

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021323\
 Data File : BF132423.D
 Acq On : 13 Feb 2023 22:23
 Operator : CG\JU
 Sample : 01328-06
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-2-BORING-1-7-14

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-BF021323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132423.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.284	409	416	426	rVB	1130369	1544463	29.43%	4.091%
2	5.660	475	480	484	rBV	3162263	3574184	68.12%	9.466%
3	6.654	643	649	652	rBV	2508054	2989405	56.97%	7.918%
4	7.031	709	713	717	rBV	1114464	860201	16.39%	2.278%
5	7.595	803	809	812	rBV	2717818	2673248	50.95%	7.080%
6	8.319	928	932	935	rBV	1816230	1476323	28.14%	3.910%
7	9.395	1109	1115	1118	rBV	5954348	5223921	99.56%	13.836%
8	10.083	1228	1232	1235	rVB	1842159	1694765	32.30%	4.489%
9	10.795	1349	1353	1356	rBV	333354	249575	4.76%	0.661%
10	10.872	1362	1366	1370	rBV	3463691	3432621	65.42%	9.091%
11	11.578	1482	1486	1489	rBV	2064724	1707954	32.55%	4.524%
12	12.089	1569	1573	1586	rBV2	241418	353458	6.74%	0.936%
13	12.807	1690	1695	1699	rBV3	87655	136527	2.60%	0.362%
14	12.877	1703	1707	1712	rBV5	51076	89481	1.71%	0.237%
15	12.966	1719	1722	1726	rVB2	120891	108546	2.07%	0.287%
16	13.030	1730	1733	1735	rBV	61615	57048	1.09%	0.151%
17	13.172	1752	1757	1760	rBV	5524646	5247154	100.00%	13.897%
18	13.730	1849	1852	1859	rVB2	45040	72952	1.39%	0.193%
19	14.236	1934	1938	1942	rBV	1518907	1345030	25.63%	3.562%
20	14.324	1947	1953	1959	rBV	1172465	1161324	22.13%	3.076%
21	14.689	2013	2015	2024	rVB3	53851	73604	1.40%	0.195%
22	14.866	2041	2045	2056	rBV	2421816	2282070	43.49%	6.044%
