

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091718\
 Data File : BF109076.D
 Acq On : 18 Sep 2018 4:55
 Operator : JU/SJ
 Sample : J4907-01
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CBH-591(1)

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-BF091418.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	4.895	432	435	447	rVB	164084	180378	4.80%	0.771%
2	5.325	504	508	511	rBV	1240194	1091816	29.07%	4.664%
3	6.348	678	682	689	rBV	937347	724732	19.30%	3.096%
4	6.489	701	706	709	rBV	2186095	2033170	54.14%	8.685%
5	6.719	742	745	749	rBV	975986	750539	19.99%	3.206%
6	6.878	768	772	775	rBV	3238357	2715383	72.31%	11.599%
7	7.283	835	841	844	rBV	2397166	2282186	60.77%	9.749%
8	8.001	959	963	966	rBV	1121067	856809	22.82%	3.660%
9	9.077	1142	1146	1149	rBV	4097073	3755214	100.00%	16.041%
10	9.466	1210	1212	1215	rBV	48019	42168	1.12%	0.180%
11	9.748	1257	1260	1264	rBV2	1020521	858794	22.87%	3.668%
12	10.530	1390	1393	1405	rBV	1535707	1536389	40.91%	6.563%
13	11.224	1508	1511	1515	rBV	955415	848233	22.59%	3.623%
14	12.648	1749	1753	1758	rBV2	35599	43625	1.16%	0.186%
15	12.812	1776	1781	1784	rBV	3933336	3752456	99.93%	16.029%
16	13.718	1931	1935	1945	rBV	54055	94909	2.53%	0.405%
17	13.854	1954	1958	1961	rBV	1007089	924203	24.61%	3.948%
18	14.636	2088	2091	2096	rBV	51061	46818	1.25%	0.200%
19	14.954	2142	2145	2150	rVB	58487	60496	1.61%	0.258%
20	15.254	2191	2196	2201	rBV	555157	642425	17.11%	2.744%
21	15.306	2202	2205	2212	rVB	52402	72241	1.92%	0.309%
22	15.712	2270	2274	2278	rVB	42207	55808	1.49%	0.238%
23	16.183	2349	2354	2359	rBV3	26198	41383	1.10%	0.177%

