

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070221\
 Data File : BF124518.D
 Acq On : 2 Jul 2021 14:40
 Operator : JU/CG
 Sample : PB137485BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB137485BL

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-BF062321.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124518.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.304	544	547	568	rBV	1218300	1156658	59.83%	11.924%
2	6.328	718	721	733	rBV	1097813	1093188	56.55%	11.270%
3	6.669	777	779	790	rBB	237918	211069	10.92%	2.176%
4	7.240	873	876	887	rBV	738667	739764	38.26%	7.626%
5	7.951	994	997	1007	rBB	318973	280786	14.52%	2.895%
6	9.034	1176	1181	1184	rBV	1778611	1622058	83.90%	16.722%
7	9.704	1292	1295	1300	rBV	439881	353820	18.30%	3.648%
8	10.498	1426	1430	1443	rBV	1234159	1061416	54.90%	10.942%
9	11.192	1545	1548	1558	rBB	455747	376220	19.46%	3.879%
10	12.780	1813	1818	1821	rBV	2175071	1933289	100.00%	19.931%
11	13.621	1954	1961	1964	rBV2	26749	37638	1.95%	0.388%
12	13.663	1964	1968	1970	rVV	34615	43178	2.23%	0.445%
13	13.698	1970	1974	1978	rVB	103304	105690	5.47%	1.090%
14	13.833	1995	1997	2007	rVB	354902	345002	17.85%	3.557%
15	15.257	2236	2239	2252	rVB	248952	308725	15.97%	3.183%
16	16.115	2377	2385	2387	rBV4	17825	31592	1.63%	0.326%

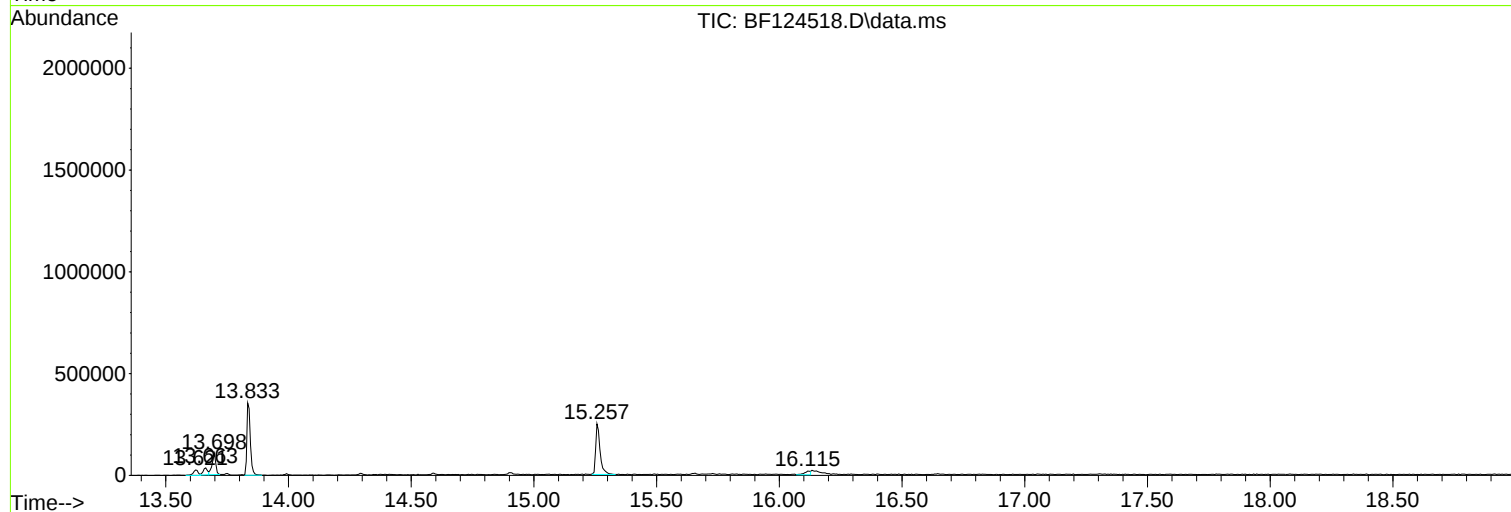
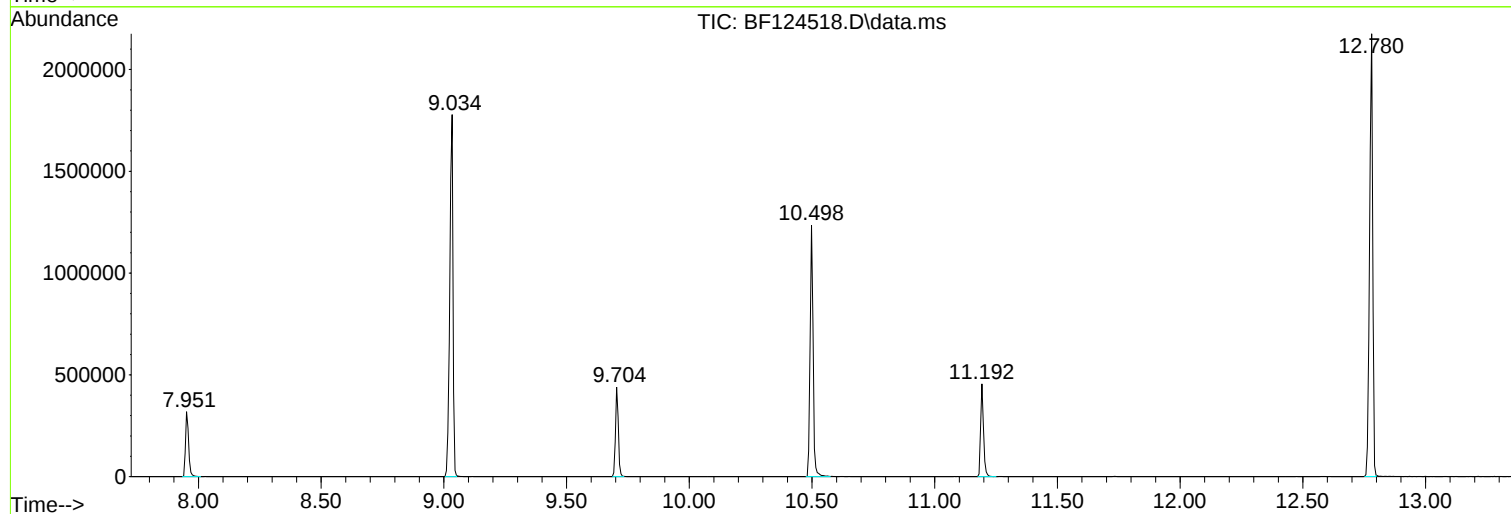
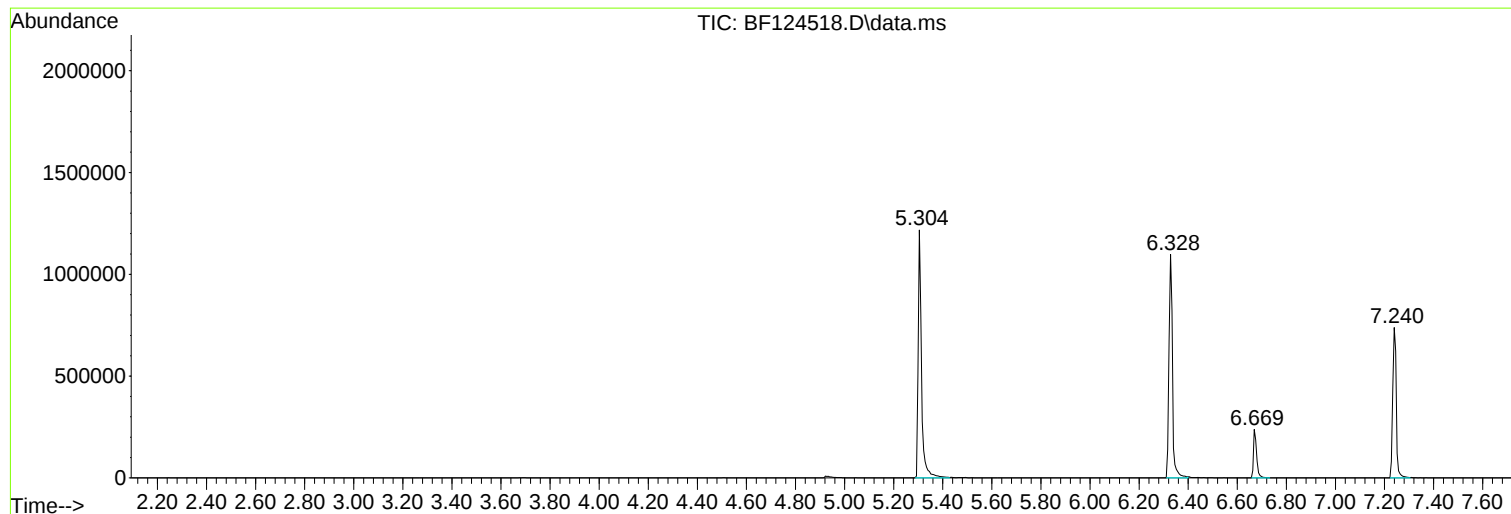
Sum of corrected areas: 9700093

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062321.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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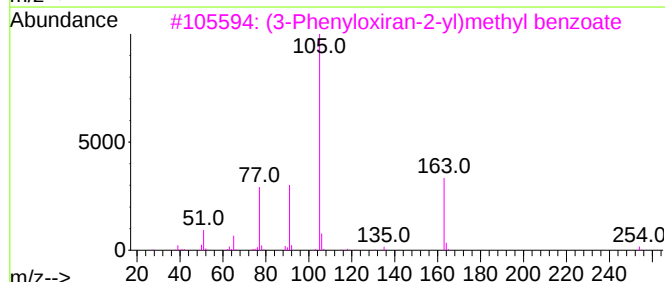
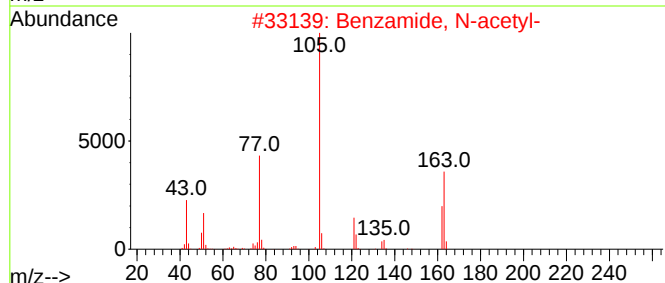
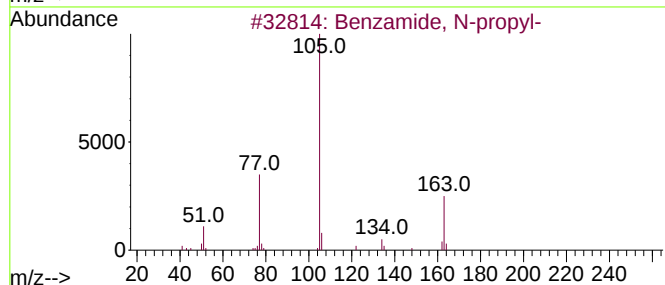
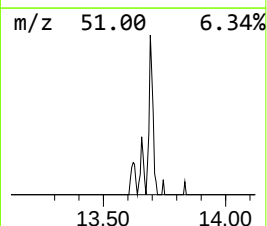
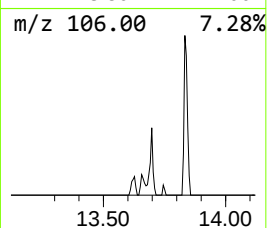
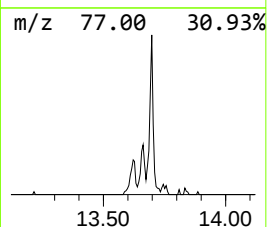
