

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF073018\
 Data File : BF107836.D
 Acq On : 31 Jul 2018 7:58
 Operator : JU/SJ
 Sample : J4221-01
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-23

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-BF073018.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	4.043	286	290	294	rVB	26092	34690	1.16%	0.175%
2	5.184	481	484	496	rBV	186277	209922	7.02%	1.060%
3	5.607	552	556	573	rBV	133559	418802	14.00%	2.114%
4	6.537	712	714	720	rVB2	39586	40106	1.34%	0.202%
5	6.613	723	727	745	rBV	186360	705742	23.59%	3.562%
6	6.737	745	748	768	rBV	798138	1227717	41.04%	6.197%
7	6.872	768	771	783	rVB4	37802	79379	2.65%	0.401%
8	6.966	783	787	793	rBV	622831	850826	28.44%	4.294%
9	7.119	809	813	836	rBV	2033255	2297689	76.81%	11.597%
10	7.531	879	883	903	rBV	951026	1811110	60.54%	9.141%
11	7.678	905	908	917	rVB2	86257	104772	3.50%	0.529%
12	7.919	941	949	955	rVB9	13815	37663	1.26%	0.190%
13	8.248	1001	1005	1021	rBV	931607	1318871	44.09%	6.657%
14	9.183	1156	1164	1166	rBV3	25656	42071	1.41%	0.212%
15	9.319	1183	1187	1202	rBV	2501835	2991348	100.00%	15.098%
16	9.707	1250	1253	1262	rVV	359786	387741	12.96%	1.957%
17	10.007	1300	1304	1317	rBV	1140810	1258671	42.08%	6.353%
18	10.801	1435	1439	1451	rBV	515449	796139	26.61%	4.018%
19	11.501	1554	1558	1570	rBV	796328	1200776	40.14%	6.061%
20	12.007	1641	1644	1648	rBV	140632	164952	5.51%	0.833%
21	13.083	1824	1827	1833	rBV	1832137	1946446	65.07%	9.824%
22	13.960	1973	1976	1979	rBV2	322118	464857	15.54%	2.346%
23	14.154	2007	2009	2013	rBV	629788	734520	24.55%	3.707%
