

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122716\
 Data File : BF091963.D
 Acq On : 27 Dec 2016 13:10
 Operator : UM/SJ
 Sample : PB95595BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB95595BL

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	4.899	243	246	255	rBV	1523169	2633953	38.47%	4.626%
2	5.367	284	287	289	rBV	5707673	6846794	100.00%	12.026%
3	6.407	375	378	380	rBV	5065097	5609008	81.92%	9.852%
4	6.510	384	387	389	rBV	5715552	5870354	85.74%	10.311%
5	6.727	404	406	408	rBV	1414111	1263133	18.45%	2.219%
6	6.887	417	420	422	rBV	4063524	4650535	67.92%	8.168%
7	7.299	452	456	458	rBV	3351188	3849251	56.22%	6.761%
8	8.019	516	519	521	rBV	1401179	1685174	24.61%	2.960%
9	9.093	610	613	616	rBV	5078865	6336005	92.54%	11.129%
10	9.768	669	672	674	rBV	2094667	1965189	28.70%	3.452%
11	10.556	738	741	744	rBV2	2850903	4116274	60.12%	7.230%
12	11.253	799	802	804	rBV	1882019	2015675	29.44%	3.540%
13	12.671	923	926	928	rBV	235169	198197	2.89%	0.348%
14	12.842	938	941	944	rBV	5731179	6030612	88.08%	10.593%
15	13.379	985	988	990	rBV	107649	137730	2.01%	0.242%
16	13.882	1030	1032	1035	rBV	1725358	1801204	26.31%	3.164%
17	15.288	1151	1155	1157	rBV	1144388	1681120	24.55%	2.953%
18	15.505	1168	1174	1187	rBV	41141	242418	3.54%	0.426%

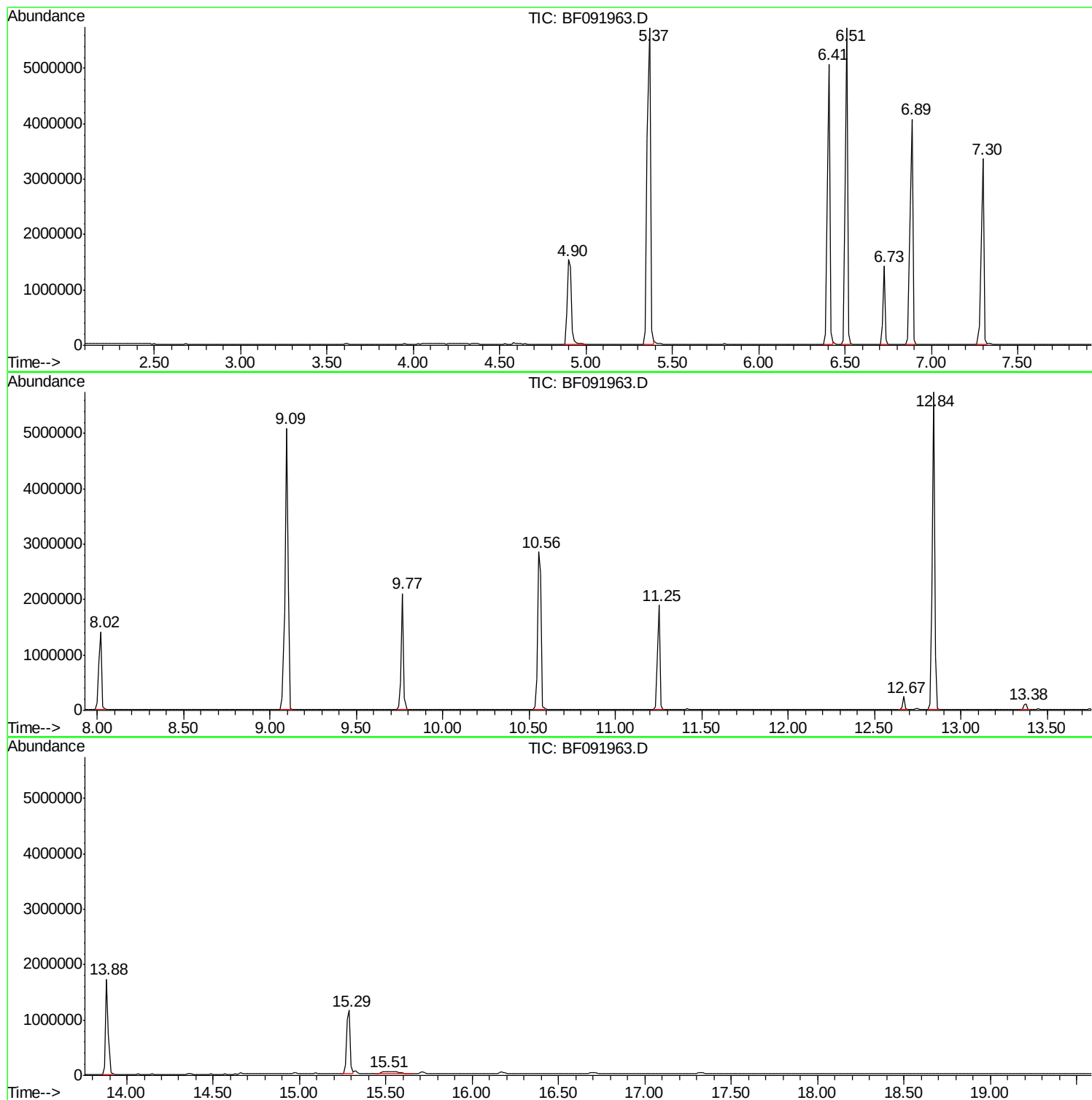
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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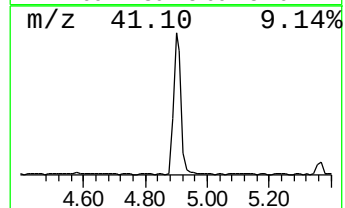
