

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
 Data File : BF102609.D
 Acq On : 29 Jan 2018 20:49
 Operator : SJ/JU
 Sample : J1344-07
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 8-SAN-4-EW-(7-8)

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:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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	4.928	480	483	493	rBV	90903	146870	3.25%	0.371%
2	5.334	547	552	574	rBV	3943754	4284550	94.67%	10.831%
3	6.363	722	727	743	rBV	3493165	4509064	99.63%	11.399%
4	6.486	743	748	751	rBV	4206670	4257743	94.08%	10.764%
5	6.710	783	786	794	rBV	1148190	1002921	22.16%	2.535%
6	6.869	808	813	816	rBV	3579953	3310909	73.16%	8.370%
7	7.286	878	884	901	rBV	2515691	2907934	64.25%	7.351%
8	7.998	1000	1005	1020	rBV	1358220	1435838	31.73%	3.630%
9	9.075	1182	1188	1191	rBV	4387228	4525878	100.00%	11.441%
10	9.469	1251	1255	1268	rVB	524786	536332	11.85%	1.356%
11	9.751	1298	1303	1317	rBV	1585324	1575362	34.81%	3.983%
12	10.174	1372	1375	1378	rVB	100716	82897	1.83%	0.210%
13	10.545	1434	1438	1449	rBV	2376364	2510097	55.46%	6.346%
14	10.645	1452	1455	1464	rVB	108934	119774	2.65%	0.303%
15	11.233	1551	1555	1565	rBV	1446020	1526286	33.72%	3.858%
16	12.633	1790	1793	1797	rBV2	65138	57405	1.27%	0.145%
17	12.821	1820	1825	1829	rBV	3613582	3992037	88.20%	10.092%
18	13.715	1973	1977	1985	rBV2	191026	302474	6.68%	0.765%
19	13.874	2001	2004	2013	rVB	1089194	1180404	26.08%	2.984%
20	13.962	2016	2019	2026	rVB	58329	61477	1.36%	0.155%
21	14.615	2127	2130	2136	rBV2	182513	220834	4.88%	0.558%
