

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
 Data File : BF132351.D
 Acq On : 07 Feb 2023 18:43
 Operator : CG\JU
 Sample : 01463-19
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-7

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-BF013123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132351.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	407	416	423	rBV	854905	1040526	28.56%	3.801%
2	5.672	477	482	485	rBV	2767313	2540526	69.73%	9.279%
3	6.666	646	651	654	rBV	2510123	2539265	69.69%	9.275%
4	7.048	713	716	720	rVB	1012752	803528	22.05%	2.935%
5	7.613	807	812	815	rBV	2020934	1721772	47.25%	6.289%
6	8.336	931	935	938	rBV	1398659	1091720	29.96%	3.988%
7	9.413	1114	1118	1121	rBV	4488347	3643620	100.00%	13.308%
8	10.101	1231	1235	1238	rBV	1602781	1286447	35.31%	4.699%
9	10.813	1352	1356	1359	rVB	248633	188977	5.19%	0.690%
10	10.889	1365	1369	1373	rBV	2679606	2381436	65.36%	8.698%
11	11.595	1485	1489	1492	rBV	1655827	1375428	37.75%	5.024%
12	11.619	1492	1493	1497	rVB	189136	107352	2.95%	0.392%
13	11.672	1497	1502	1504	rBV2	52760	67805	1.86%	0.248%
14	12.107	1571	1576	1578	rBV2	309370	318125	8.73%	1.162%
15	12.213	1590	1594	1596	rBV2	46007	50200	1.38%	0.183%
16	12.819	1693	1697	1700	rBV	296750	264020	7.25%	0.964%
17	12.895	1706	1710	1716	rBV2	62039	75354	2.07%	0.275%
18	13.048	1729	1736	1742	rBV	324976	346512	9.51%	1.266%
19	13.189	1755	1760	1763	rBV	4117207	3556168	97.60%	12.989%
20	14.077	1905	1911	1923	rBV4	183672	400763	11.00%	1.464%
21	14.254	1936	1941	1944	rBV	1001393	952118	26.13%	3.478%
