

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
 Data File : BF134366.D
 Acq On : 19 Jul 2023 19:12
 Operator : CG\JU
 Sample : 03637-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A508

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: BF134366.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	10	15	rBV	1355205	1775865	64.68%	11.970%
2	2.193	15	18	23	rVB2	40348	56590	2.06%	0.381%
3	5.081	506	509	515	rBV	23019	28568	1.04%	0.193%
4	5.475	573	576	592	rBV	1034838	961778	35.03%	6.483%
5	6.475	743	746	756	rBV	656380	566944	20.65%	3.821%
6	6.839	804	808	813	rBV	446907	406401	14.80%	2.739%
7	7.404	899	904	907	rBV	1605535	1471780	53.61%	9.920%
8	8.116	1021	1025	1028	rBV	691448	534461	19.47%	3.602%
9	8.927	1159	1163	1169	rVB	45475	41132	1.50%	0.277%
10	9.198	1204	1209	1211	rBV	2916304	2745504	100.00%	18.505%
11	9.774	1302	1307	1314	rBV3	20162	30165	1.10%	0.203%
12	9.874	1314	1324	1327	rVV	694835	584886	21.30%	3.942%
13	9.904	1327	1329	1334	rVB	55416	49110	1.79%	0.331%
14	10.080	1355	1359	1363	rBV	30334	29501	1.07%	0.199%
15	10.422	1414	1417	1421	rVB2	42653	41244	1.50%	0.278%
16	10.669	1455	1459	1463	rBV	1717105	1581596	57.61%	10.660%
17	10.816	1480	1484	1494	rVB	60314	63562	2.32%	0.428%
18	11.174	1542	1545	1549	rVB	32688	29538	1.08%	0.199%
19	11.369	1574	1578	1580	rBV	598711	494205	18.00%	3.331%
20	11.392	1580	1582	1585	rVB	86513	68238	2.49%	0.460%
21	11.604	1612	1618	1622	rBV	41103	50114	1.83%	0.338%
22	11.898	1664	1668	1672	rBV	213614	195984	7.14%	1.321%
23	12.592	1783	1786	1791	rBV	31552	33671	1.23%	0.227%
24	12.686	1799	1802	1808	rBV2	109635	113606	4.14%	0.766%
25	12.968	1845	1850	1853	rBV	2459524	2125408	77.41%	14.326%
26	13.898	2005	2008	2013	rVB5	28468	39082	1.42%	0.263%
27	14.033	2027	2031	2035	rBV	395051	374899	13.66%	2.527%