23	15.389	2131	2134	2140	rVB2	54550	65218	1.24%	0.173%
24	15.801	2199	2204	2212	rVB2	941472	1252902	23.88%	3.318%
25	16.289	2283	2287	2302	rVB4	33878	84898	1.62%	0.225%

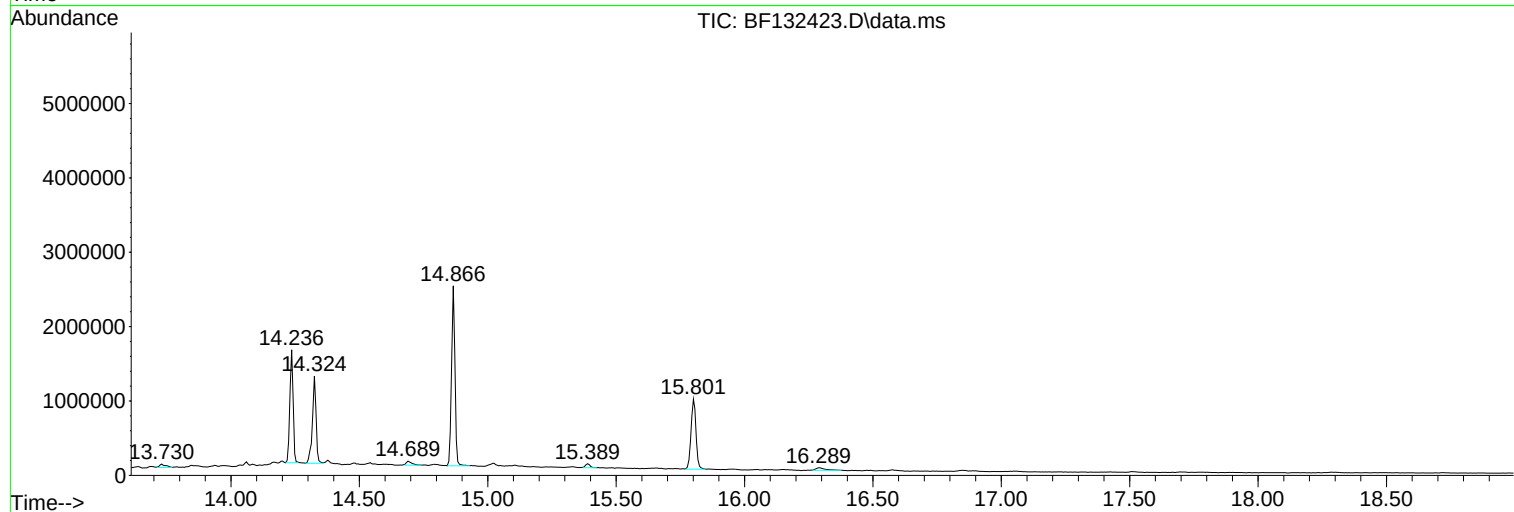
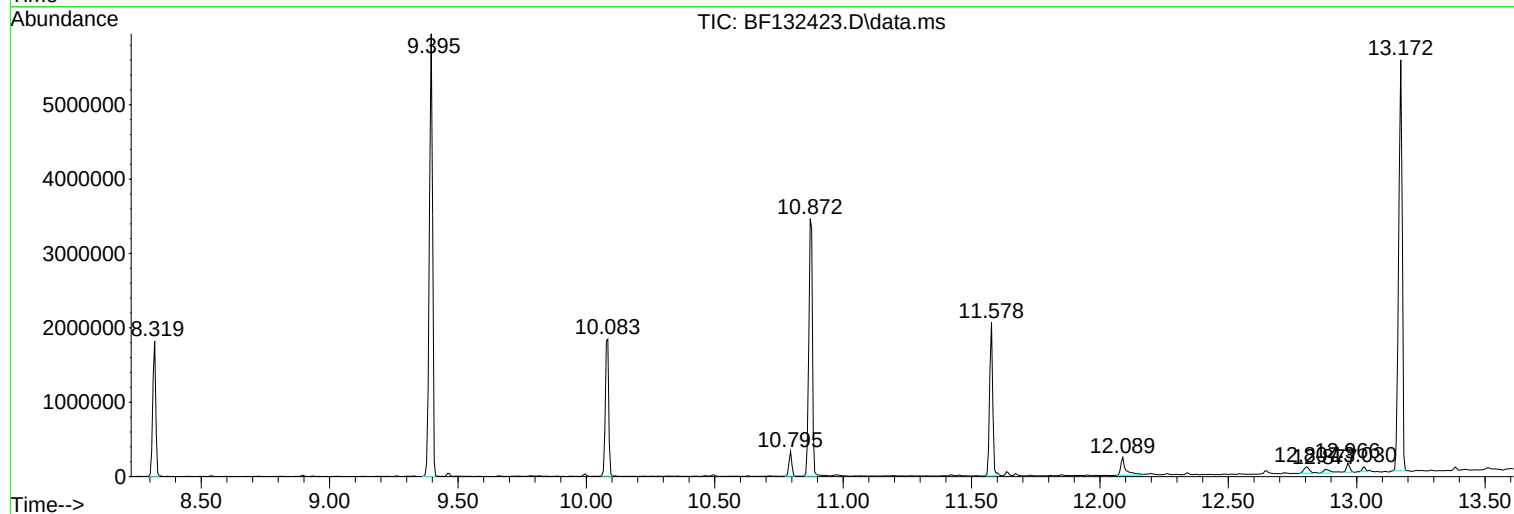
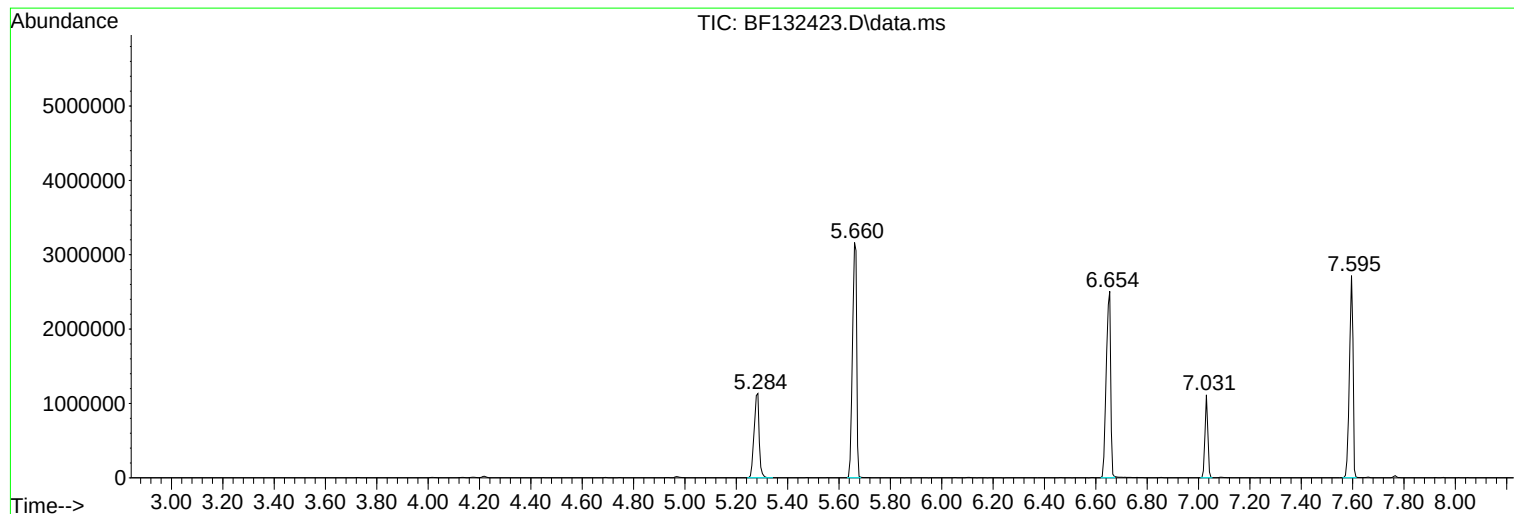
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Instrument :
BNA_F
ClientSampleId :
COMP-2-BORING-1-7-14

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021323.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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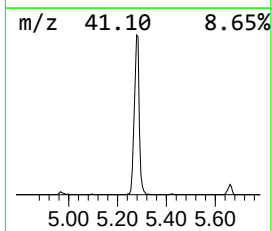
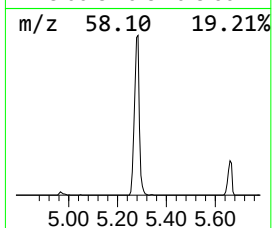
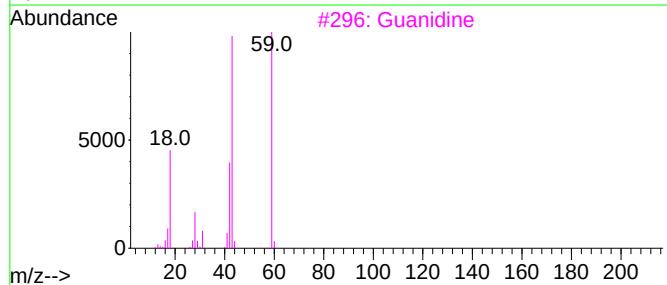
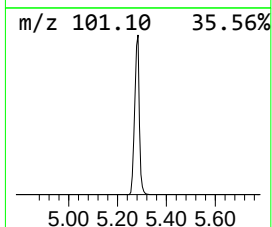
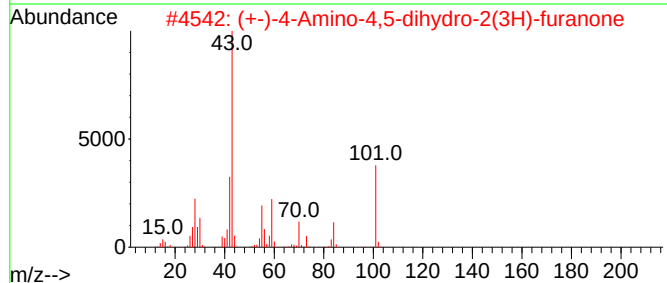
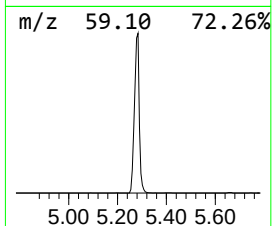
