

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072718\
 Data File : BF107755.D
 Acq On : 27 Jul 2018 19:28
 Operator : JU/SJ
 Sample : J4193-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-035

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-BF072018.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	5.190	482	485	498	rBV	264740	370657	12.63%	1.471%
2	5.596	550	554	592	rBV	1178590	2325337	79.21%	9.228%
3	6.596	720	724	744	rBV	1287161	2360435	80.41%	9.367%
4	6.731	744	747	783	rVV	1928104	2935622	100.00%	11.650%
5	6.960	783	786	808	rVV	472788	893447	30.43%	3.546%
6	7.113	808	812	833	rVV	1651459	1966544	66.99%	7.804%
7	7.525	879	882	905	rBV	789097	1527018	52.02%	6.060%
8	8.242	1000	1004	1023	rBV	812885	1152360	39.25%	4.573%
9	9.313	1182	1186	1208	rBV	2318805	2714666	92.47%	10.773%
10	9.707	1249	1253	1264	rBV	102264	125542	4.28%	0.498%
11	10.001	1299	1303	1319	rBV	1052374	1176798	40.09%	4.670%
12	10.795	1434	1438	1462	rBV	1072450	1608571	54.79%	6.384%
13	11.495	1553	1557	1580	rBV	782005	1069155	36.42%	4.243%
14	12.001	1639	1643	1646	rBV	34876	42457	1.45%	0.168%
15	13.077	1822	1826	1838	rBV	1901929	2059705	70.16%	8.174%
16	13.954	1972	1975	1982	rBV2	94447	115936	3.95%	0.460%
17	14.142	2003	2007	2018	rBV	850271	1107256	37.72%	4.394%
18	14.271	2026	2029	2034	rBV2	27623	33511	1.14%	0.133%
19	14.577	2078	2081	2086	rBV	47738	65416	2.23%	0.260%
20	14.895	2132	2135	2138	rBV	45588	49810	1.70%	0.198%
21	14.977	2146	2149	2154	rVB	44532	49161	1.67%	0.195%
22	15.248	2192	2195	2201	rVB	86680	98620	3.36%	0.391%
23	15.677	2259	2268	2280	rBV	617963	1167555	39.77%	4.633%
24	16.107	2337	2341	2346	rVB2	68025	104063	3.54%	0.413%
