

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
 Data File : BF085164.D
 Acq On : 3 Mar 2016 18:57
 Operator : SJ/UM
 Sample : PB88646BL
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB88646BL

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-BF030316.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	5.190	251	254	261	rBV	632374	820008	18.67%	2.318%
2	5.590	286	289	291	rBV	3561466	3850006	87.65%	10.885%
3	6.596	374	377	380	rBV	3170218	3244726	73.87%	9.174%
4	6.744	387	390	392	rBV	3920946	3709932	84.46%	10.489%
5	6.973	408	410	412	rBV	901065	906483	20.64%	2.563%
6	7.133	422	424	427	rVB	3286115	2859612	65.10%	8.085%
7	7.293	437	438	439	rBV	109196	74856	1.70%	0.212%
8	7.533	456	459	462	rBV	2012736	2258778	51.42%	6.386%
9	7.842	485	486	487	rBV	226399	155625	3.54%	0.440%
10	8.265	520	523	525	rBV	1215968	1251369	28.49%	3.538%
11	8.367	530	532	535	rBV	82906	89604	2.04%	0.253%
12	9.339	614	617	619	rBV	4446270	4392572	100.00%	12.419%
13	10.013	674	676	679	rBV	1201250	1302361	29.65%	3.682%
14	10.802	742	745	748	rBV	2419236	2419949	55.09%	6.842%
15	11.499	804	806	809	rBV	1547281	1375903	31.32%	3.890%
16	12.676	907	909	911	rVB	267281	183532	4.18%	0.519%
17	13.088	942	945	947	rBV	4528496	4299317	97.88%	12.155%
18	13.477	977	979	980	rVB2	79436	54883	1.25%	0.155%
19	14.139	1034	1037	1039	rBV	997513	1139675	25.95%	3.222%
20	15.602	1162	1165	1168	rBV	583356	783796	17.84%	2.216%
21	16.688	1249	1260	1268	rBV4	34156	197496	4.50%	0.558%

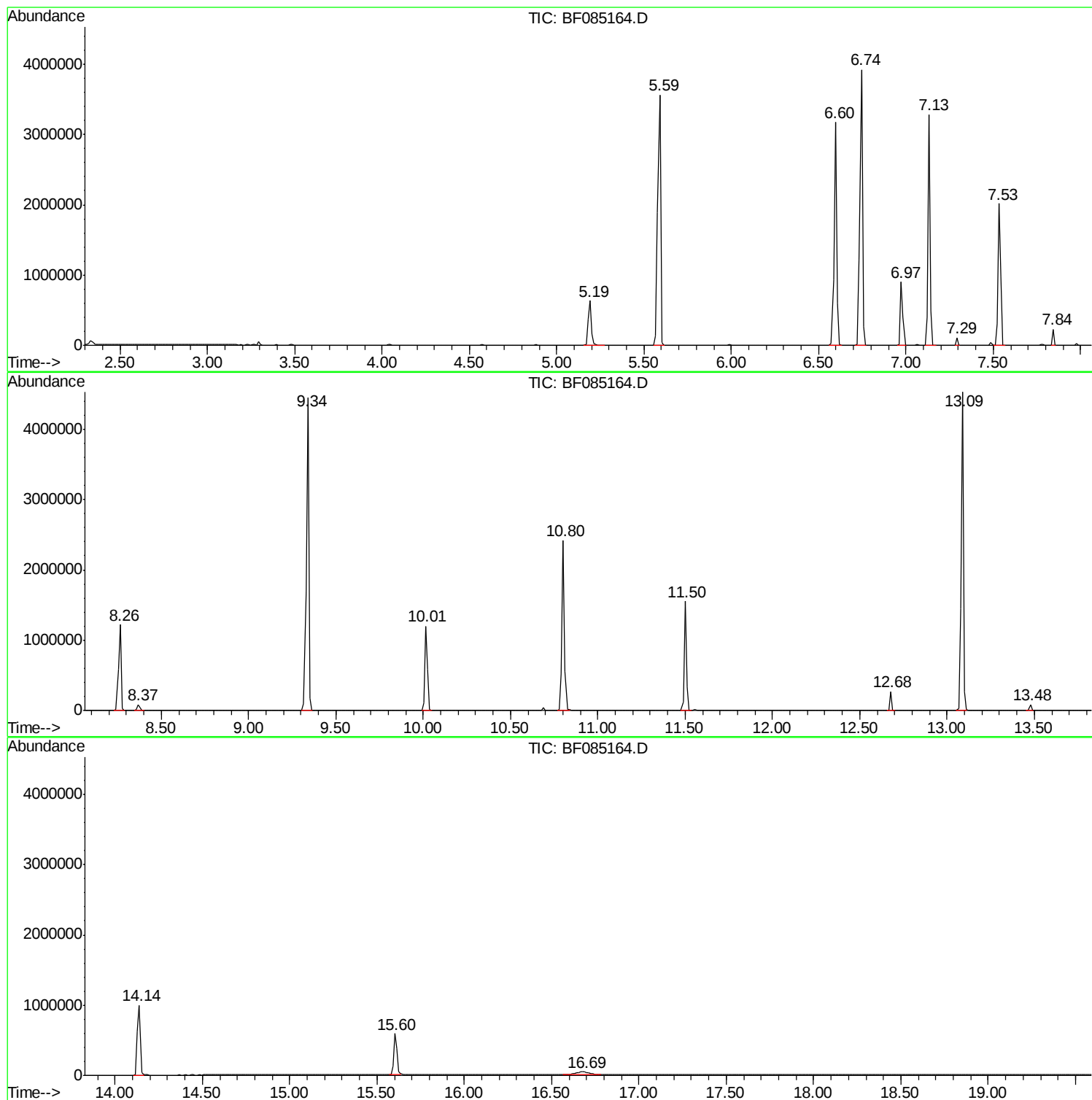
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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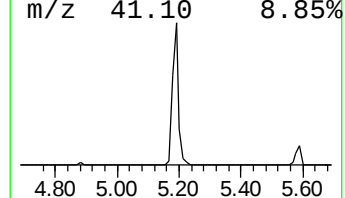