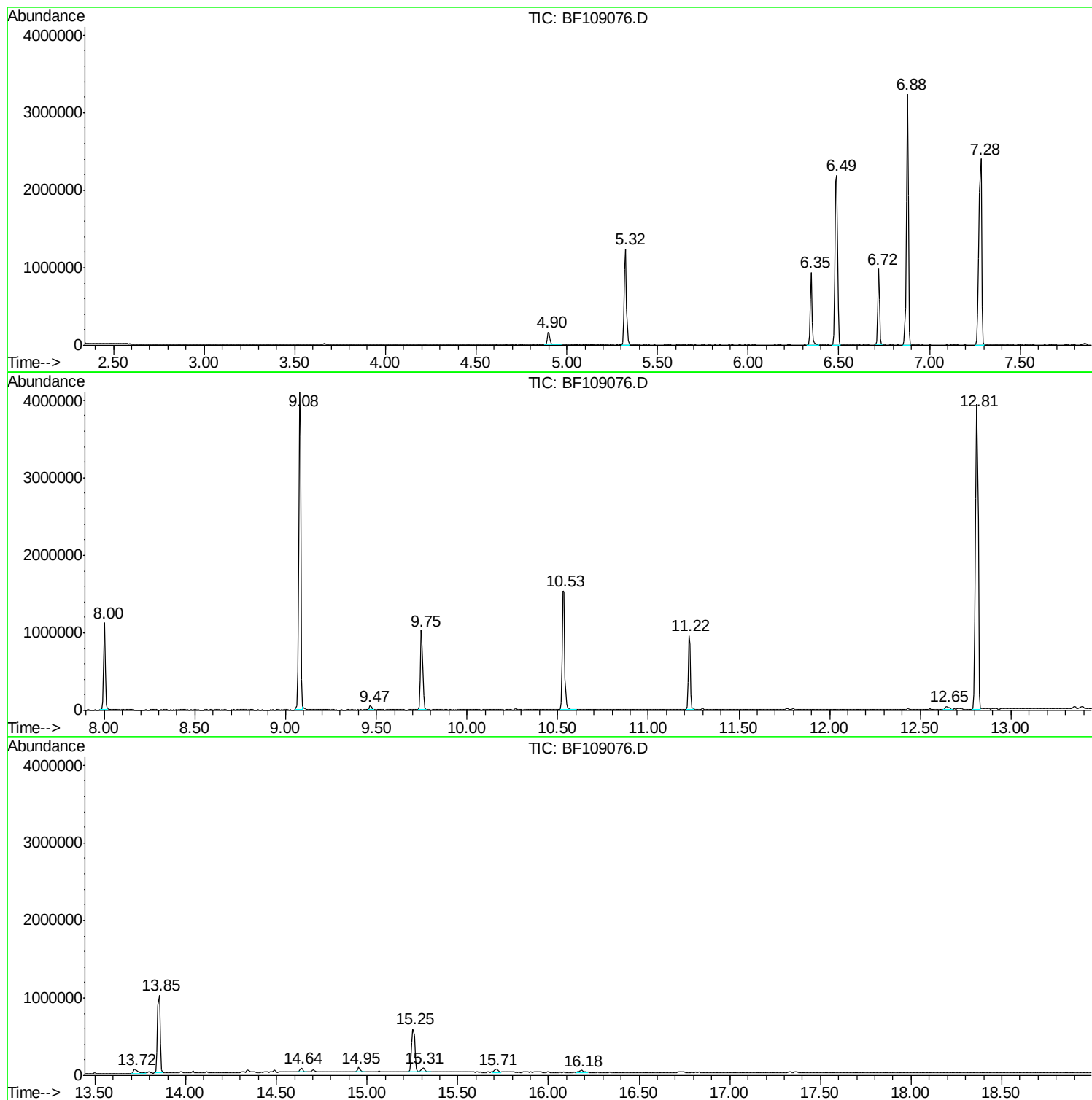
Sum of corrected areas: 23410175

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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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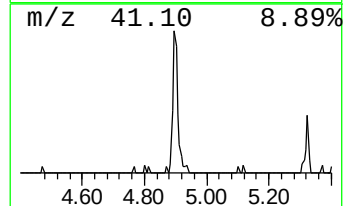
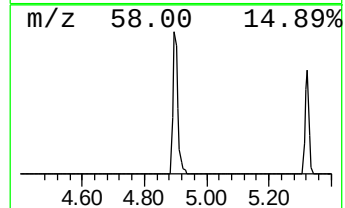
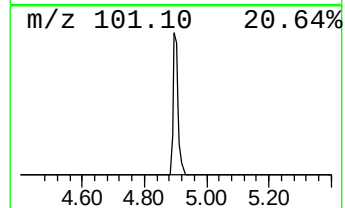
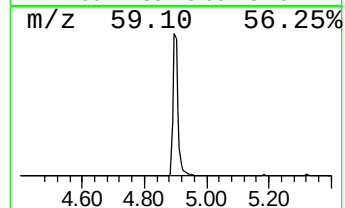
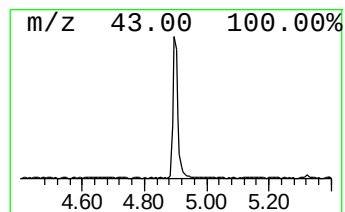
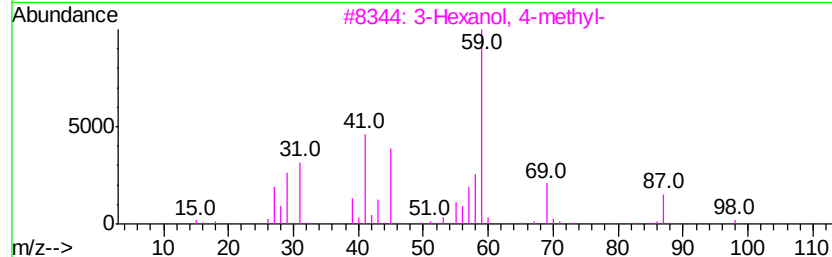
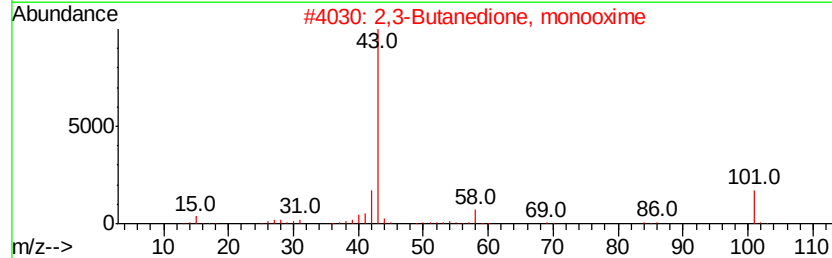
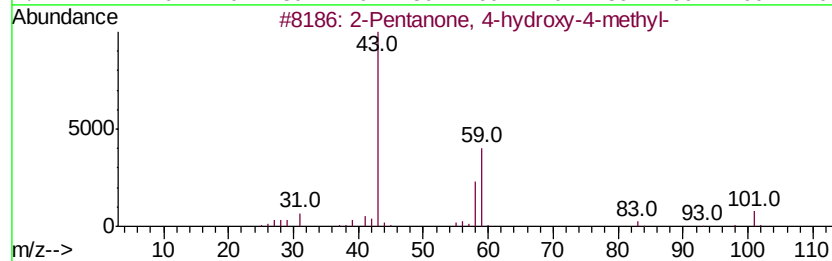
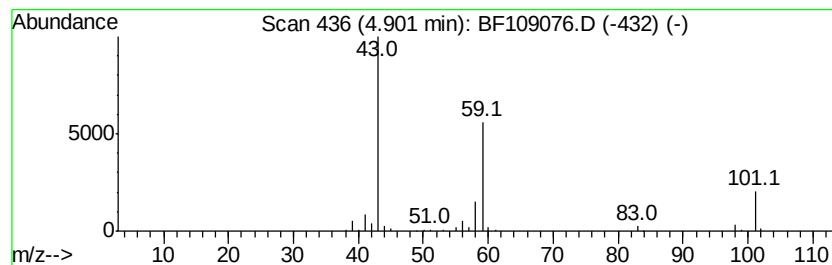
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	4.81 ng	180378	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9