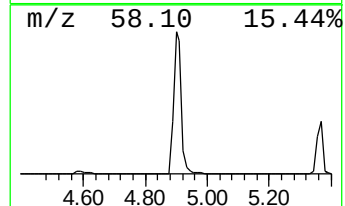
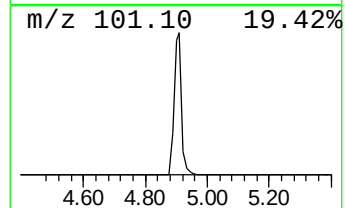
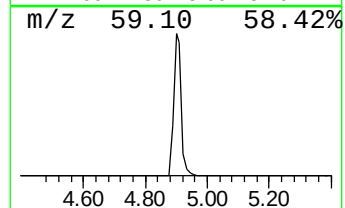
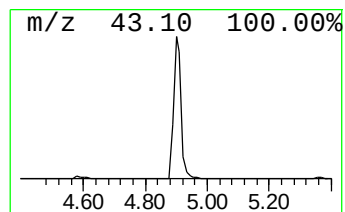
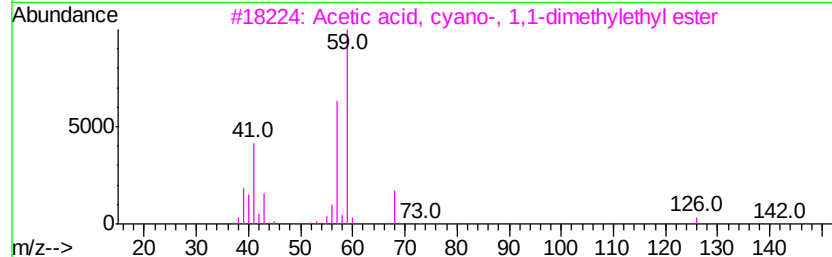
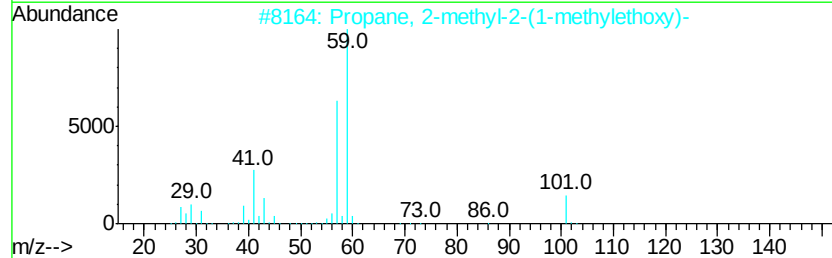
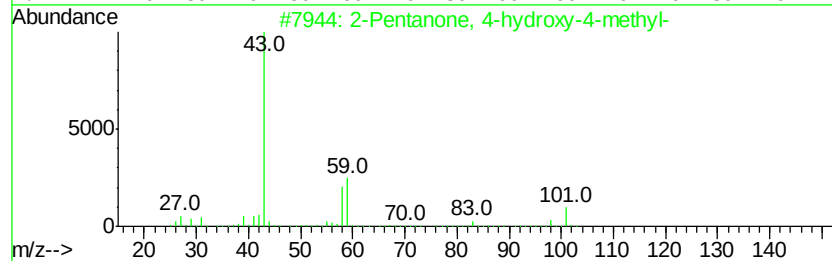
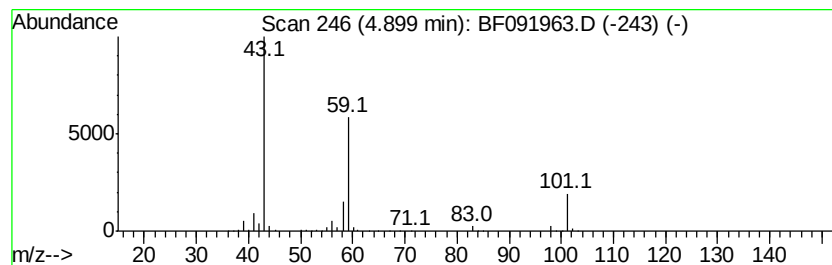
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.90	41.71 ng	2633950	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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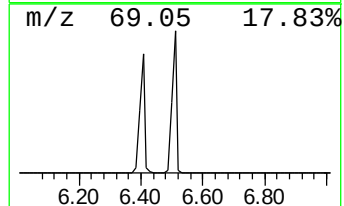
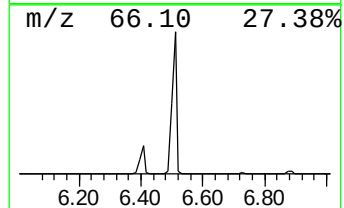
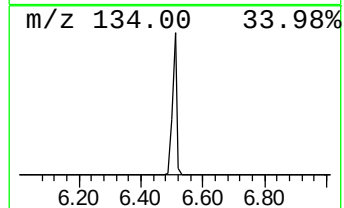
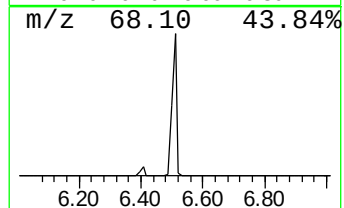
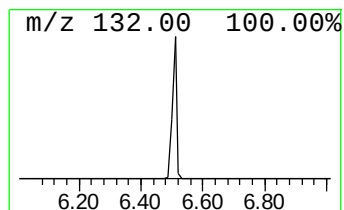