25	16.642	2429	2432	2438	rVB	52054	78783	2.68%	0.313%

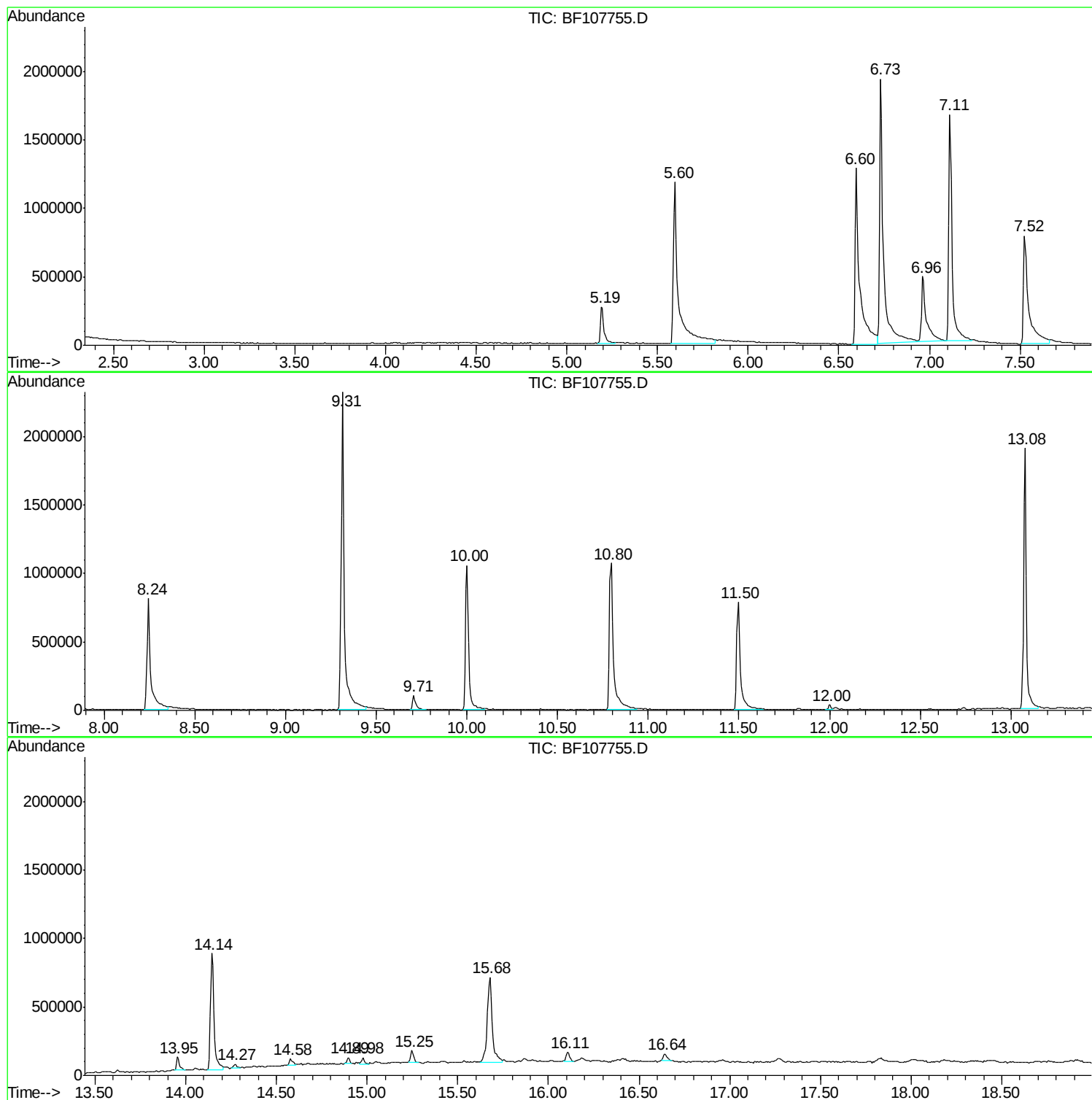
Sum of corrected areas: 25198425

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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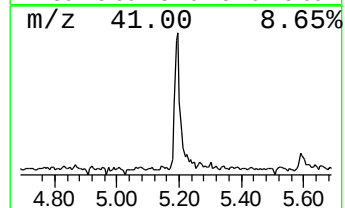
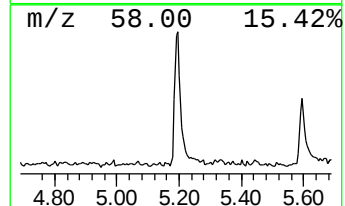
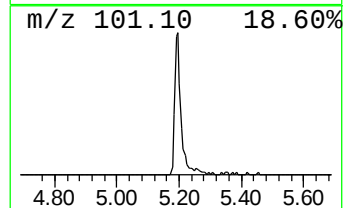
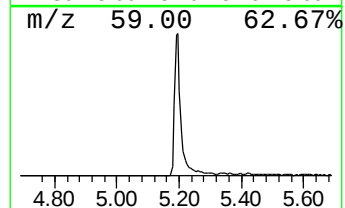
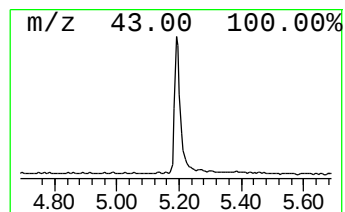
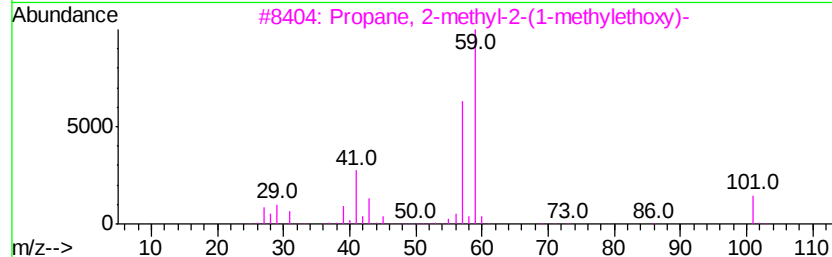
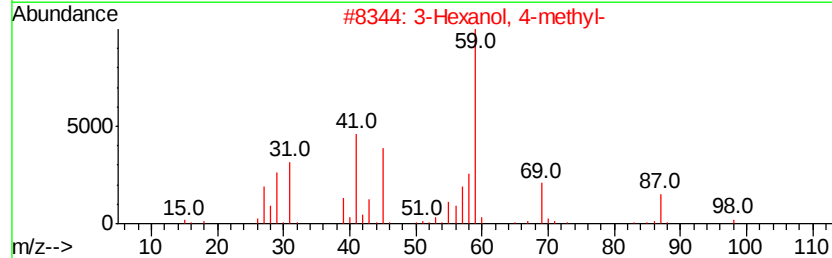
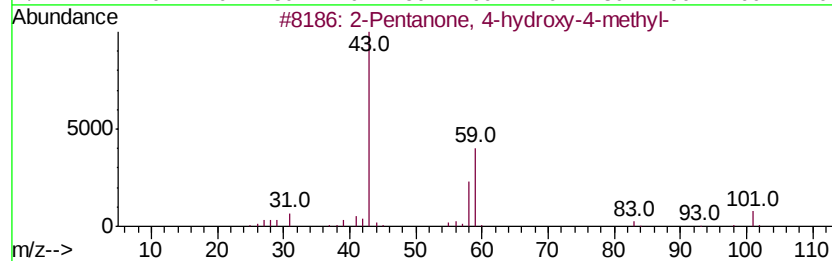
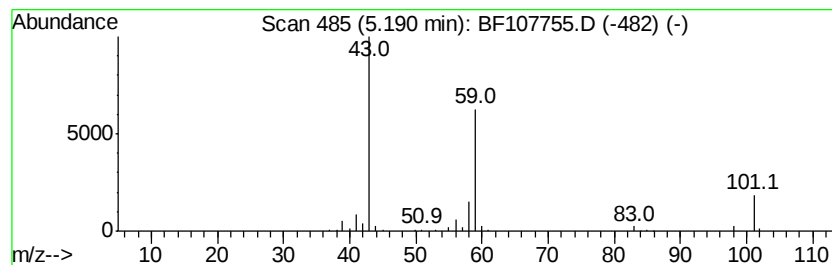
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	8.30 ng	370657	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25



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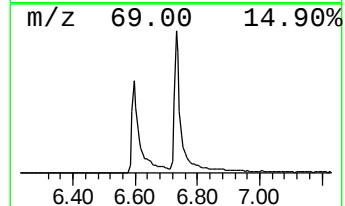
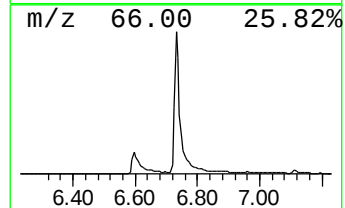
