

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022317\
 Data File : BF093099.D
 Acq On : 23 Feb 2017 10:12
 Operator : SJ/MA
 Sample : PB97103BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB97103BL

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-BF013017.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	3.767	144	147	155	rVB	69985	116761	2.53%	0.318%
2	5.013	253	256	272	rVB	1111232	1686176	36.52%	4.596%
3	5.436	291	293	296	rBV	3202698	3811797	82.56%	10.391%
4	6.476	381	384	387	rBV	3105931	3685716	79.83%	10.047%
5	6.613	393	396	398	rBV	3193550	4090725	88.61%	11.151%
6	6.842	414	416	418	rBV	924303	898572	19.46%	2.449%
7	7.002	427	430	432	rBV	2419454	3168441	68.63%	8.637%
8	7.413	463	466	468	rBV	2464956	2726602	59.06%	7.433%
9	8.133	526	529	531	rBV	822175	1161390	25.16%	3.166%
10	9.208	619	623	625	rBV	3878538	4616789	100.00%	12.585%
11	9.882	679	682	684	rBV	971680	1275917	27.64%	3.478%
12	10.659	748	750	753	rBV2	1604481	2275309	49.28%	6.202%
13	11.356	809	811	814	rBV	1510214	1280152	27.73%	3.490%
14	12.945	947	950	952	rBV	3637361	3928180	85.08%	10.708%
15	13.985	1039	1041	1044	rBV	723955	891515	19.31%	2.430%
16	14.145	1047	1055	1063	rVV2	18244	79818	1.73%	0.218%
17	15.414	1164	1166	1173	rVB	564190	718270	15.56%	1.958%
18	15.608	1175	1183	1192	rVV4	21776	109359	2.37%	0.298%
19	15.963	1208	1214	1221	rBV3	25352	96829	2.10%	0.264%
20	19.197	1490	1497	1507	rVB10	11063	65633	1.42%	0.179%

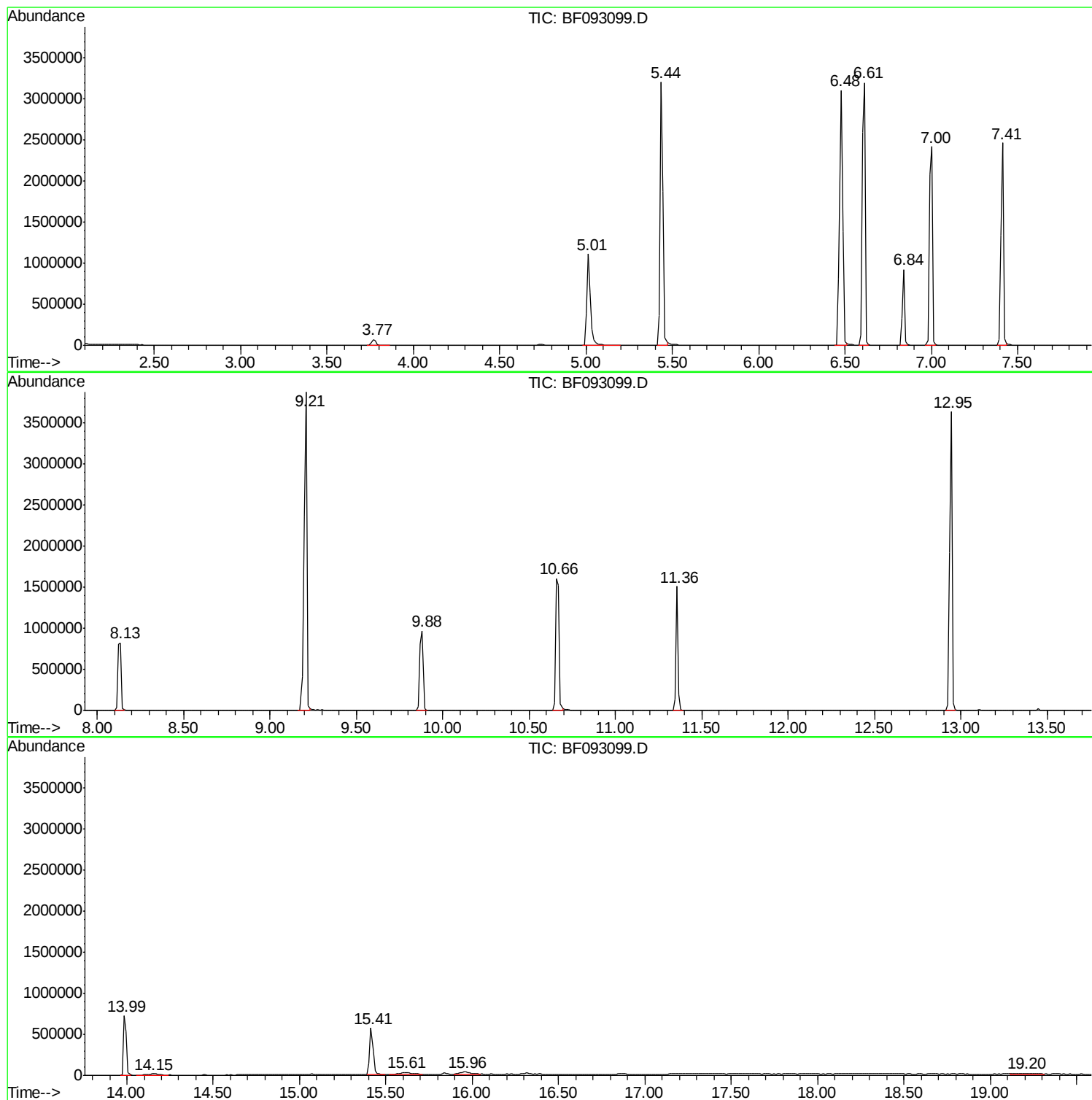
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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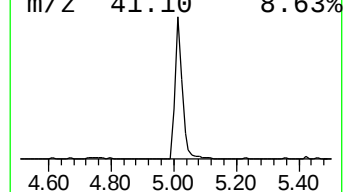
