

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082420\
 Data File : BF121413.D
 Acq On : 24 Aug 2020 22:32
 Operator : JU/CG
 Sample : L3719-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20200510-AMENDED-COMP-A

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BF081920.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.875	470	474	491	rVB	215011	285142	10.56%	1.319%
2	5.310	544	548	569	rBV	1722150	1915725	70.93%	8.860%
3	6.345	720	724	741	rBV	2189057	2290340	84.80%	10.592%
4	6.534	753	756	768	rVB	34868	42514	1.57%	0.197%
5	6.693	780	783	787	rBV	1050840	851239	31.52%	3.937%
6	7.263	875	880	890	rBV	1462540	1471525	54.48%	6.806%
7	7.410	901	905	908	rBV	136309	114419	4.24%	0.529%
8	7.975	998	1001	1017	rVB	1269866	1165132	43.14%	5.389%
9	8.151	1026	1031	1039	rBV3	12005	37045	1.37%	0.171%
10	9.051	1180	1184	1187	rBV	2894681	2556171	94.64%	11.822%
11	9.116	1192	1195	1202	rVB2	47697	47458	1.76%	0.219%
12	9.445	1248	1251	1259	rBV	294552	264619	9.80%	1.224%
13	9.569	1264	1272	1279	rVB	25470	38899	1.44%	0.180%
14	9.728	1295	1299	1302	rBV	1645349	1347845	49.90%	6.234%
15	10.516	1430	1433	1443	rBV	937078	900346	33.33%	4.164%
16	10.633	1450	1453	1462	rVB	138591	120502	4.46%	0.557%
17	10.786	1471	1479	1482	rBV4	35104	81423	3.01%	0.377%
18	10.892	1493	1497	1503	rBV3	16949	31101	1.15%	0.144%
19	11.092	1523	1531	1540	rBV6	25303	61913	2.29%	0.286%
20	11.210	1547	1551	1555	rBV	1718446	1491001	55.20%	6.896%
21	12.798	1816	1821	1824	rBV	2829907	2700917	100.00%	12.491%
22	13.033	1857	1861	1868	rBV2	31927	43775	1.62%	0.202%
23	13.292	1898	1905	1909	rBV	76605	89083	3.30%	0.412%
24	13.704	1968	1975	1989	rBV2	315927	664372	24.60%	3.073%
25	13.851	1996	2000	2003	rBV	1502705	1369374	50.70%	6.333%
26	14.016	2025	2028	2031	rBV	57300	51570	1.91%	0.239%
27	14.321	2077	2080	2082	rBV	62824	49930	1.85%	0.231%
28	14.363	2082	2087	2093	rVV6	20380	39162	1.45%	0.181%
