

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
 Data File : BF134123.D
 Acq On : 07 Jul 2023 06:54
 Operator : CG\JU
 Sample : PB153945BL
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB153945BL

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134123.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	16	20	30	rVB	66862	96803	2.36%	0.391%
2	2.316	35	39	47	rVB	49120	66779	1.63%	0.269%
3	5.105	508	513	524	rBV	161282	242219	5.90%	0.977%
4	5.487	573	578	581	rBV	3196748	3257788	79.39%	13.147%
5	6.481	742	747	750	rBV	2878370	3302111	80.47%	13.326%
6	6.846	805	809	822	rBV	723898	660731	16.10%	2.666%
7	7.410	899	905	908	rBV	2297413	2148672	52.36%	8.671%
8	8.122	1022	1026	1039	rBV	1029291	851353	20.75%	3.436%
9	9.204	1204	1210	1213	rBV	4487271	3880883	94.57%	15.661%
10	9.881	1321	1325	1337	rBV	1156138	946682	23.07%	3.820%
11	10.675	1456	1460	1476	rBV	2672029	2678907	65.28%	10.811%
12	11.375	1575	1579	1597	rBV	1155602	1016839	24.78%	4.103%
13	12.975	1846	1851	1854	rBV	4139061	4103666	100.00%	16.560%
14	14.033	2027	2031	2043	rBV	838284	799547	19.48%	3.227%
15	15.539	2281	2287	2299	rBV	448889	658735	16.05%	2.658%
16	17.521	2612	2624	2625	rBV4	28752	68504	1.67%	0.276%

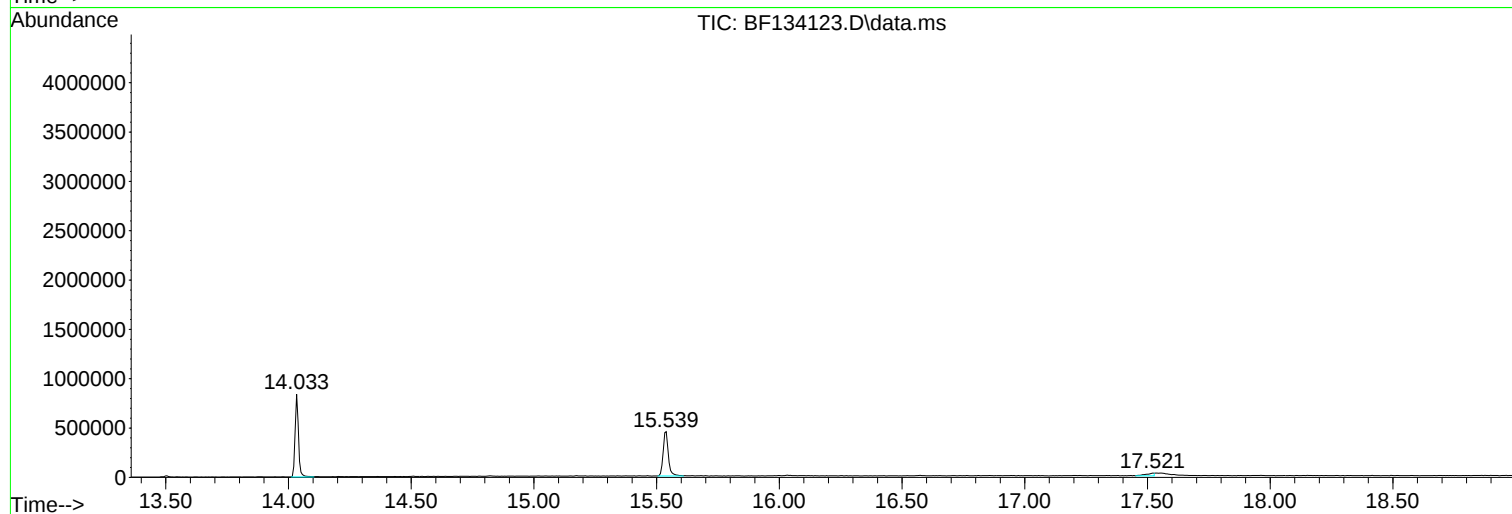
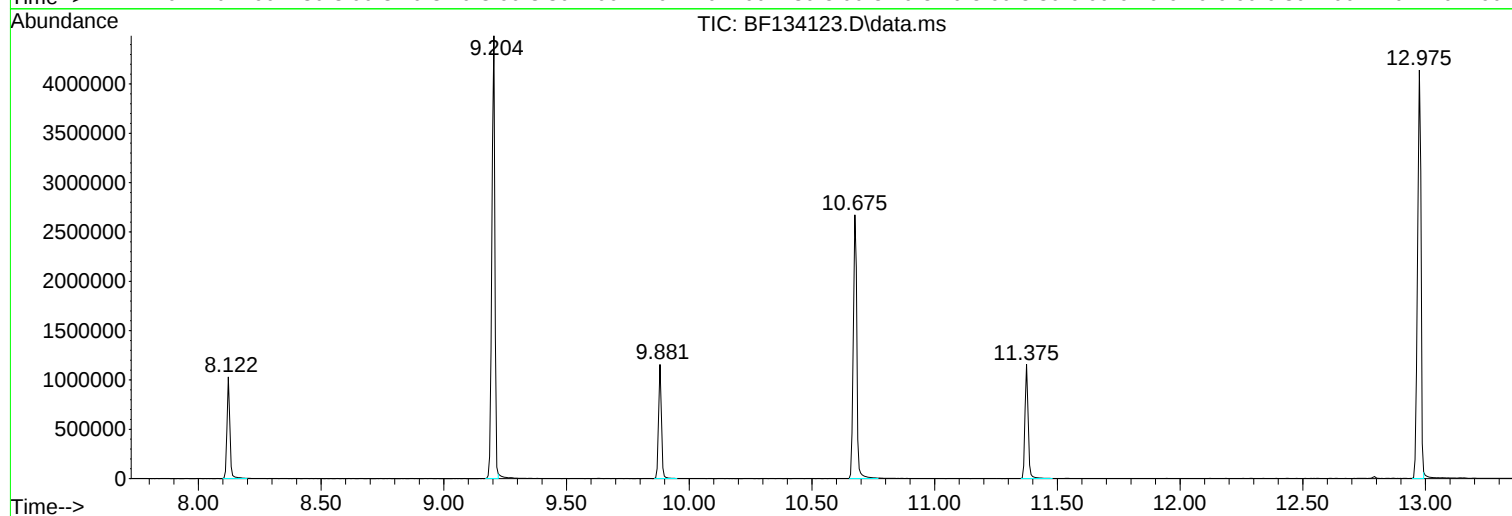
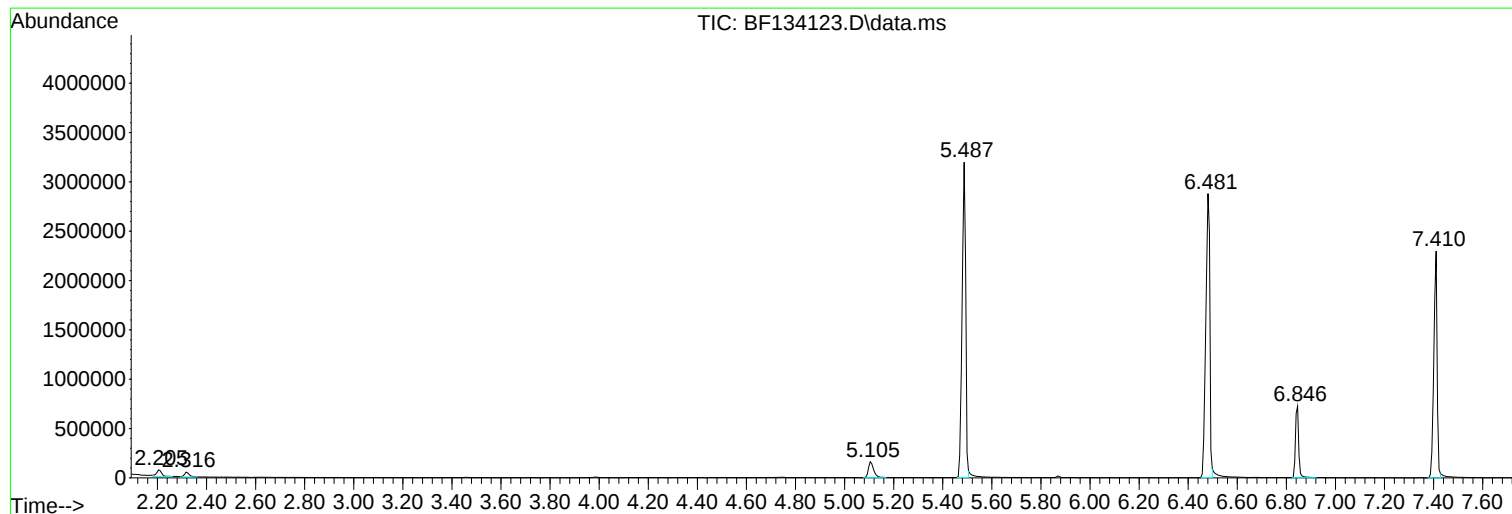
Sum of corrected areas: 24780219

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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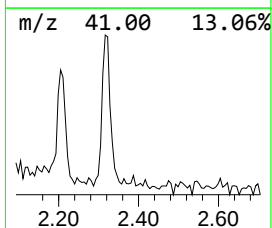