22	15.309	2243	2248	2257	rBV	728887	1009979	22.32%	2.553%

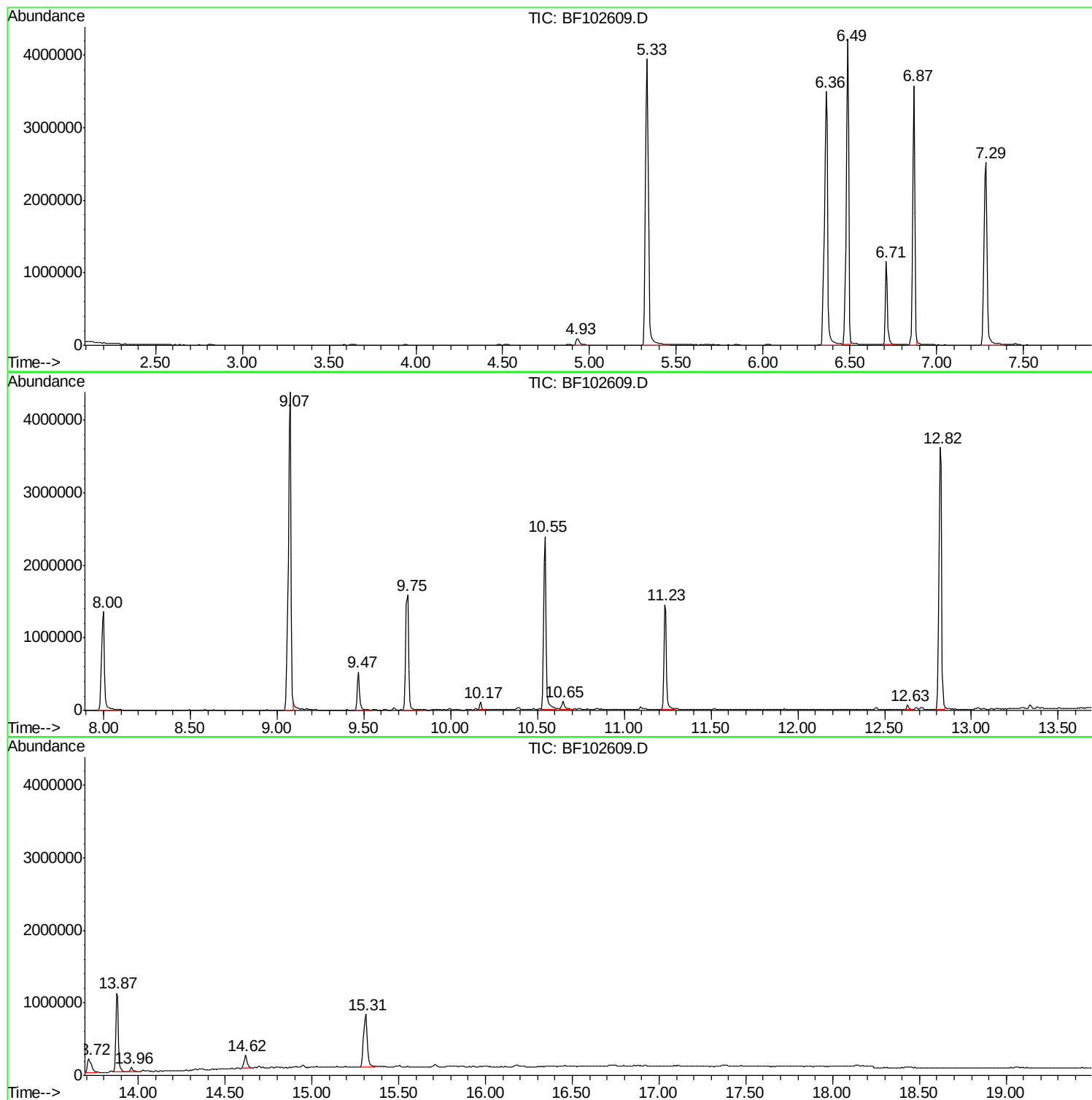
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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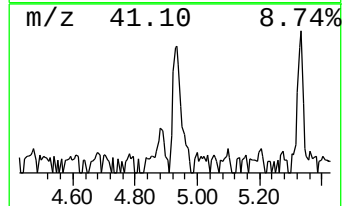
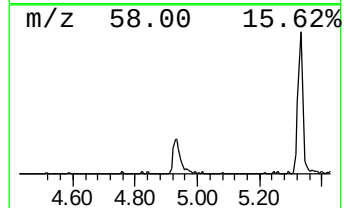
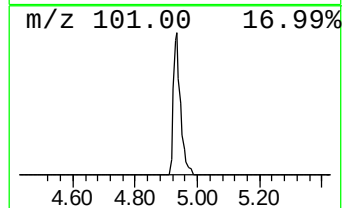
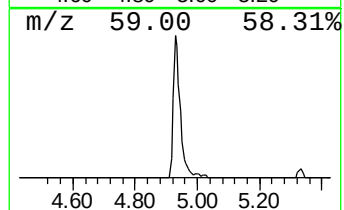
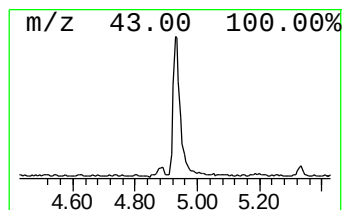
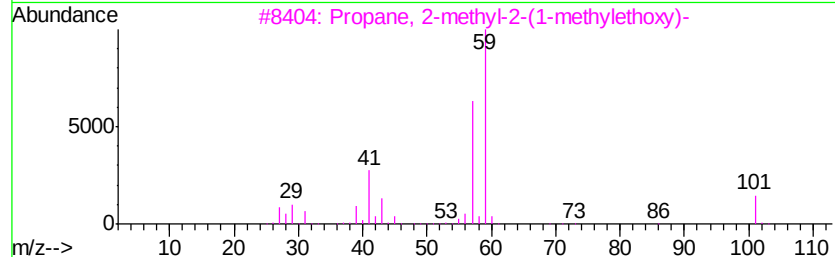
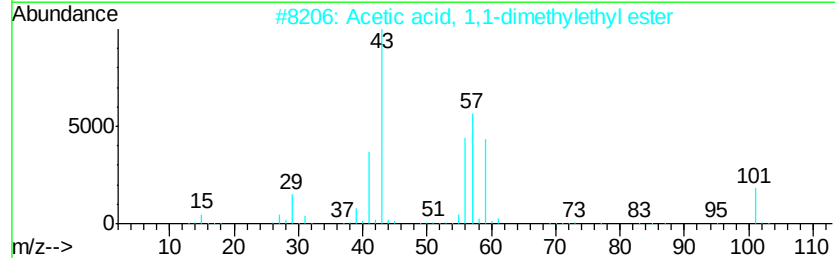
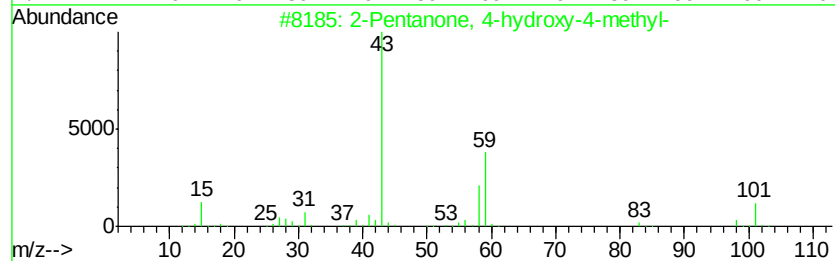
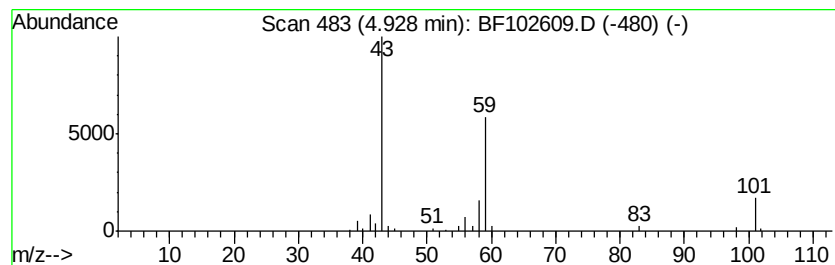
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.93	2.93 ng	146870	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		3-Octanol	130	C8H18O	000589-98-0	33