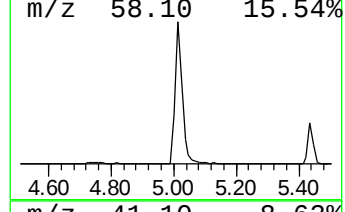
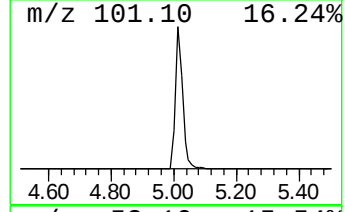
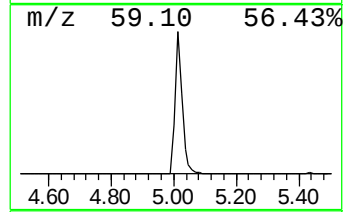
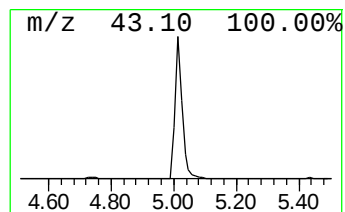
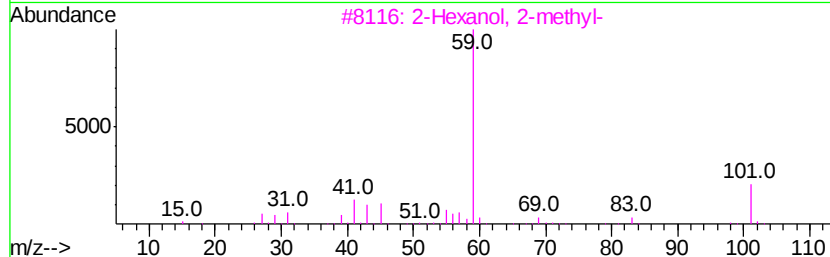
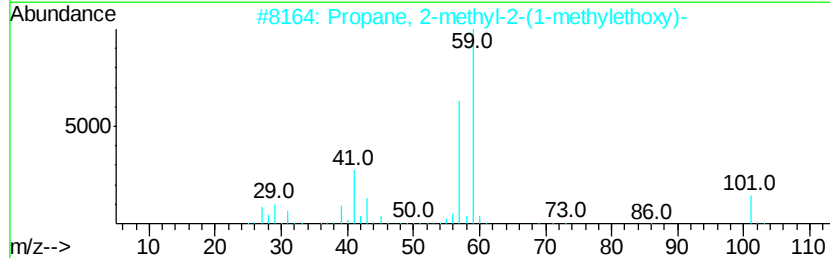
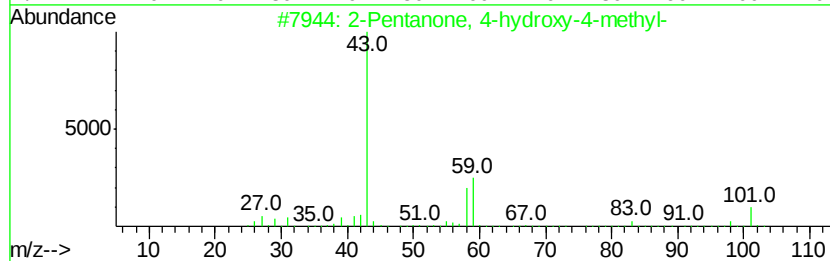
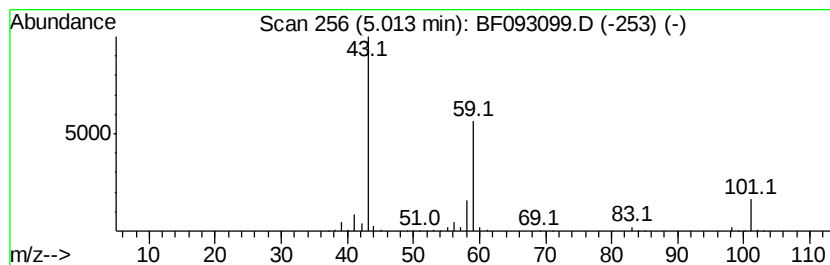
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	37.53 ng	1686180	1,4-Dichlorobenzene-d4	6.84

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



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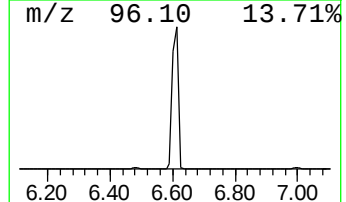
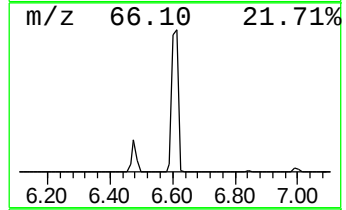
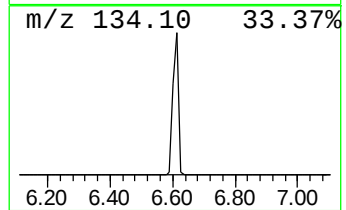
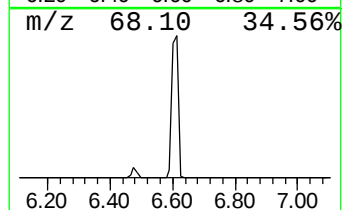
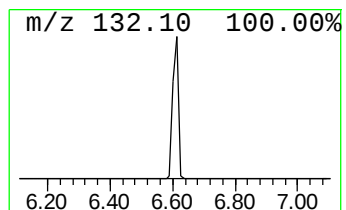
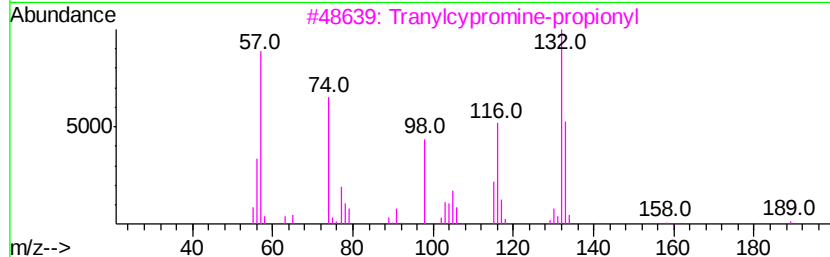
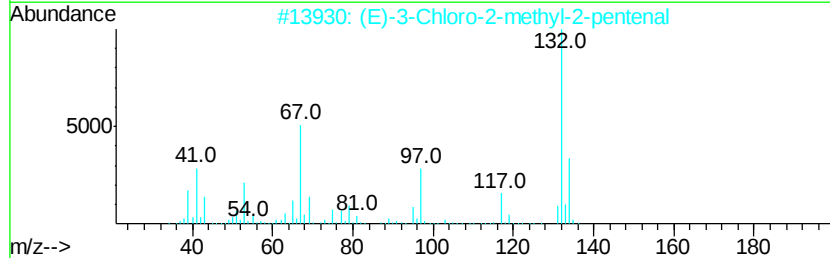
