

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061121\
 Data File : BF124258.D
 Acq On : 11 Jun 2021 13:33
 Operator : JU/CG
 Sample : PB136924BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB136924BL

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124258.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	10	15	20	rVB	38932	49783	2.48%	0.458%
2	2.281	27	33	37	rBB	28156	35286	1.76%	0.324%
3	5.087	506	510	517	rBB2	34307	51269	2.55%	0.471%
4	5.481	573	577	580	rBV	1487675	1317628	65.61%	12.115%
5	6.487	743	748	751	rBV	1300629	1277213	63.59%	11.743%
6	6.840	805	808	812	rBB	348721	264397	13.16%	2.431%
7	7.404	899	904	907	rBV	849108	879184	43.78%	8.084%
8	8.122	1022	1026	1030	rBV	379902	336381	16.75%	3.093%
9	9.204	1204	1210	1213	rBV	2113170	1732049	86.24%	15.925%
10	9.880	1320	1325	1329	rBV	529059	427144	21.27%	3.927%
11	10.675	1455	1460	1463	rBV	1446408	1247290	62.10%	11.468%
12	11.369	1574	1578	1582	rBV	569042	454154	22.61%	4.176%
13	12.963	1843	1849	1852	rBV	2164847	2008405	100.00%	18.466%
14	13.874	2001	2004	2008	rVB	28437	30540	1.52%	0.281%
15	14.016	2024	2028	2031	rVB	423547	363005	18.07%	3.338%
16	15.492	2274	2279	2285	rVB	234678	297789	14.83%	2.738%
17	16.998	2525	2535	2541	rBV7	32060	104544	5.21%	0.961%

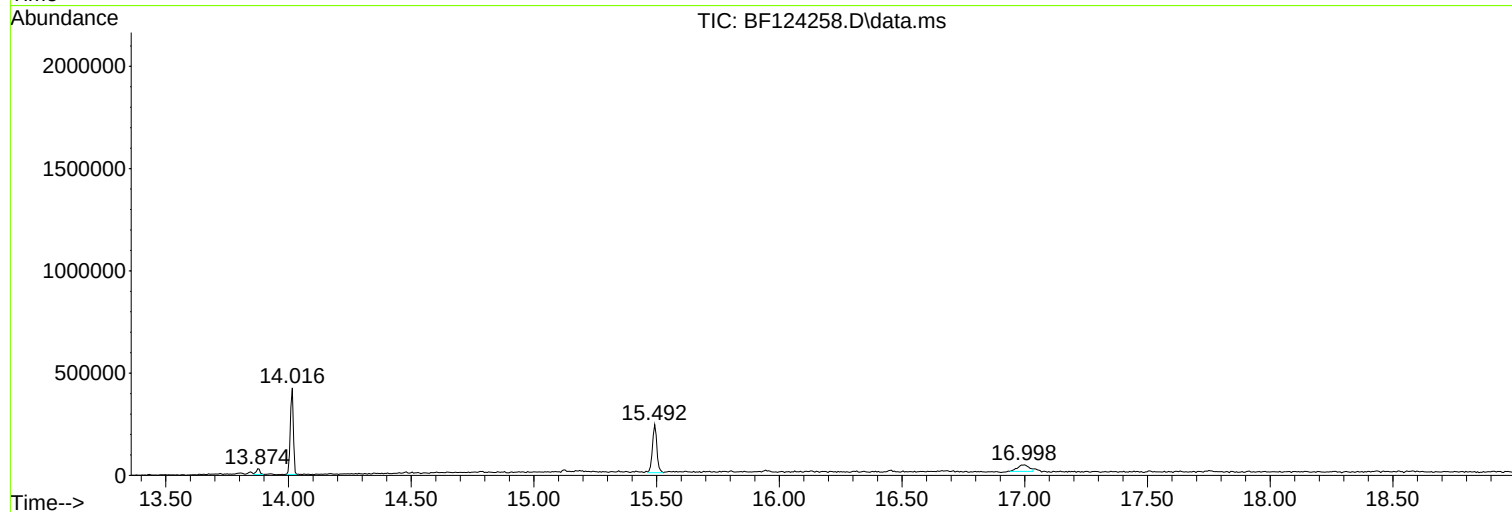
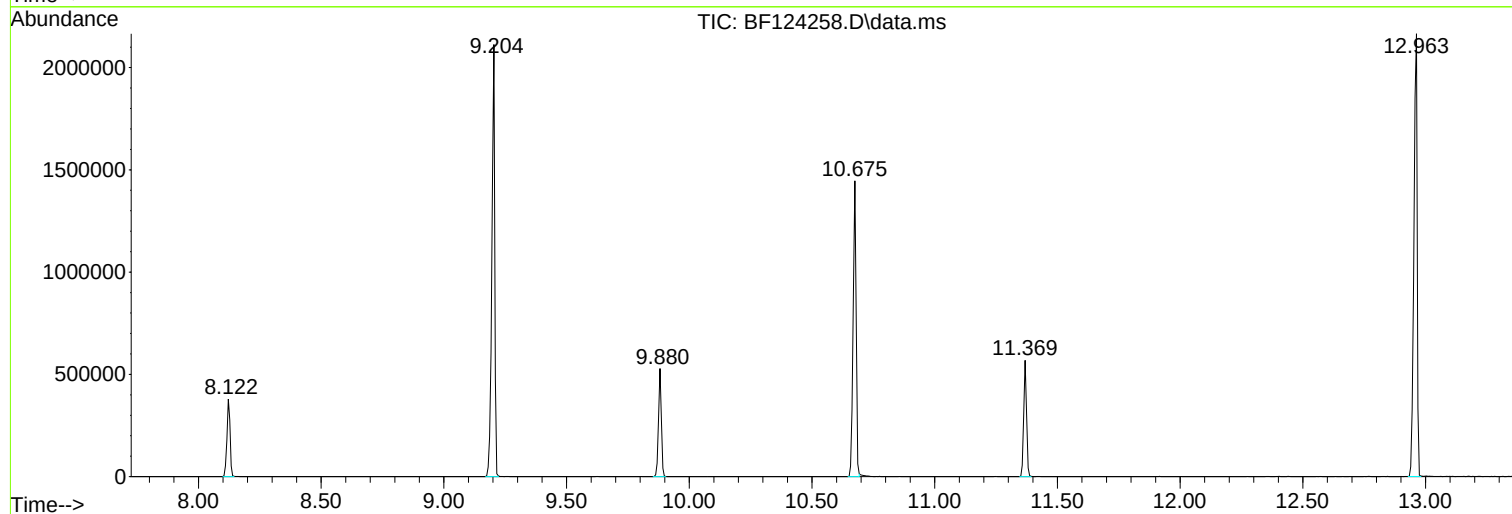
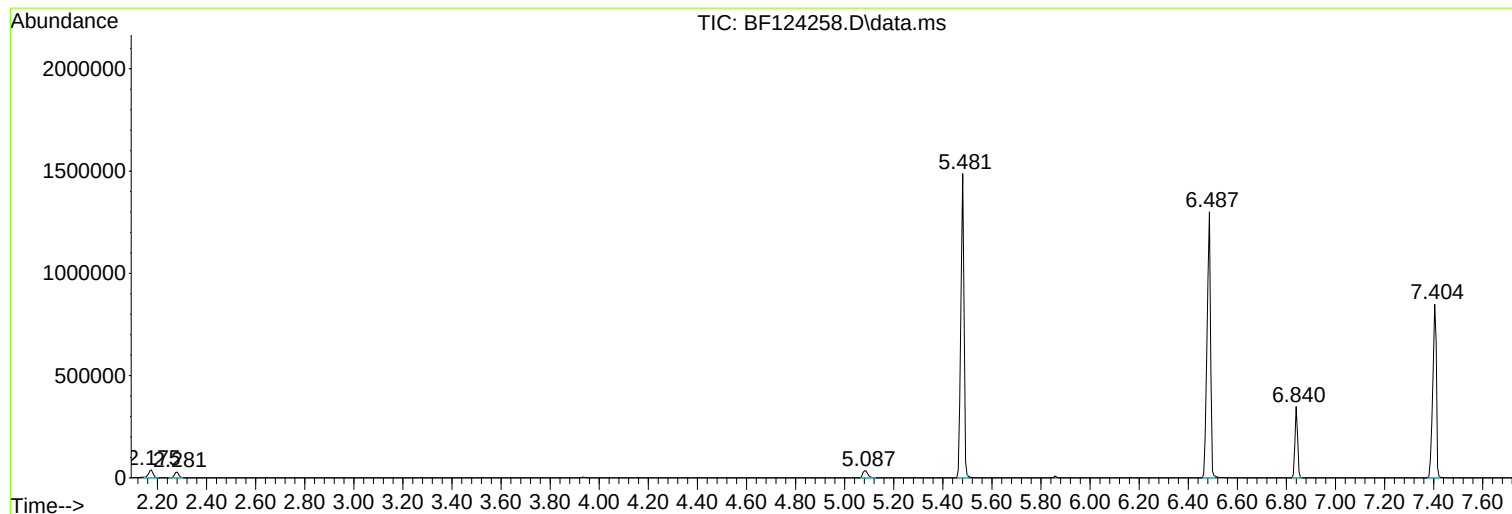
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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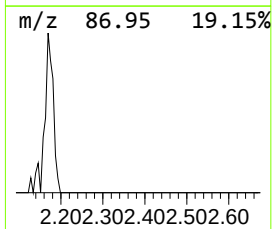
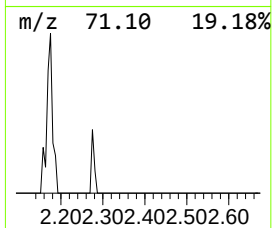
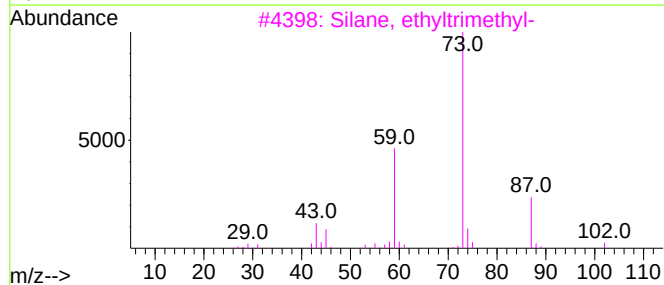
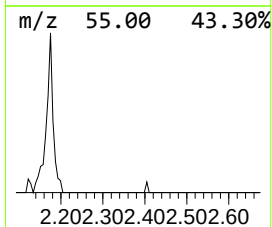