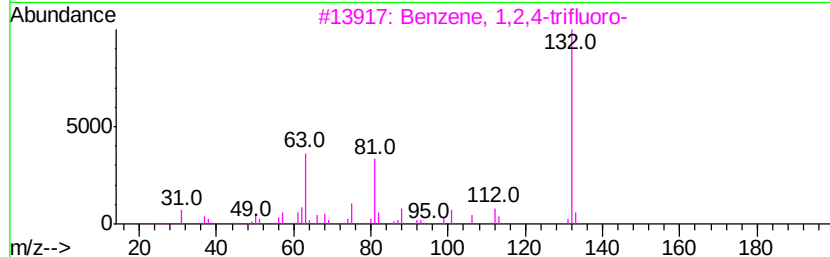
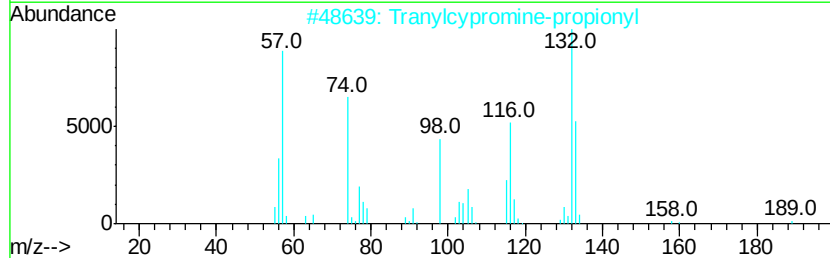
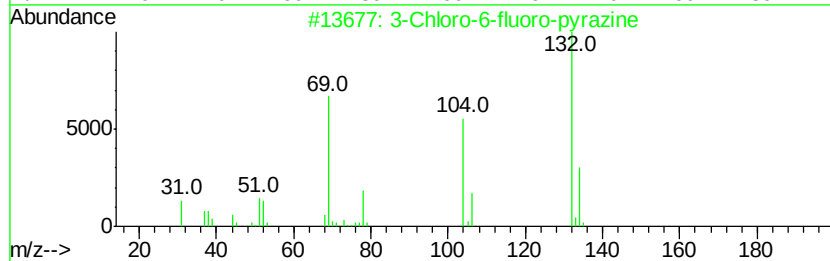
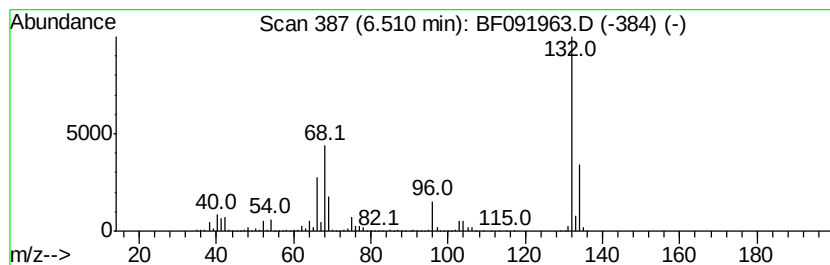
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Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	92.95 ng	5870350	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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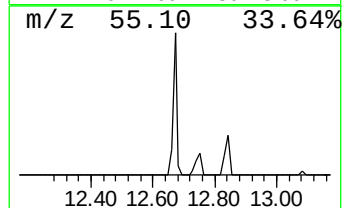
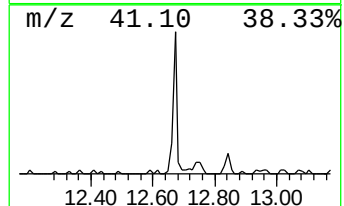
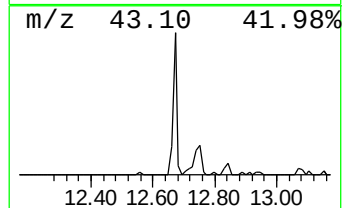
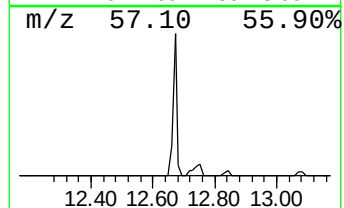
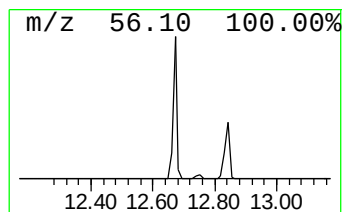
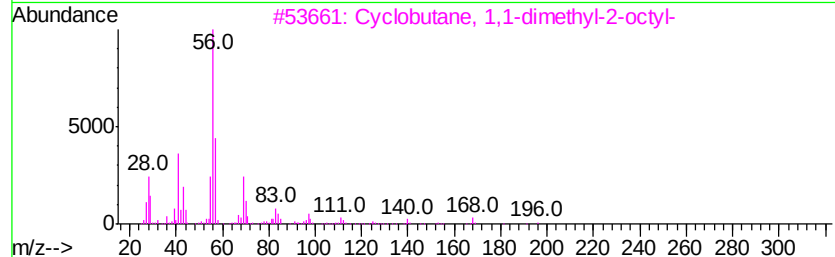
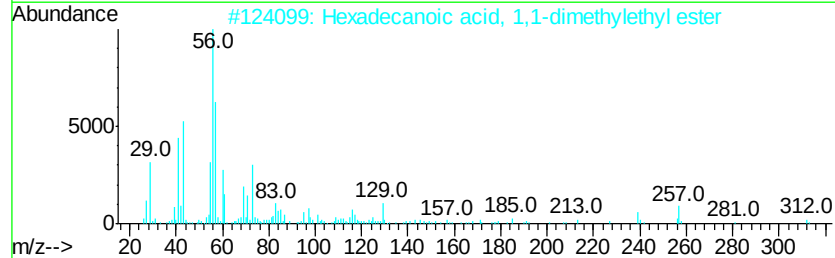
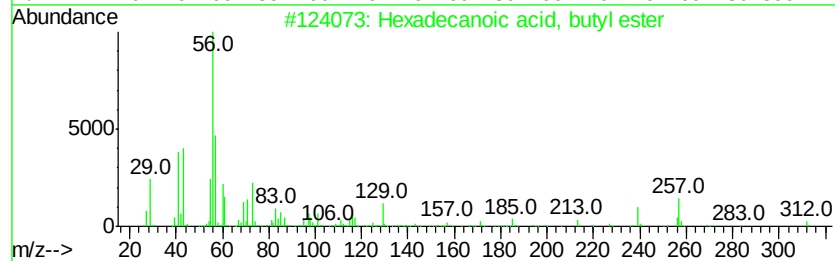
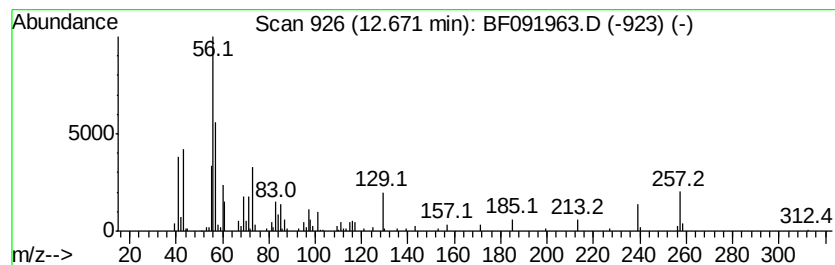