29	14.610	2126	2129	2135	rVB2	105036	128116	4.74%	0.593%
30	14.933	2180	2184	2189	rBV	57785	61592	2.28%	0.285%
31	15.263	2235	2240	2250	rVB	1063939	1254955	46.46%	5.804%
32	15.680	2308	2311	2318	rVB2	39161	55098	2.04%	0.255%

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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-BF081920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

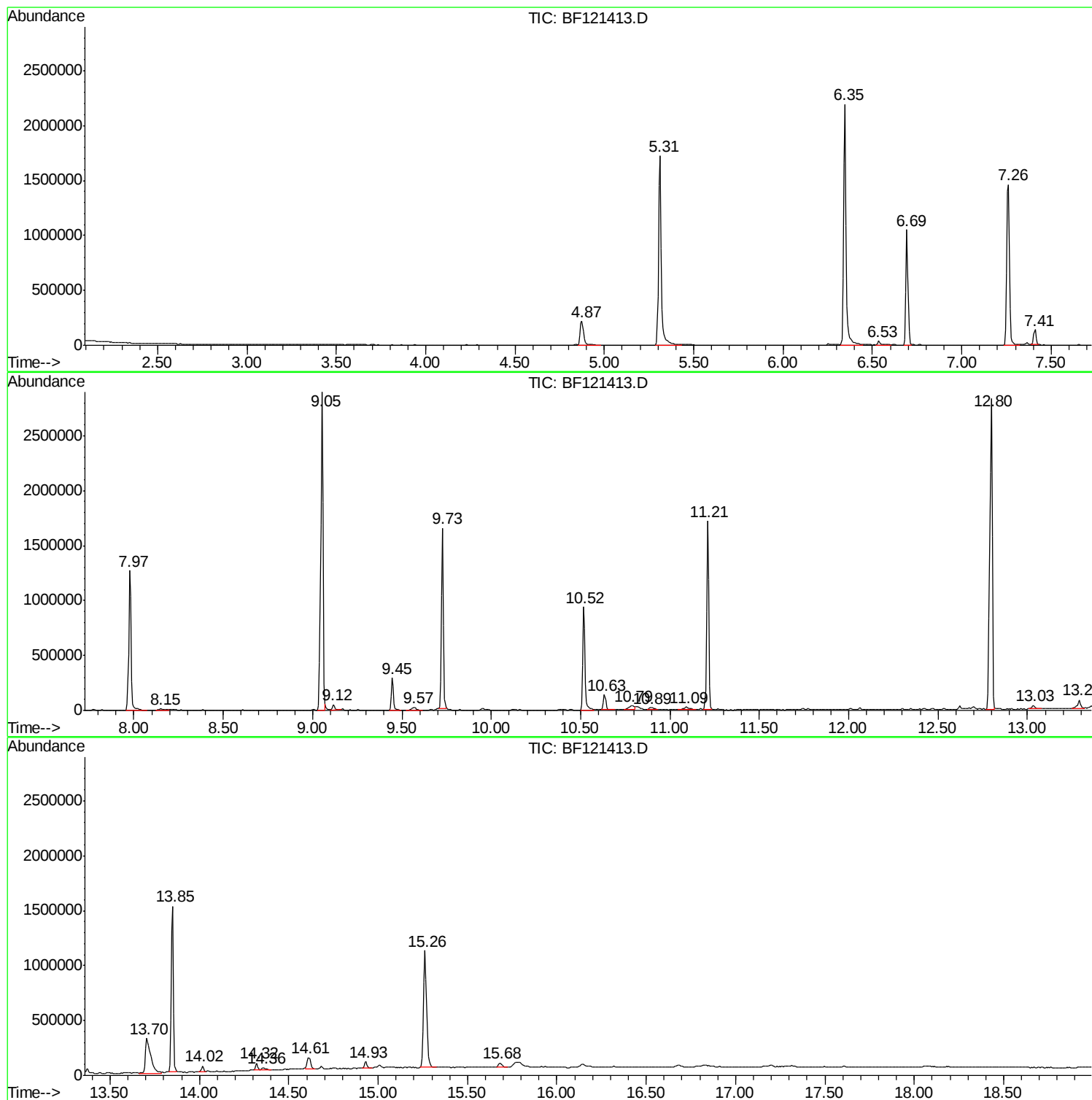
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF081920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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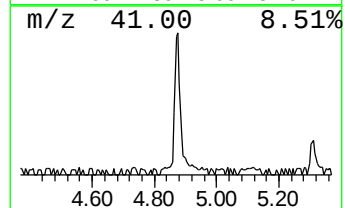
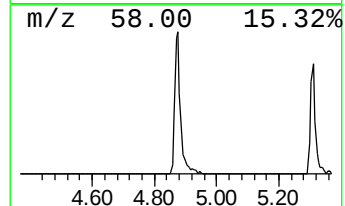
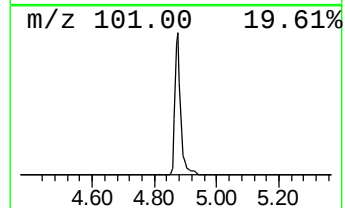
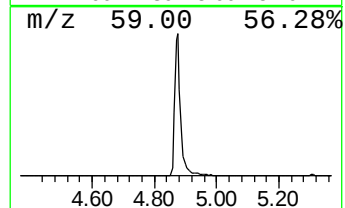
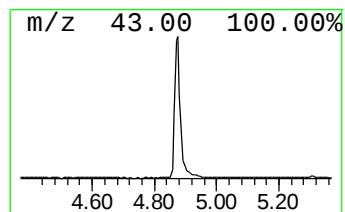
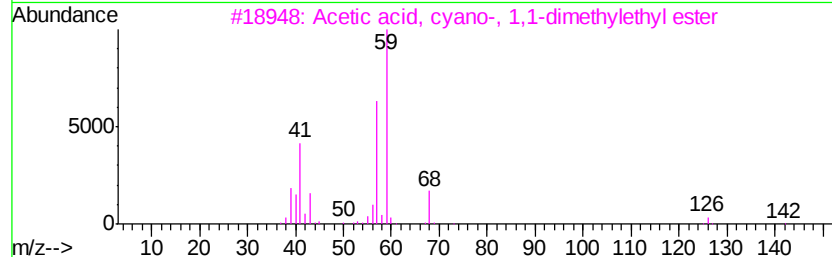
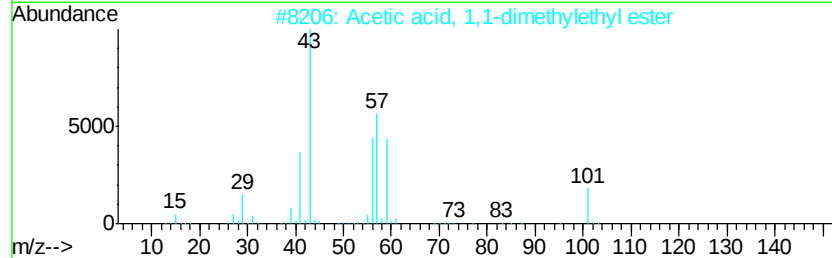
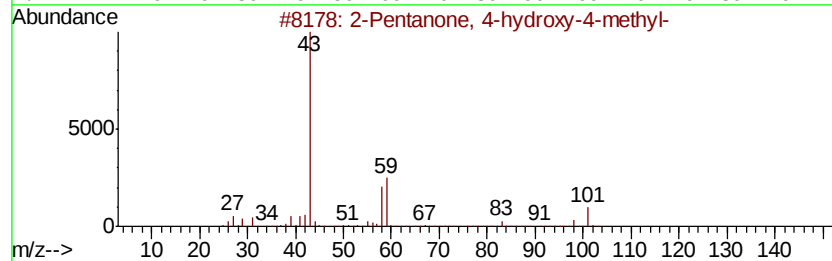
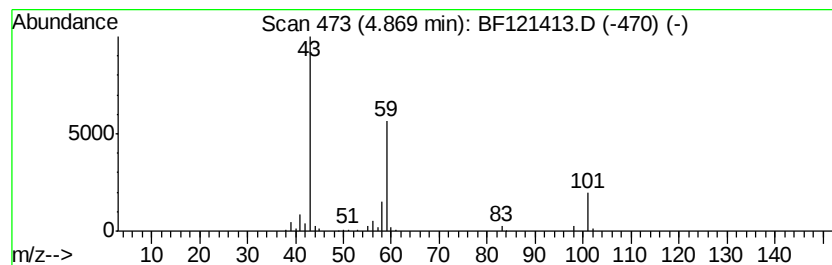