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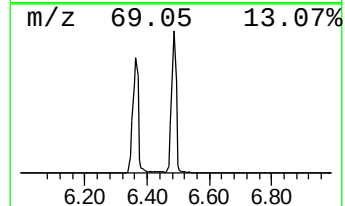
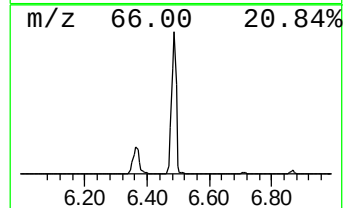
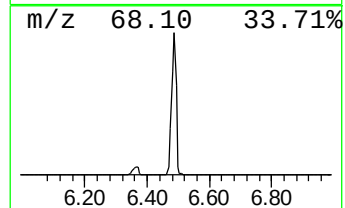
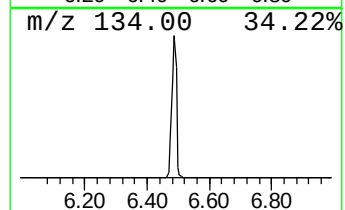
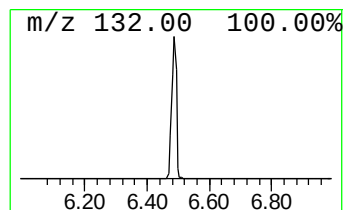
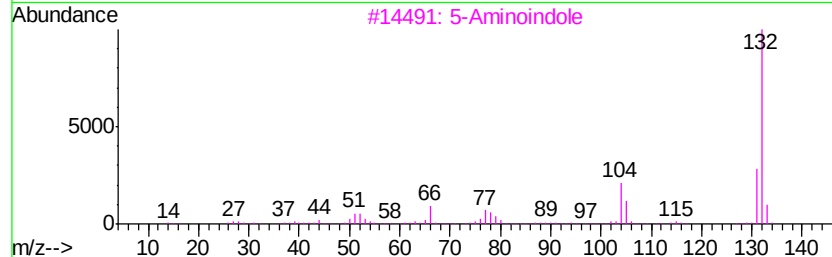
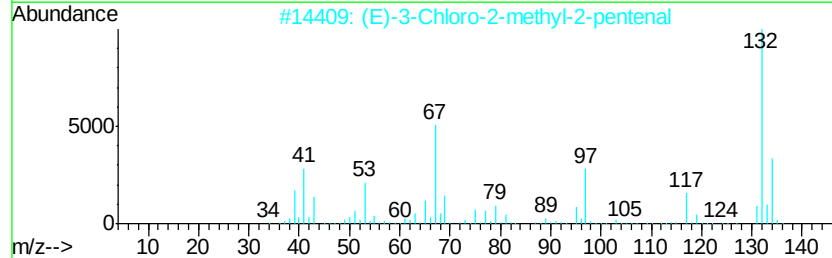
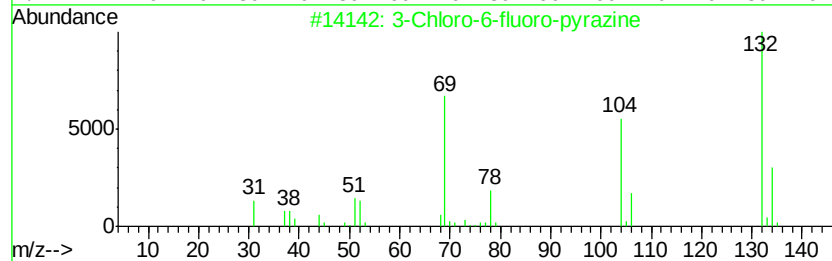
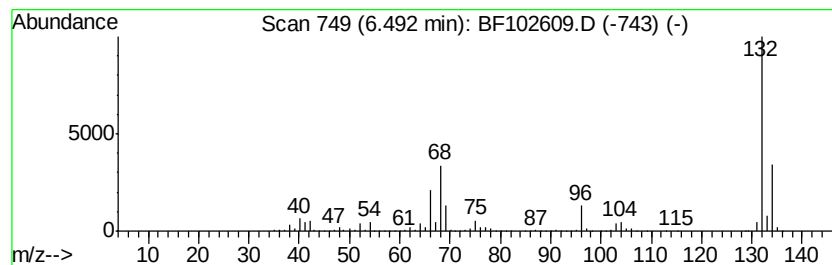
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	84.91 ng	4257740	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
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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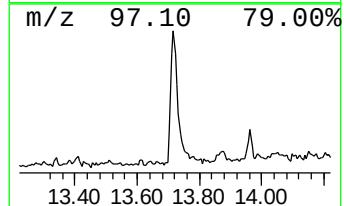
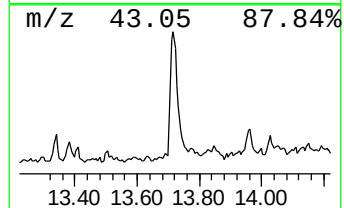
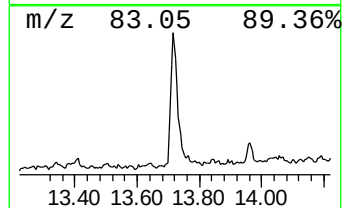
