473361	26.39%	4.007%
11	10.568	739	742	745	rBV2	3581618	5362742	57.23%	8.689%
12	11.265	800	803	805	rBV	2644016	2612327	27.88%	4.233%
13	12.682	924	927	929	rBV	353246	326171	3.48%	0.528%
14	12.854	939	942	944	rBV	6851435	7442595	79.42%	12.059%
15	13.379	986	988	990	rBV	200974	208399	2.22%	0.338%
16	13.894	1030	1033	1036	rBV	2216849	2087015	22.27%	3.381%
17	15.288	1152	1155	1158	rBV	1089922	1557034	16.62%	2.523%
18	15.551	1171	1178	1188	rVB3	31328	167421	1.79%	0.271%

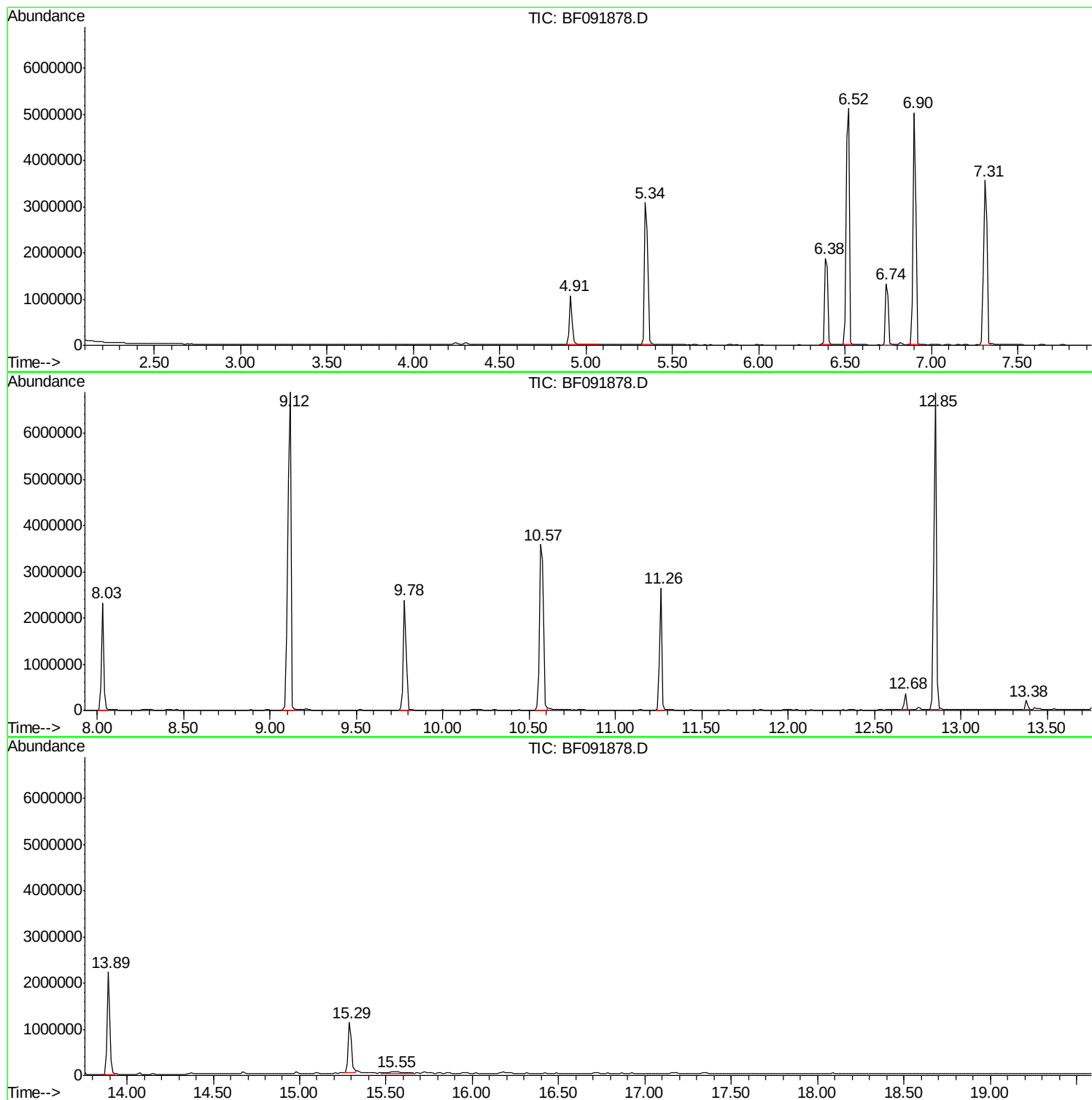
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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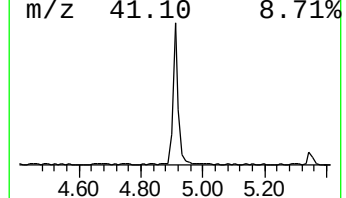