22	14.277	1944	1945	1951	rVB	114386	92721	2.54%	0.339%
23	14.342	1951	1956	1962	rBV	911959	917495	25.18%	3.351%
24	15.130	2087	2090	2094	rVB	69559	68890	1.89%	0.252%
25	15.354	2124	2128	2131	rBV	98601	150645	4.13%	0.550%
26	15.689	2182	2185	2191	rVB	61321	78363	2.15%	0.286%
27	15.760	2192	2197	2203	rVV	83816	120700	3.31%	0.441%
28	15.830	2204	2209	2223	rVB2	713961	994325	27.29%	3.632%
29	16.324	2290	2293	2297	rVB	32535	42707	1.17%	0.156%
30	17.454	2479	2485	2497	rBV2	39058	90853	2.49%	0.332%
31	17.948	2564	2569	2579	rVB2	30556	69880	1.92%	0.255%

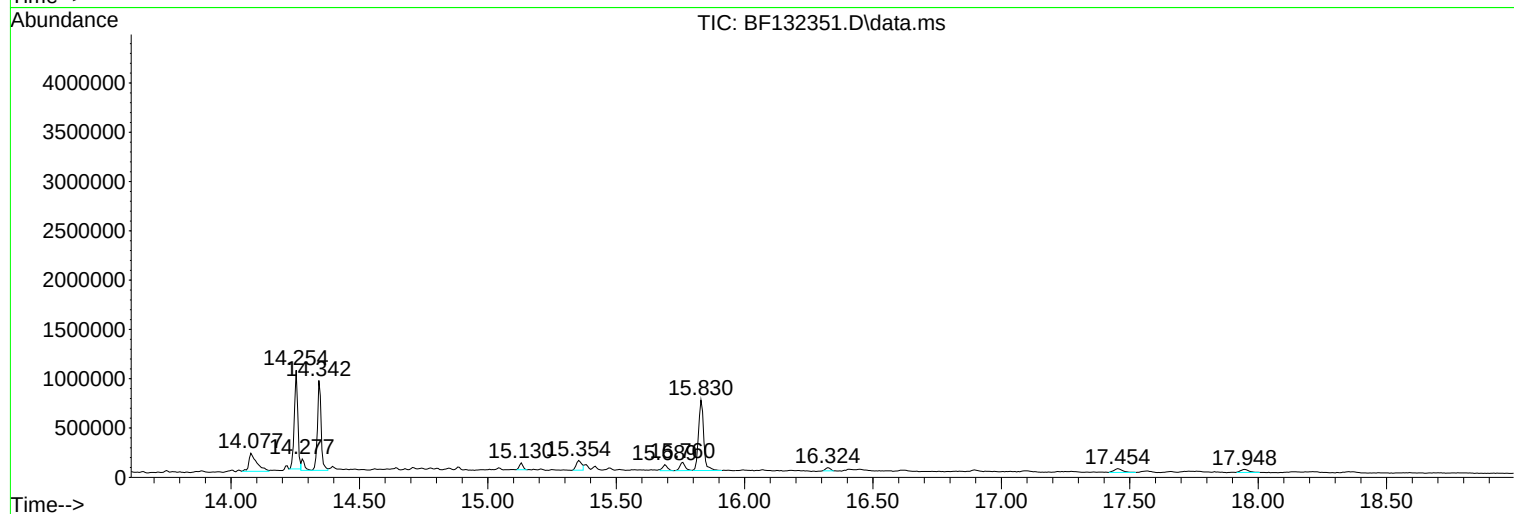
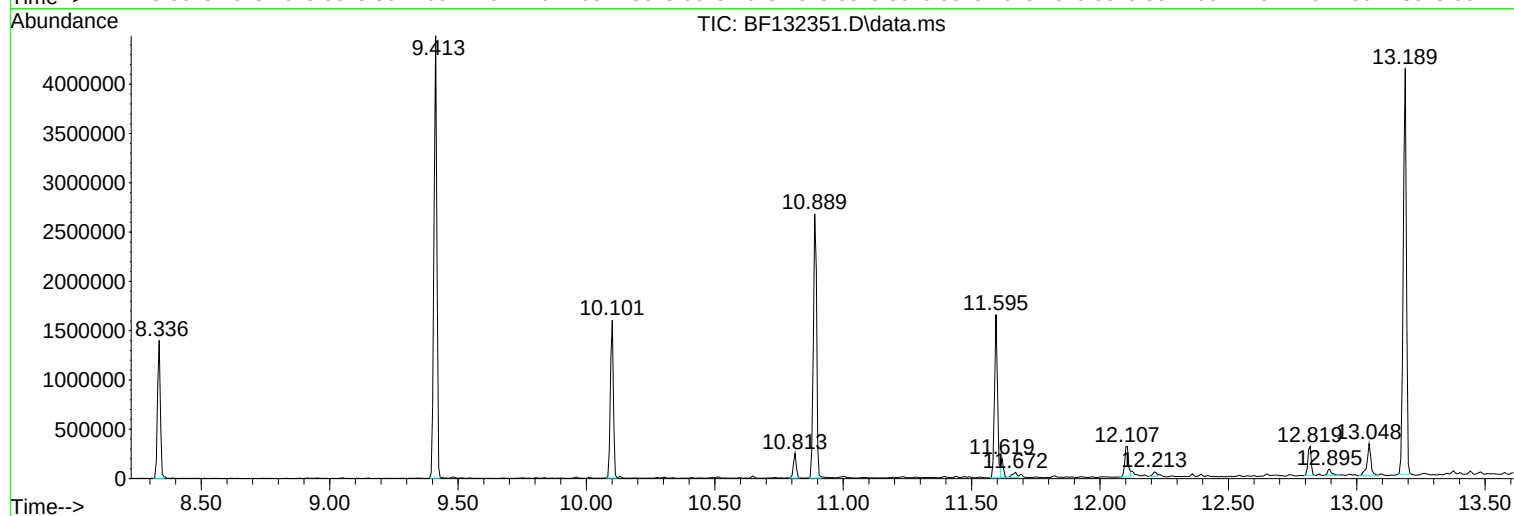
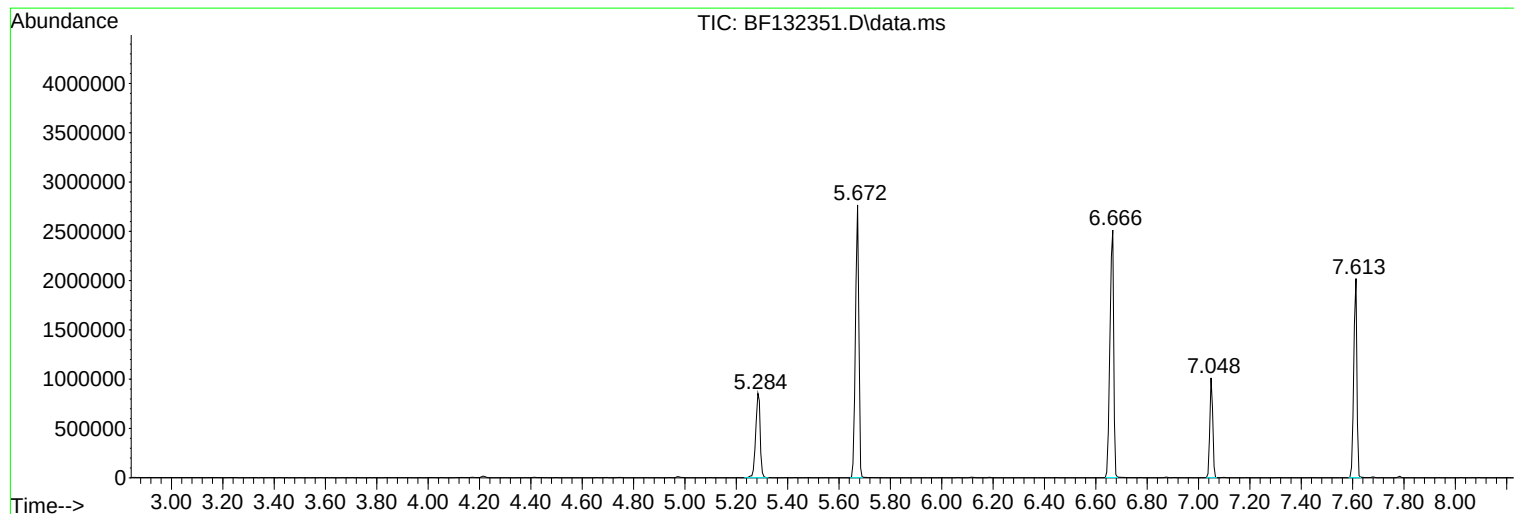
