

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
 Data File : BF122370.D
 Acq On : 18 Nov 2020 16:29
 Operator : JU/CG
 Sample : L4737-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MS-MSD

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-BF110920.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122370.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	34	rVB	2291508	3092786	36.89%	5.821%
2	5.469	570	575	578	rBV	3432715	3030356	36.15%	5.703%
3	6.475	742	746	755	rBV	2311478	2088921	24.92%	3.931%
4	6.687	779	782	791	rBV	122259	115336	1.38%	0.217%
5	6.863	808	812	815	rBV	1809135	1390782	16.59%	2.617%
6	7.428	902	908	911	rBV	4621854	4484211	53.49%	8.439%
7	8.145	1026	1030	1034	rBV	1964880	1838482	21.93%	3.460%
8	9.228	1209	1214	1217	rBV	8478625	7960647	94.96%	14.982%
9	9.616	1276	1280	1291	rVB	786423	669825	7.99%	1.261%
10	9.904	1325	1329	1341	rVB	2629146	2241009	26.73%	4.218%
11	10.692	1458	1463	1466	rBV	5930877	5558837	66.31%	10.462%
12	11.386	1577	1581	1585	rBV	2598672	2387132	28.48%	4.493%
13	11.922	1667	1672	1686	rBV2	817735	1098459	13.10%	2.067%
14	12.374	1745	1749	1752	rBV	208406	188510	2.25%	0.355%
15	12.627	1786	1792	1797	rBV3	60621	101943	1.22%	0.192%
16	12.704	1802	1805	1810	rBV	455553	495451	5.91%	0.932%
17	12.980	1847	1852	1855	rBV	8656398	8383106	100.00%	15.777%
18	13.598	1954	1957	1960	rBV	182059	171719	2.05%	0.323%
19	13.880	2001	2005	2015	rBV	837423	1293429	15.43%	2.434%
20	14.027	2025	2030	2033	rBV	2949939	2588115	30.87%	4.871%
21	14.198	2056	2059	2066	rBV	162713	165897	1.98%	0.312%
22	14.504	2106	2111	2113	rBV	211222	200668	2.39%	0.378%
23	14.810	2160	2163	2169	rVB	211799	213435	2.55%	0.402%