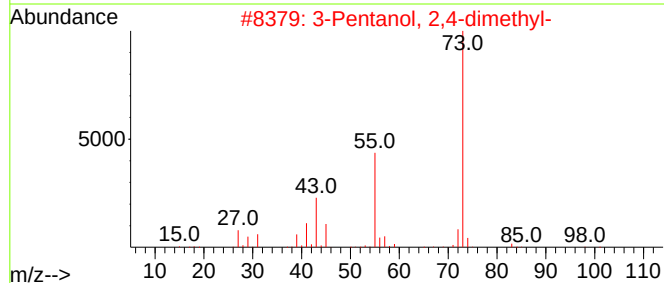
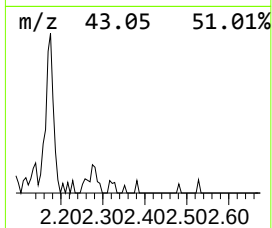
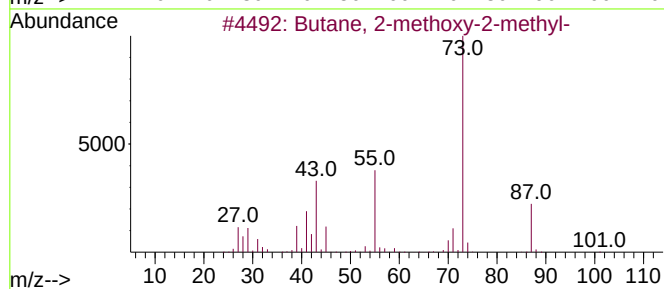
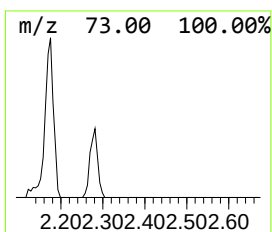
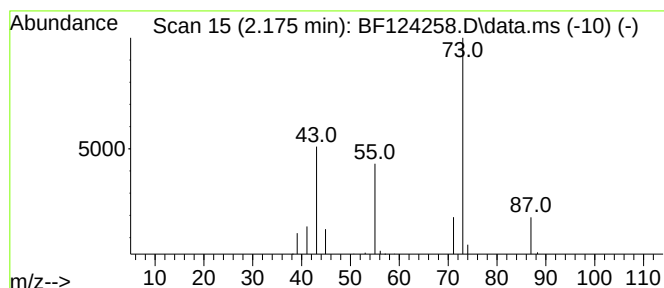
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	3.77 ng	49783	1,4-Dichlorobenzene-d4	6.840

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	25
4		1-Propene-1-thiol	74	C3H6S	000925-89-3	12
5		1-Pentanamine	87	C5H13N	000110-58-7	9



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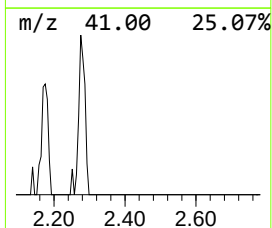
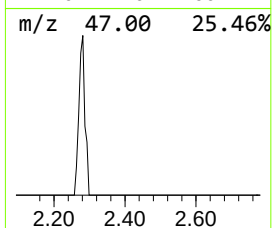
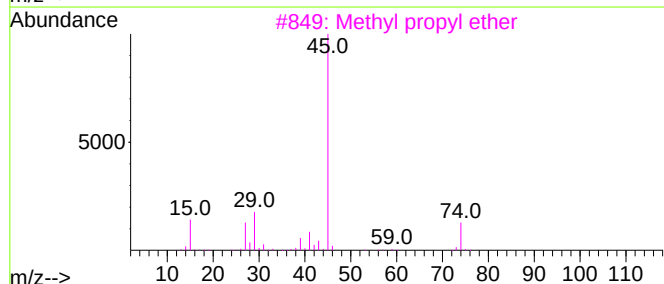
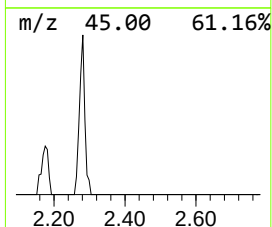
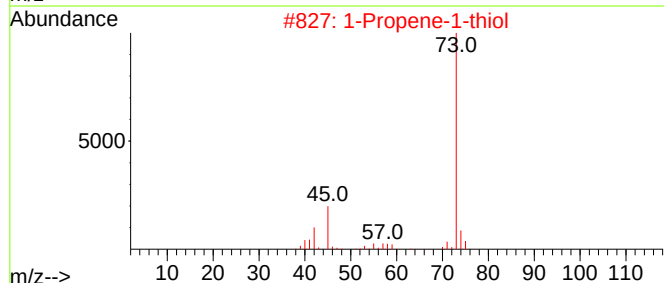
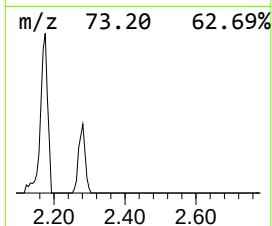
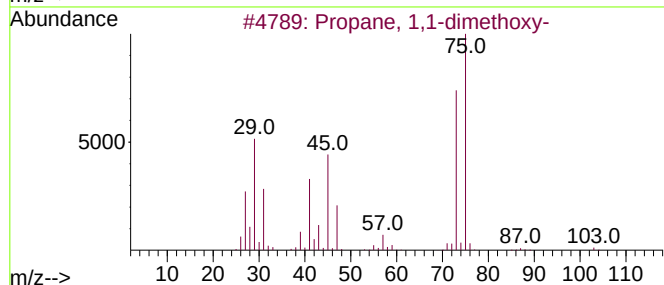