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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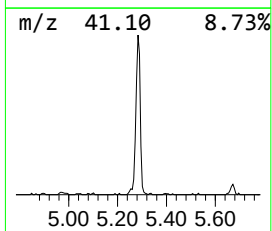
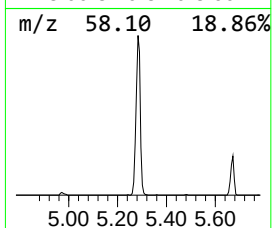
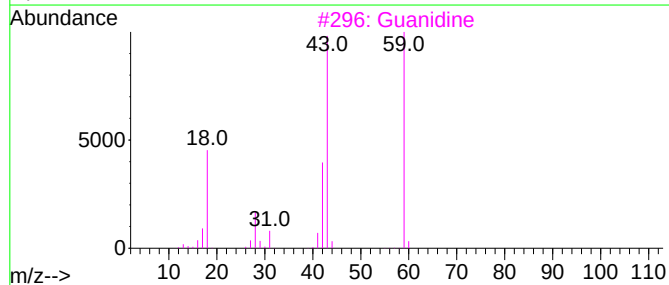
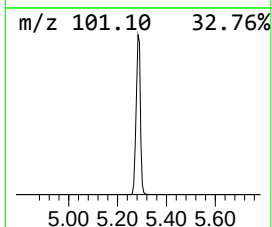
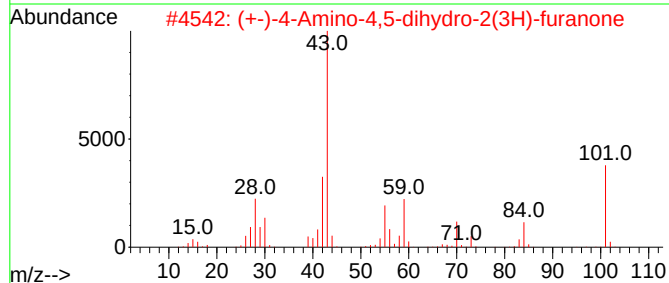
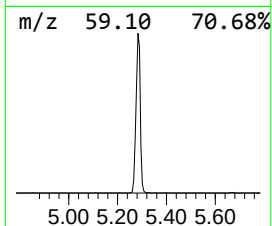
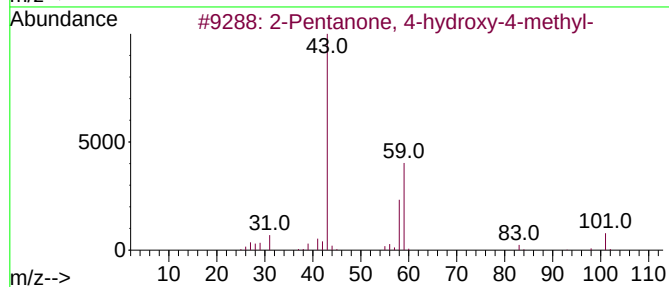
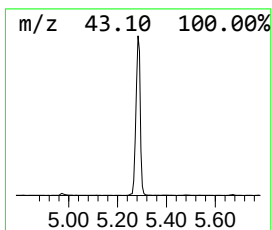
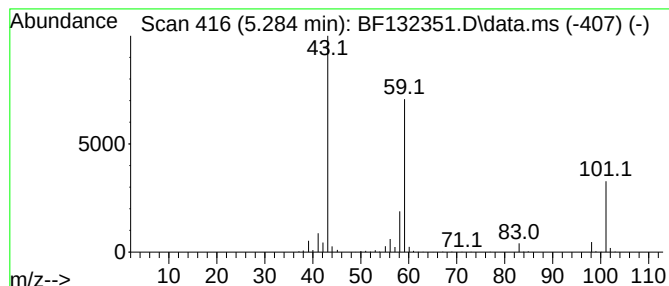
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.284	25.90 ng	1040530	1,4-Dichlorobenzene-d4	7.048

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3			Guanidine	59	CH5N3	000113-00-8	43
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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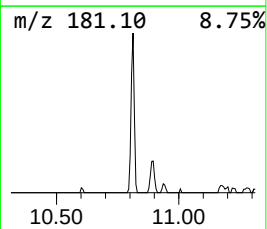