24	15.151	2217	2221	2227	rBV	193366	224631	2.68%	0.423%
25	15.498	2274	2280	2284	rBV	1839884	2454582	29.28%	4.619%
26	15.539	2284	2287	2294	rVB	176415	227553	2.71%	0.428%
27	15.980	2357	2362	2367	rVB	104571	154472	1.84%	0.291%
28	16.045	2367	2373	2380	rBV5	65587	191183	2.28%	0.360%
29	16.486	2443	2448	2452	rBV3	59623	123820	1.48%	0.233%

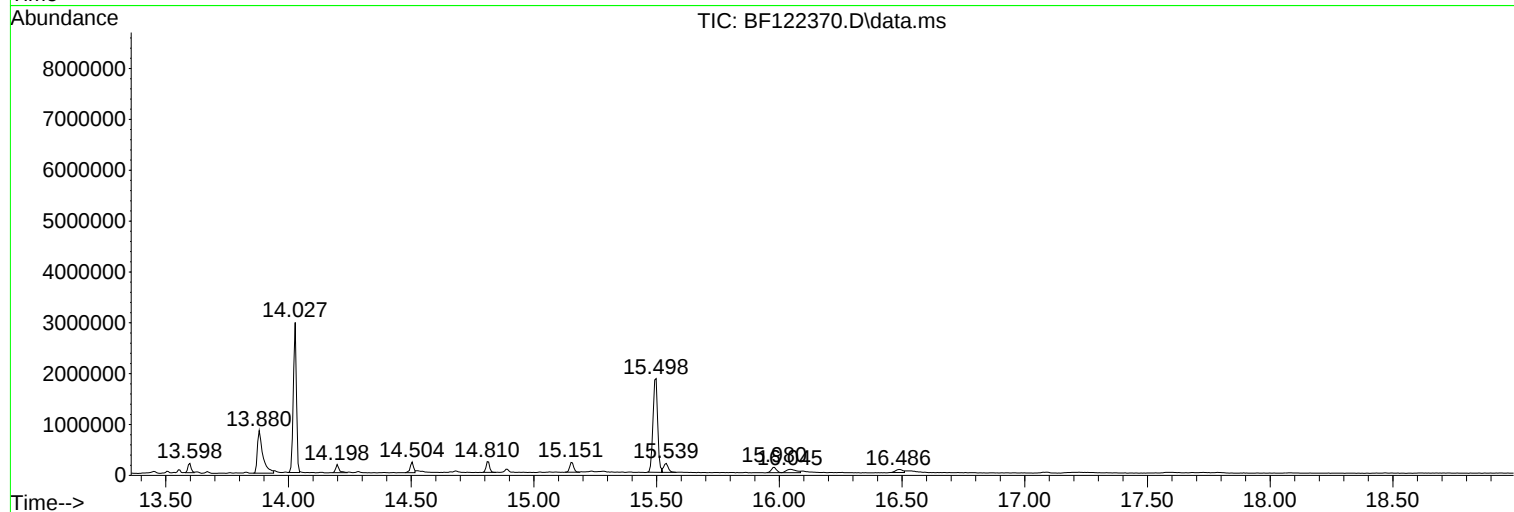
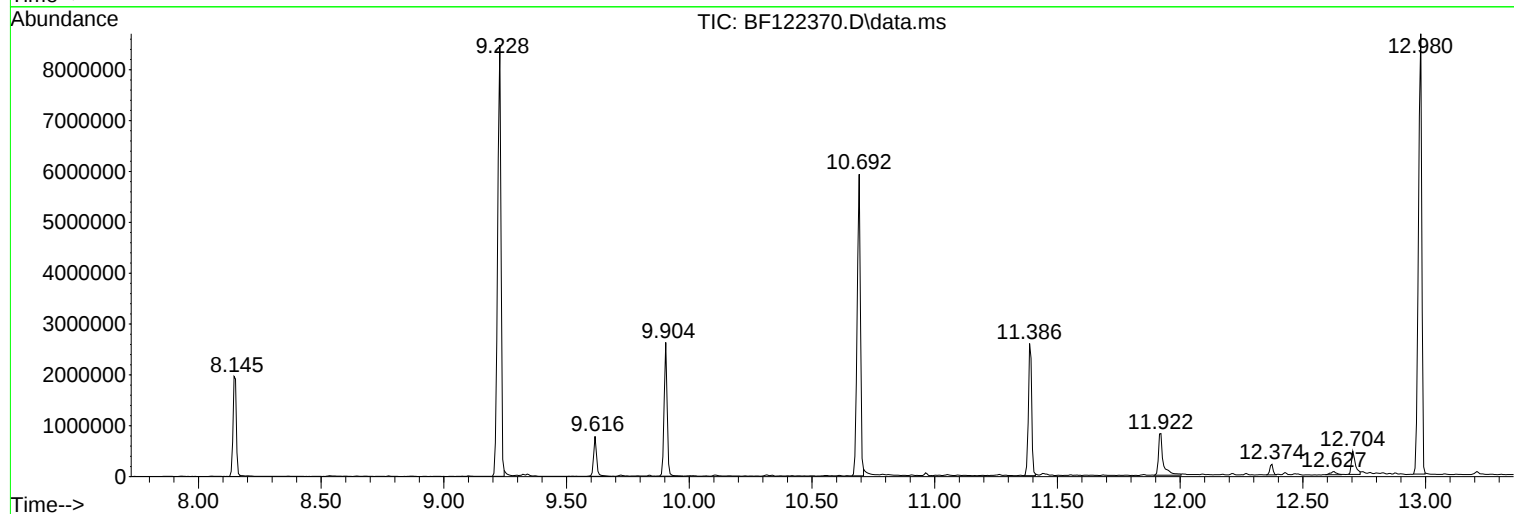
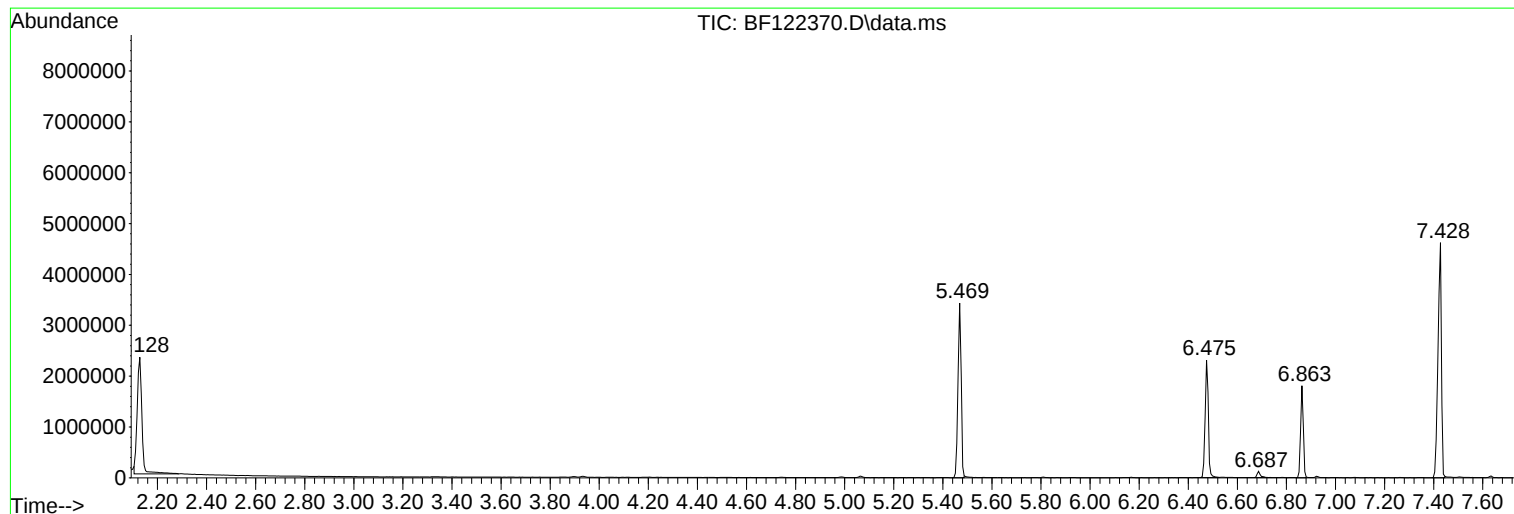
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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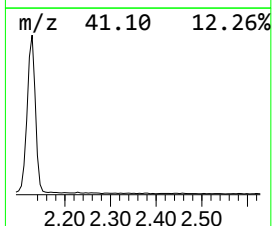
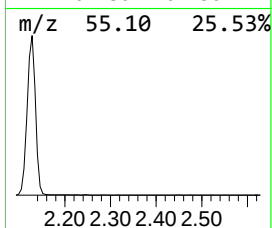
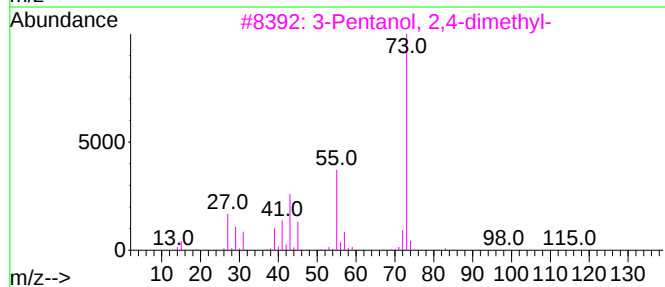
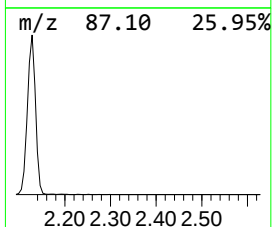
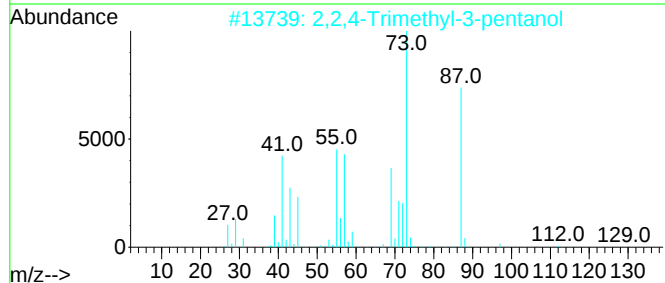
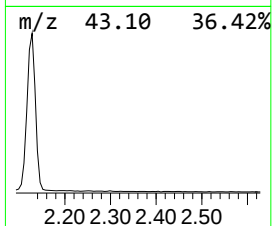