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	2.20 ng	198197	Chrysene-d12	13.88

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		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
4		Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	30
5		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	27



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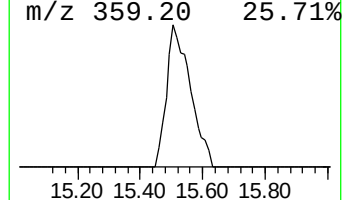
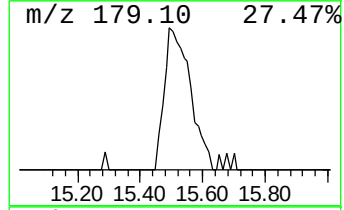
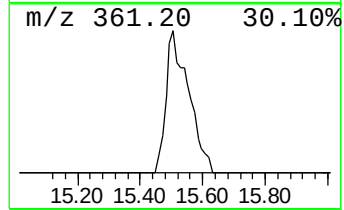
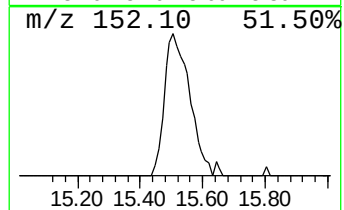
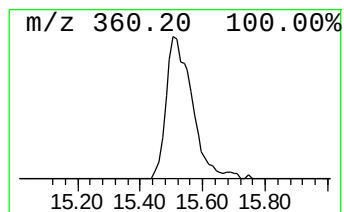
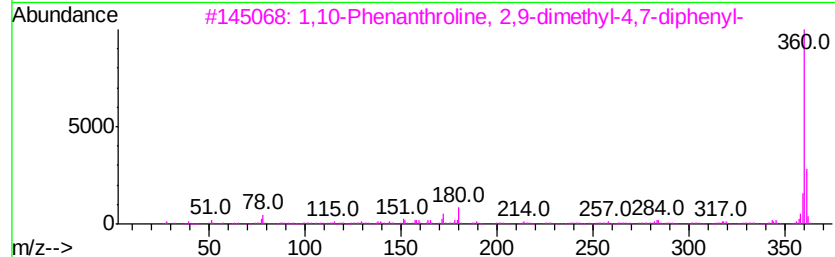
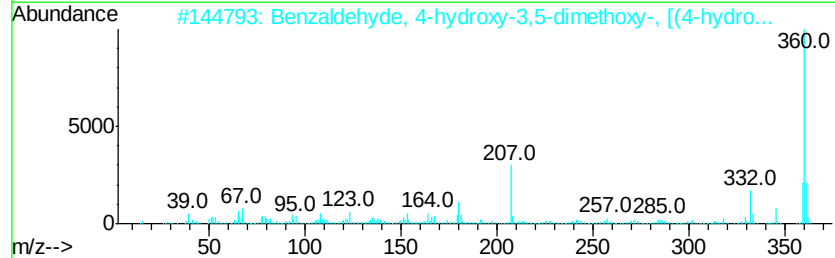
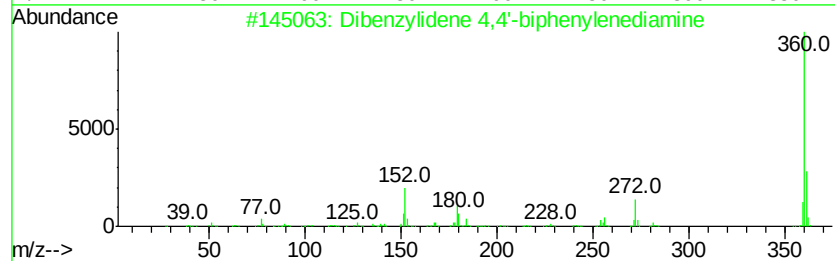