28	14.127	2044	2047	2051	rVB	27360	30004	1.09%	0.202%
29	15.539	2282	2287	2294	rBV	240319	312692	11.39%	2.108%

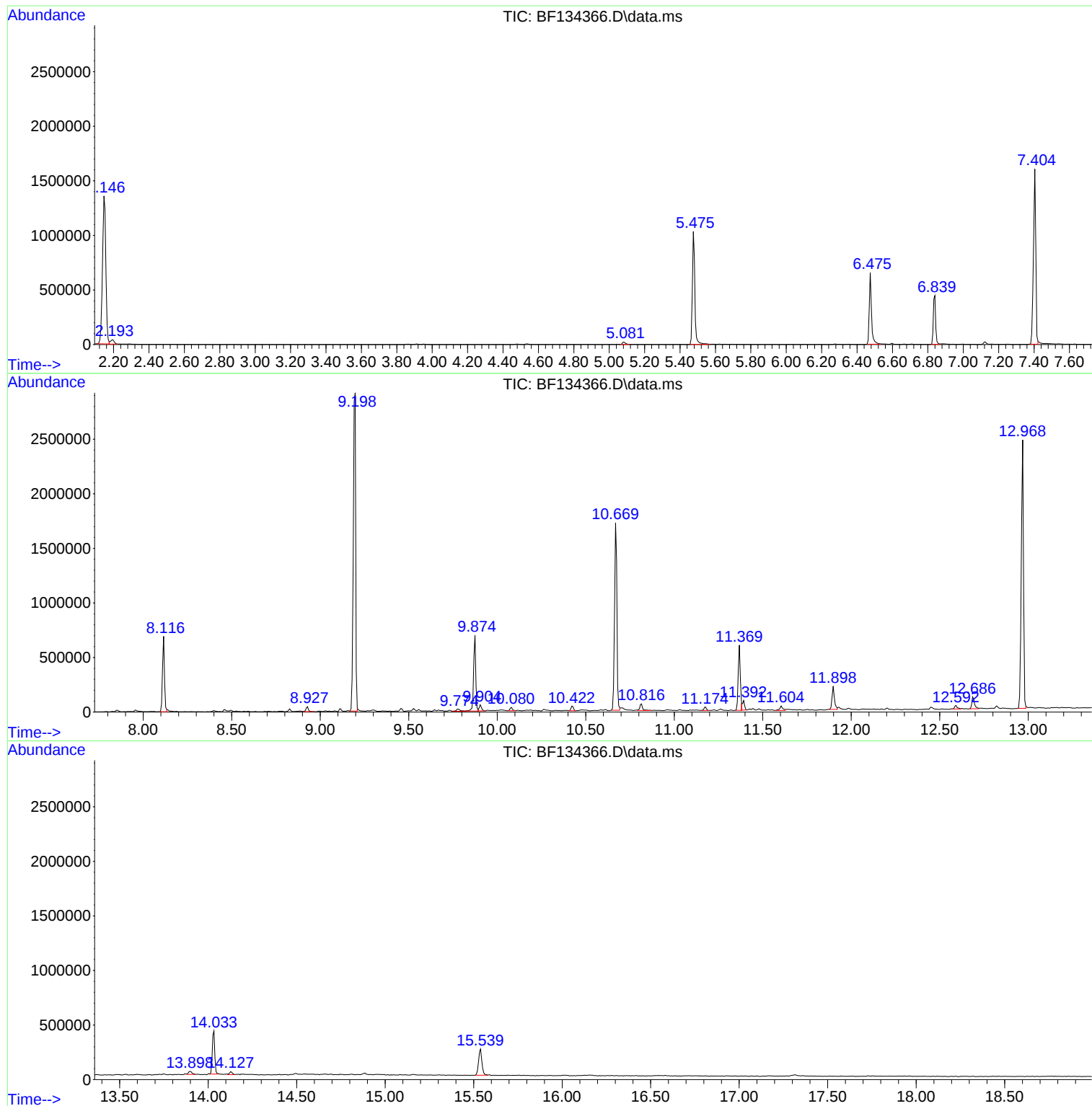
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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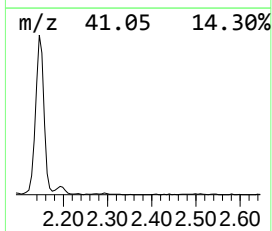
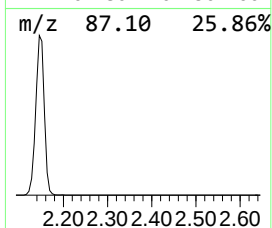
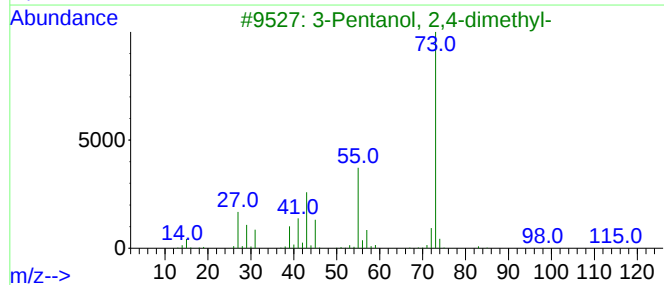
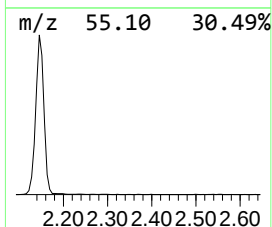
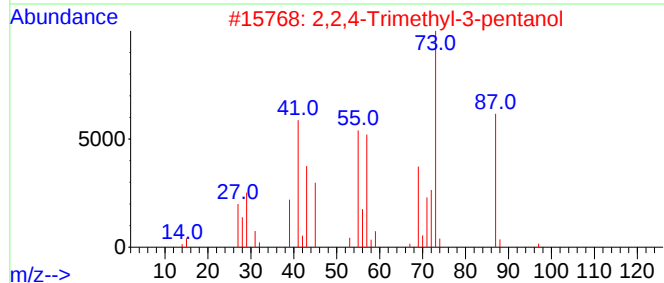
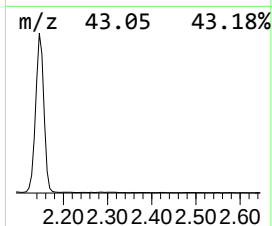
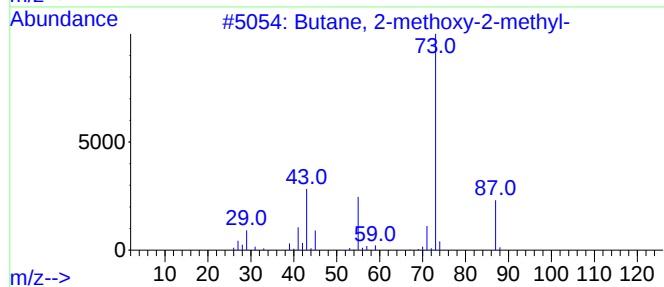
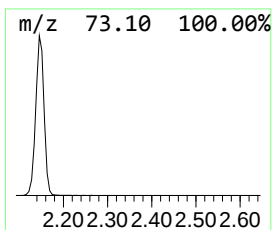
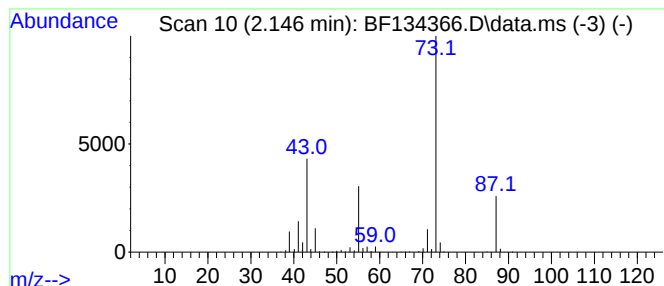
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	87.39 ng	1775870	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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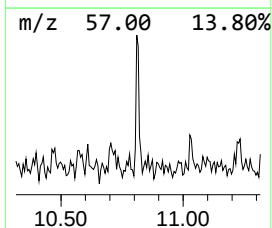