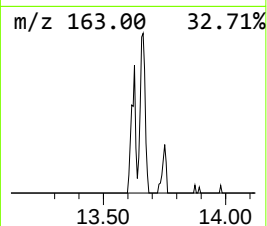
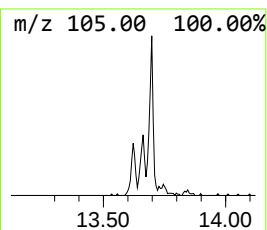
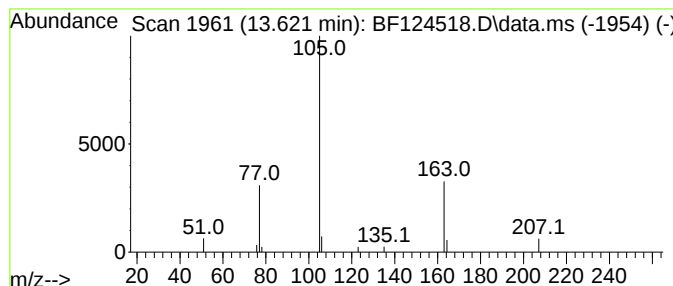
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzamide, N-propyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.621	2.18 ng	37638	Chrysene-d12	13.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	78
2			Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	56
3			(3-Phenylloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	43
4			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	40
5			N-Benzoylglycine ethyl ester	207	C11H13NO3	001499-53-2	28



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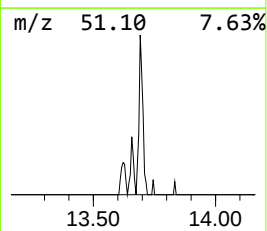
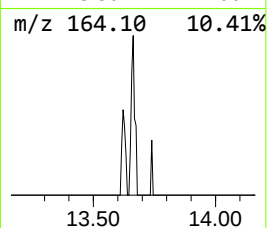
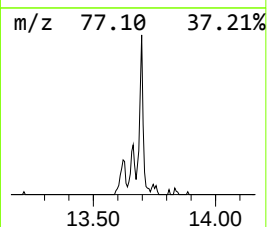
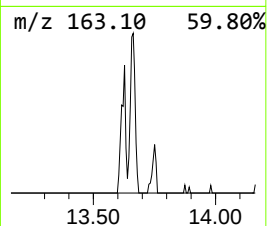
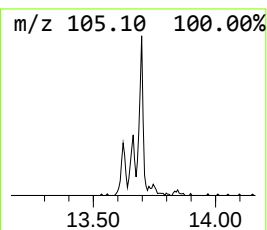
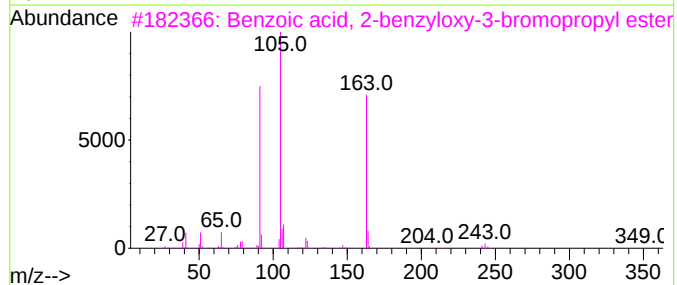