24	14.983	2148	2150	2159	rVB	663056	687594	22.99%	3.471%

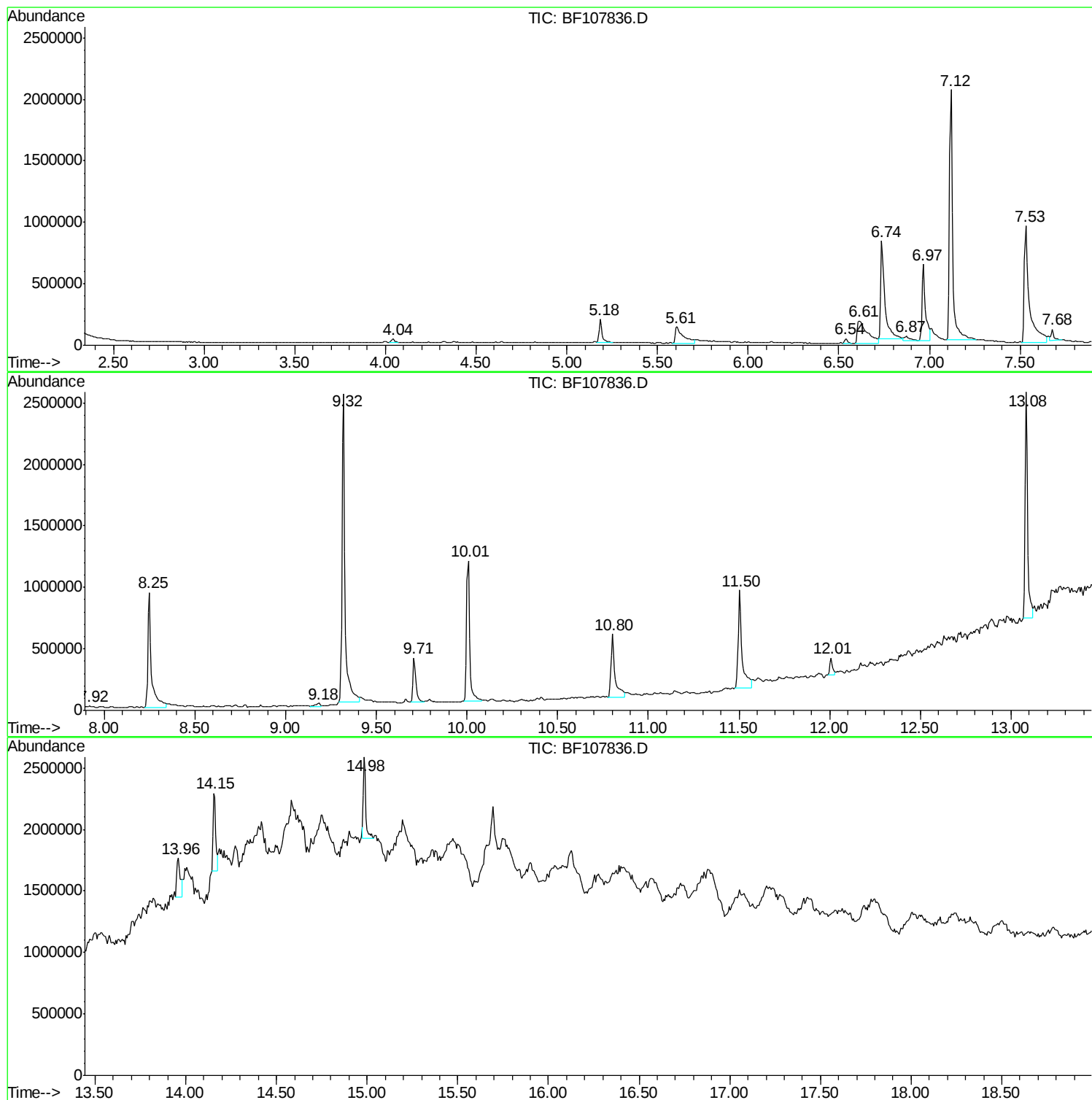
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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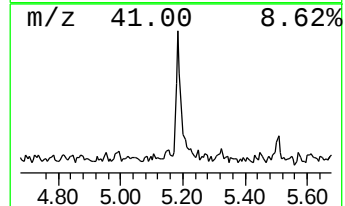
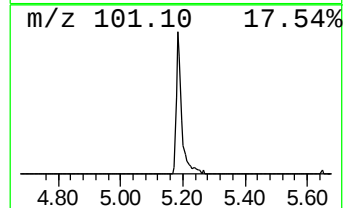
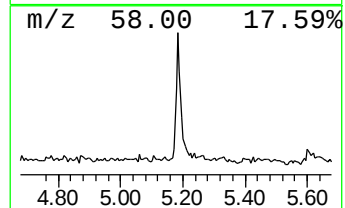
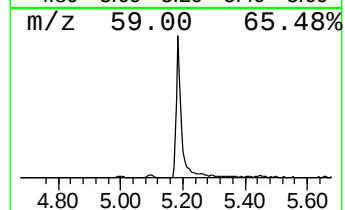
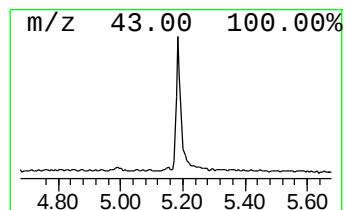
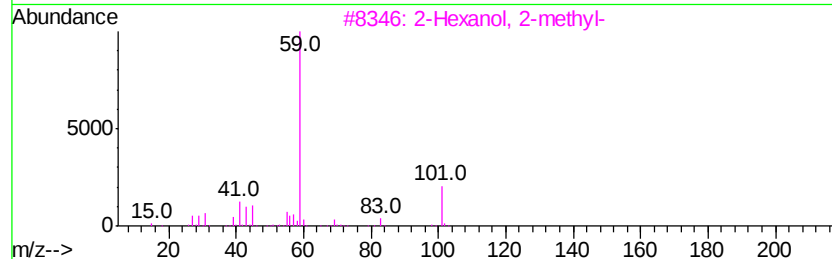
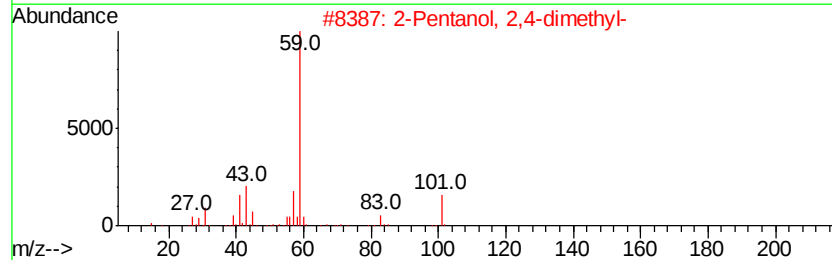
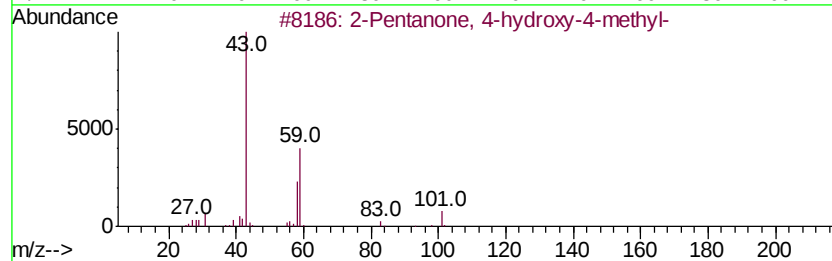
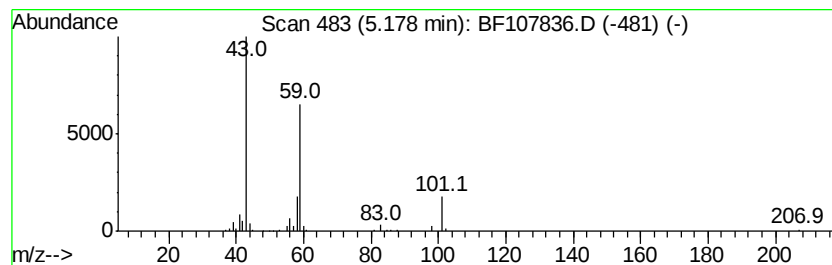
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	4.93 ng	209922	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
4		Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	36
5		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32