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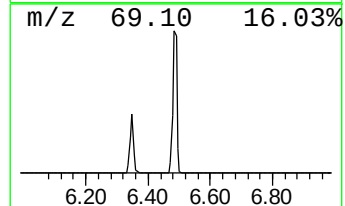
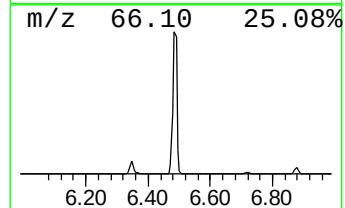
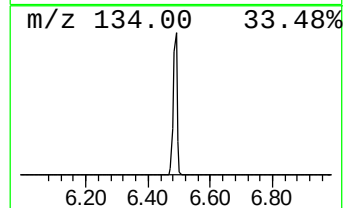
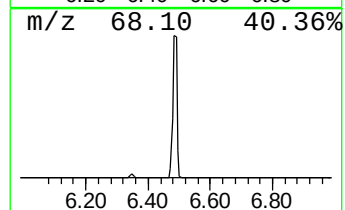
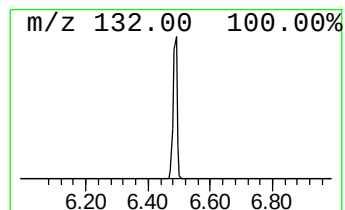
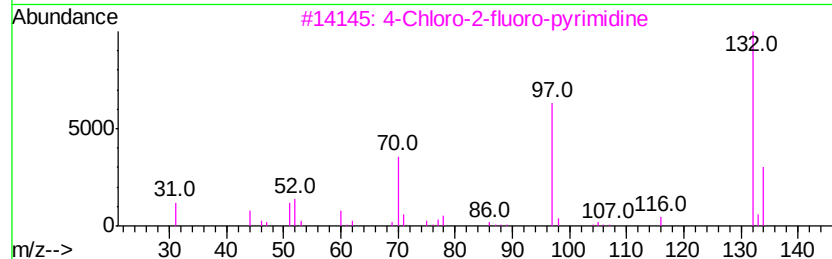
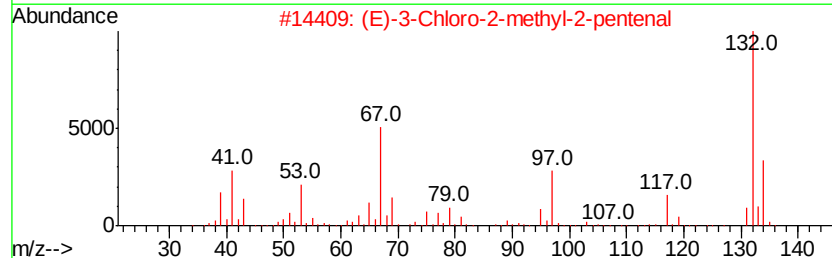
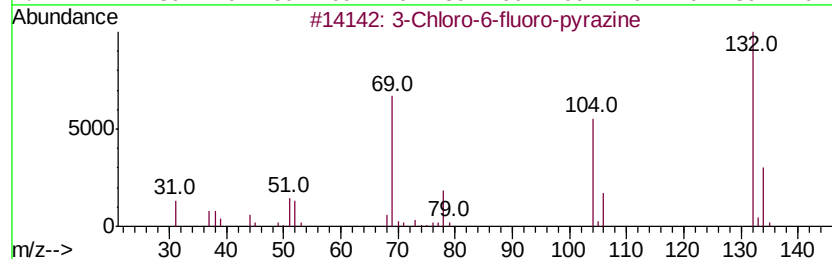
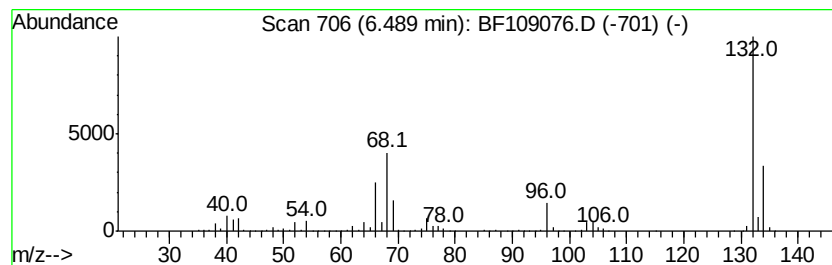
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Peak Number 2 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	54.18 ng	2033170	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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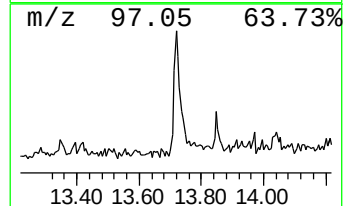
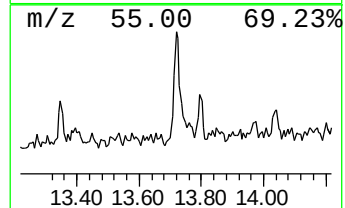
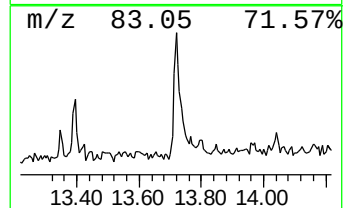
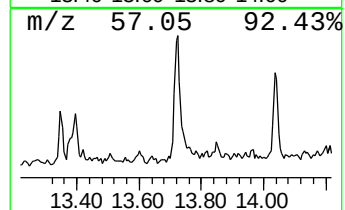