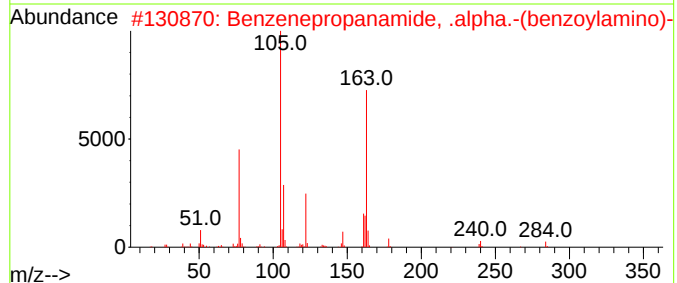
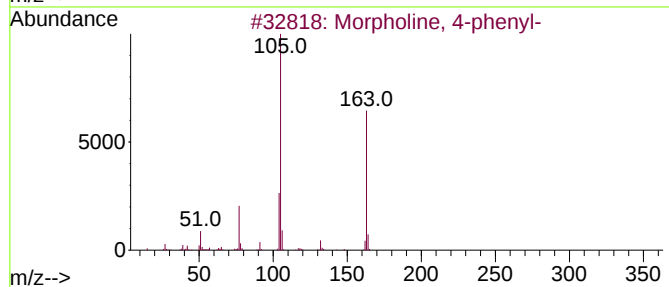
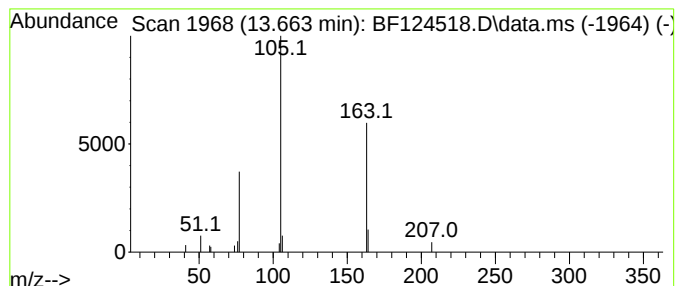
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Morpholine, 4-phenyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.663	2.50 ng	43178	Chrysene-d12	13.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	59
2			Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	56
3			Benzoic acid, 2-benzyloxy-3-brom...	348	C17H17BrO3	1000191-33-3	45
4			.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	43
5			1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	40



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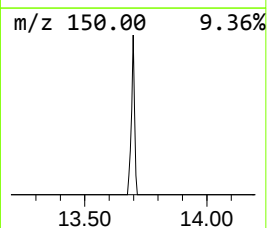
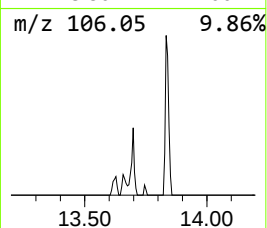
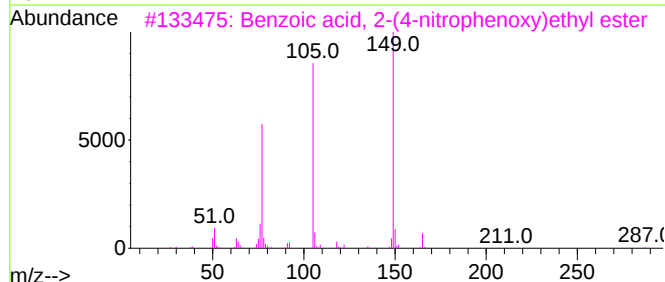
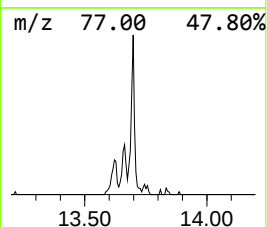
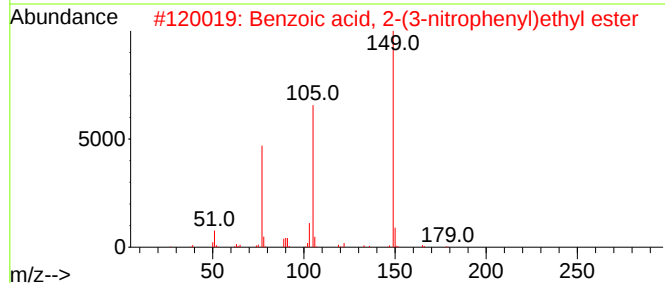
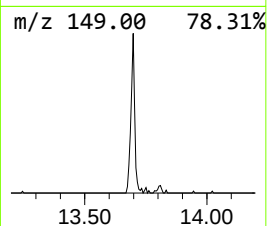
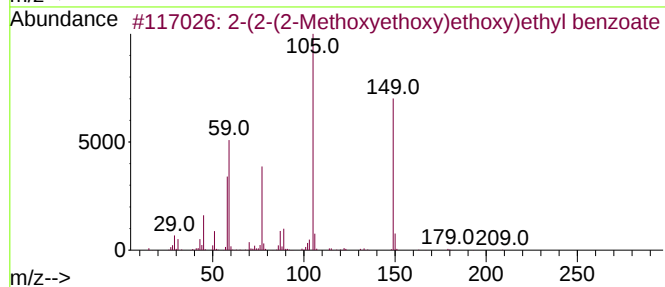