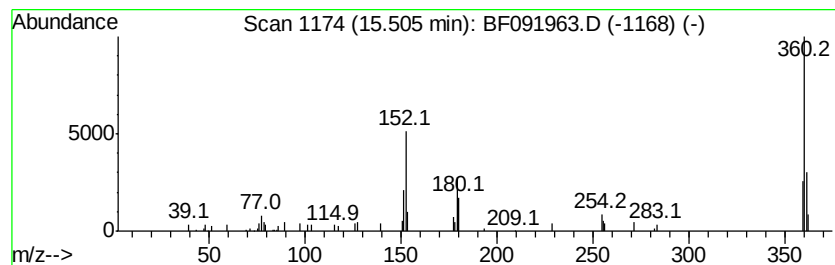
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Peak Number 5 Dibenzylidene 4,4'-biphenyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.51	2.88 ng	242418	Perylene-d12	15.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	90
2		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	46
3		1,10-Phenanthroline, 2,9-dimethv...	360	C26H20N2	004733-39-5	46
4		1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	43
5		N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	41.7	ng	2633950	1	6.73	1263130	20.0
unknown6.51	6.51	93.0	ng	5870350	1	6.73	1263130	20.0
Hexadecanoic acid...	12.67	2.2	ng	198197	5	13.88	1801200	20.0
Dibenzylidene 4,4...	15.51	2.9	ng	242418	6	15.29	1681120	20.0