

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112322\
 Data File : BF131367.D
 Acq On : 23 Nov 2022 18:19
 Operator : CG\JU
 Sample : N5765-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-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-BF112122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131367.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	13	rVB2	49983	75949	2.50%	0.322%
2	2.334	35	42	48	rBV	941208	1186535	39.03%	5.032%
3	2.446	57	61	67	rVB	51387	65363	2.15%	0.277%
4	5.187	522	527	535	rVB	523912	638099	20.99%	2.706%
5	5.569	586	592	595	rBV	2676409	2624581	86.34%	11.130%
6	6.563	755	761	764	rBV	2174922	2687685	88.42%	11.397%
7	6.951	823	827	830	rVB	889906	759765	24.99%	3.222%
8	7.516	917	923	926	rBV	1648565	1731277	56.96%	7.342%
9	8.239	1040	1046	1049	rBV	1082938	1002124	32.97%	4.250%
10	8.816	1138	1144	1148	rBV2	24274	31033	1.02%	0.132%
11	9.322	1223	1230	1233	rBV	3059054	3039682	100.00%	12.890%
12	9.392	1237	1242	1245	rBV	34333	30788	1.01%	0.131%
13	9.916	1327	1331	1337	rBV2	47952	53952	1.77%	0.229%
14	10.004	1339	1346	1349	rBV	1373814	1172099	38.56%	4.970%
15	10.722	1462	1468	1473	rBV	59619	55801	1.84%	0.237%
16	10.798	1473	1481	1484	rBV	2116201	2017672	66.38%	8.556%
17	11.498	1594	1600	1604	rBV	1302165	1188049	39.08%	5.038%
18	11.604	1615	1618	1621	rBV	40460	31802	1.05%	0.135%
19	12.086	1697	1700	1705	rBV	87991	72777	2.39%	0.309%
20	12.274	1729	1732	1740	rBV4	39683	55681	1.83%	0.236%
21	13.098	1867	1872	1875	rBV	3210412	2819261	92.75%	11.955%
22	13.992	2020	2024	2034	rBV2	105270	203227	6.69%	0.862%
23	14.157	2048	2052	2055	rVB	1011364	905207	29.78%	3.839%