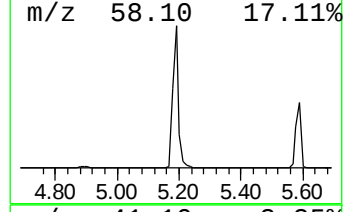
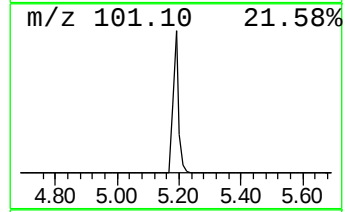
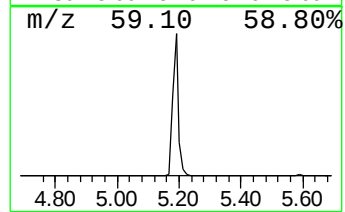
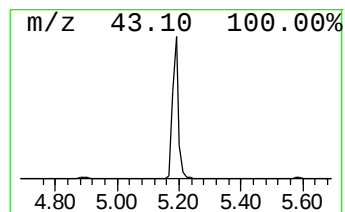
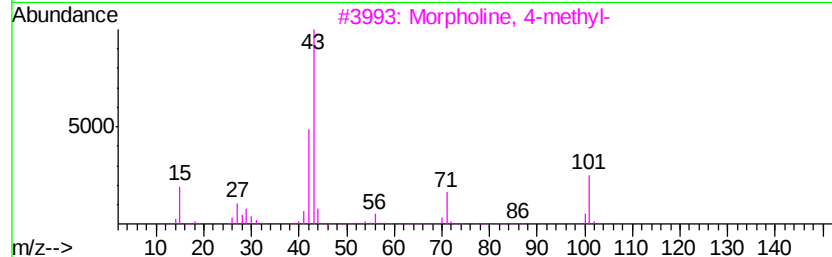
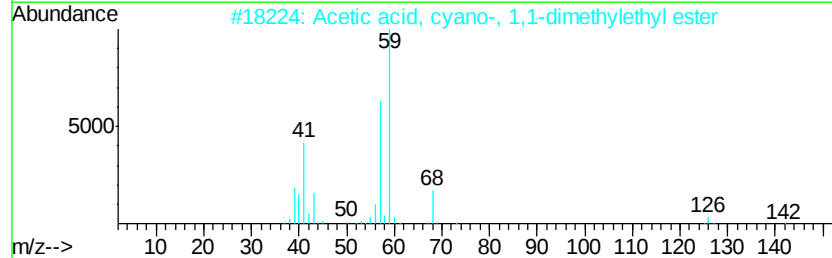
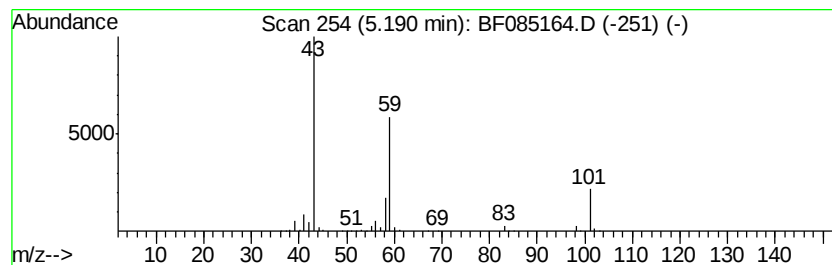
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	18.09 ng	820008	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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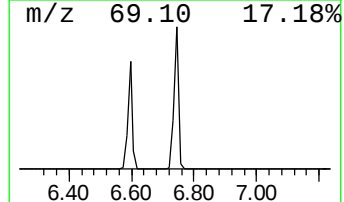
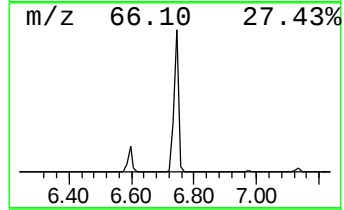
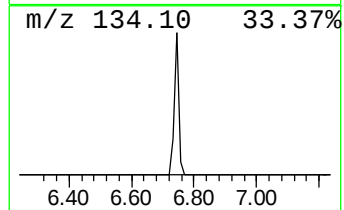
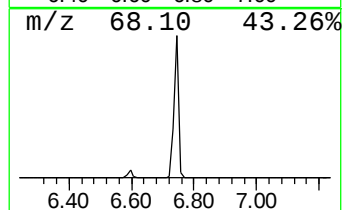
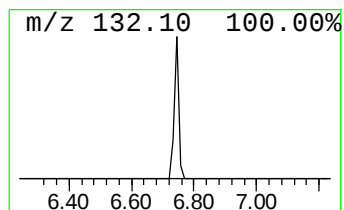
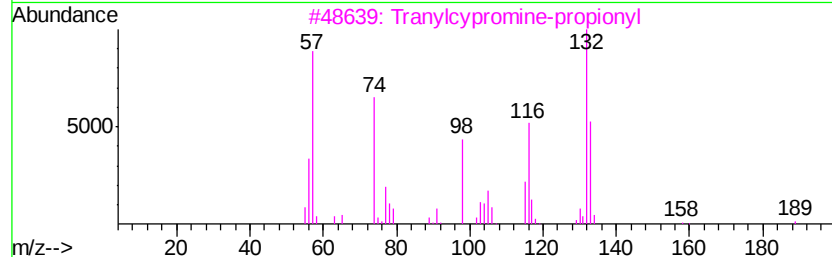
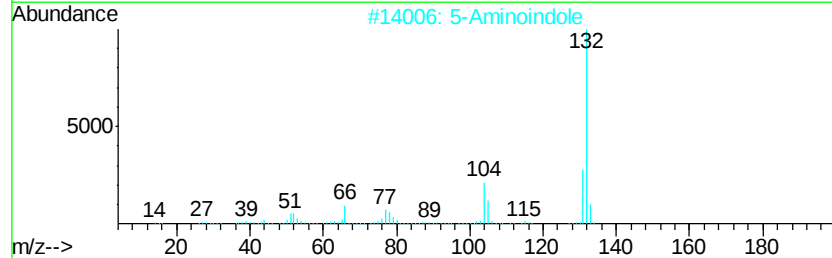
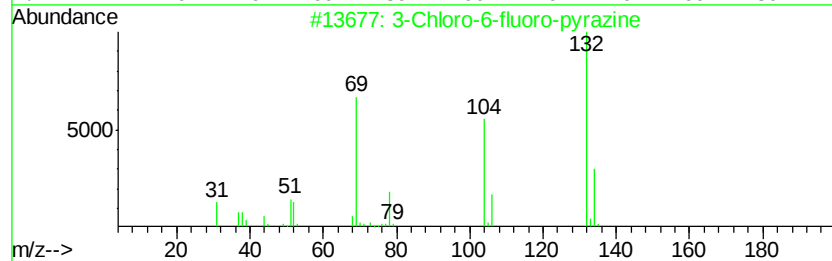