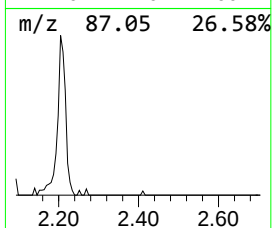
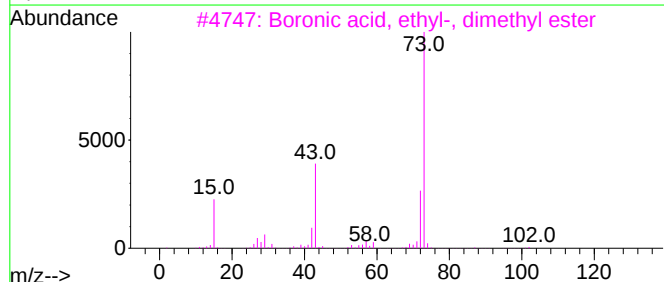
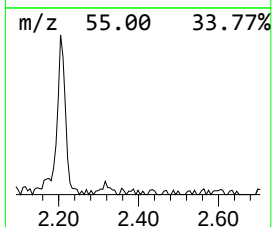
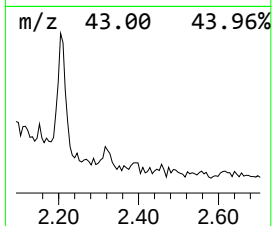
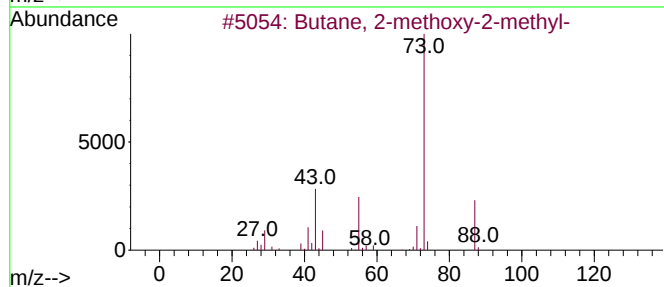
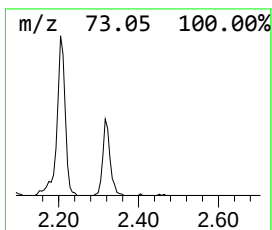
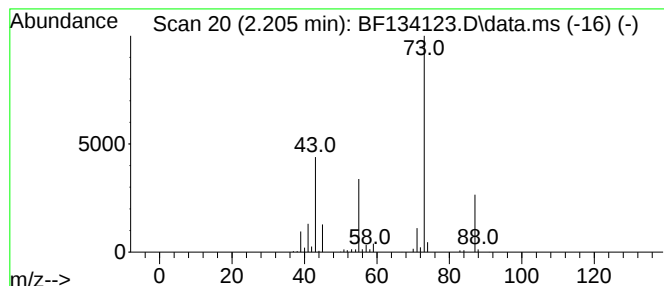
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.205	2.93 ng	96803	1,4-Dichlorobenzene-d4	6.846

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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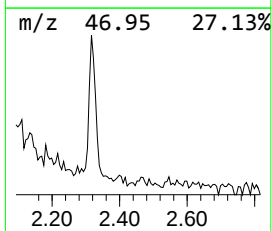
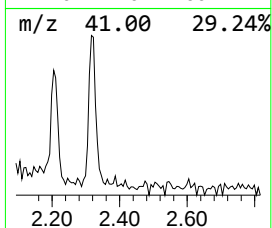
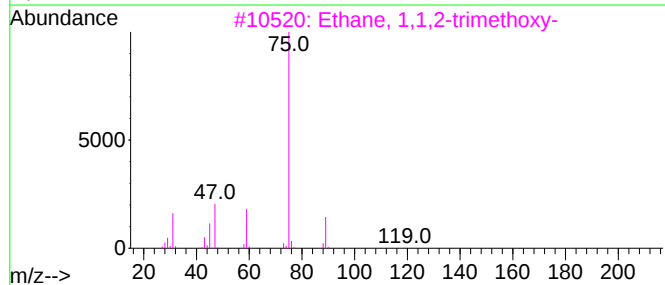
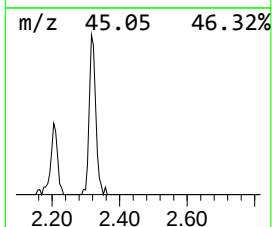
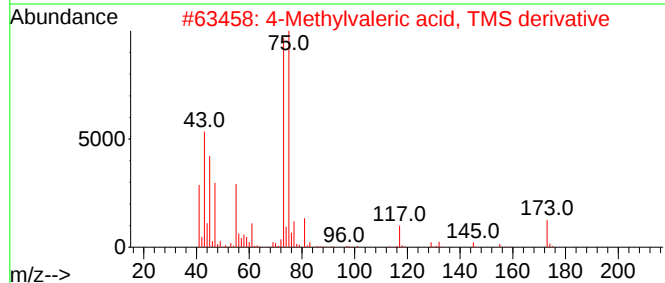
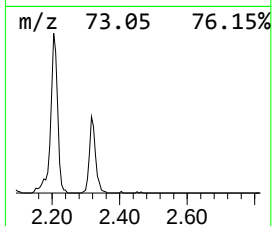