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.87	6.70 ng	285142	1,4-Dichlorobenzene-d4	6.69	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethv...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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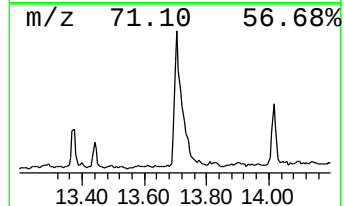
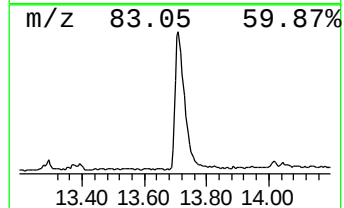
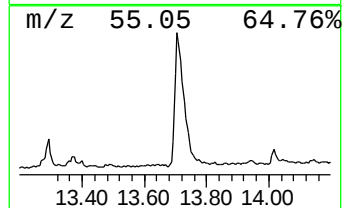
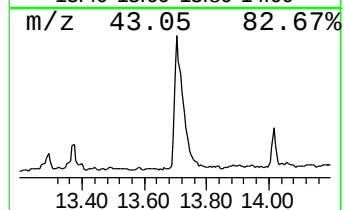
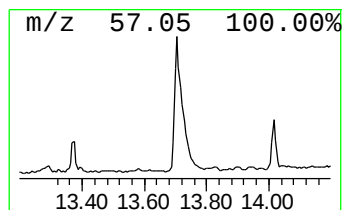
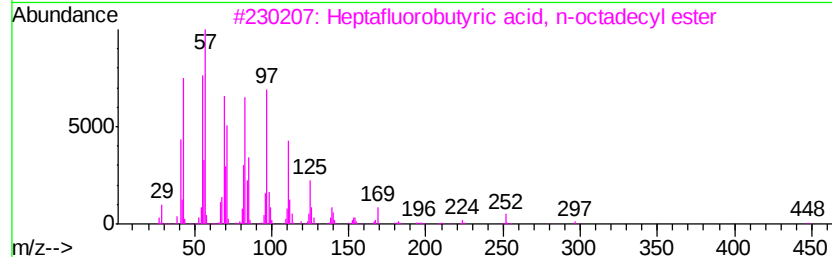
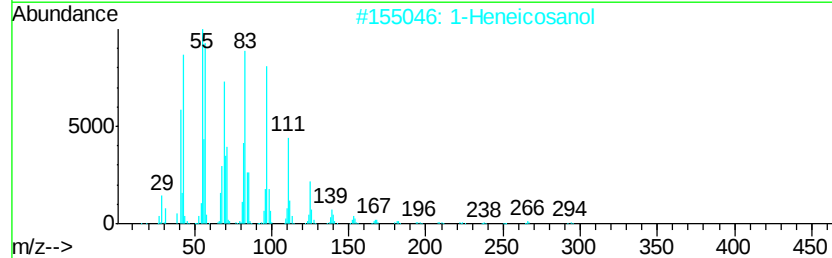
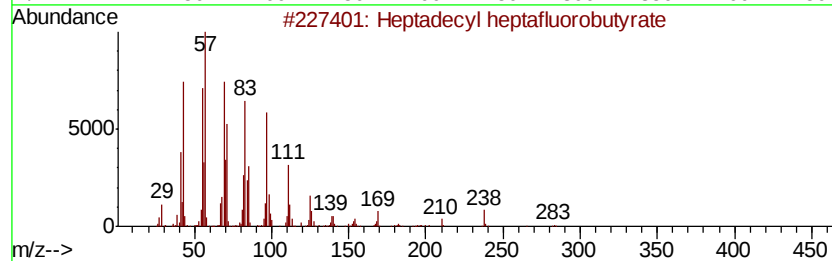
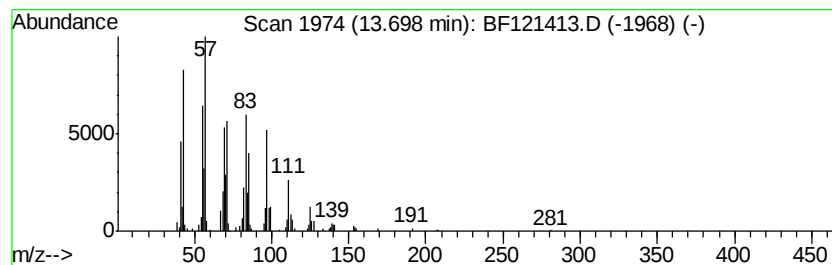
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Heptadecyl heptafluorobutyrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.70	9.70 ng	664372	Chrysene-d12	13.85	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	91
4	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91