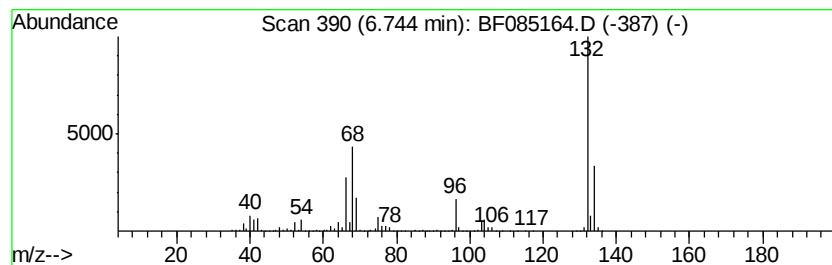
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	81.85 ng	3709930	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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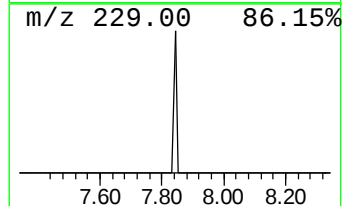
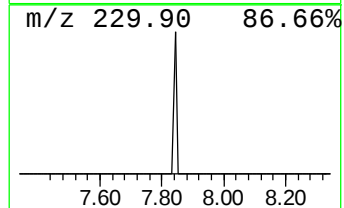
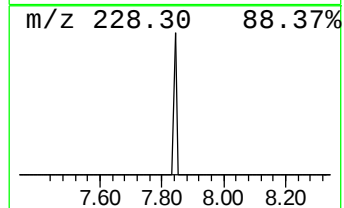
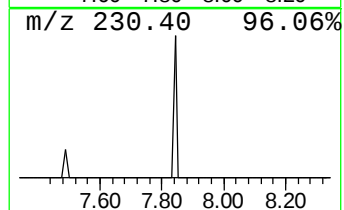
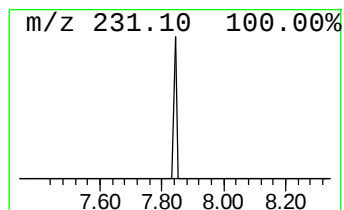
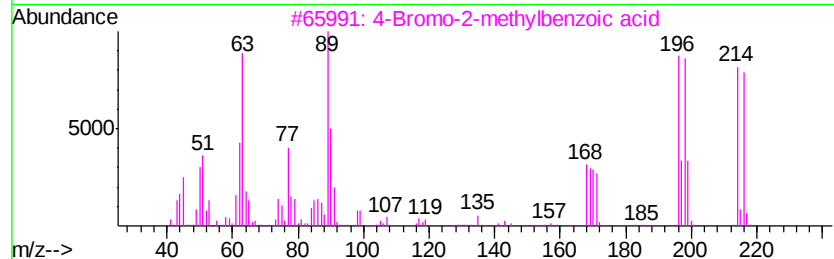
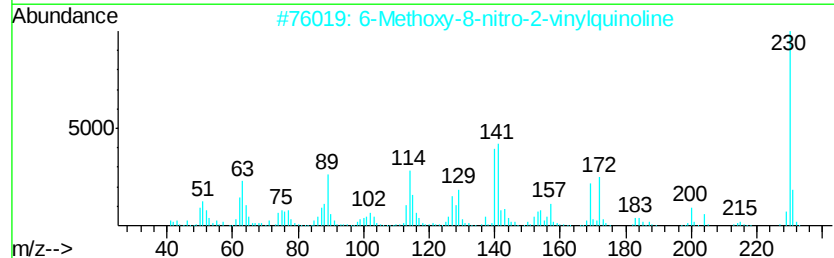
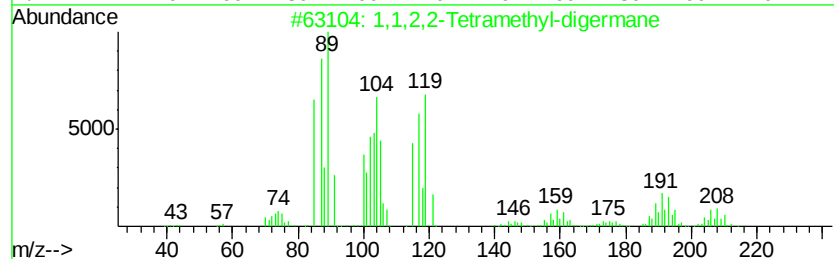
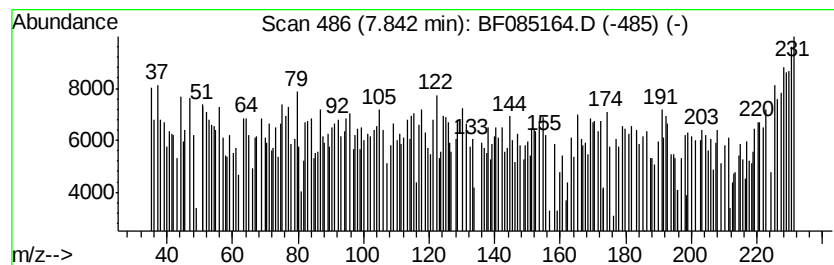
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Peak Number 4 1,1,2,2-Tetramethyl-digermene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.84	2.49 ng	155625	Napthalene-d8	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1,2,2-Tetramethyl-digermene	210	C4H14Ge2	1000296-51-6	81