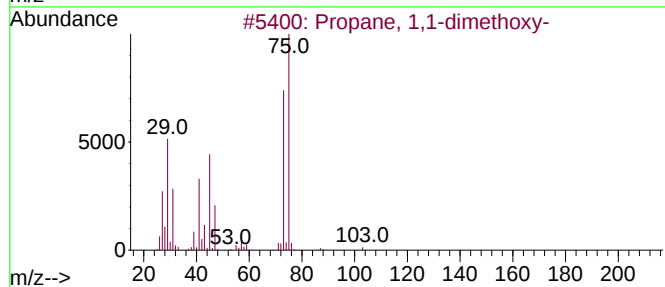
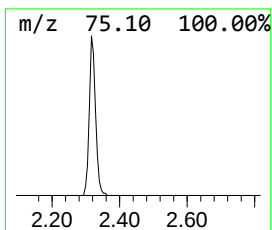
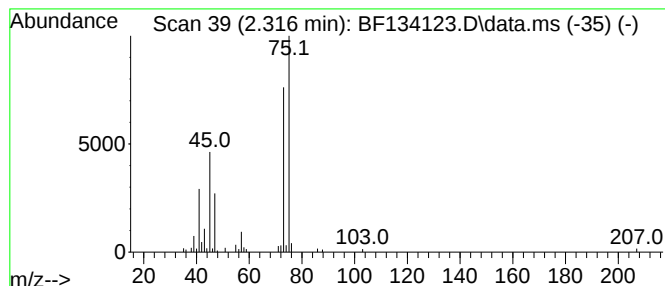
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.316	2.02 ng	66779	1,4-Dichlorobenzene-d4	6.846

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			4-Methylvaleric acid, TMS deriva...	188	C9H20O2Si	959048-10-3	40
3			Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	40
4			Hexane, 1-(2,2-dimethoxyethoxy)-	190	C10H22O3	017597-95-4	30
5			Methane, trimethoxy-	106	C4H10O3	000149-73-5	28



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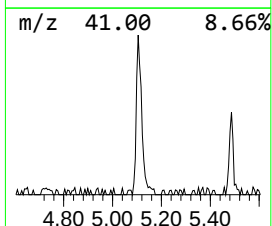
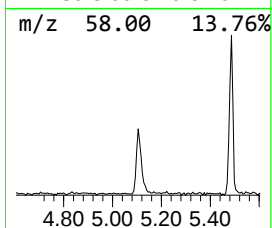
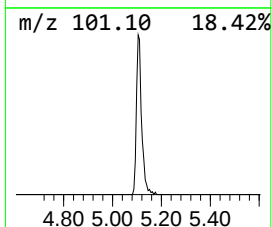
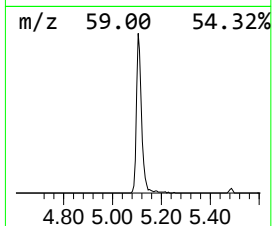