24	14.315	2075	2079	2086	rVB	32358	32261	1.06%	0.137%
25	14.933	2180	2184	2186	rBV	76542	87969	2.89%	0.373%
26	15.315	2245	2249	2255	rVB	40388	46849	1.54%	0.199%
27	15.692	2307	2313	2317	rBV	566237	713616	23.48%	3.026%
28	15.727	2317	2319	2327	rVB2	45366	55840	1.84%	0.237%
29	16.204	2395	2400	2405	rBV	35486	56702	1.87%	0.240%
30	16.751	2489	2493	2501	rVB2	31439	59235	1.95%	0.251%
31	17.403	2597	2604	2610	rBV2	18389	39456	1.30%	0.167%
32	18.162	2728	2733	2745	rVB4	16336	41232	1.36%	0.175%

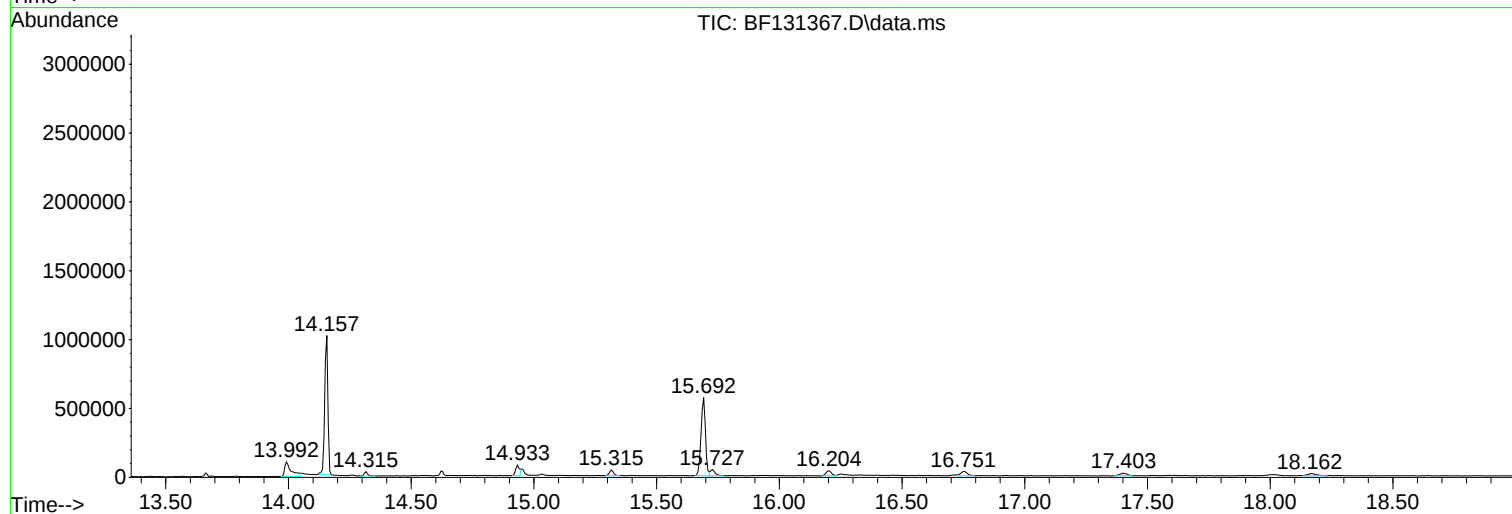
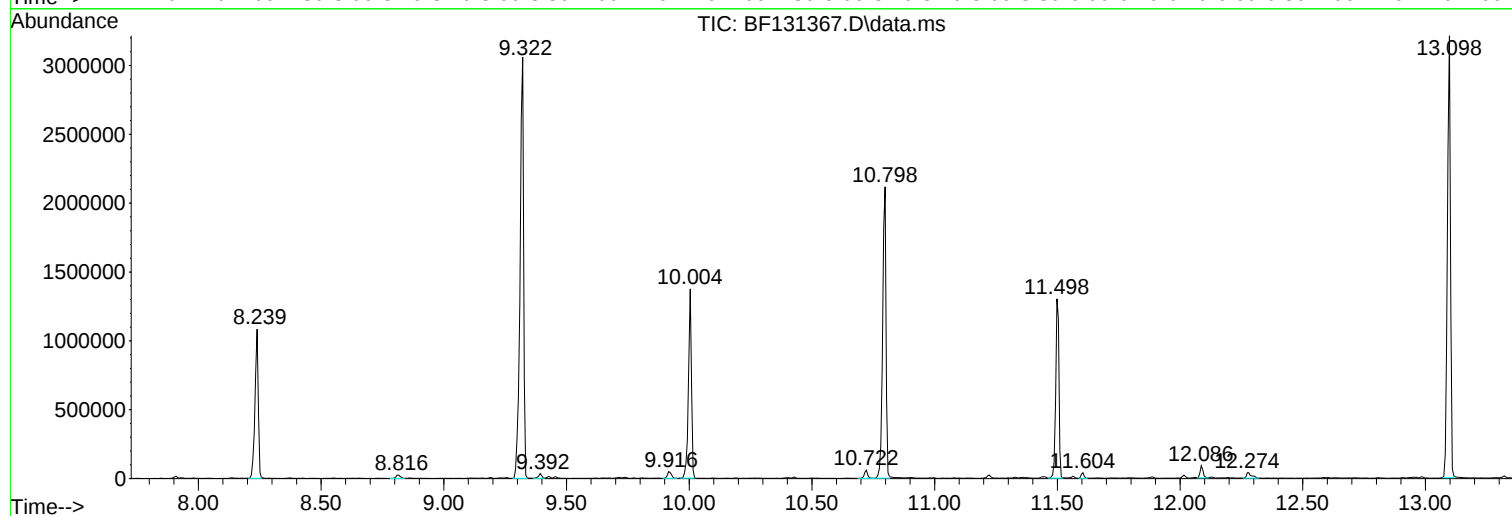
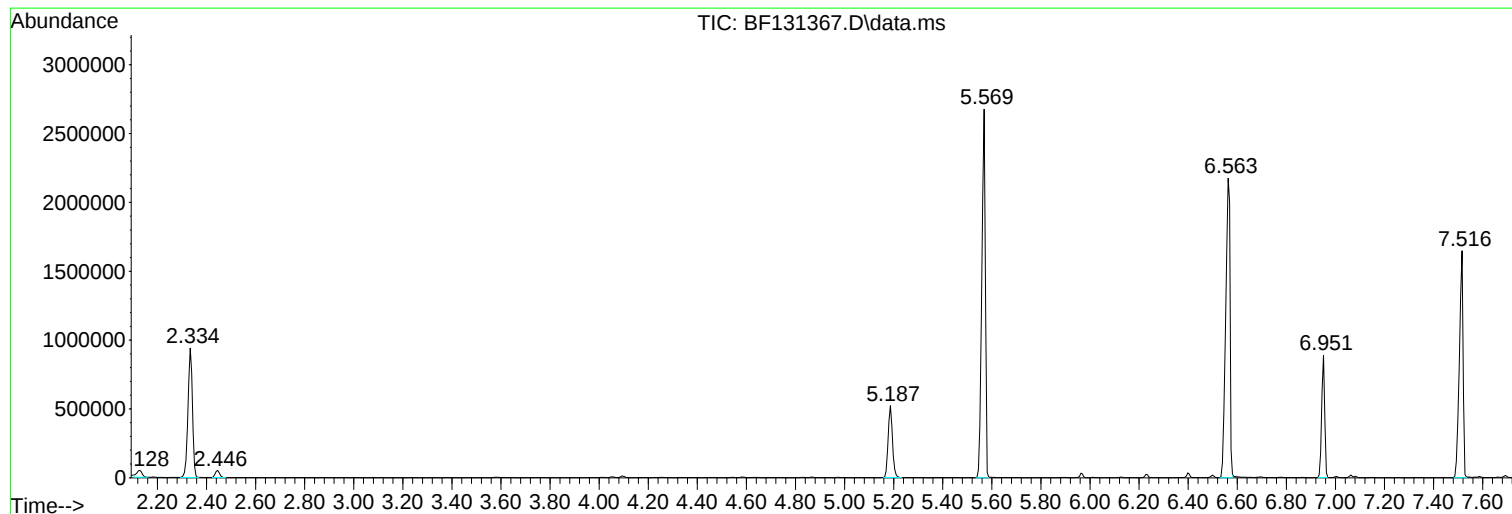
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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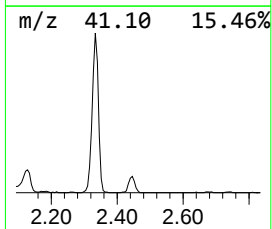