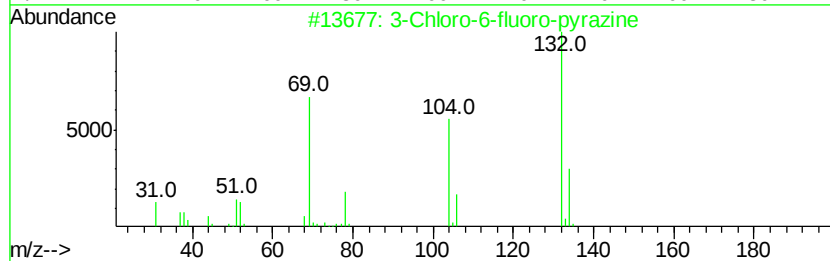
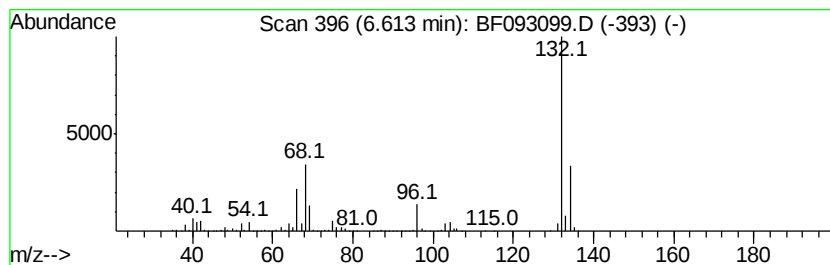
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Peak Number 3 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	91.05 ng	4090730	1,4-Dichlorobenzene-d4	6.84

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	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	16
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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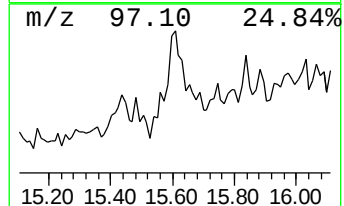
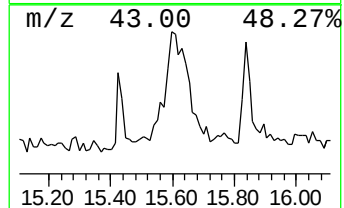
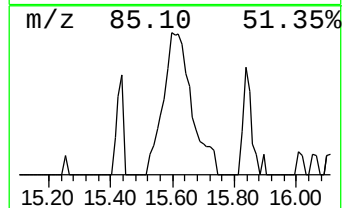
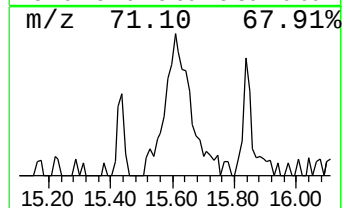
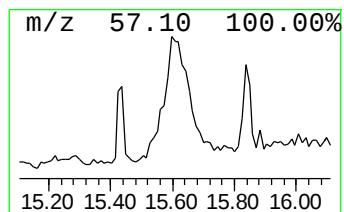
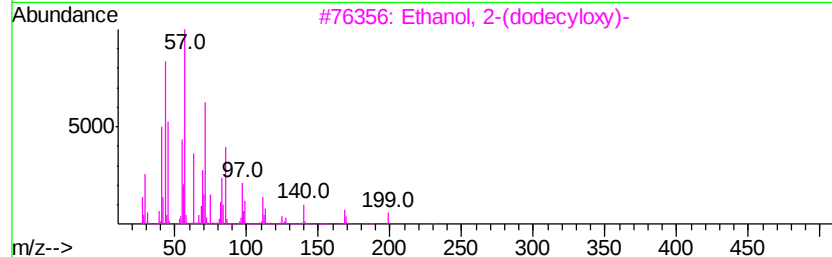
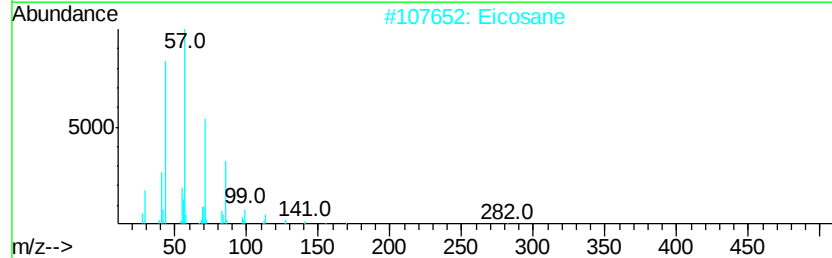
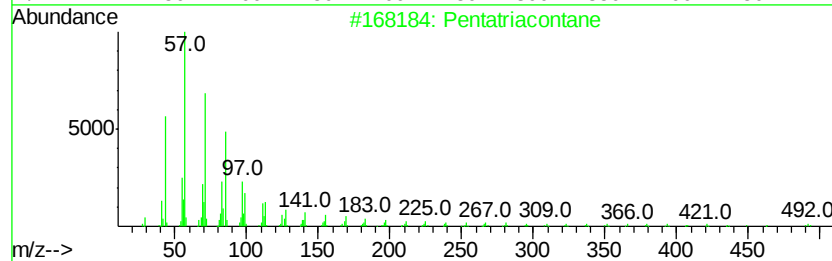