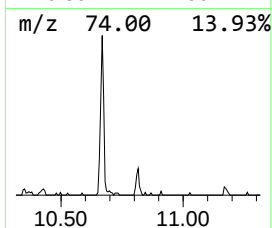
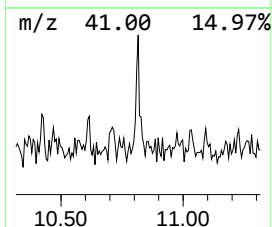
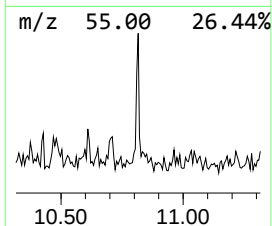
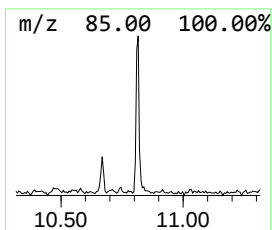
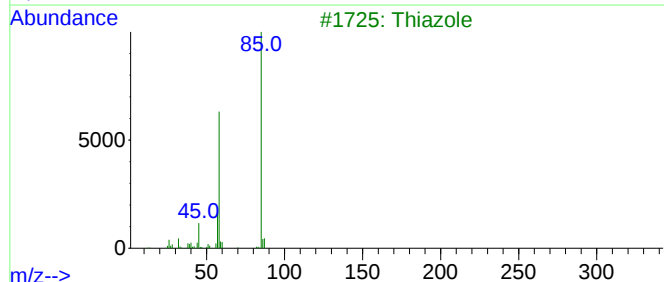
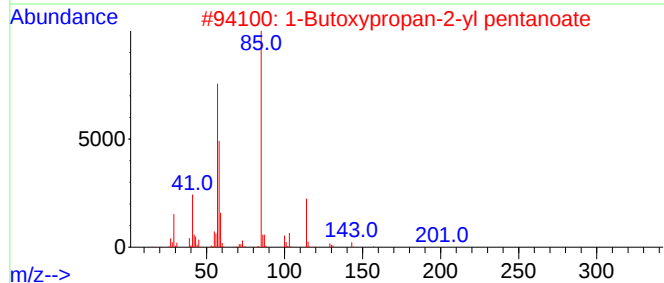
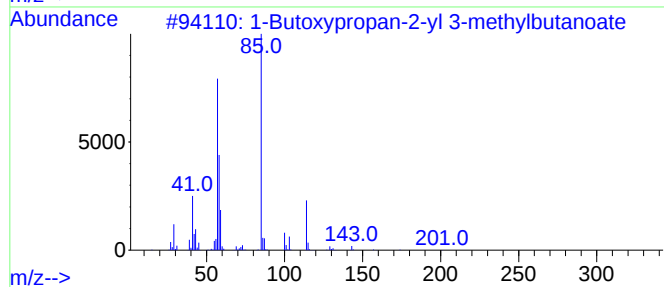
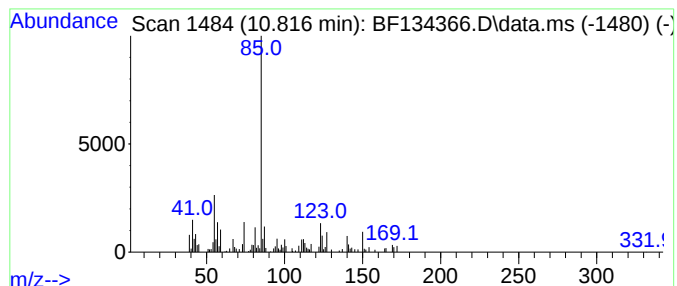
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1-Butoxypropan-2-yl 3-methy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.816	2.57 ng	63562	Phenanthrene-d10	11.368	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butoxypropan-2-yl 3-methylbuta...	216	C12H24O3	1000367-11-9	50
2	1-Butoxypropan-2-yl pentanoate	216	C12H24O3	1000367-12-0	50
3	Thiazole	85	C3H3NS	000288-47-1	47
4	Pentanoic acid, 2-propenyl ester	142	C8H14O2	006321-45-5	47
5	2(3H)-Furanone, 5-hexyldihydro-	170	C10H18O2	000706-14-9	43