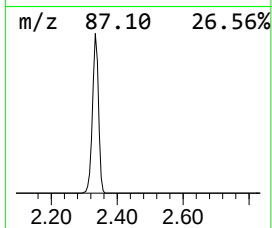
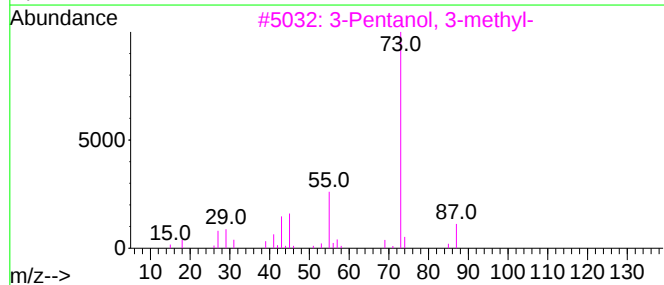
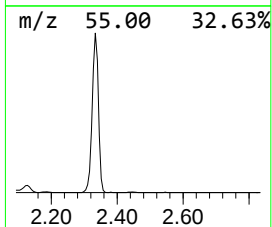
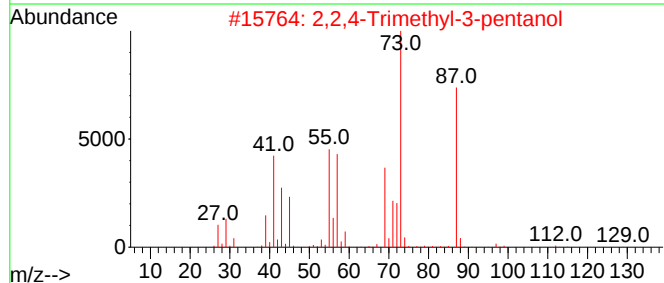
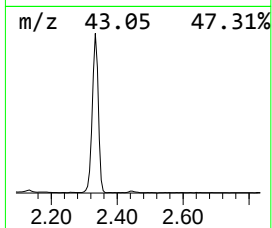
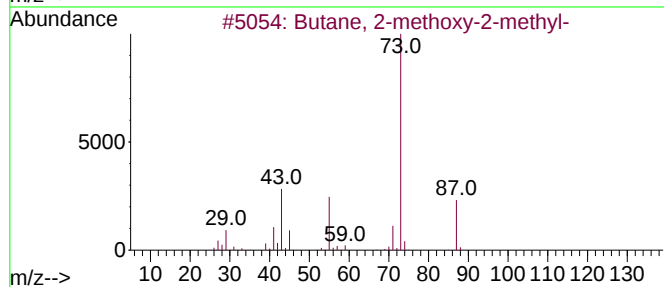
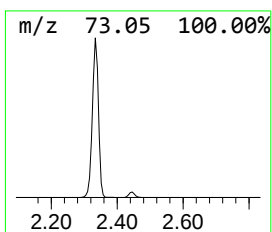
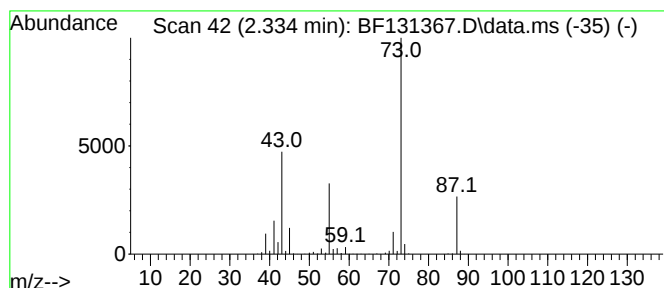
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.334	31.23 ng	1186540	1,4-Dichlorobenzene-d4	6.951

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, 3-methyl-	102	C6H14O	000077-74-7	38
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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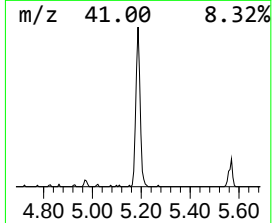
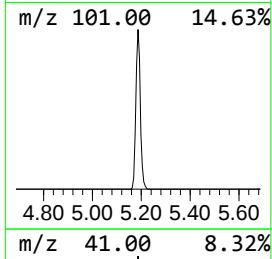
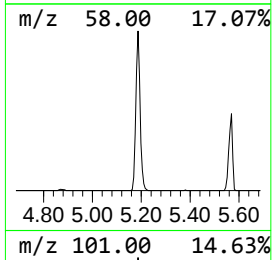
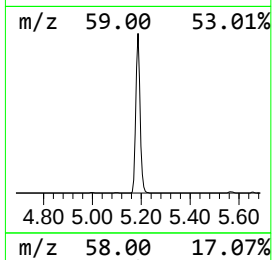
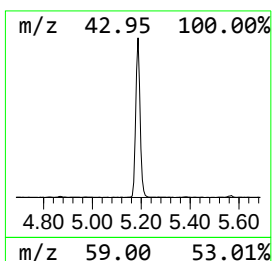