2		6-Methoxy-8-nitro-2-vinylquinoline	230	C12H10N2O3	064992-64-9	62
3		4-Bromo-2-methylbenzoic acid	214	C8H7BrO2	068837-59-2	60
4		Furoxan, 4-nitro-3-phenyl-, 2-oxide	207	C8H5N3O4	049558-03-4	45
5		2,3-Dichloro-6-methylquinoxaline	212	C9H6Cl2N2	039267-05-5	41



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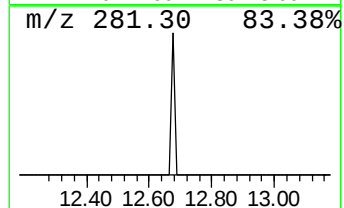
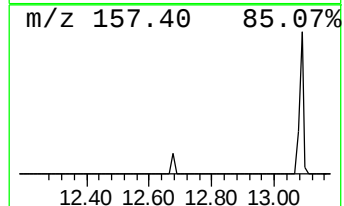
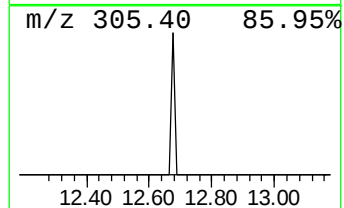
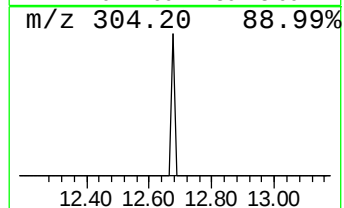
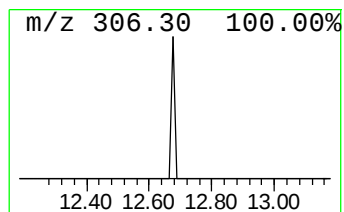
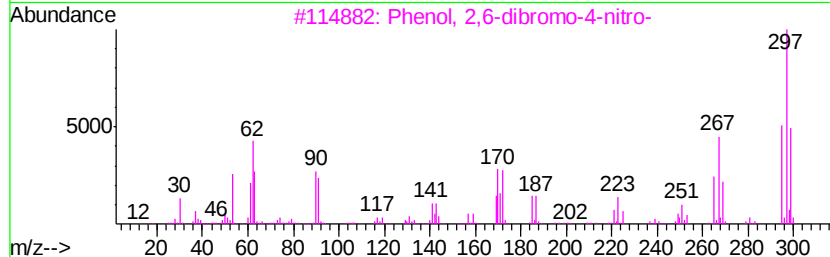
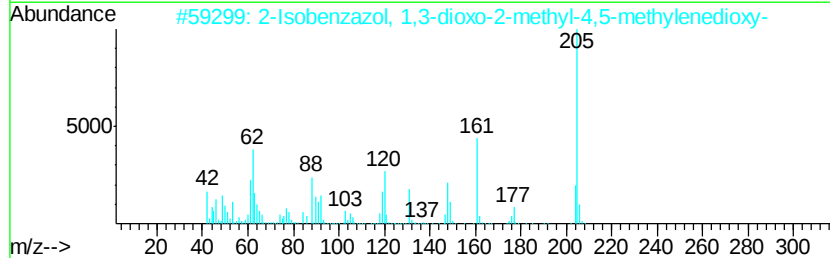
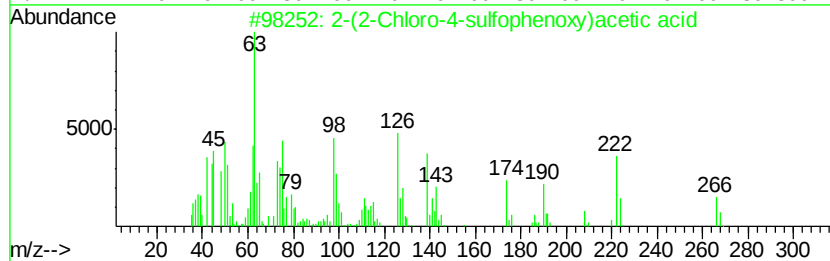
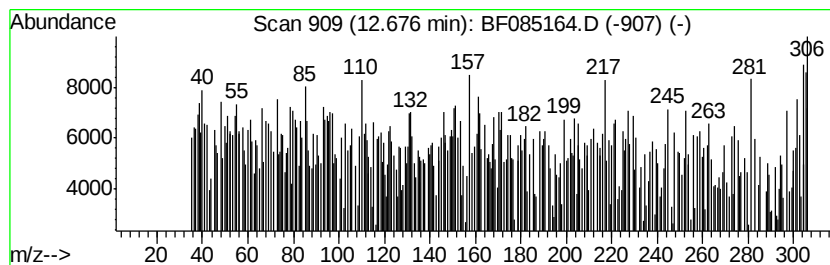