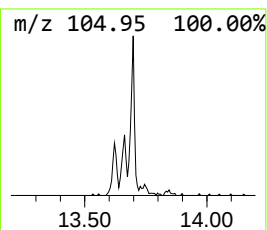
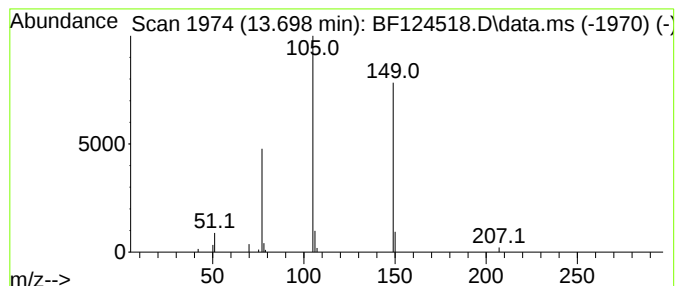
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Peak Number 3 2-(2-(2-Methoxyethoxy)ethox... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.698	6.13 ng	105690	Chrysene-d12	13.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	83		
2	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	83		
3	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	74		
4	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	64		
5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64		



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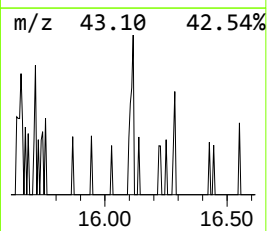
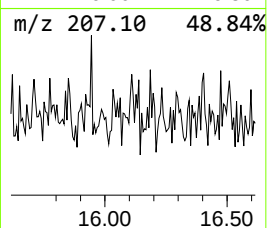
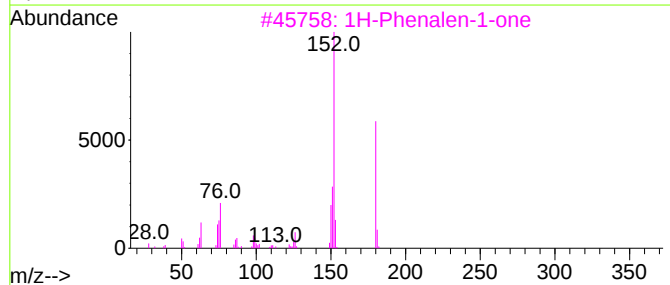
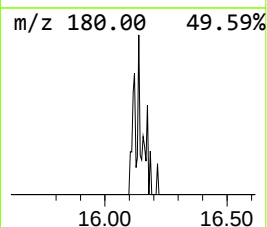
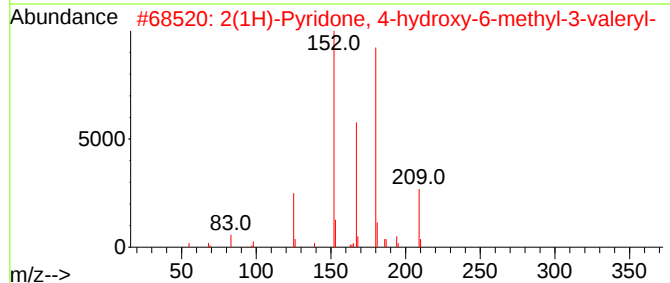
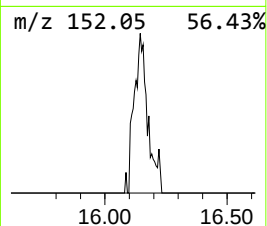
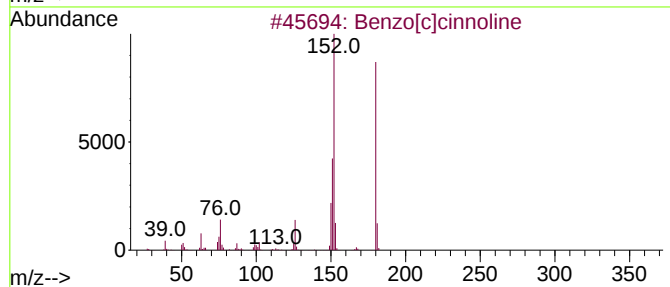