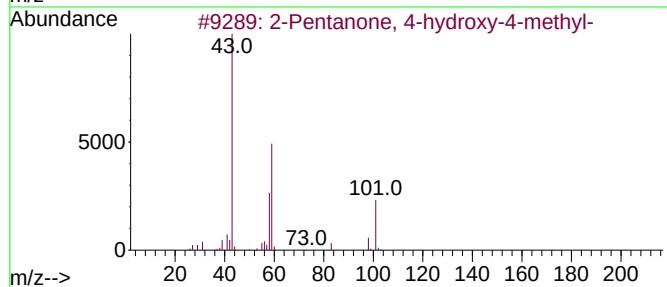
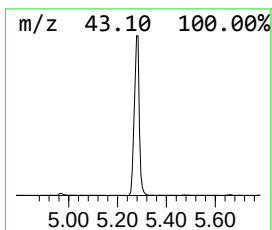
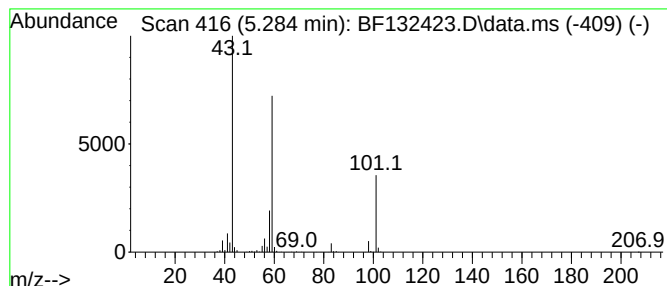
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.284	35.91 ng	1544460	1,4-Dichlorobenzene-d4	7.031

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3			Guanidine	59	CH5N3	000113-00-8	38
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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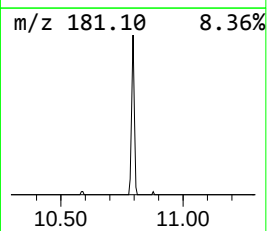
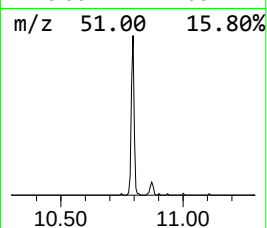
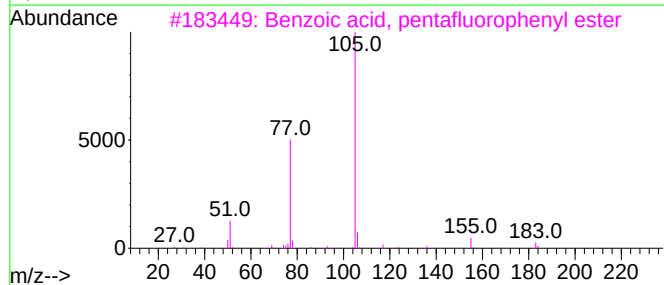
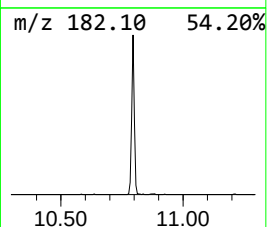
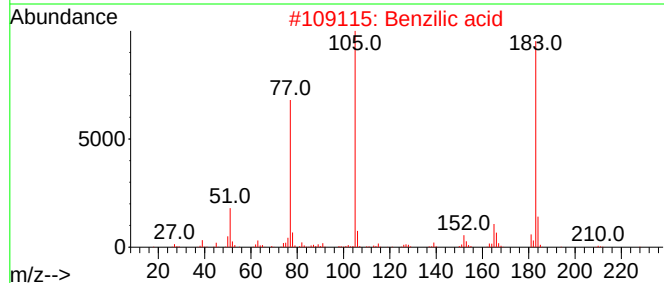
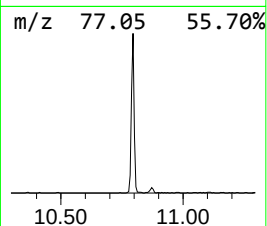
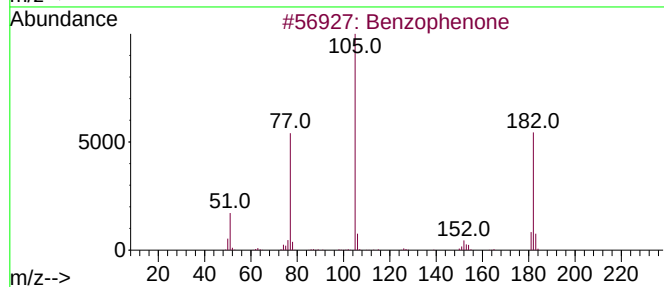
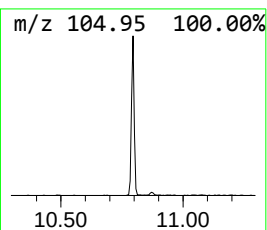
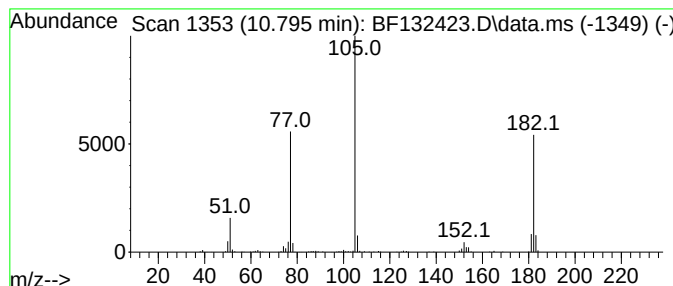