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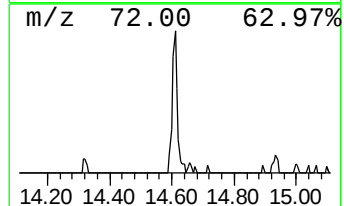
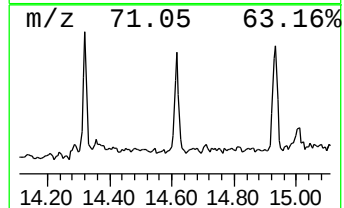
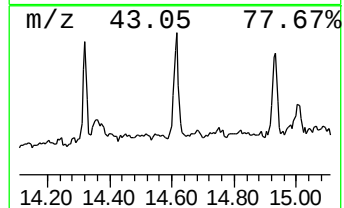
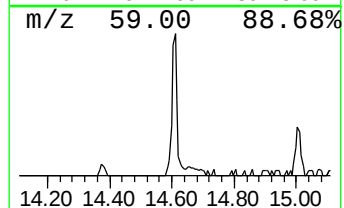
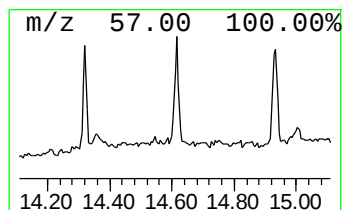
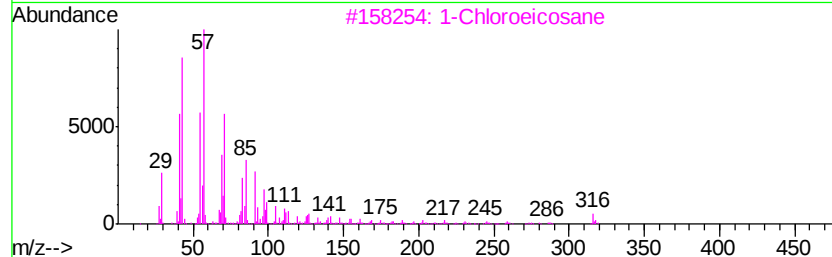
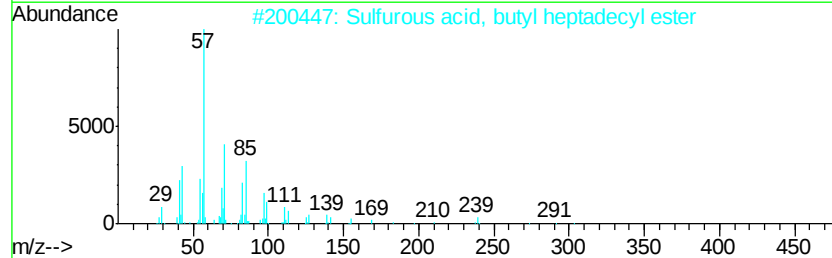
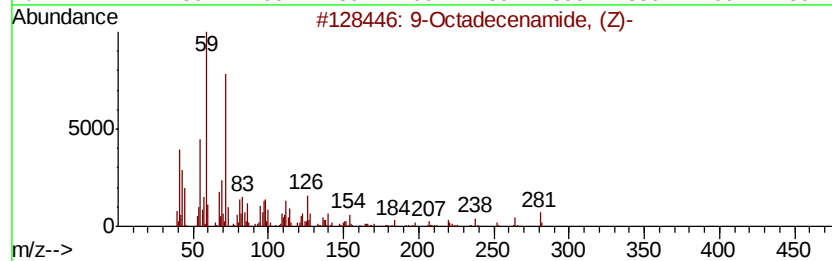
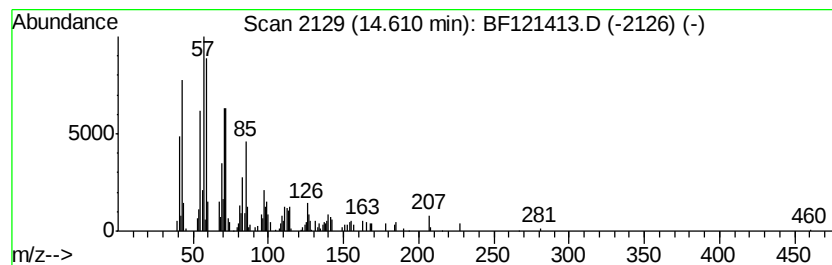
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown14.61 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	2.04 ng	128116	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	46
2		Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	42
3		1-Chloroeicosane	316	C20H41Cl	042217-02-7	41
4		Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	38
5		1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.87	6.7	ng	285142	1	6.69	851239	20.0
Heptadecyl heptaf...	13.70	9.7	ng	664372	5	13.85	1369370	20.0
unknown14.61	14.61	2.0	ng	128116	6	15.26	1254960	20.0