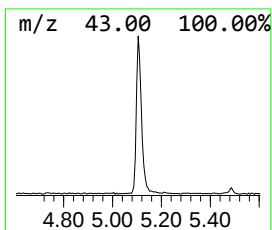
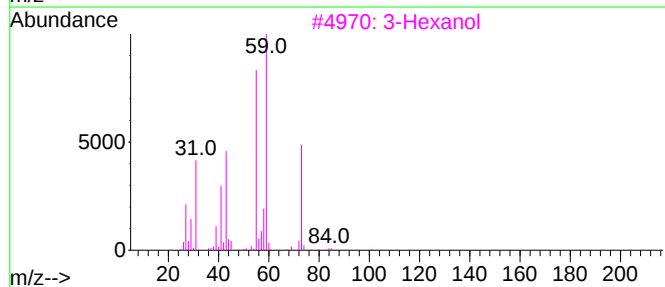
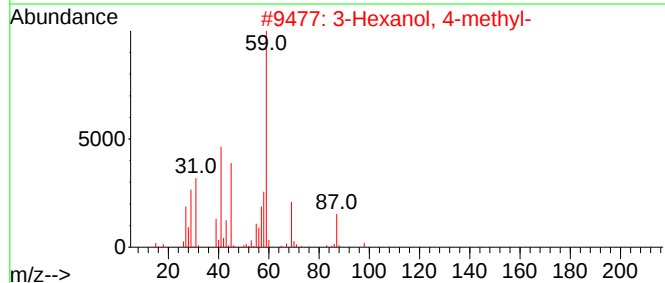
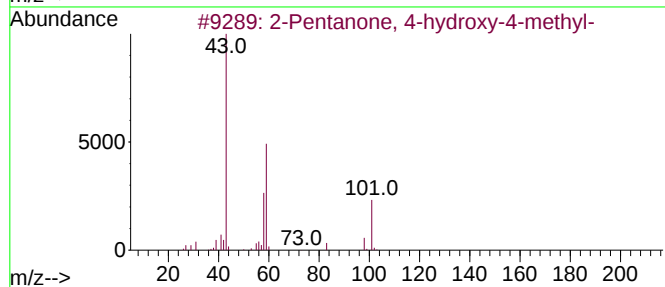
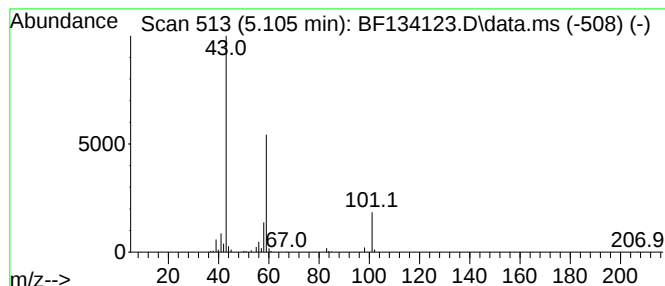
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.105	7.33 ng	242219	1,4-Dichlorobenzene-d4			6.846
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
3	3-Hexanol		102	C6H14O	000623-37-0	33
4	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	16



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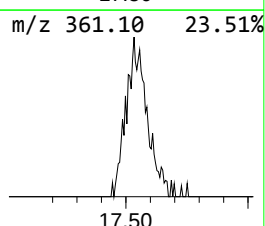
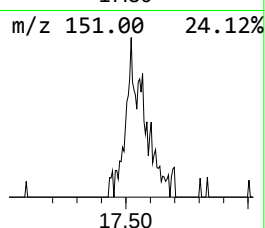
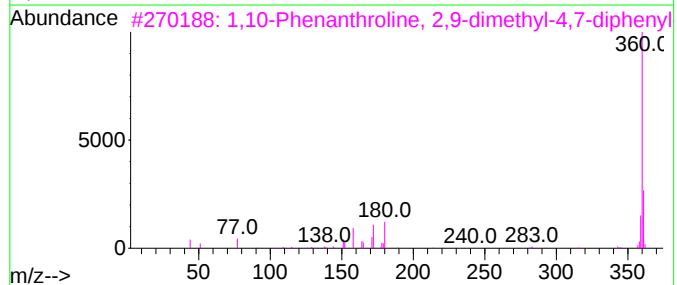
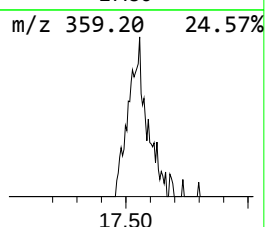
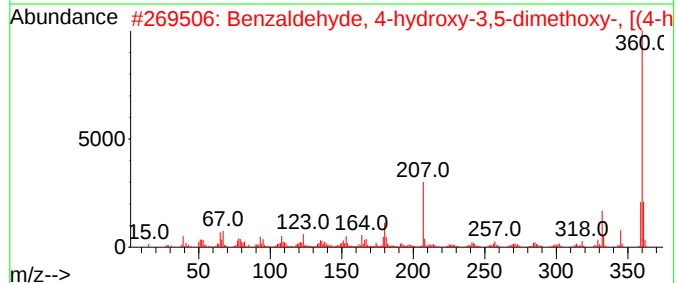
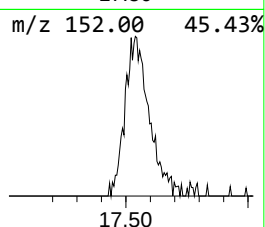