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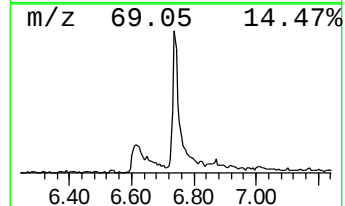
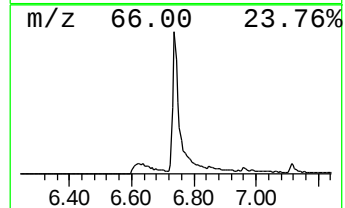
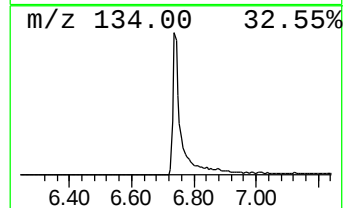
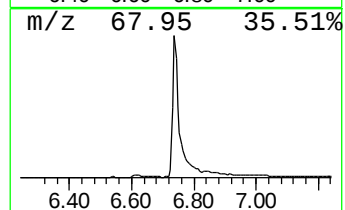
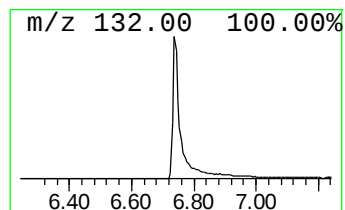
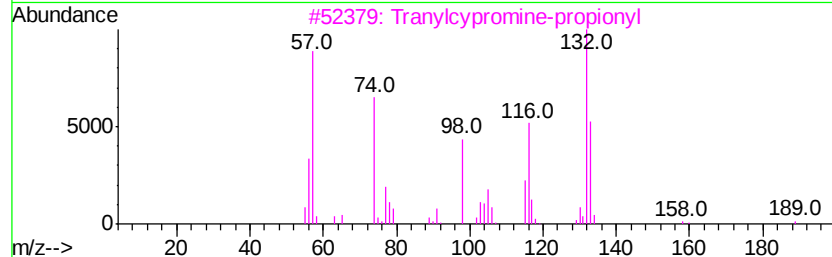
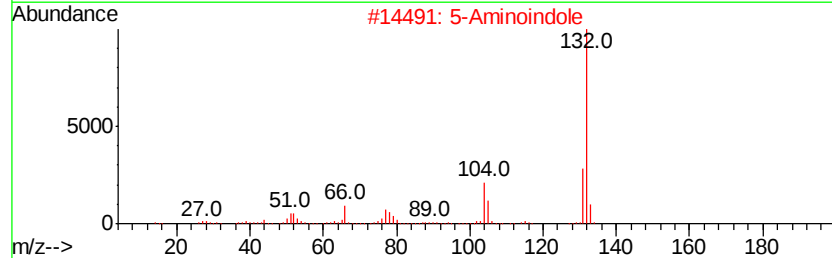
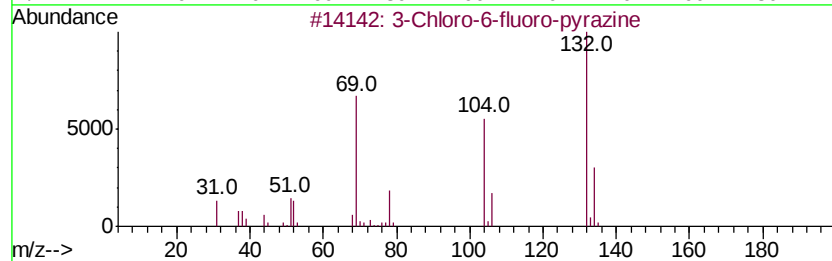
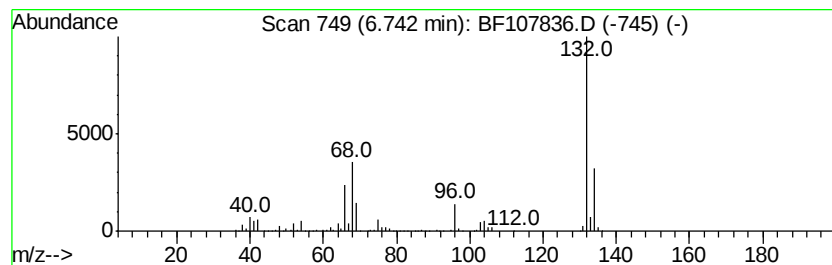
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Peak Number 2 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	28.86 ng	1227720	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	10
5			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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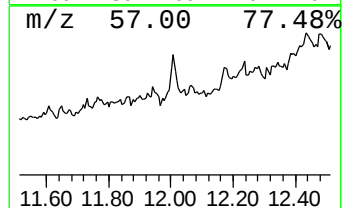