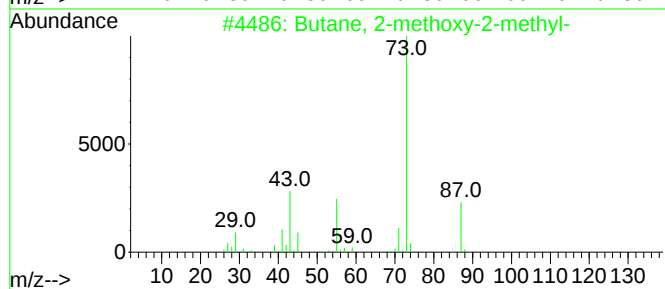
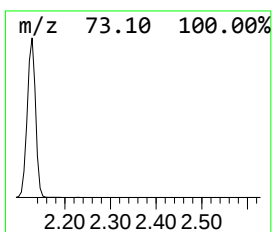
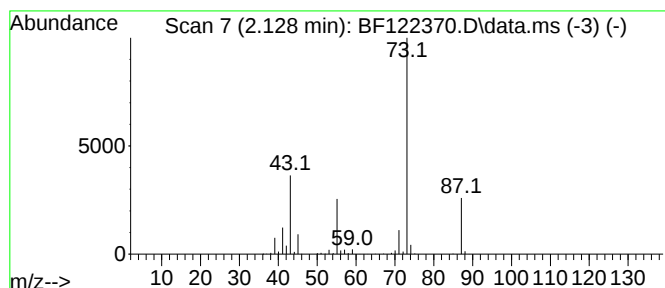
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
2.128	44.48 ng	3092790	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
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	37
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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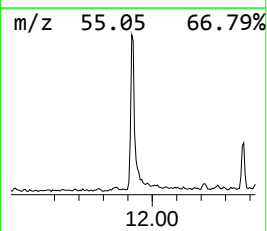
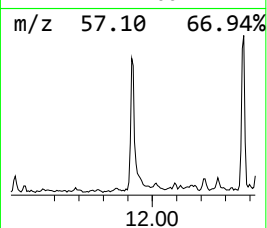
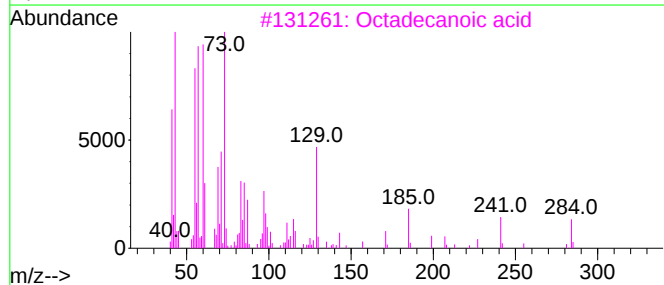
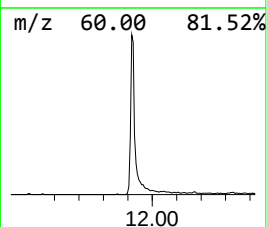
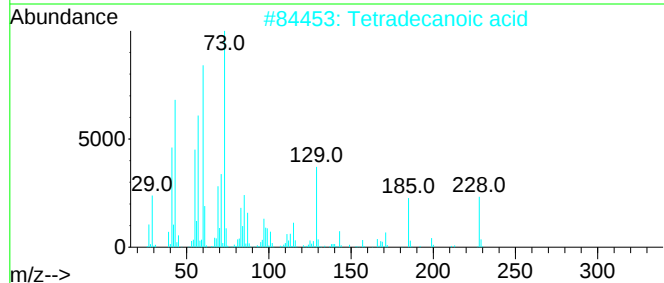
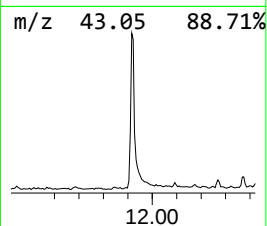
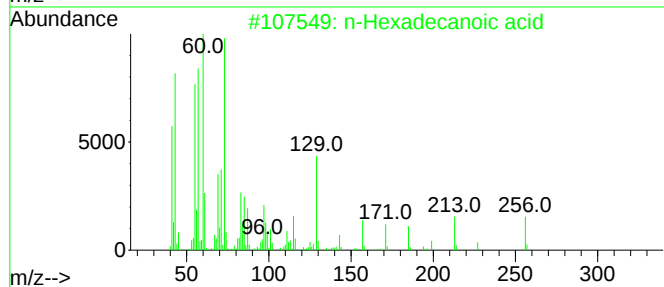
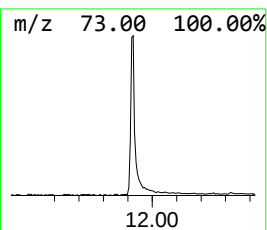
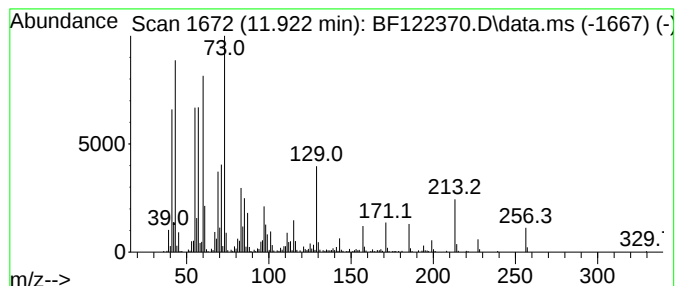