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.795	2.95 ng	249575	Acenaphthene-d10	10.084

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzilic acid	228	C14H12O3	000076-93-7	50
3			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47
4			Methyl benzilate	242	C15H14O3	000076-89-1	47
5			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	43



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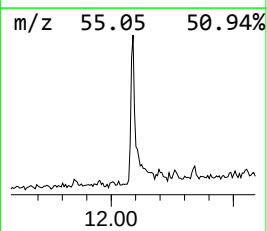
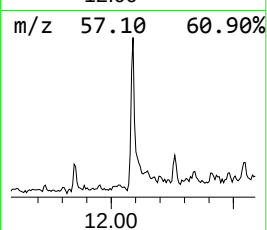
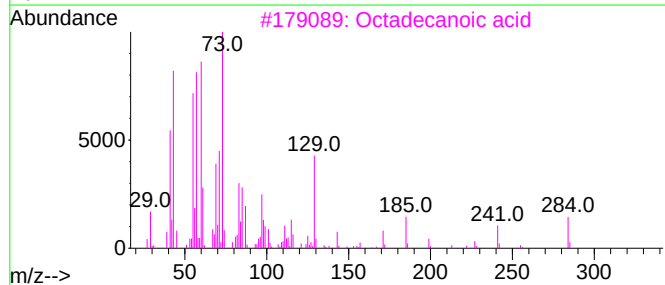
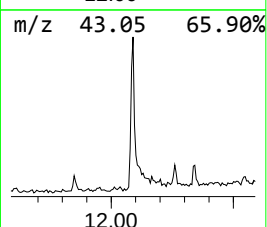
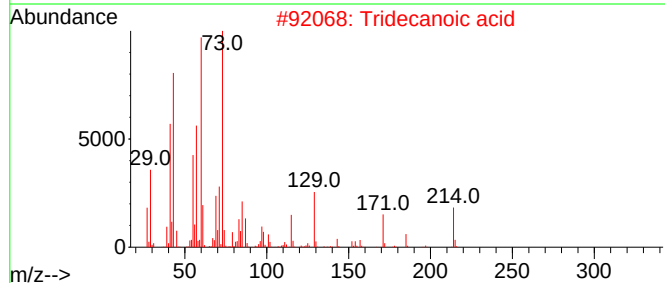
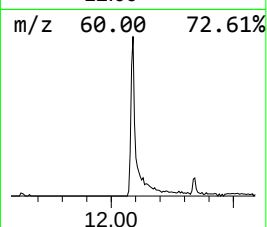
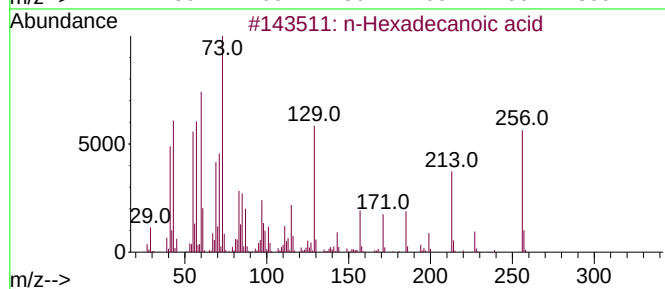
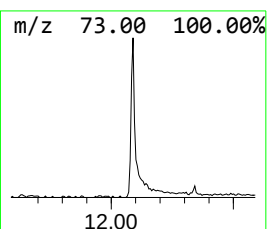
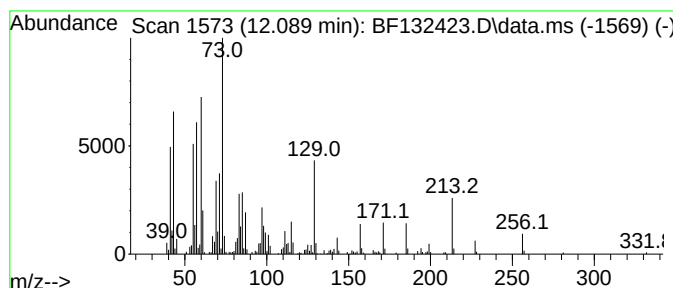
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.089	4.14 ng	353458	Phenanthrene-d10	11.578