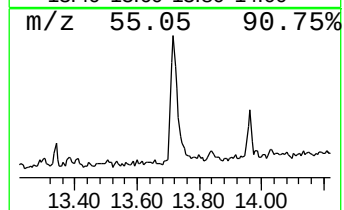
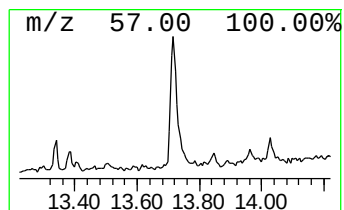
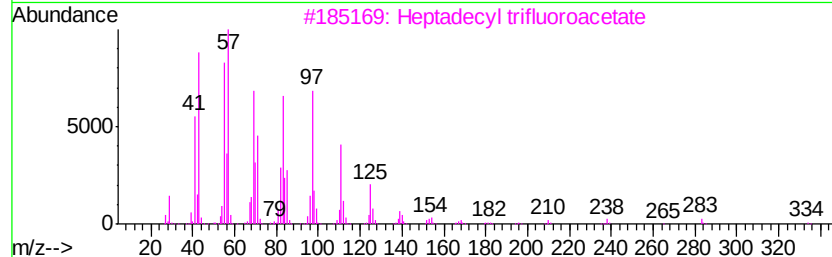
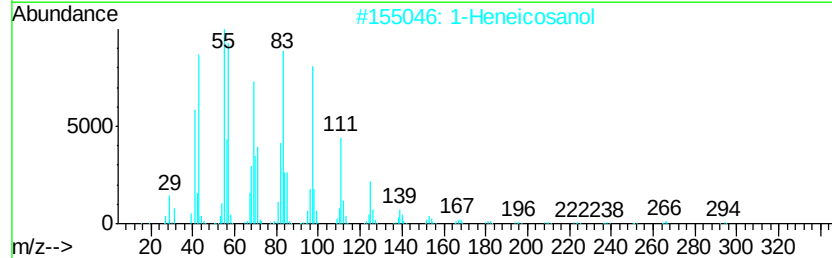
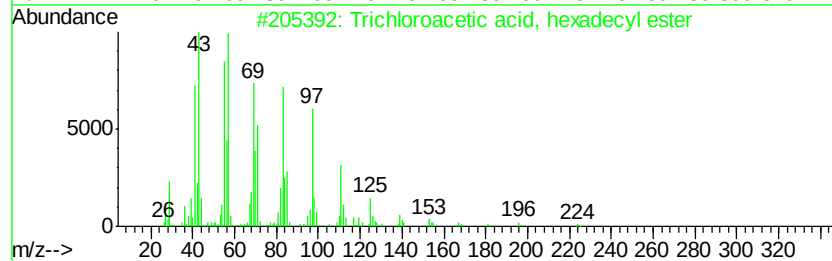
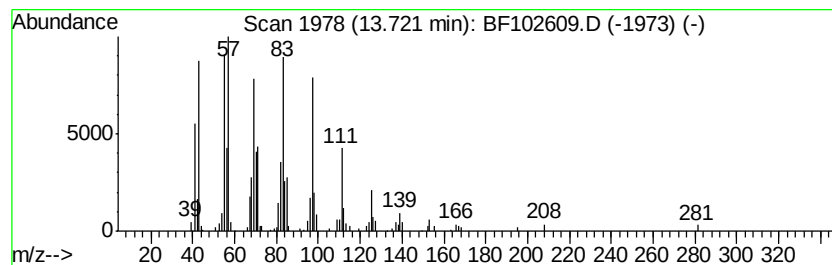
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Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	5.12 ng	302474	Chrysene-d12	13.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
5		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91



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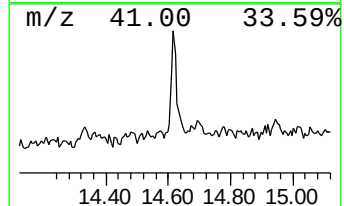
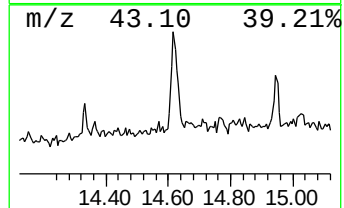
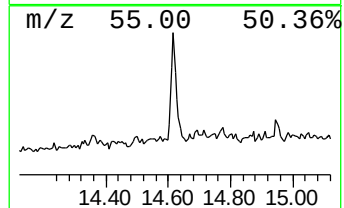
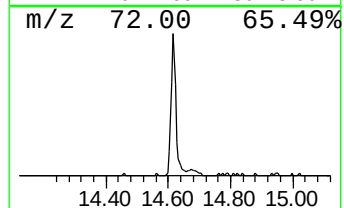
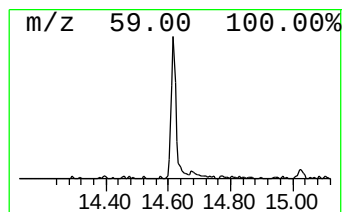