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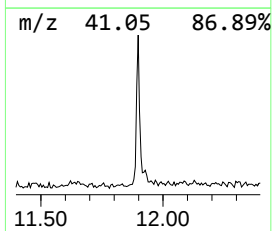
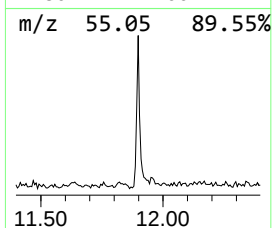
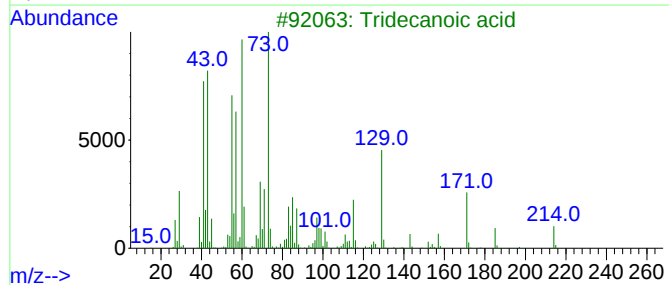
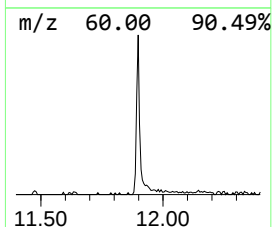
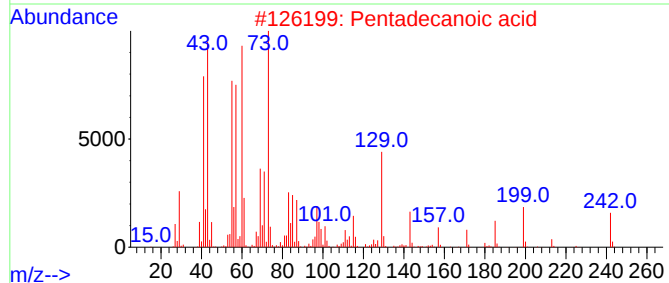
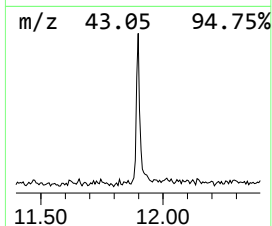
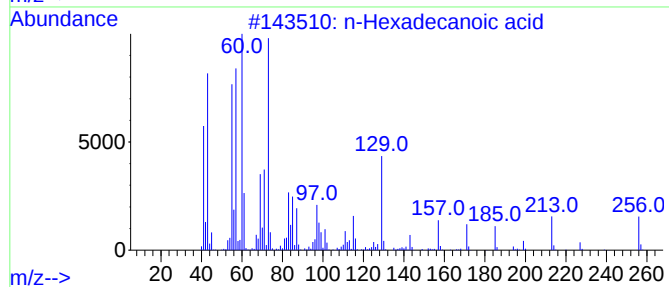
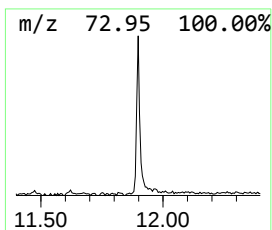
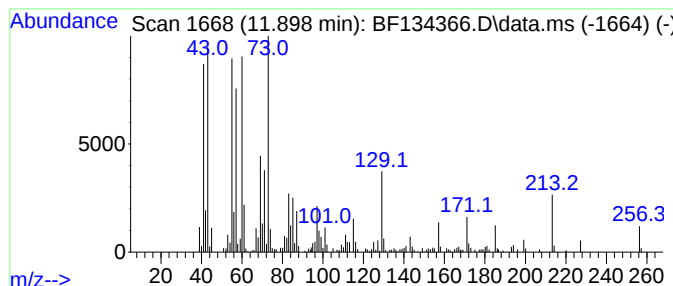
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	7.93 ng	195984	Phenanthrene-d10	11.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Undecanoic acid	186	C11H22O2	000112-37-8	70
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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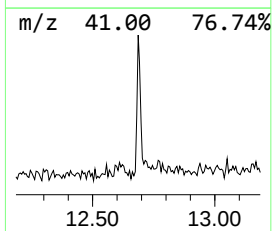
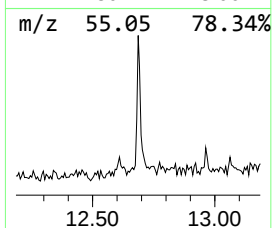
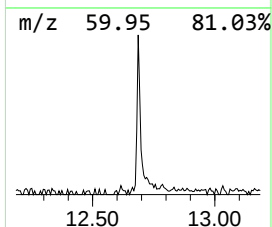
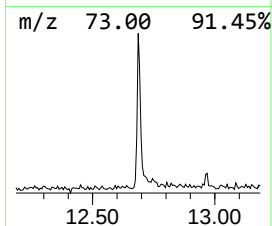
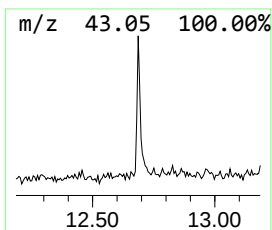