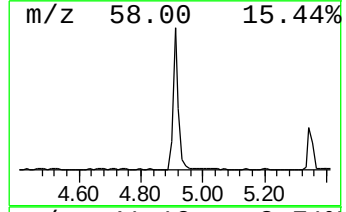
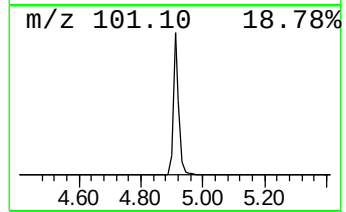
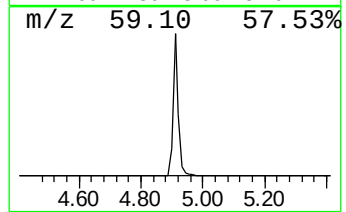
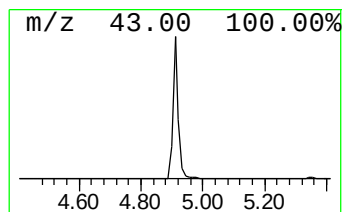
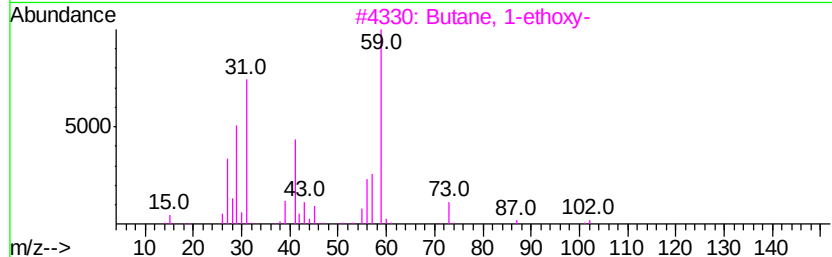
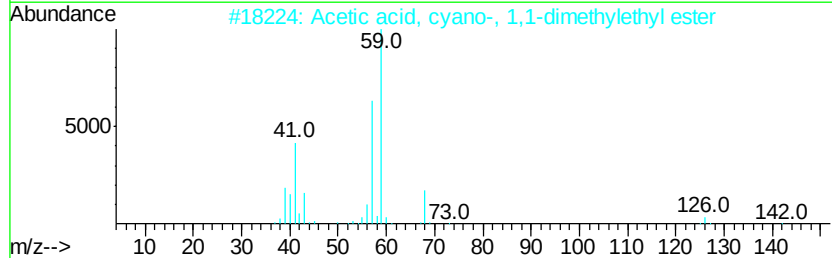
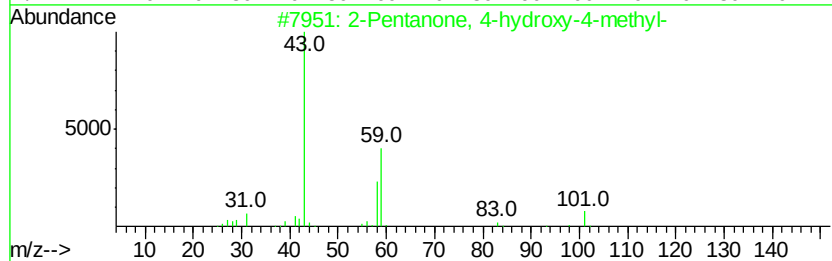
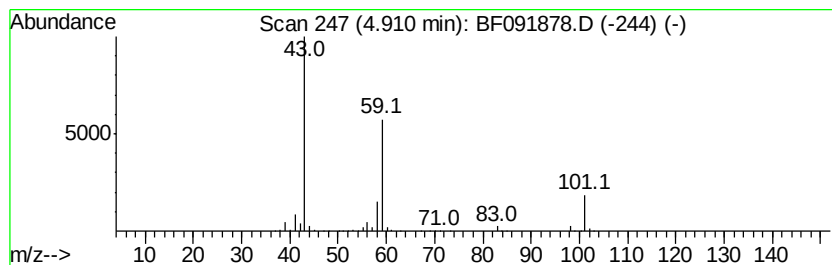
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	15.13 ng	1273000	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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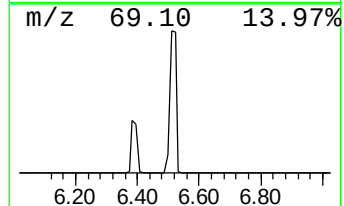