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	9.20 ng	1098460	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Octadecanoic acid	284	C18H36O2	000057-11-4	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			Tridecanoic acid	214	C13H26O2	000638-53-9	87



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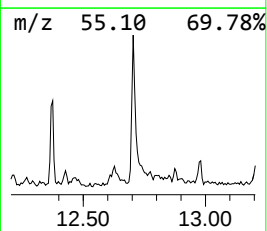
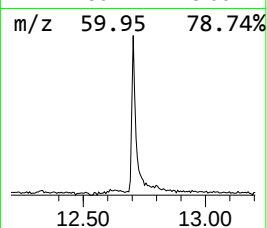
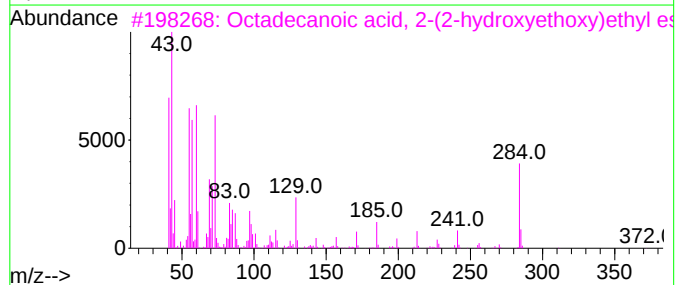
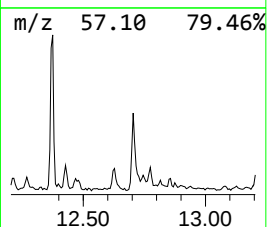
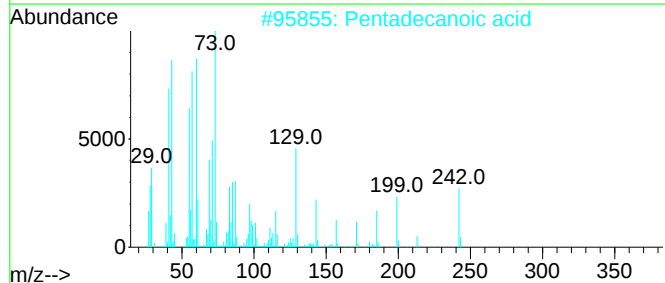
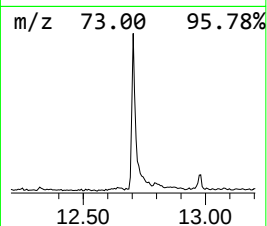
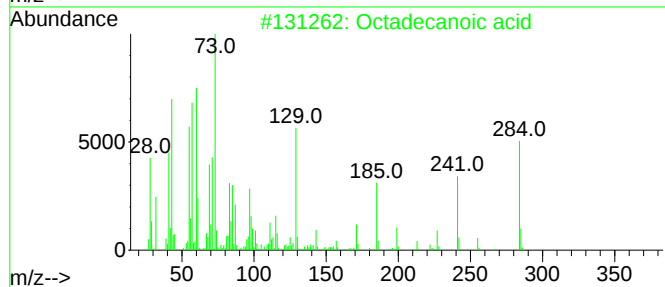
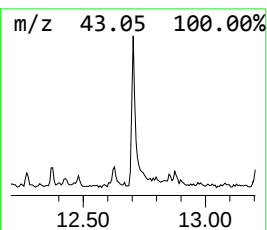
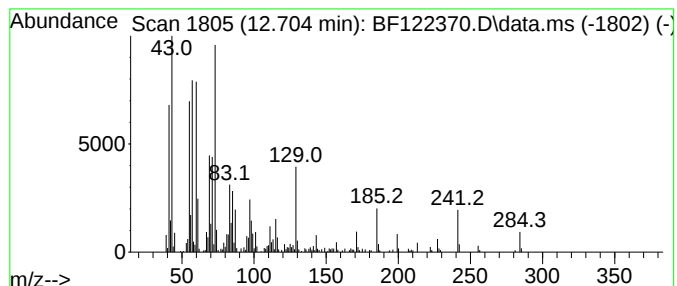
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	4.15 ng	495451	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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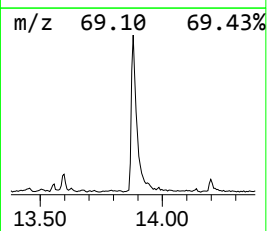