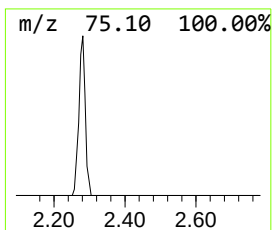
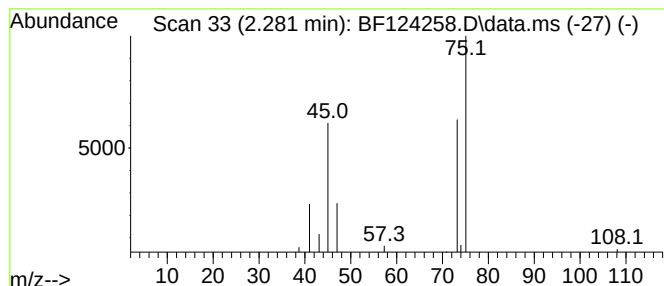
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown2.281 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.281	2.67 ng	35286	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	9
2			1-Propene-1-thiol	74	C3H6S	000925-89-3	4
3			Methyl propyl ether	74	C4H10O	000557-17-5	4
4			Propane, 2-chloro-1-methoxy-	108	C4H9ClO	005390-71-6	4
5			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	4



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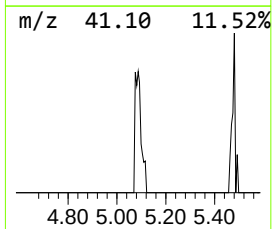
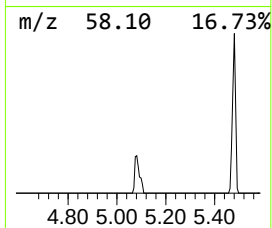
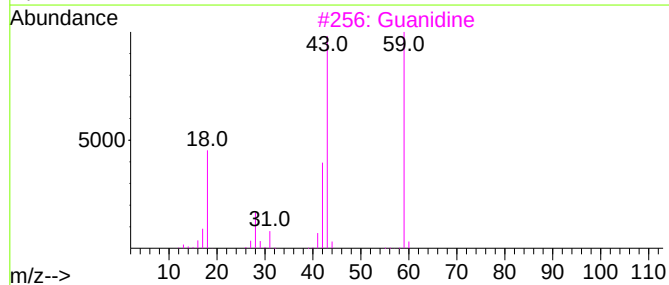
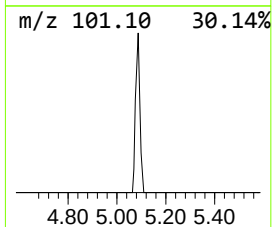
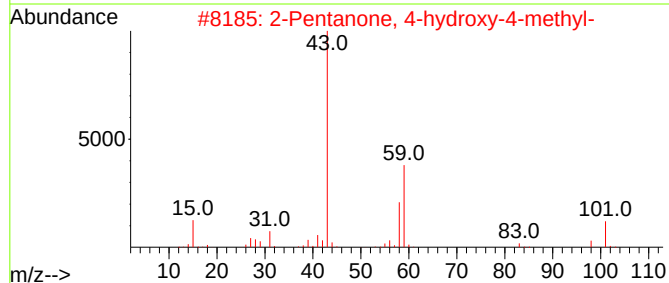
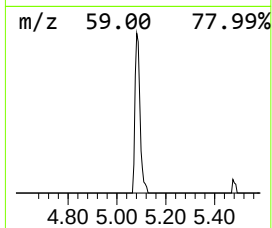
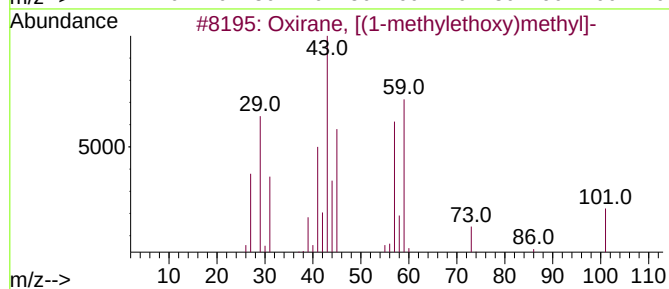