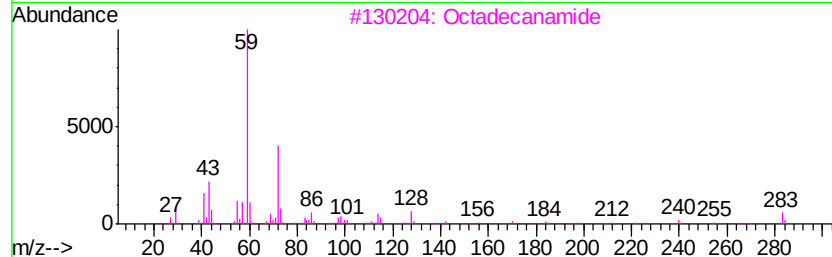
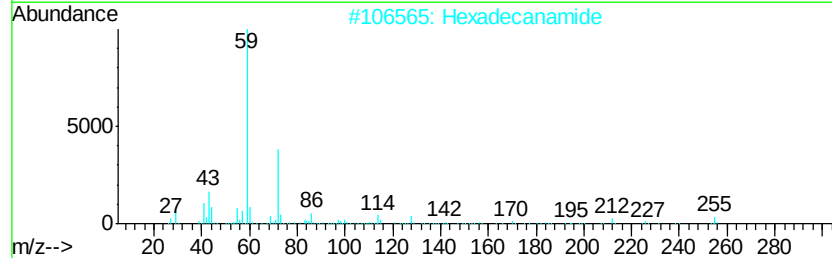
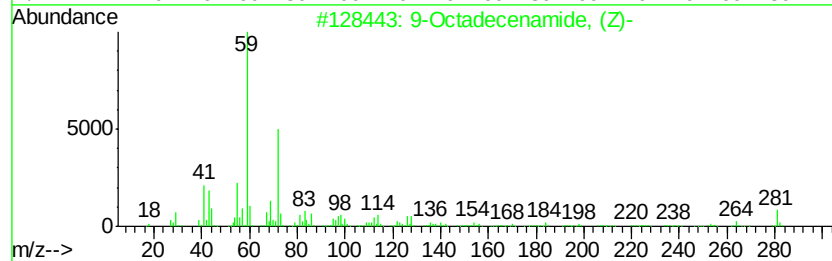
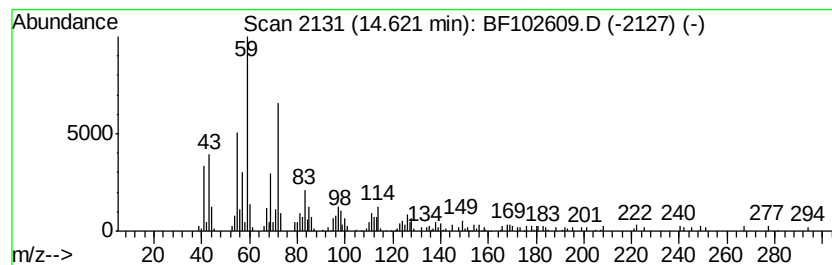
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	4.37 ng	220834	Perylene-d12	15.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		Hexadecanamide	255	C16H33NO	000629-54-9	64
3		Octadecanamide	283	C18H37NO	000124-26-5	53
4		trans-2,7-Dimethyl-4,6-octadien-...	154	C10H18O	1000281-69-5	46
5		2-Methyl-tridecane-2,12-diol	230	C14H30O2	1000187-03-5	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	2.9	ng	146870	1	6.71	1002920	20.0
unknown6.49	6.49	84.9	ng	4257740	1	6.71	1002920	20.0
Trichloroacetic a...	13.72	5.1	ng	302474	5	13.88	1180400	20.0
9-Octadecenamide,...	14.62	4.4	ng	220834	6	15.31	1009980	20.0