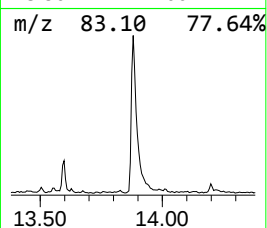
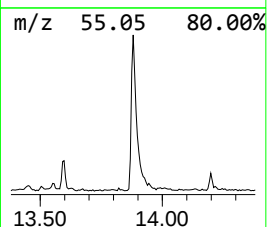
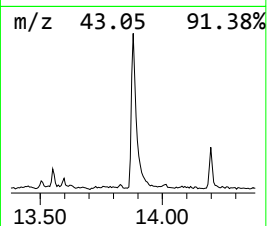
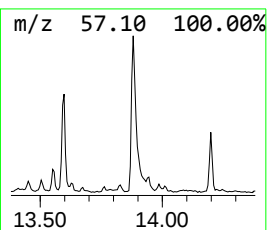
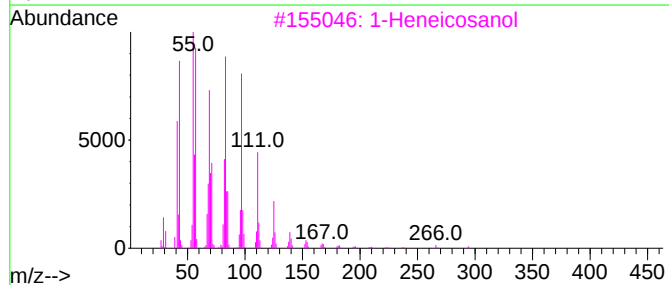
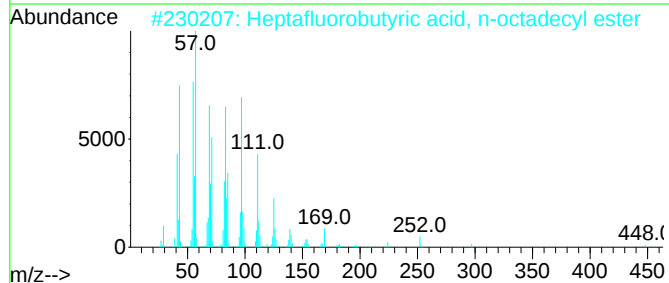
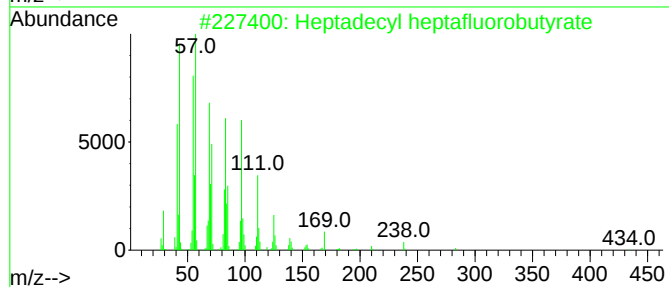
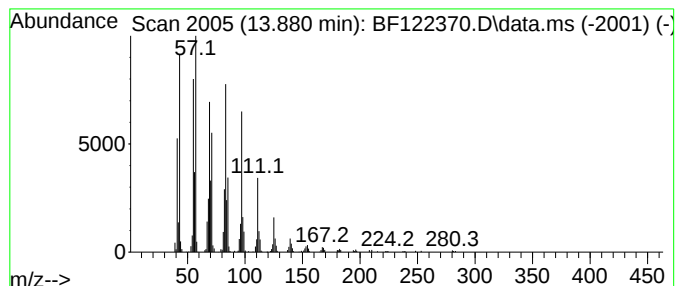
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Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	10.00 ng	1293430	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	91
5			Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.128	44.5	ng	3092790	1	6.863	1390780	20.0
n-Hexadecanoic ...	11.922	9.2	ng	1098460	4	11.386	2387130	20.0
Octadecanoic acid	12.704	4.2	ng	495451	4	11.386	2387130	20.0
Heptadecyl hept...	13.880	10.0	ng	1293430	5	14.027	2588120	20.0