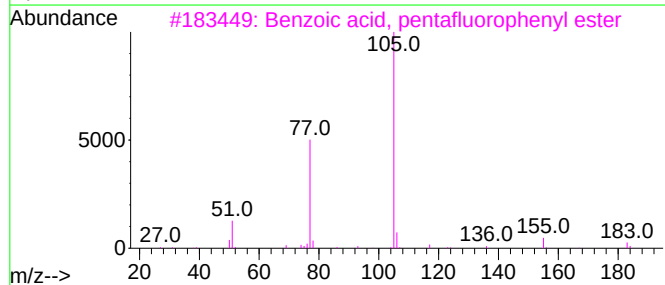
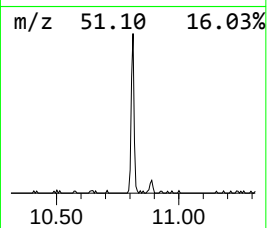
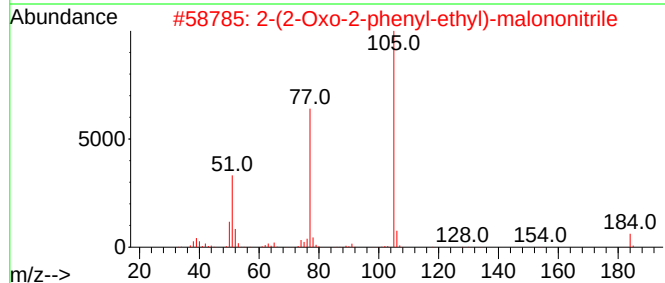
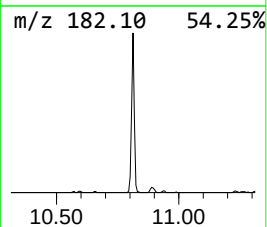
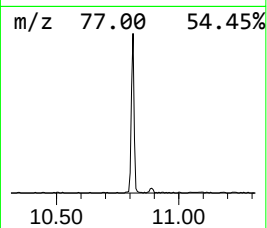
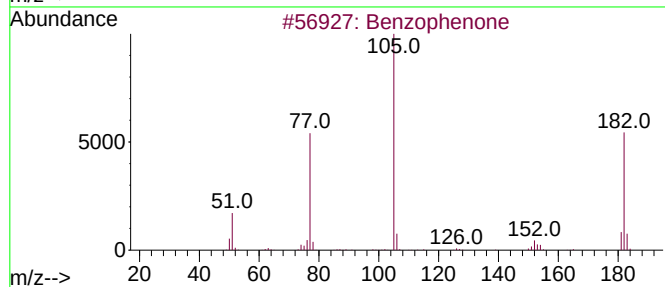
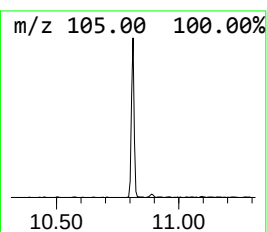
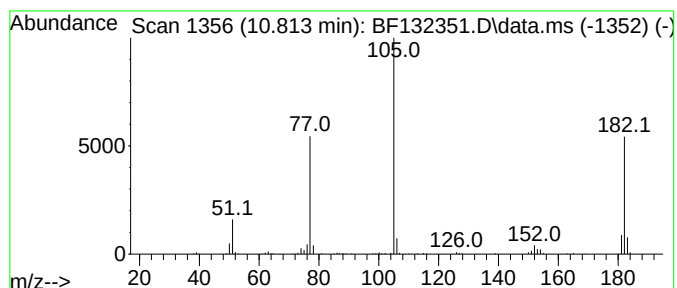
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.813	2.94 ng	188977	Acenaphthene-d10	10.101

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
3			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
5			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46



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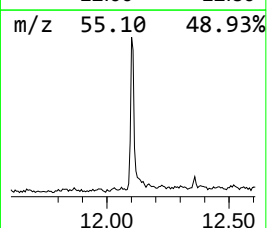
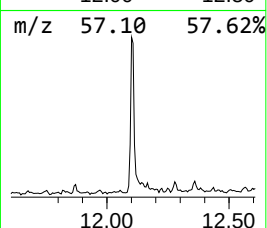
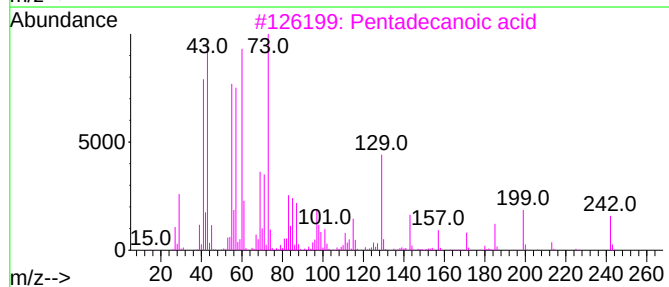