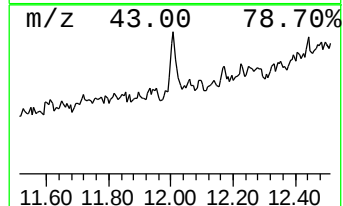
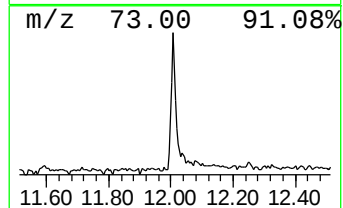
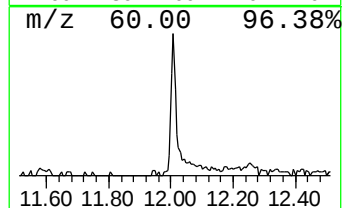
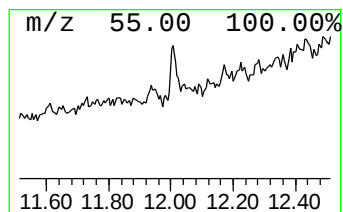
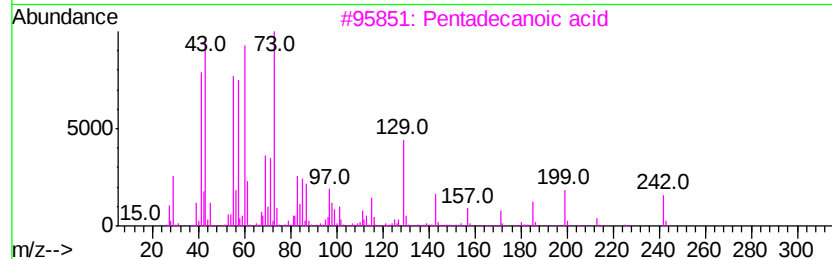
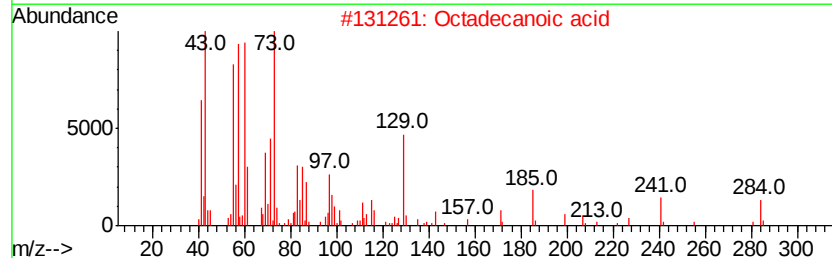
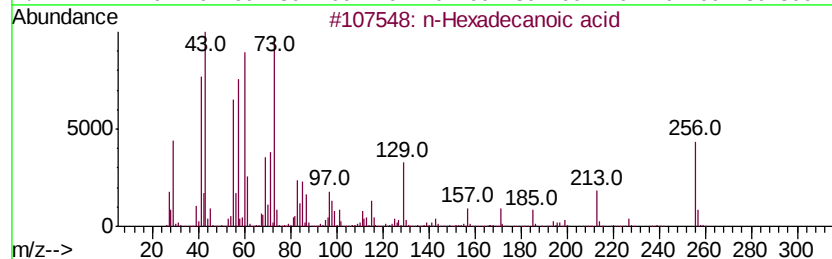
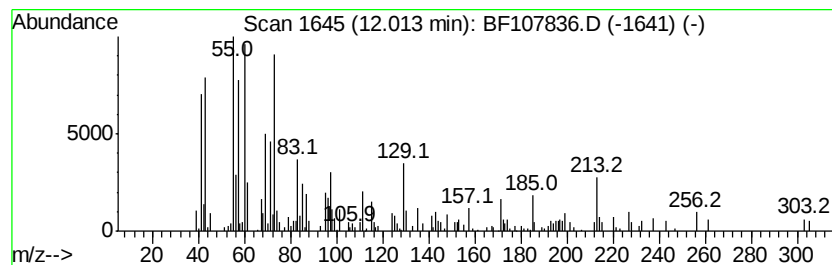
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	2.75 ng	164952	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72



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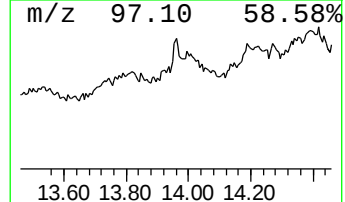
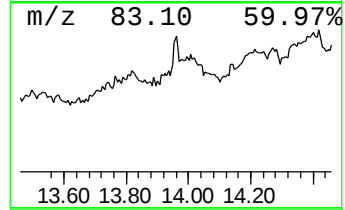
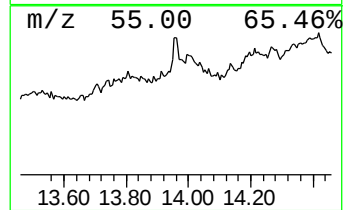
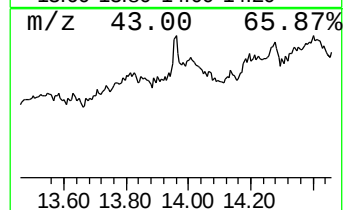
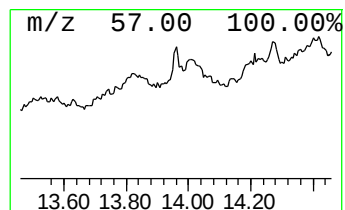
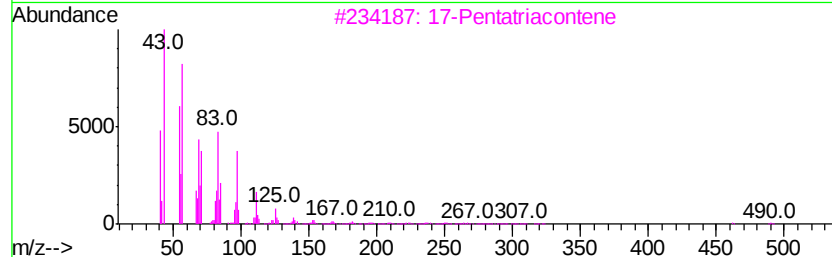
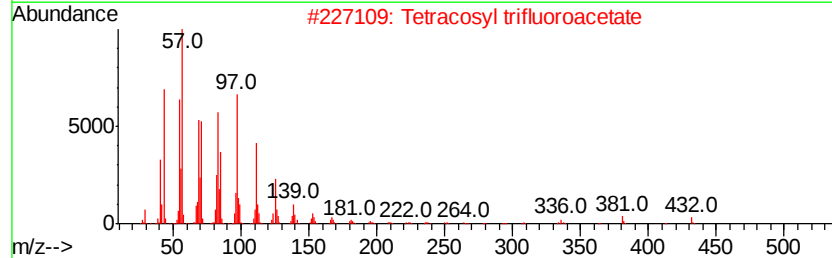