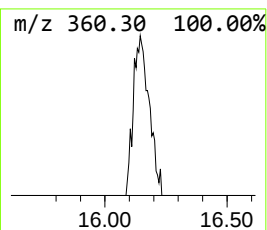
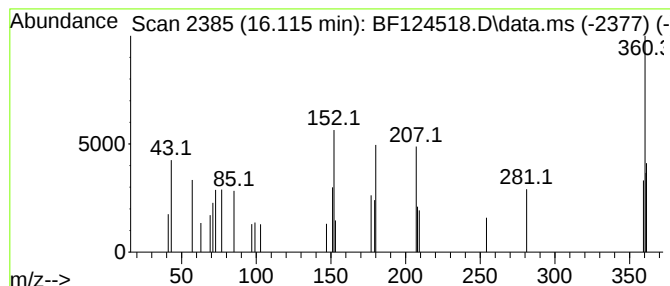
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TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown16.115 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.115	2.05 ng	31592	Perylene-d12	15.257

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]cinnoline	180	C12H8N2	000230-17-1	11
2			2(1H)-Pyridone, 4-hydroxy-6-meth...	209	C11H15NO3	007135-84-4	10
3			1H-Phenalen-1-one	180	C13H8O	000548-39-0	9
4			[.mu.-Fulvalene]bis(cyclopentadi...	360	C20H18V2	1000163-45-2	5
5			1,2-Bis(3,4,5-trimethoxyphenyl)e...	360	C20H24O6	061240-22-0	5



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzamide, N-pr...	13.621	2.2	ng	37638	5	13.833	345002	20.0
Morpholine, 4-p...	13.663	2.5	ng	43178	5	13.833	345002	20.0
2-(2-(2-Methoxy...	13.698	6.1	ng	105690	5	13.833	345002	20.0
unknown16.115	16.115	2.0	ng	31592	6	15.257	308725	20.0