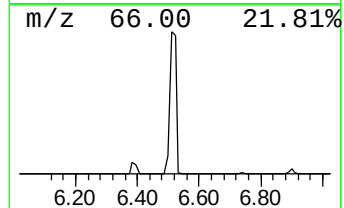
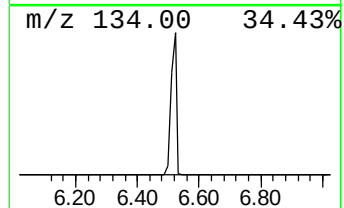
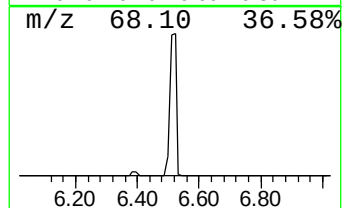
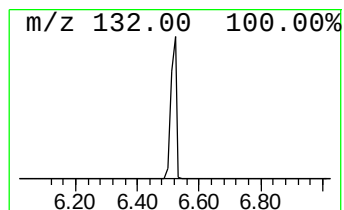
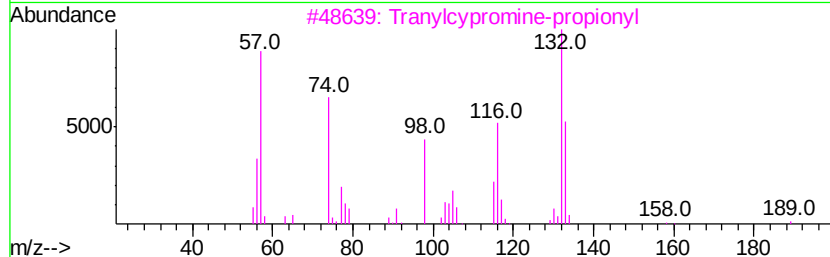
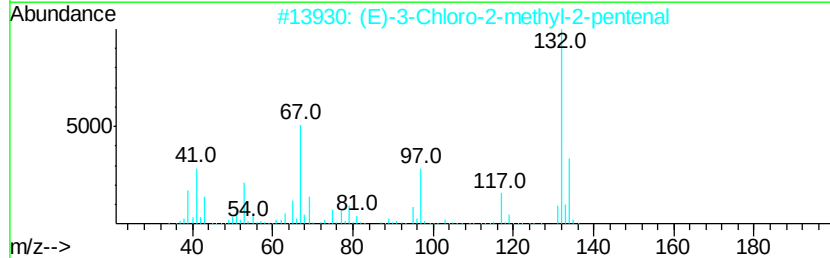
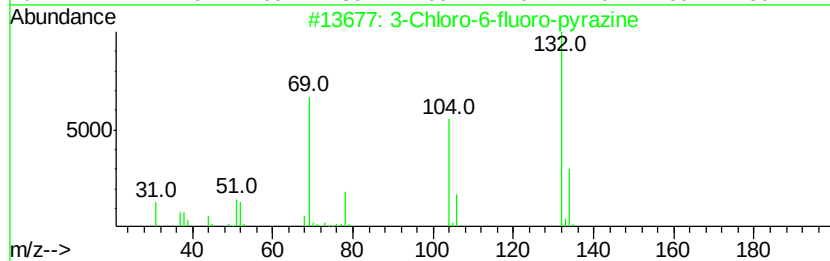
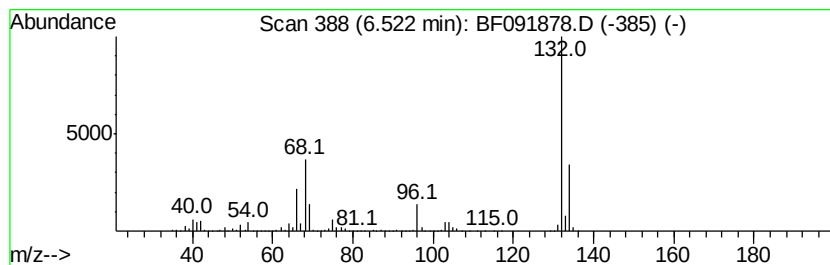
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Peak Number 2 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	82.71 ng	6958100	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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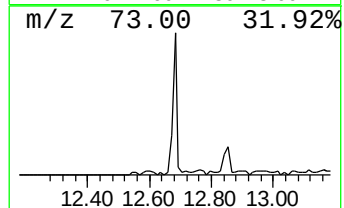