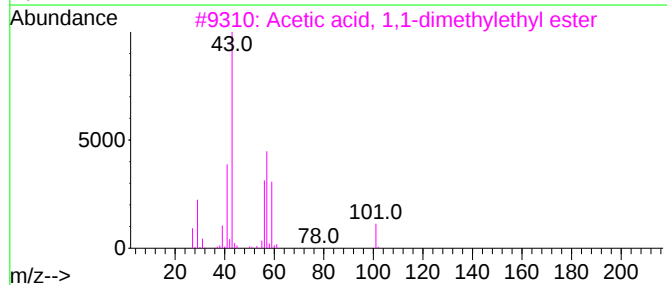
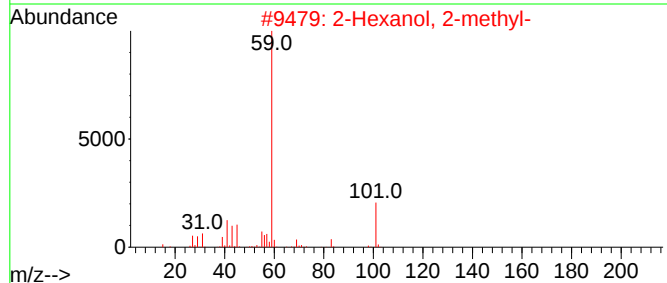
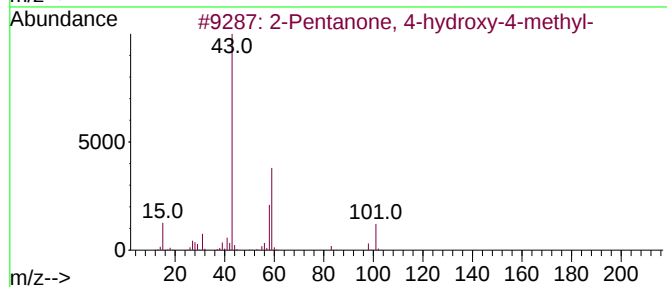
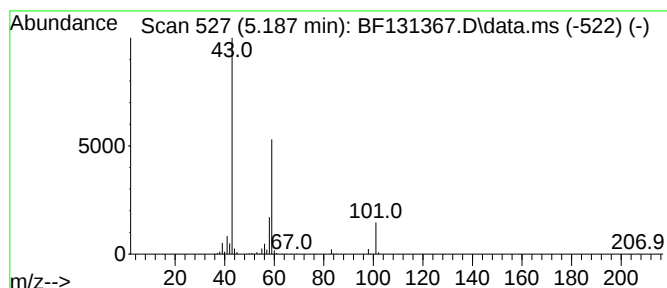
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.187	16.80 ng	638099	1,4-Dichlorobenzene-d4	6.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	32
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



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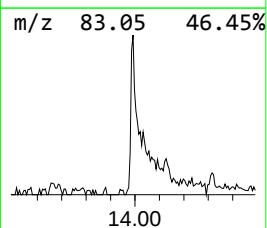
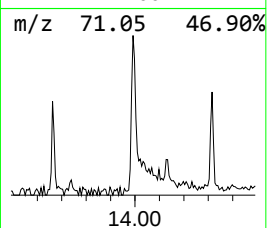
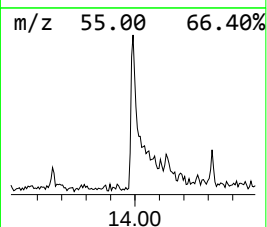
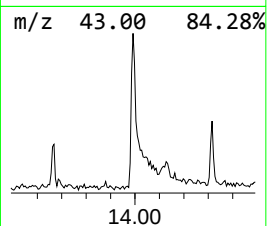
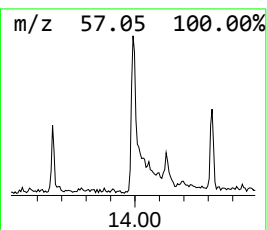
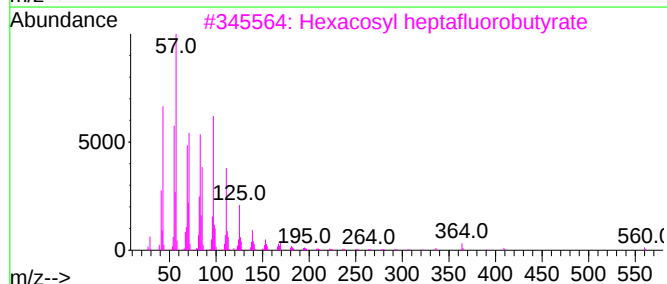
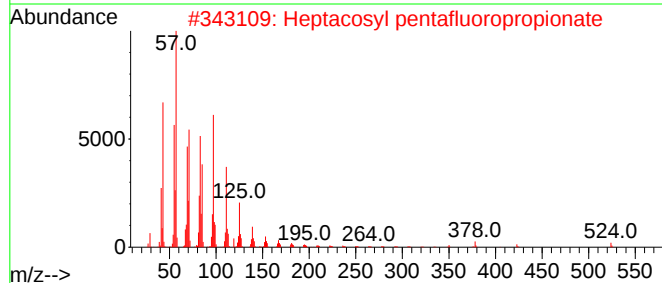
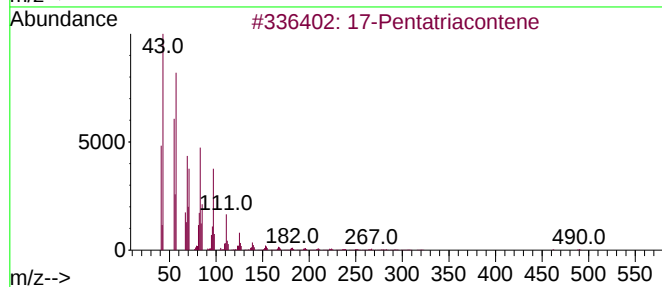
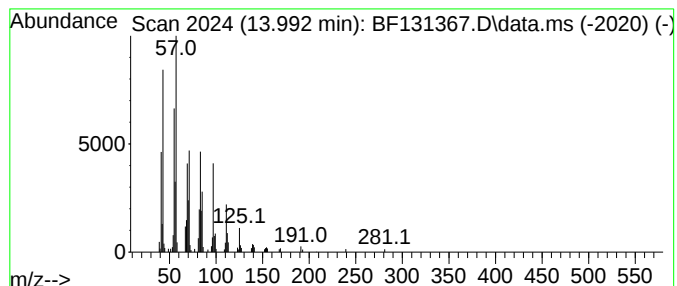