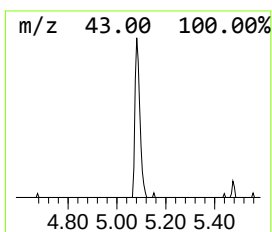
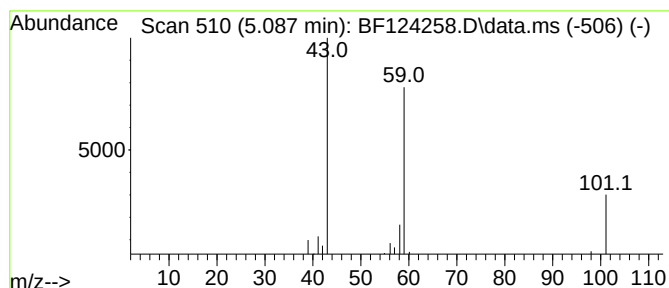
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Peak Number 3 unknown5.087 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	3.88 ng	51269	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	40
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	36
3			Guanidine	59	CH5N3	000113-00-8	9
4			1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	9
5			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9



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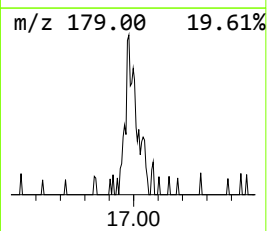
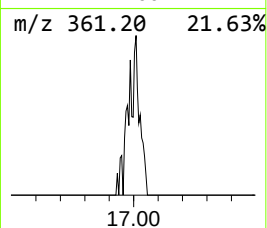
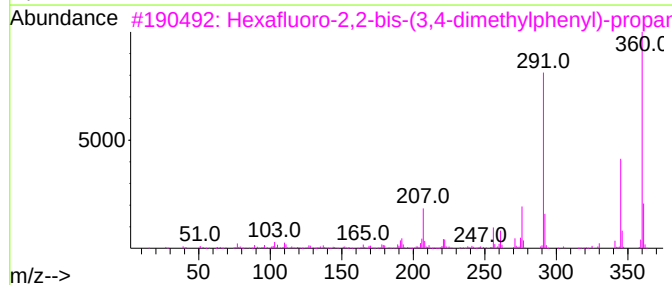
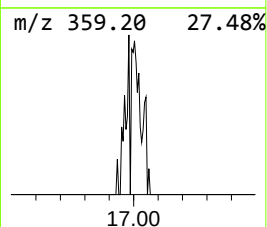
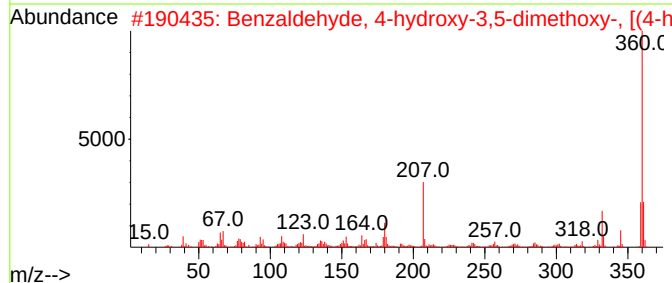
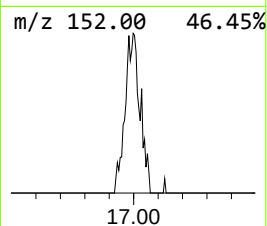