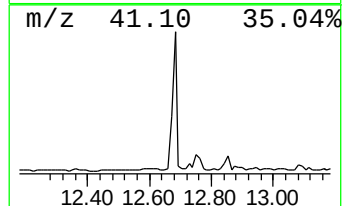
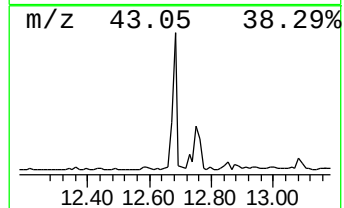
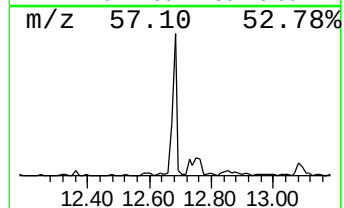
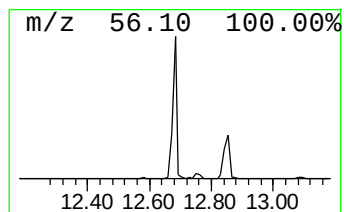
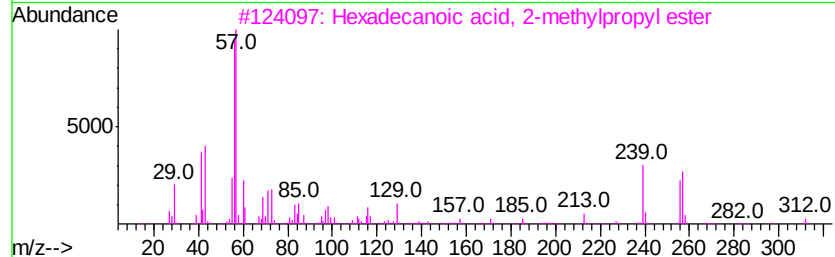
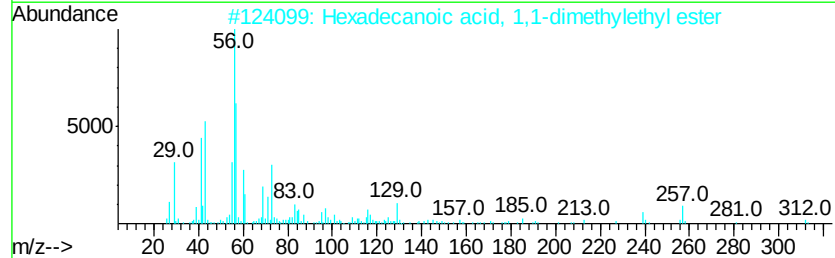
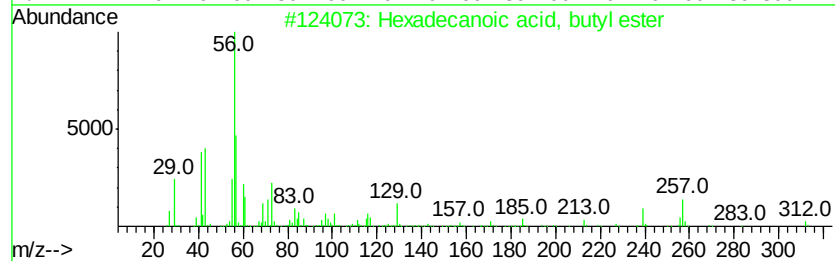
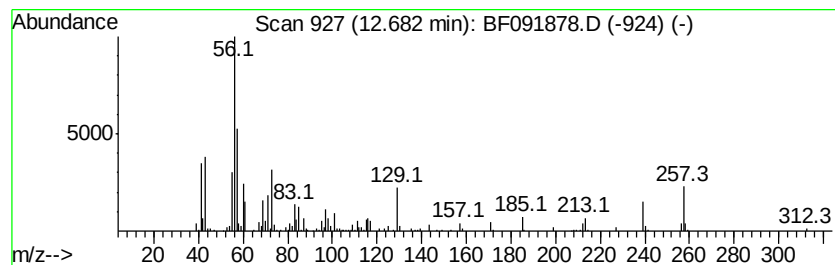
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	3.13 ng	326171	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	94
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	68
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	64
4		Nipecotic acid	129	C6H11NO2	000498-95-3	50