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 2-(2-Chloro-4-sulfophenoxy)... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	2.67 ng	183532	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-(2-Chloro-4-sulfophenoxy)aceti...	266	C8H7ClO6S	303096-94-8	56
2		2-Isobenzazol, 1,3-dioxo-2-methy...	205	C10H7N04	1000111-66-6	56
3		Phenol, 2,6-dibromo-4-nitro-	295	C6H3Br2NO3	000099-28-5	53
4		Pyridine 1-oxide, 3,5-dibromo-	251	C5H3Br2NO	002402-99-5	50
5		1,9-Dioxa-4,6,12,14-tetraazacycl...	292	C10H20N4O2S2	074804-39-0	46



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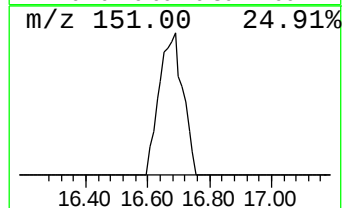
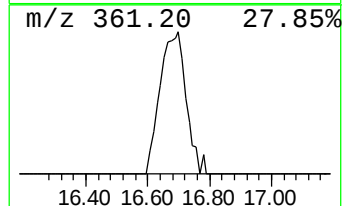
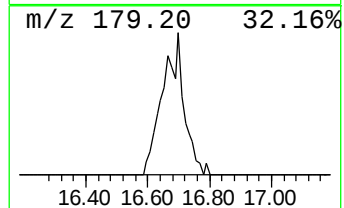
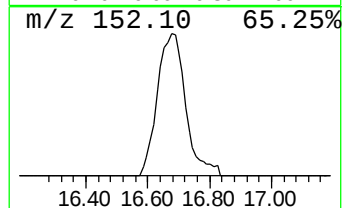
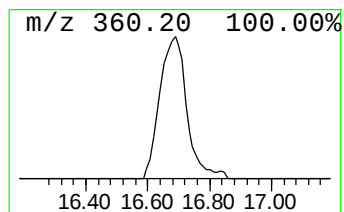
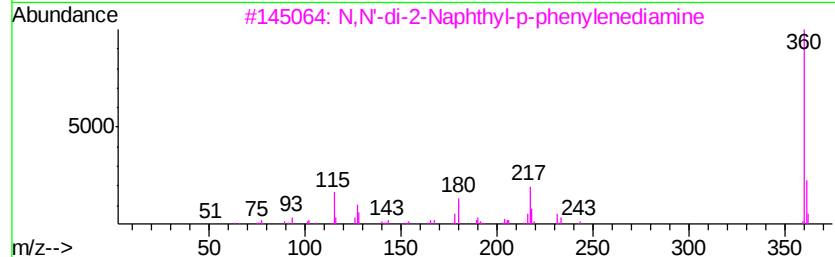
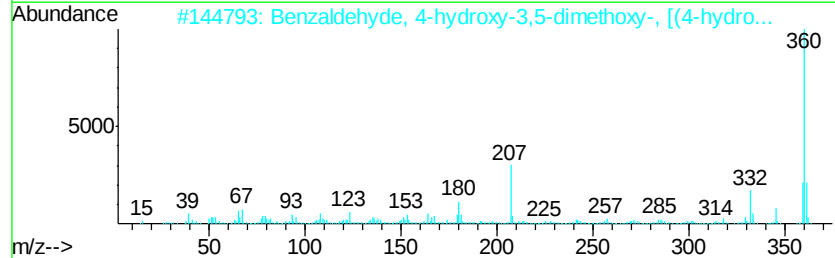