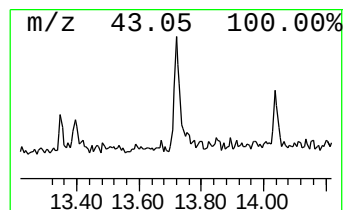
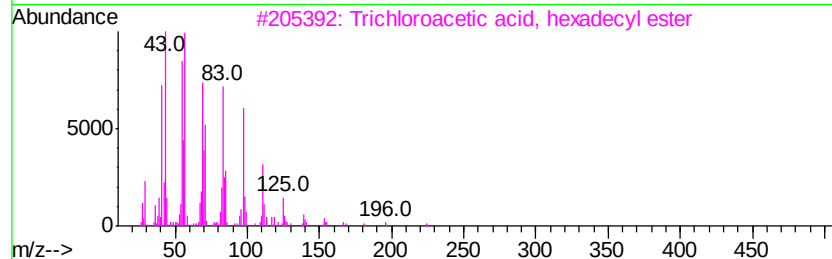
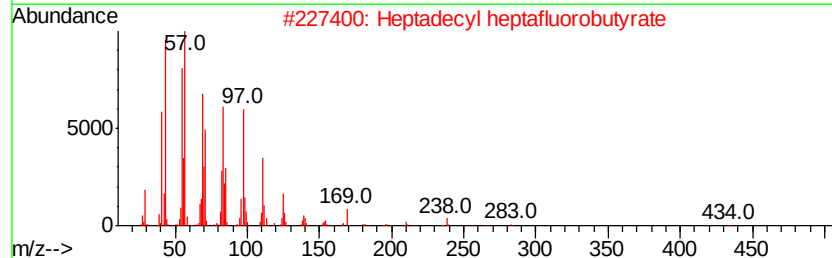
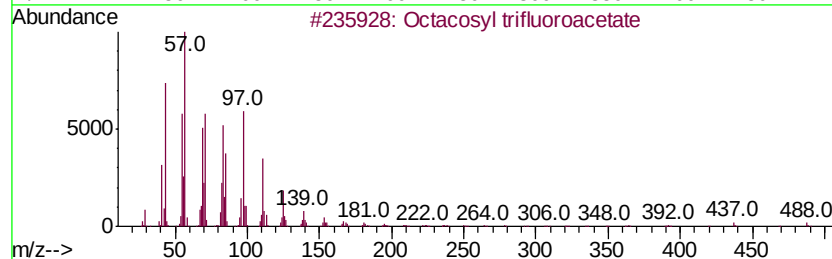
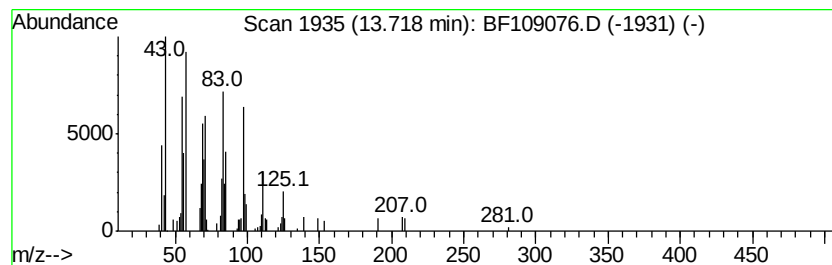
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Peak Number 4 Octacosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	2.05 ng	94909	Chrysene-d12	13.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
4		Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	87
5		Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	87



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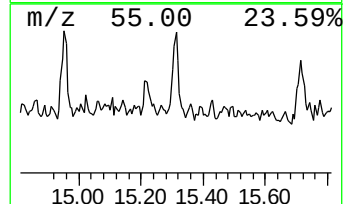
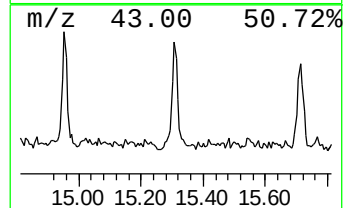
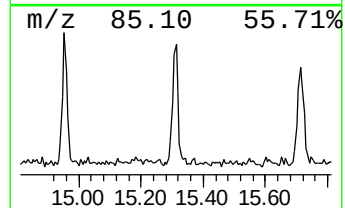
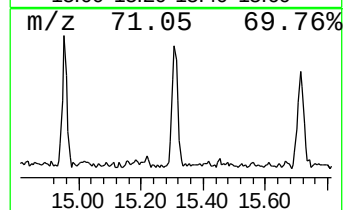
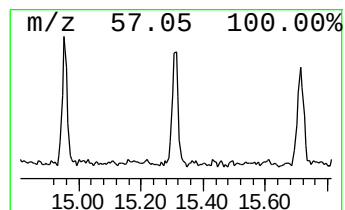