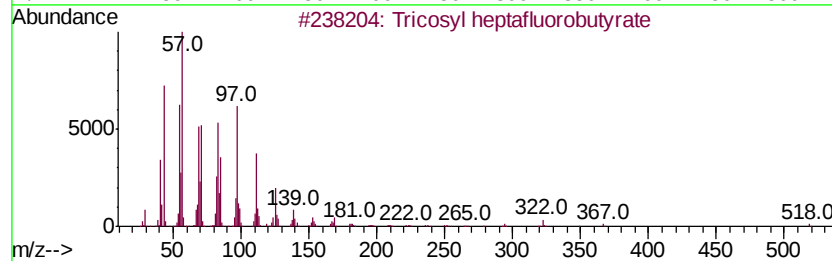
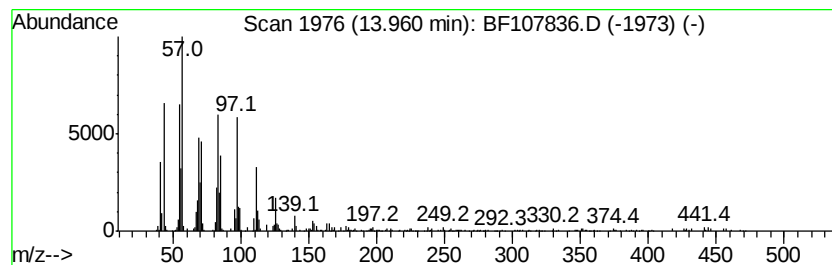
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Peak Number 5 Tricosyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	12.66 ng	464857	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
2		Tetracosyl trifluoroacetate	450	C26H49F3O2	1000351-76-4	91
3		17-Pentatriacontene	491	C35H70	006971-40-0	91
4		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
5		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91



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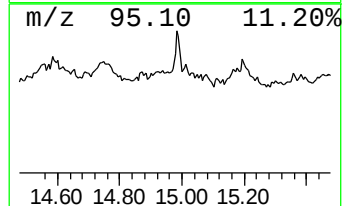
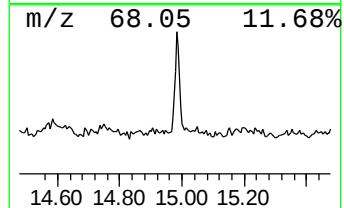
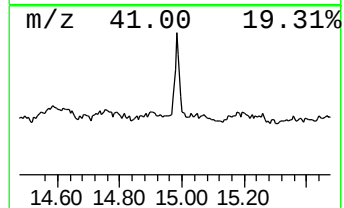
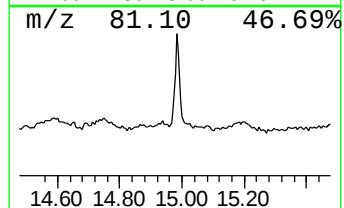
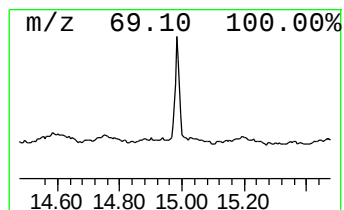
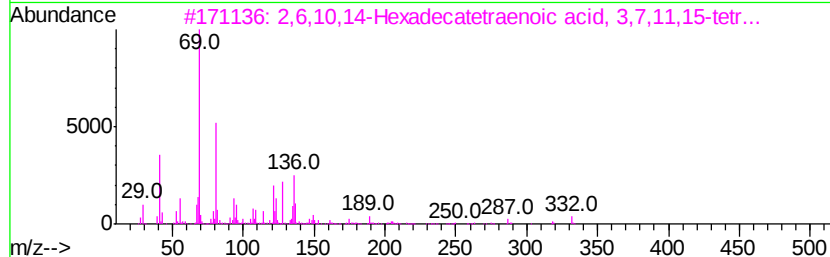