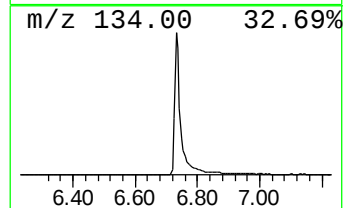
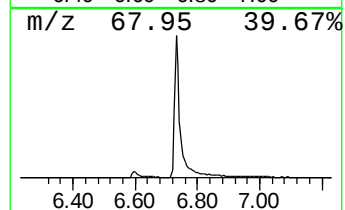
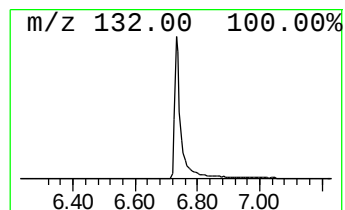
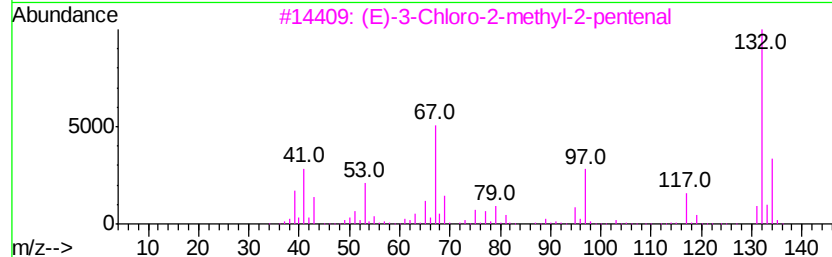
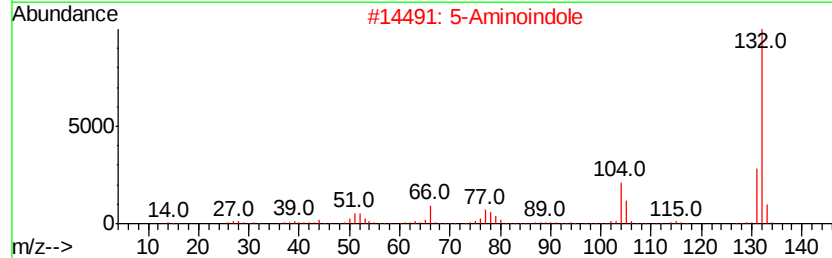
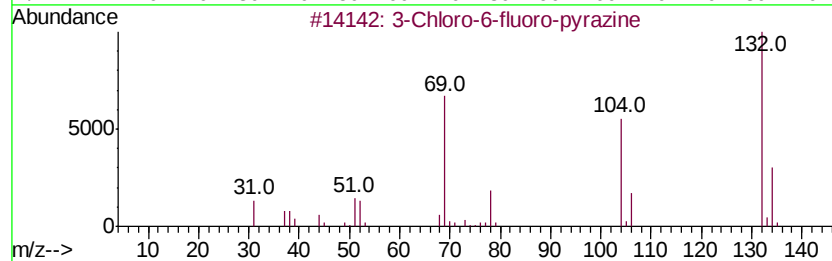
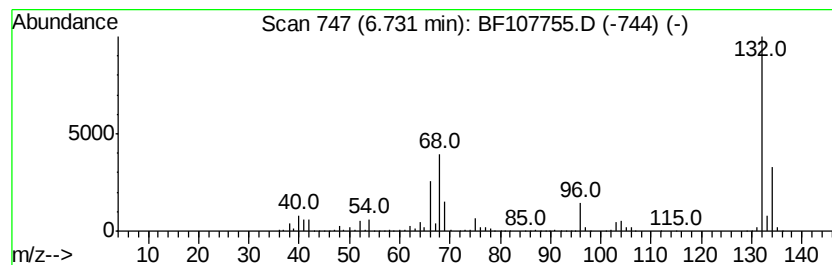
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Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	65.71 ng	2935620	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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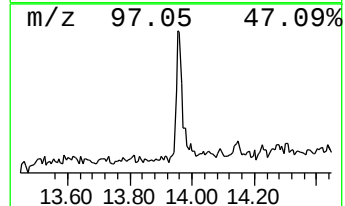
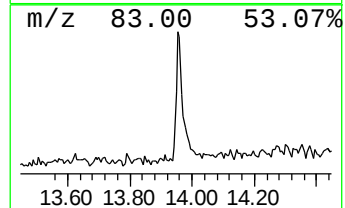
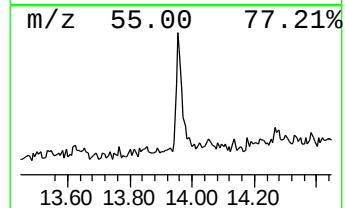
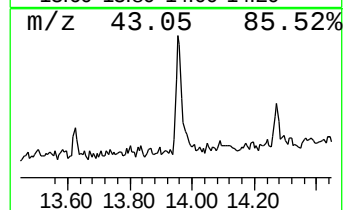
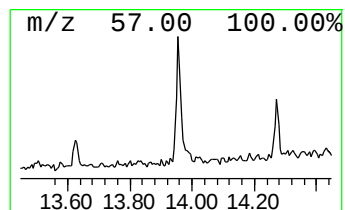
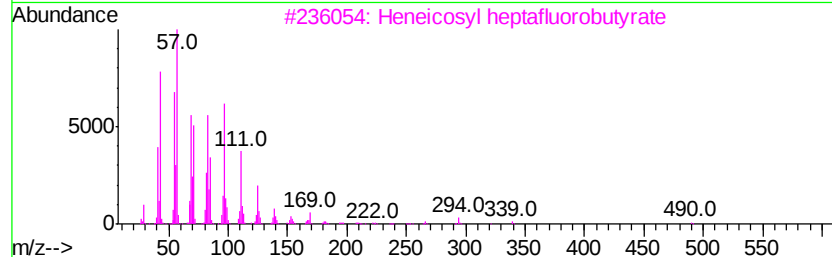
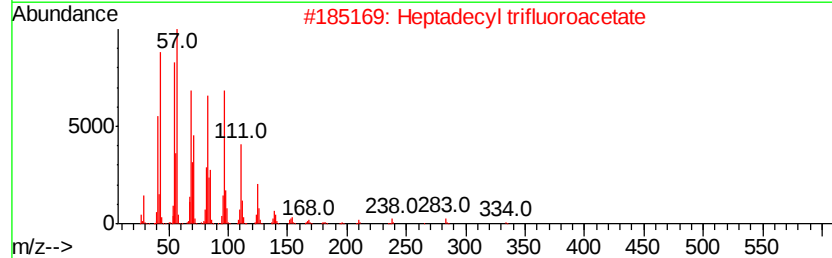