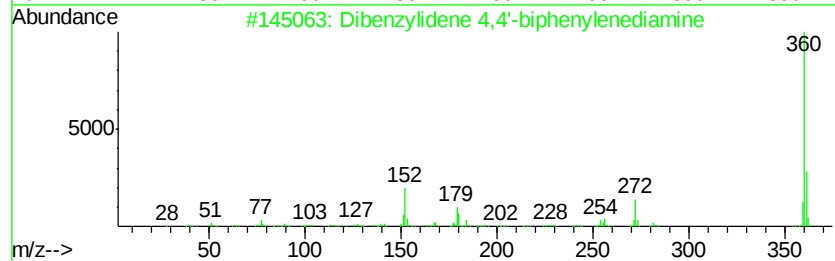
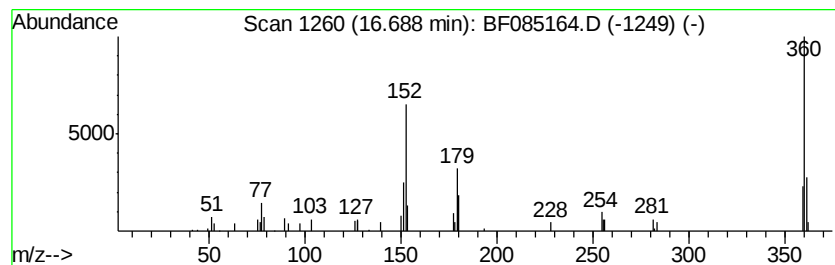
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Peak Number 6 Dibenzylidene 4,4'-biphenyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	5.04 ng	197496	Perylene-d12	15.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	93
2		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	43
3		N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	43
4		1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	43
5		1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.19	18.1	ng	820008	1	6.97	906483	20.0
unknown6.74	6.74	81.8	ng	3709930	1	6.97	906483	20.0
1,1,2,2-Tetrameth...	7.84	2.5	ng	155625	2	8.26	1251370	20.0
2-(2-Chloro-4-sul...	12.68	2.7	ng	183532	4	11.50	1375900	20.0
Dibenzylidene 4,4...	16.69	5.0	ng	197496	6	15.60	783796	20.0