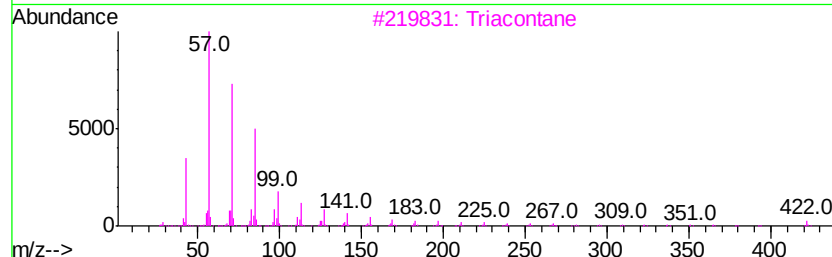
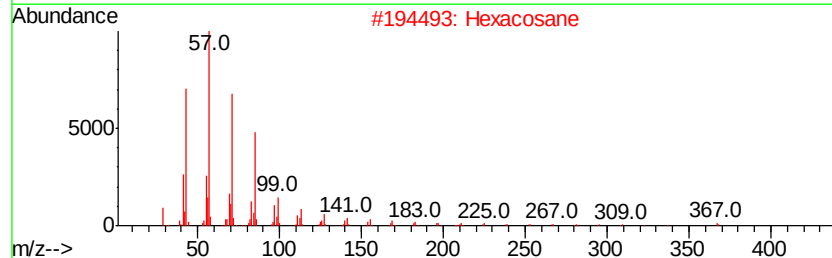
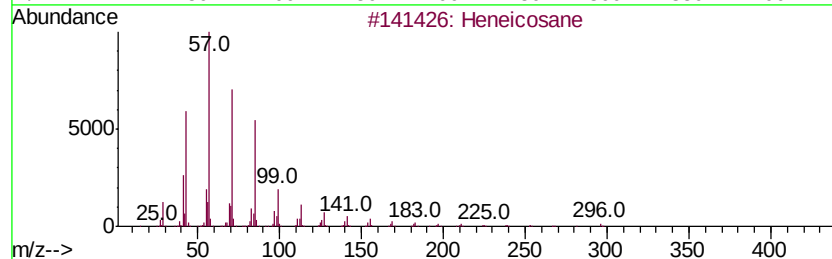
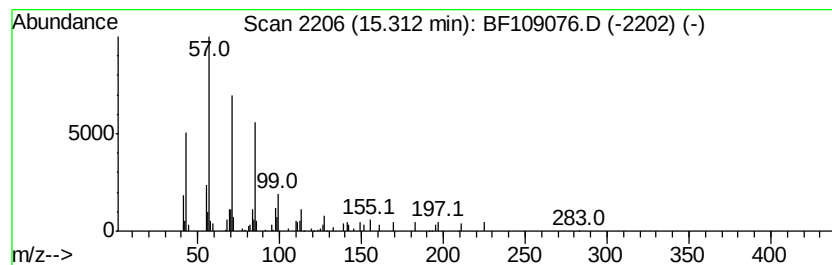
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Peak Number 5 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	2.25 ng	72241	Perylene-d12	15.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Hexacosane		366	C26H54	000630-01-3	90
3	Triacontane		422	C30H62	000638-68-6	90
4	Octadecane		254	C18H38	000593-45-3	87
5	Hexadecane		226	C16H34	000544-76-3	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	4.8	ng	180378	1	6.72	750539	20.0
unknown6.49	6.49	54.2	ng	2033170	1	6.72	750539	20.0
Octacosyl trifluo...	13.72	2.0	ng	94909	5	13.85	924203	20.0
Heneicosane	15.31	2.3	ng	72241	6	15.25	642425	20.0