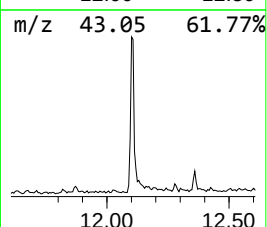
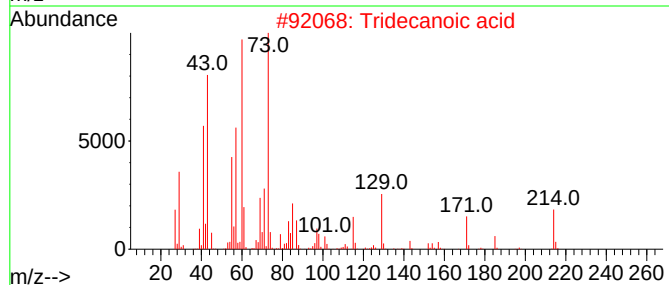
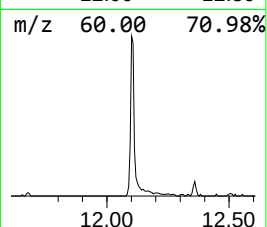
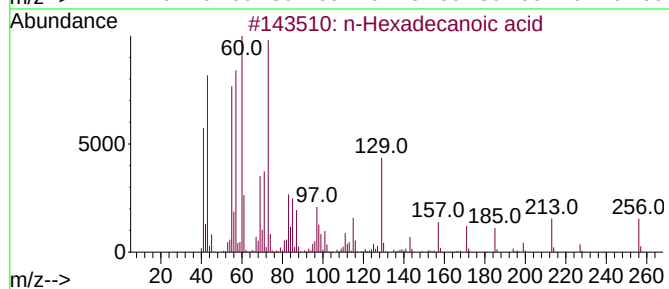
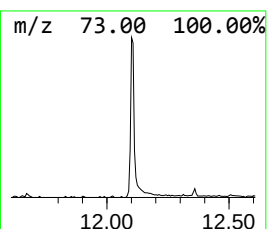
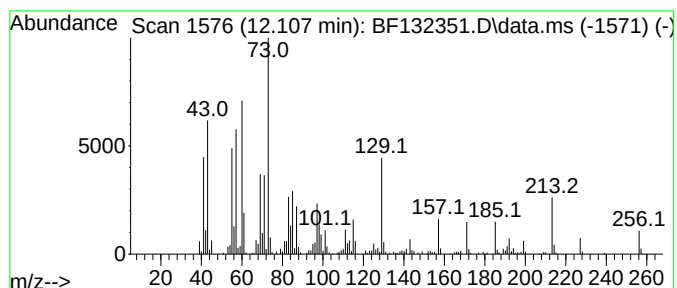
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.107	4.63 ng	318125	Phenanthrene-d10	11.595

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	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5		n-Decanoic acid	172	C10H20O2	000334-48-5	53



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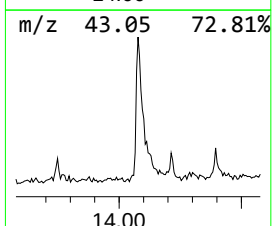
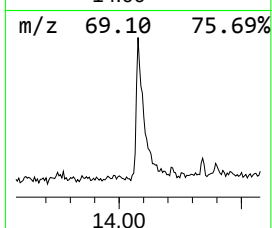
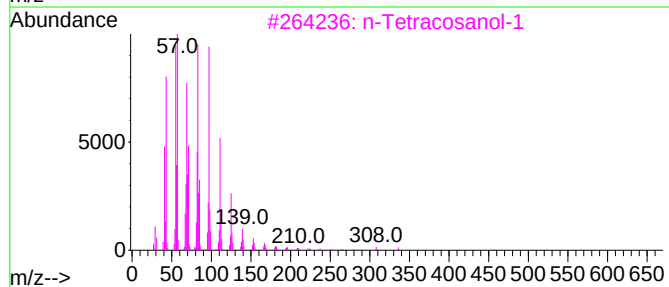
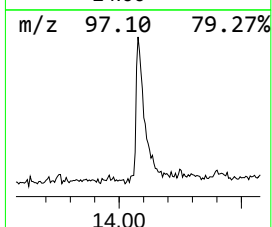
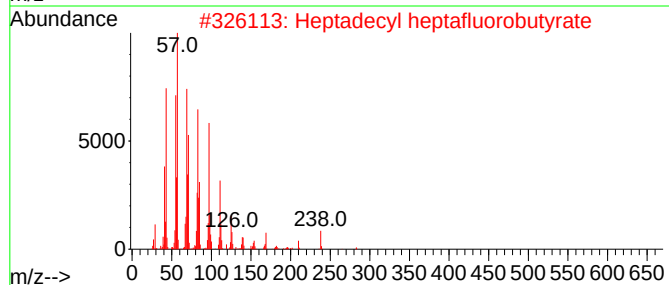