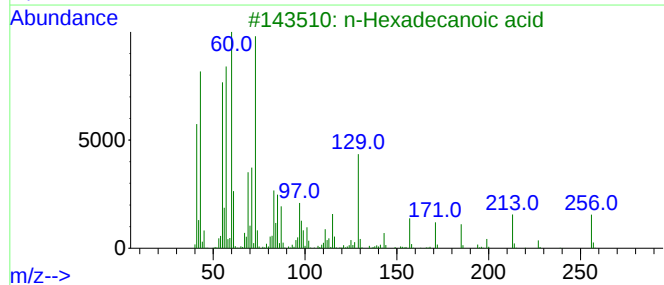
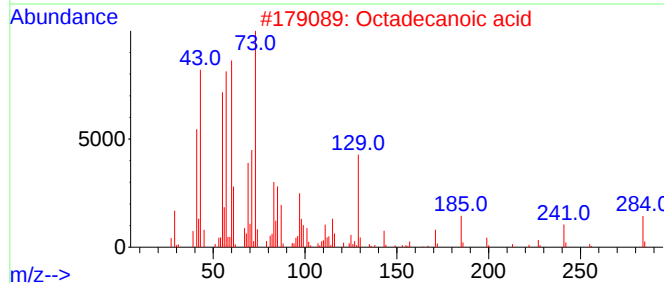
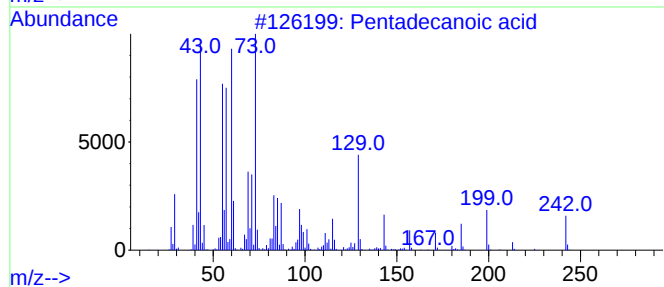
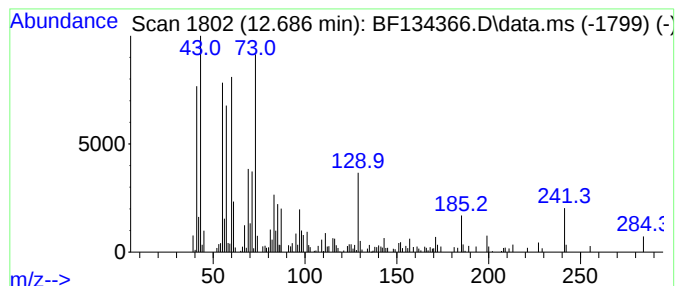
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 Pentadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.686	4.60 ng	113606	Phenanthrene-d10	11.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
2			Octadecanoic acid	284	C18H36O2	000057-11-4	90
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	70



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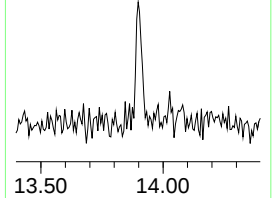
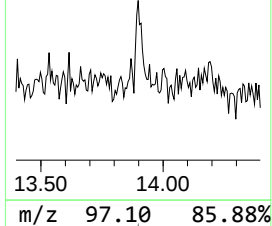
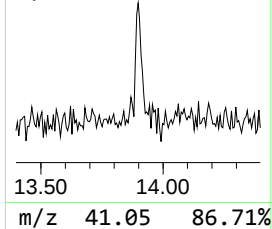
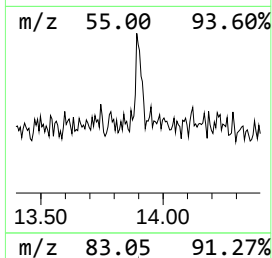
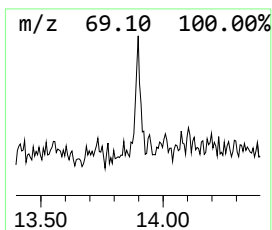
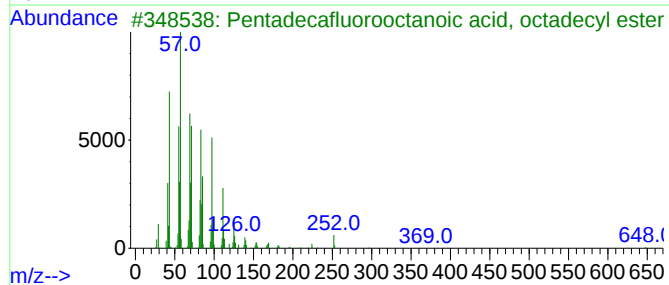
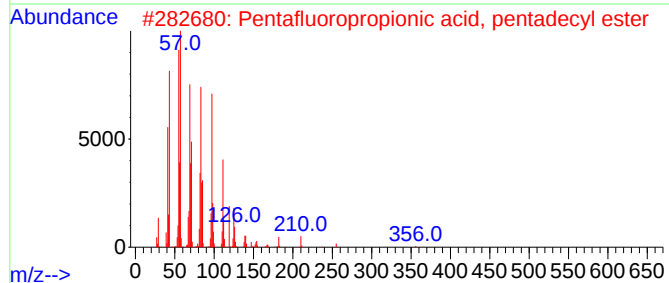
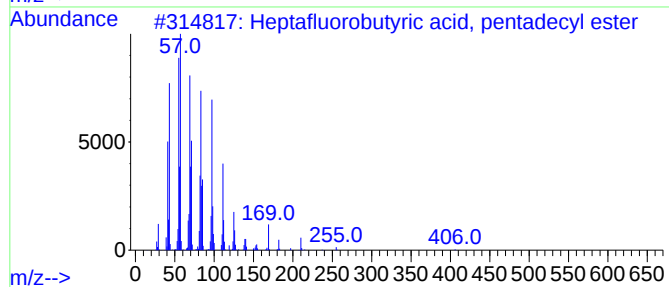