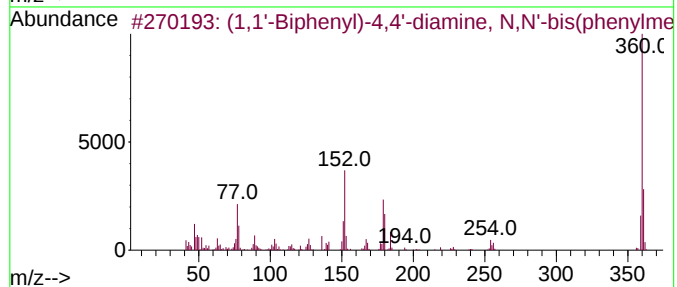
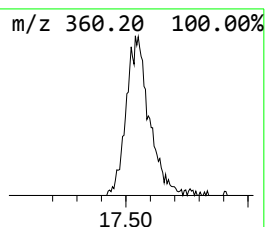
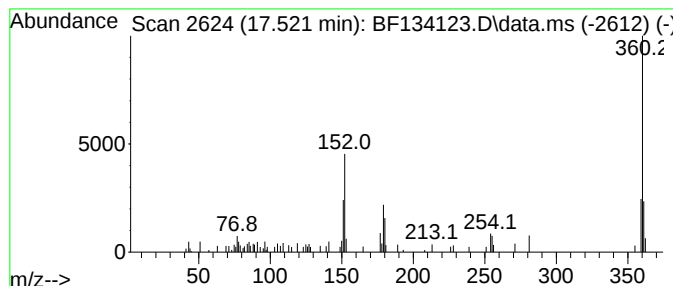
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Peak Number 4 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.521	2.08 ng	68504	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	91
2			Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	47
3			1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	43
4			Jaceidin	360	C18H16O8	010173-01-0	43
5			1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.205	2.9	ng	96803	1	6.846	660731	20.0
Propane, 1,1-di...	2.316	2.0	ng	66779	1	6.846	660731	20.0
2-Pentanone, 4-...	5.105	7.3	ng	242219	1	6.846	660731	20.0
(1,1'-Biphenyl)...	17.521	2.1	ng	68504	6	15.539	658735	20.0