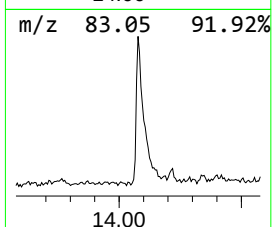
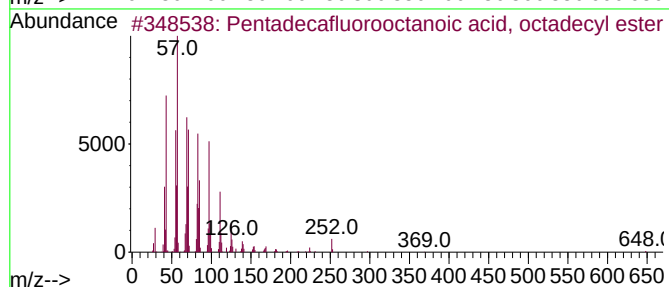
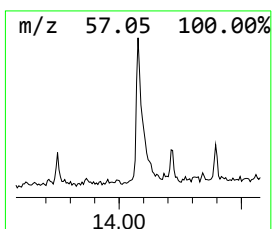
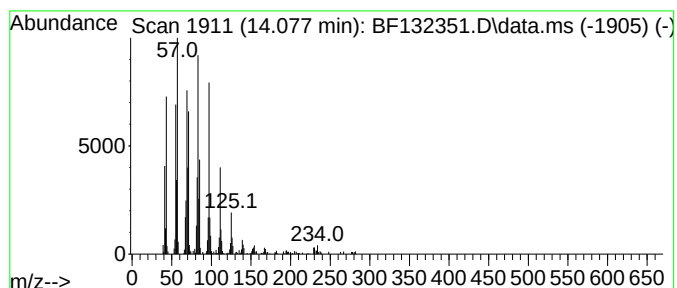
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Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.077	8.42 ng	400763	Chrysene-d12	14.254

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5			9-Eicosene, (E)-	280	C20H40	074685-29-3	91



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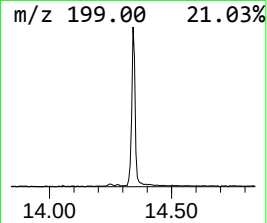
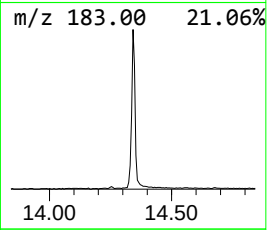
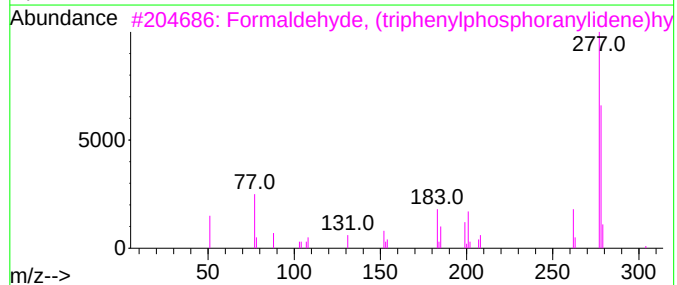
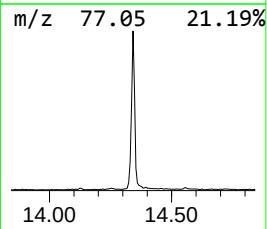
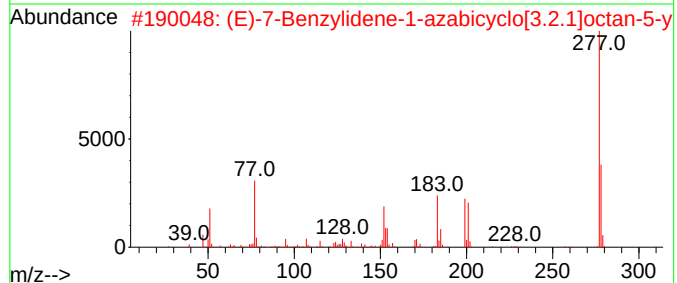
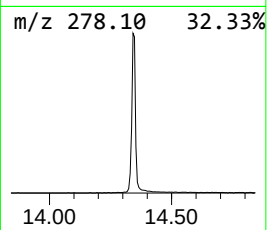
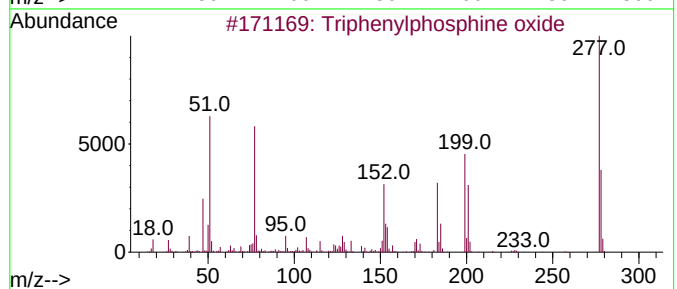