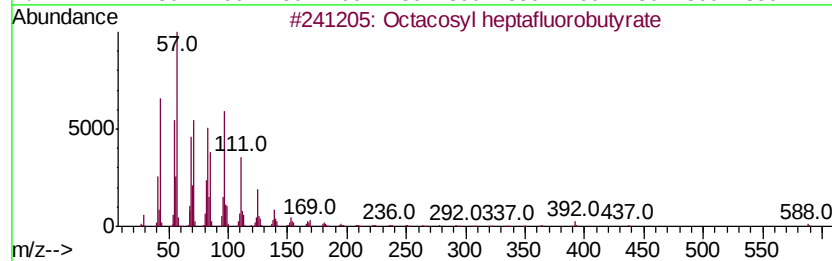
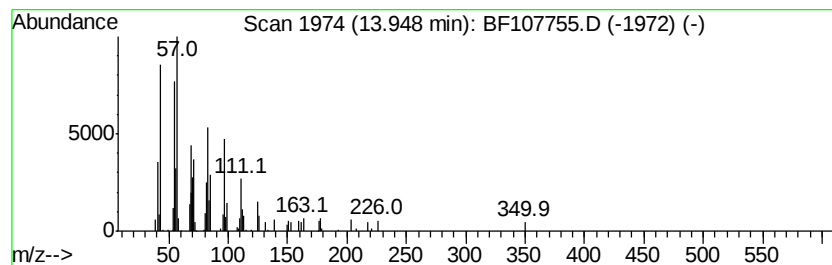
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Octacosyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.95	2.09 ng	115936	Chrysene-d12		14.14		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl heptafluorobutvrate	606	C32H57F7O2	1000351-83-6	91
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3			Heneicosyl heptafluorobutvrate	508	C25H43F7O2	1000351-83-8	91
4			Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	91
5			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91



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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-hy...	5.19	8.3	ng	370657	1	6.96	893447	20.0
unknown6.73	6.73	65.7	ng	2935620	1	6.96	893447	20.0
Octacosyl heptafl...	13.95	2.1	ng	115936	5	14.14	1107260	20.0