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Octadecanoic acid	284	C18H36O2	000057-11-4	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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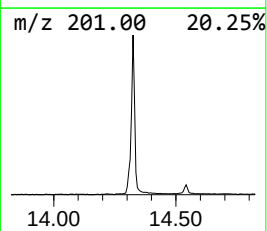
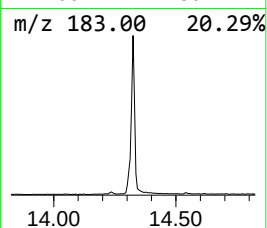
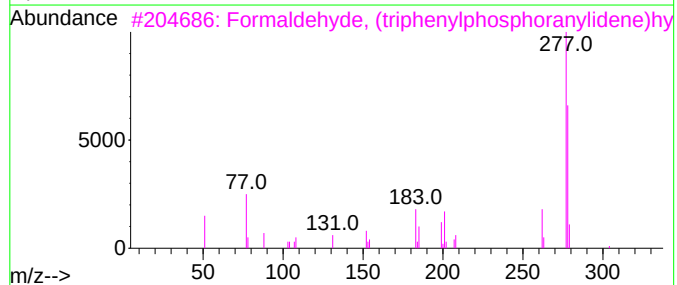
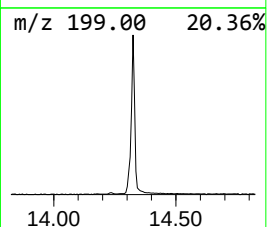
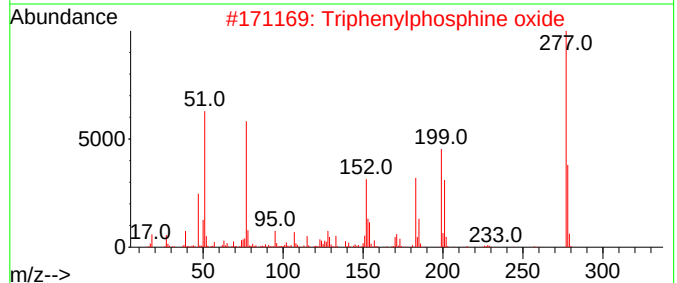
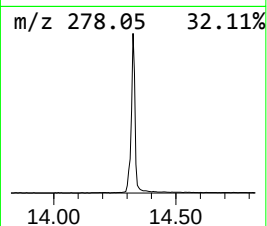
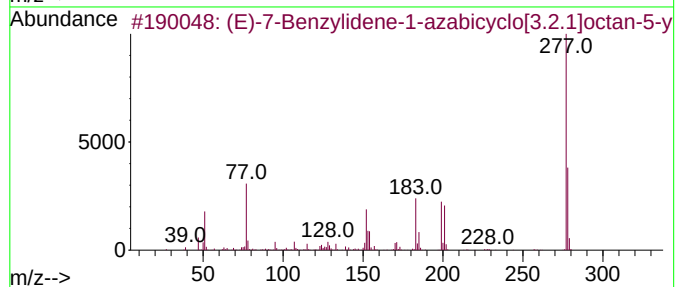
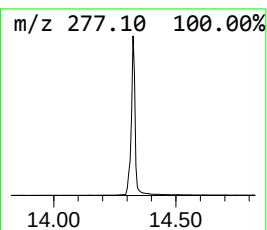
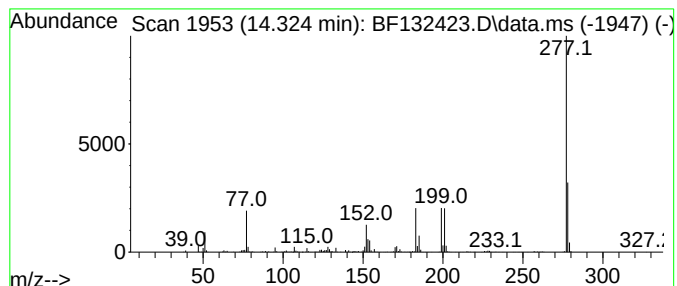
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Peak Number 4 (E)-7-Benzylidene-1-azabicy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.324	17.27 ng	1161320	Chrysene-d12	14.236