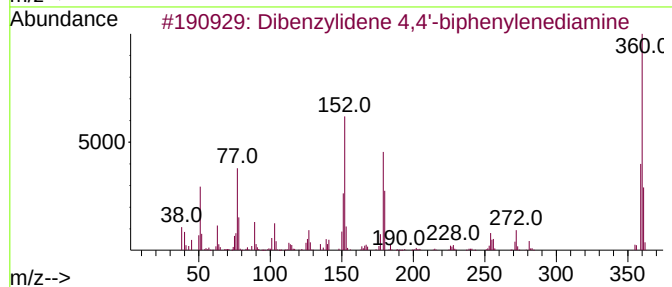
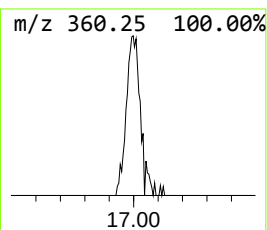
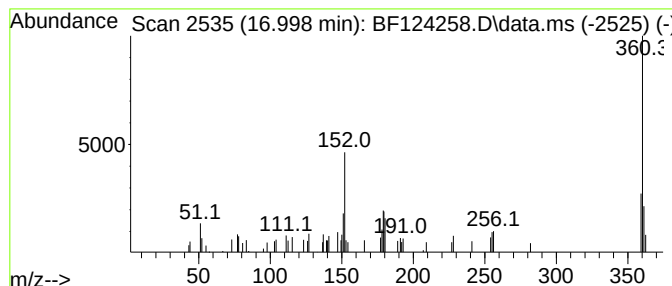
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Dibenzylidene 4,4'-biphenyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.998	7.02 ng	104544	Perylene-d12	15.492	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	86
2	Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	38
3	Hexafluoro-2,2-bis-(3,4-dimethyl...	360	C19H18F6	065294-20-4	38
4	N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	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
Butane, 2-metho...	2.175	3.8	ng	49783	1	6.840	264397	20.0
unknown2.281	2.281	2.7	ng	35286	1	6.840	264397	20.0
unknown5.087	5.087	3.9	ng	51269	1	6.840	264397	20.0
Dibenzylidene 4...	16.998	7.0	ng	104544	6	15.492	297789	20.0