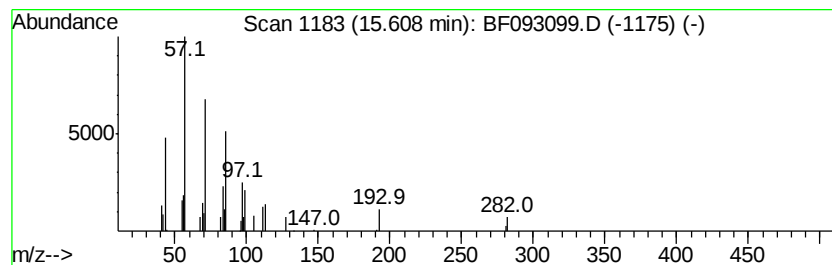
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Peak Number 5 Pentatriacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	3.05 ng	109359	Perylene-d12	15.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentatriacontane	493	C35H72	000630-07-9	86
2		Eicosane	282	C20H42	000112-95-8	76
3		Ethanol, 2-(dodecyl-oxo)-	230	C14H30O2	004536-30-5	72
4		Tetratriacontane	479	C34H70	014167-59-0	64
5		Heneicosane	296	C21H44	000629-94-7	58



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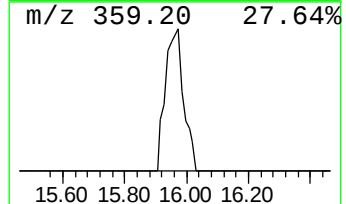
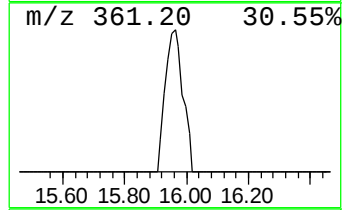
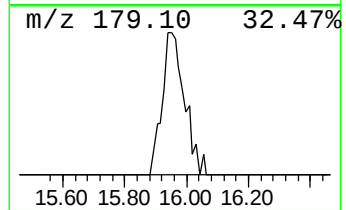
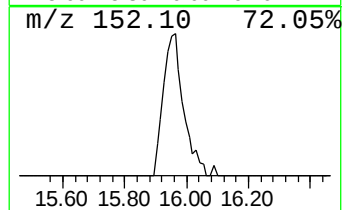
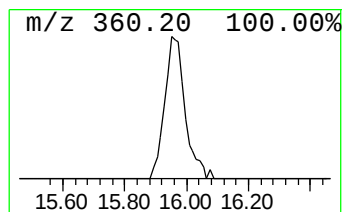
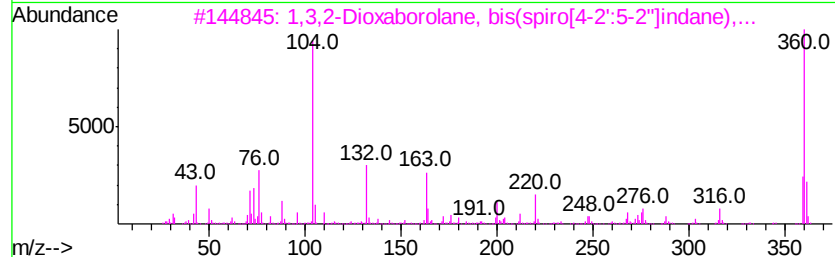
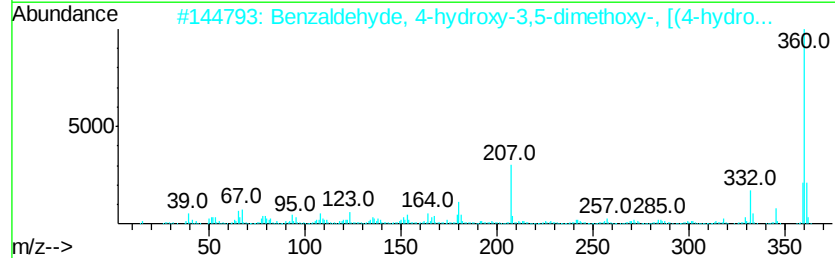