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Peak Number 3 17-Pentatriacontene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.992	4.49 ng	203227	Chrysene-d12	14.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	91
2			Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	91
3			Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	91
4			Triacetyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	91
5			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	91



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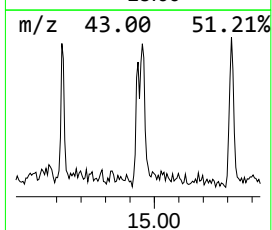
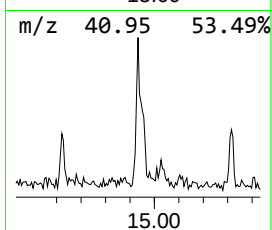
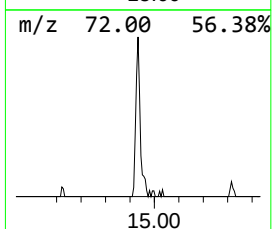
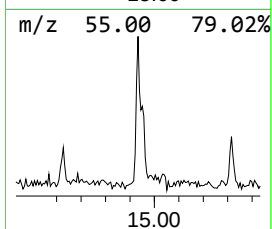
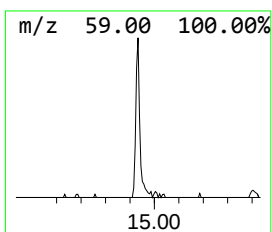
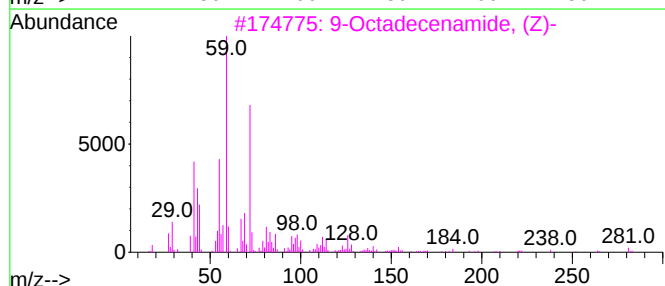