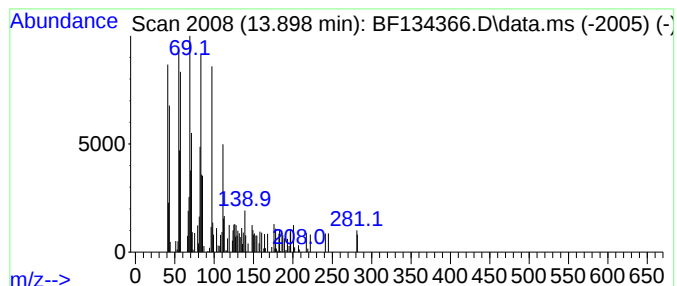
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TIC Library : C:\Database\NIST20.L
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Peak Number 7 Heptafluorobutyric acid, pe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	2.08 ng	39082	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	87
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	87
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	83
4			1-Hexacosene	364	C26H52	018835-33-1	83
5			1-Tetracosene	336	C24H48	010192-32-2	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.146	87.4	ng	1775870	1	6.839	406401	20.0
1-Butoxypropan-...	10.816	2.6	ng	63562	4	11.368	494205	20.0
n-Hexadecanoic ...	11.898	7.9	ng	195984	4	11.368	494205	20.0
Pentadecanoic acid	12.686	4.6	ng	113606	4	11.368	494205	20.0
Heptafluorobuty...	13.898	2.1	ng	39082	5	14.033	374899	20.0