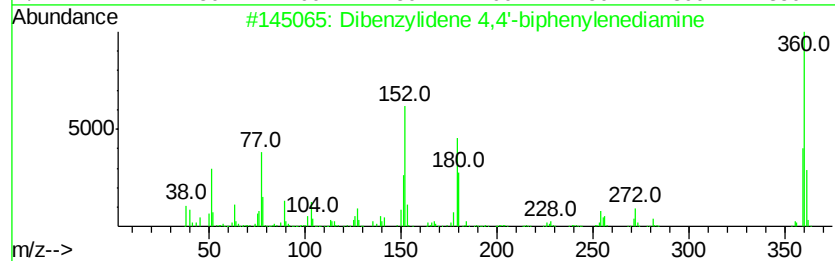
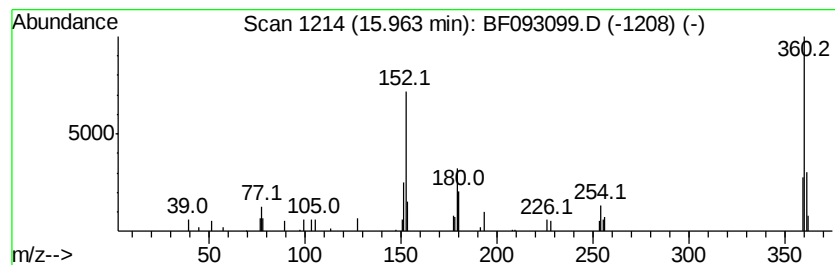
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Peak Number 6 Dibenzylidene 4,4'-biphenyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	2.70 ng	96829	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	95
2		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	47
3		1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	38
4		N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	32
5		[2-(4-Methoxy-phenyl)-2H-benzo[g...	360	C22H20N2O3	1000188-59-8	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	37.5	ng	1686180	1	6.84	898572	20.0
unknown6.61	6.61	91.0	ng	4090730	1	6.84	898572	20.0
Pentatriacontane	15.61	3.0	ng	109359	6	15.41	718270	20.0
Dibenzylidene 4,4...	15.96	2.7	ng	96829	6	15.41	718270	20.0