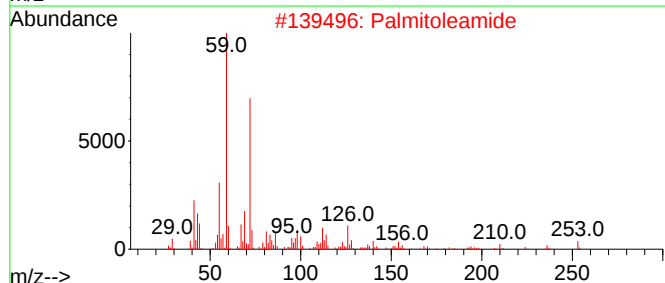
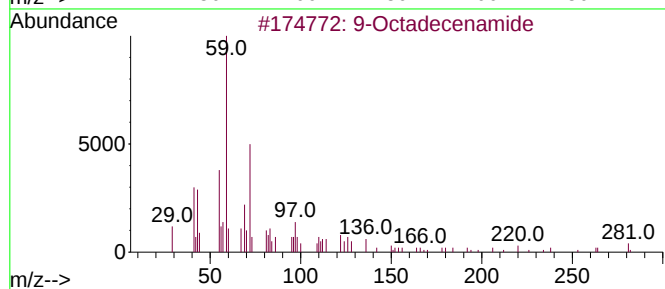
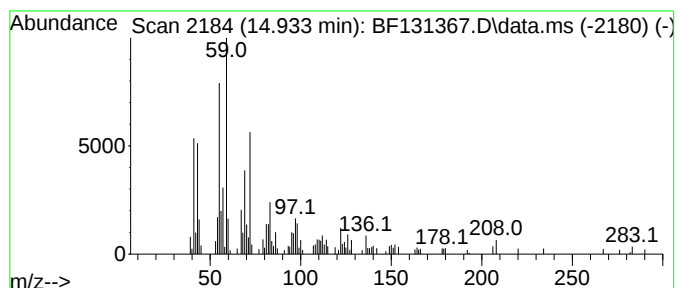
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Peak Number 4 9-Octadecenamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	2.47 ng	87969	Perylene-d12	15.692

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide	281	C18H35NO	003322-62-1	83
2			Palmitoleamide	253	C16H31NO	106010-22-4	72
3			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
4			Octadecanamide	283	C18H37NO	000124-26-5	58
5			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.334	31.2	ng	1186540	1	6.951	759765	20.0
2-Pentanone, 4-...	5.187	16.8	ng	638099	1	6.951	759765	20.0
17-Pentatriacon...	13.992	4.5	ng	203227	5	14.157	905207	20.0
9-Octadecenamide	14.933	2.5	ng	87969	6	15.692	713616	20.0