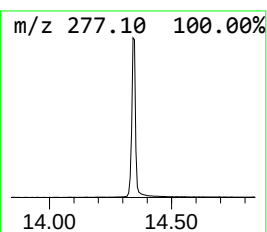
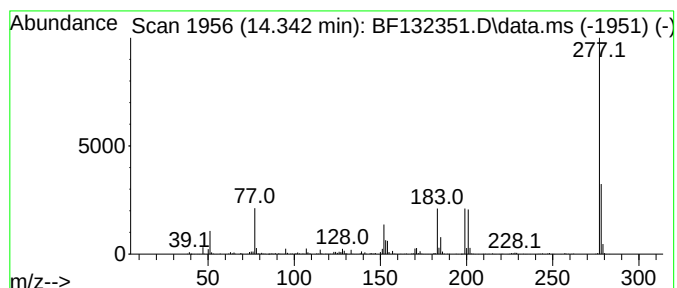
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.342	19.27 ng	917495	Chrysene-d12	14.254

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	92
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	42
4			Cobalt, (.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	17
5			4-Nitro-4'-methyldiphenylsulfone	277	C13H11N04S	004094-37-5	12



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.284	25.9	ng	1040530	1	7.048	803528	20.0
Benzophenone	10.813	2.9	ng	188977	3	10.101	1286450	20.0
n-Hexadecanoic ...	12.107	4.6	ng	318125	4	11.595	1375430	20.0
Pentadecafluoro...	14.077	8.4	ng	400763	5	14.254	952118	20.0
Triphenylphosph...	14.342	19.3	ng	917495	5	14.254	952118	20.0