5		Oxan-4-one, 2-trifluoromethyl-2-...	212	C8H11F3O3	212615-80-0	38



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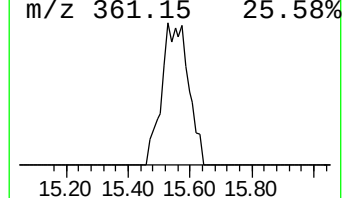
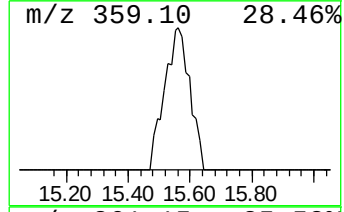
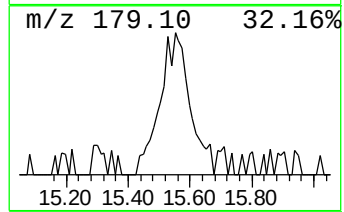
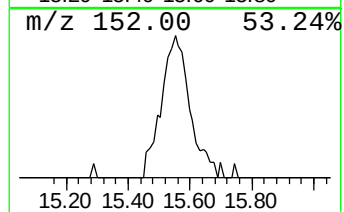
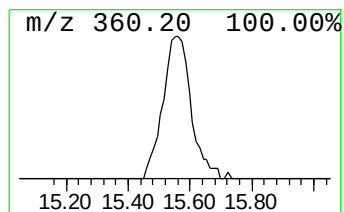
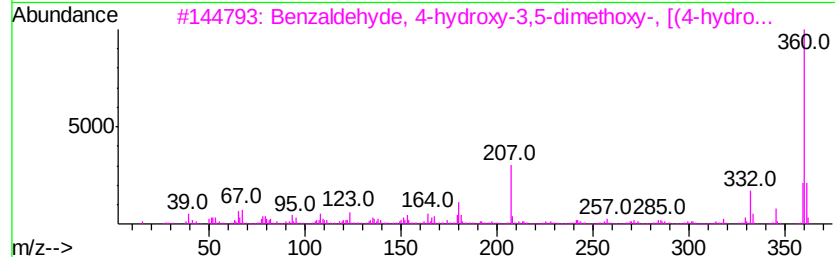
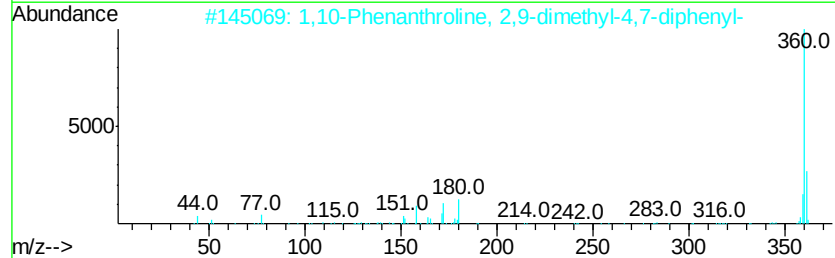
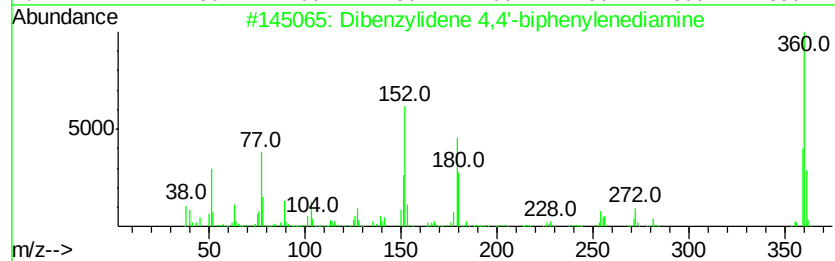
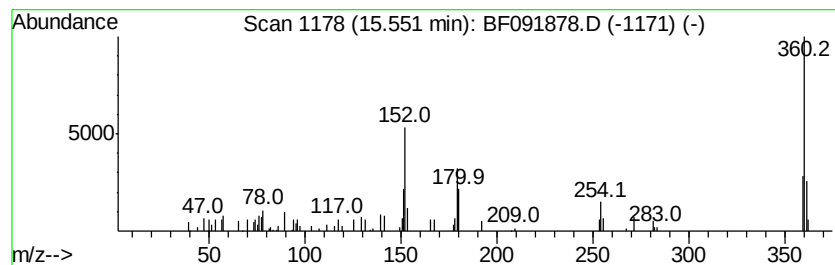
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Peak Number 5 Dibenzylidene 4,4'-biphenyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.55	2.15 ng	167421	Perylene-d12	15.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	94
2		1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	47
3		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	43
4		Benzo[1,2-b:4,3-b']dipyrrole-1,8...	360	C18H20N2O6	174832-71-4	38
5		1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.91	15.1	ng	1273000	1	6.74	1682450	20.0
unknown6.52	6.52	82.7	ng	6958100	1	6.74	1682450	20.0
Hexadecanoic acid...	12.68	3.1	ng	326171	5	13.89	2087020	20.0
Dibenzylidene 4,4...	15.55	2.1	ng	167421	6	15.29	1557030	20.0