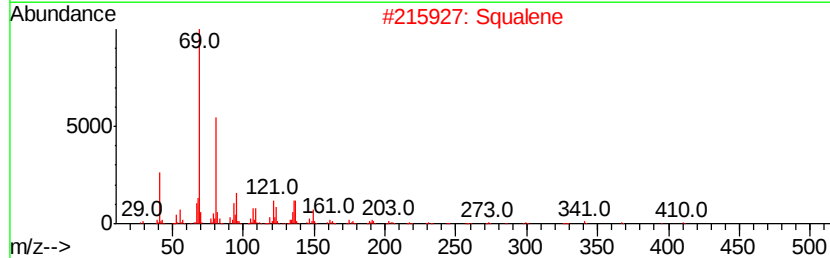
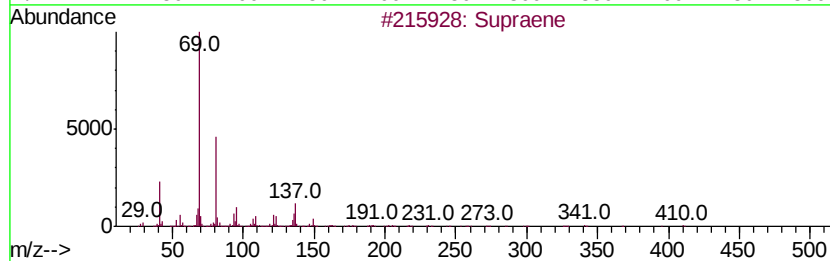
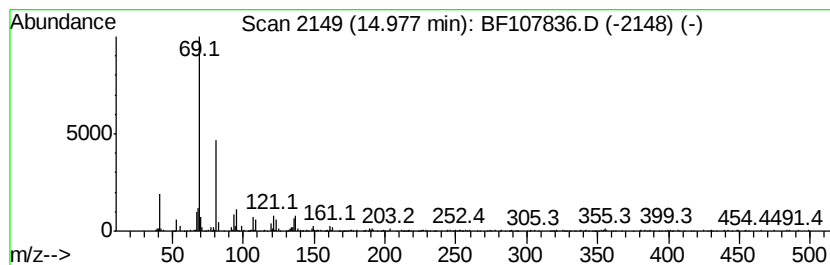
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Peak Number 6 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	20.00 ng	687594	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	98
2		Squalene	410	C30H50	000111-02-4	87
3		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5		2,6-Octadiene, 1-(2-bromophenoxy...	308	C16H21BrO	1000163-04-5	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.18	4.9	ng	209922	1	6.97	850826	20.0
unknown6.74	6.74	28.9	ng	1227720	1	6.97	850826	20.0
n-Hexadecanoic acid	12.01	2.8	ng	164952	4	11.50	1200780	20.0
Tricosyl heptaflu...	13.96	12.7	ng	464857	5	14.15	734520	20.0
Supraene	14.98	20.0	ng	687594	6	15.69	687594	20.0