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		(E)-7-Benzylidene-1-azabicyclo[3...]	293 C15H19NO3S	1000483-83-4 91
2		Triphenylphosphine oxide	278 C18H15OP	000791-28-6 91
3		Formaldehyde, (triphenylphosphor...	304 C19H17N2P	015990-54-2 40
4		Vanadium, cycloheptatrienyl-(pen...	277 C17H22V	1000155-20-5 25
5		5-Methyl-8-phenylfuro[3',2':5,6]...	277 C16H11N3O2	1000460-07-9 25



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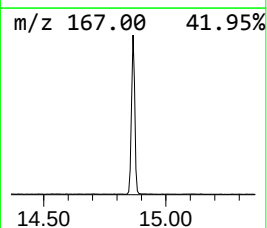
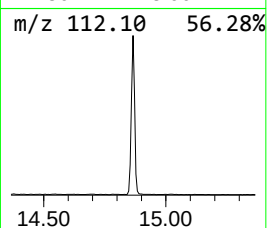
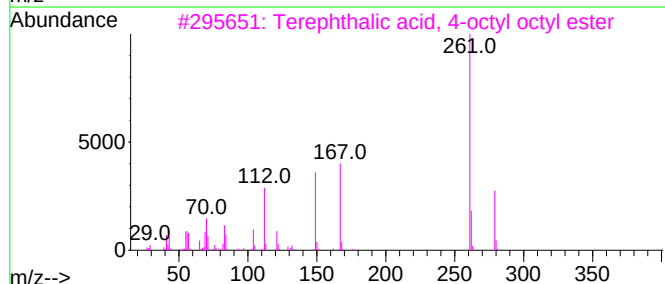
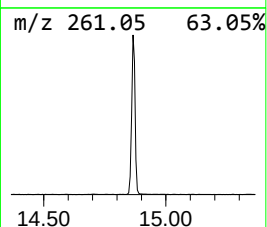
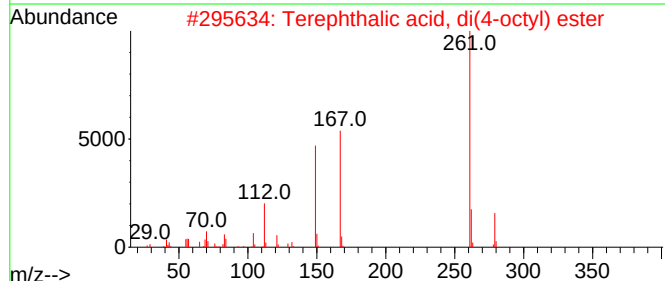
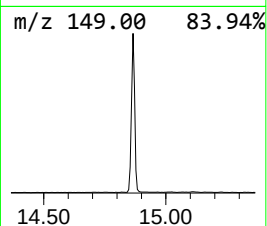
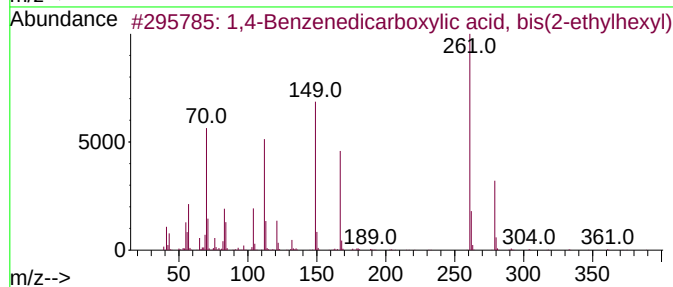
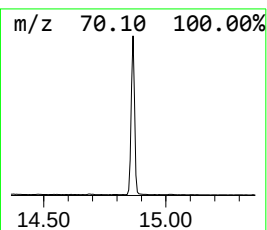
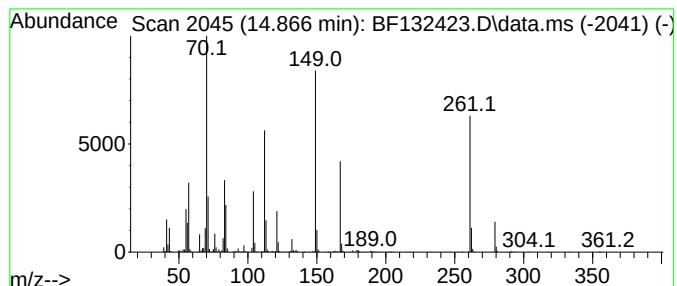
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TIC Integration Parameters: LSCINT.P

Peak Number 5 1,4-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.866	33.93 ng	2282070	Chrysene-d12	14.236	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	87
2	Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	81
3	Terephthalic acid, 4-octyl octyl...	390	C24H38O4	1000323-73-7	68
4	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	64
5	Isophthalic acid, 3-methylbut-2-...	348	C21H32O4	1000344-72-4	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.284	35.9	ng	1544460	1	7.031	860201	20.0
Benzophenone	10.795	3.0	ng	249575	3	10.084	1694770	20.0
n-Hexadecanoic ...	12.089	4.1	ng	353458	4	11.578	1707950	20.0
(E)-7-Benzylide...	14.324	17.3	ng	1161320	5	14.236	1345030	20.0
1,4-Benzenedica...	14.866	33.9	ng	2282070	5	14.236	1345030	20.0