

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051622\
 Data File : BG053574.D
 Acq On : 16 May 2022 19:36
 Operator : CG/JU
 Sample : N2847-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PSC-124019

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_G\Methods\8270-BG050522.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053574.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.655	379	386	401	rBV	394586	655388	57.93%	8.396%
2	7.253	651	658	668	rBV	419171	754207	66.67%	9.662%
3	8.087	794	800	809	rVB	90753	155338	13.73%	1.990%
4	9.250	990	998	1009	rBV	253673	474791	41.97%	6.082%
5	10.895	1269	1278	1288	rBV	124495	233384	20.63%	2.990%
6	13.333	1687	1693	1701	rBV	570160	884421	78.18%	11.330%
7	14.713	1918	1928	1937	rBV	225289	368337	32.56%	4.719%
8	16.199	2174	2181	2192	rBV	593505	965056	85.31%	12.363%
9	17.457	2389	2395	2401	rBV	284487	435499	38.50%	5.579%
10	18.344	2541	2546	2560	rBV2	117420	254700	22.51%	3.263%
11	19.513	2738	2745	2752	rBV6	20039	54272	4.80%	0.695%
12	19.607	2757	2761	2774	rBV2	174235	365971	32.35%	4.688%
13	20.059	2833	2838	2844	rVB	851057	1131250	100.00%	14.492%
14	21.363	3056	3060	3073	rBV2	63529	139868	12.36%	1.792%
15	21.739	3118	3124	3131	rVB2	268161	456940	40.39%	5.854%
16	25.023	3674	3683	3695	rVB2	166602	476719	42.14%	6.107%

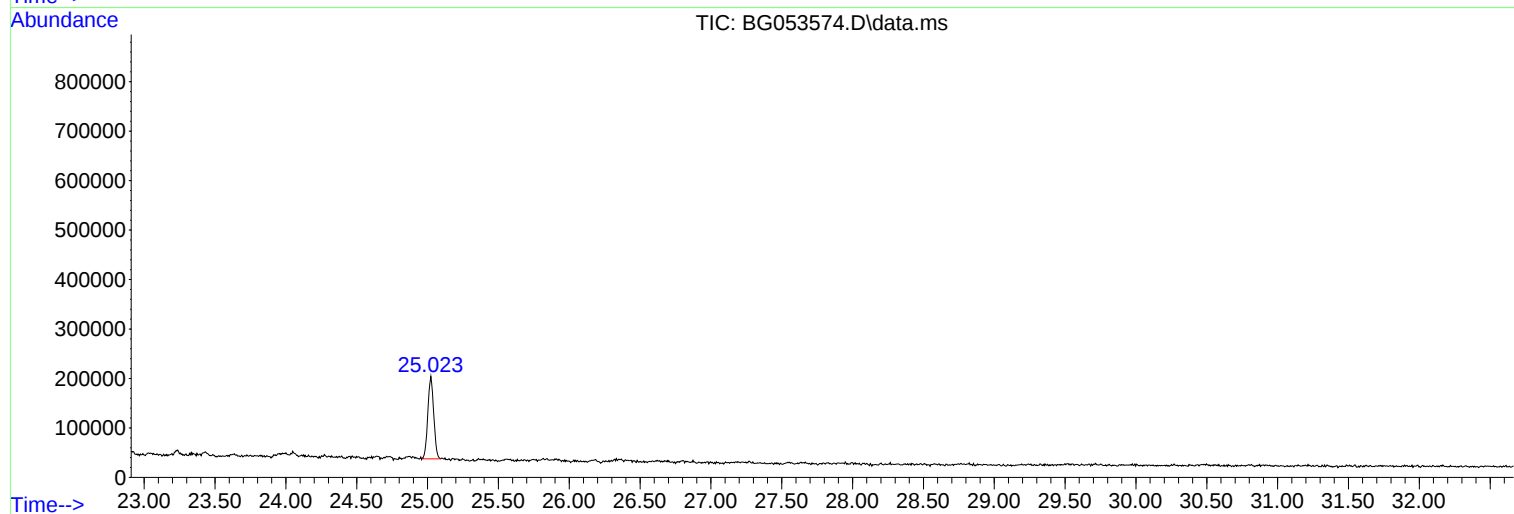
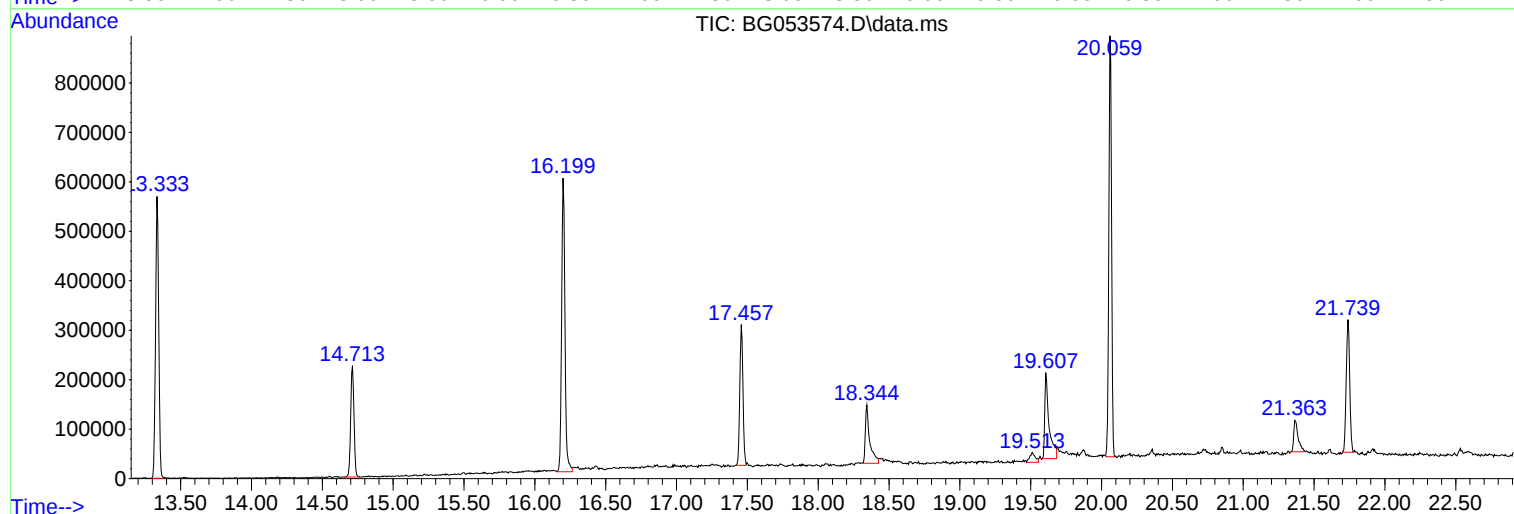
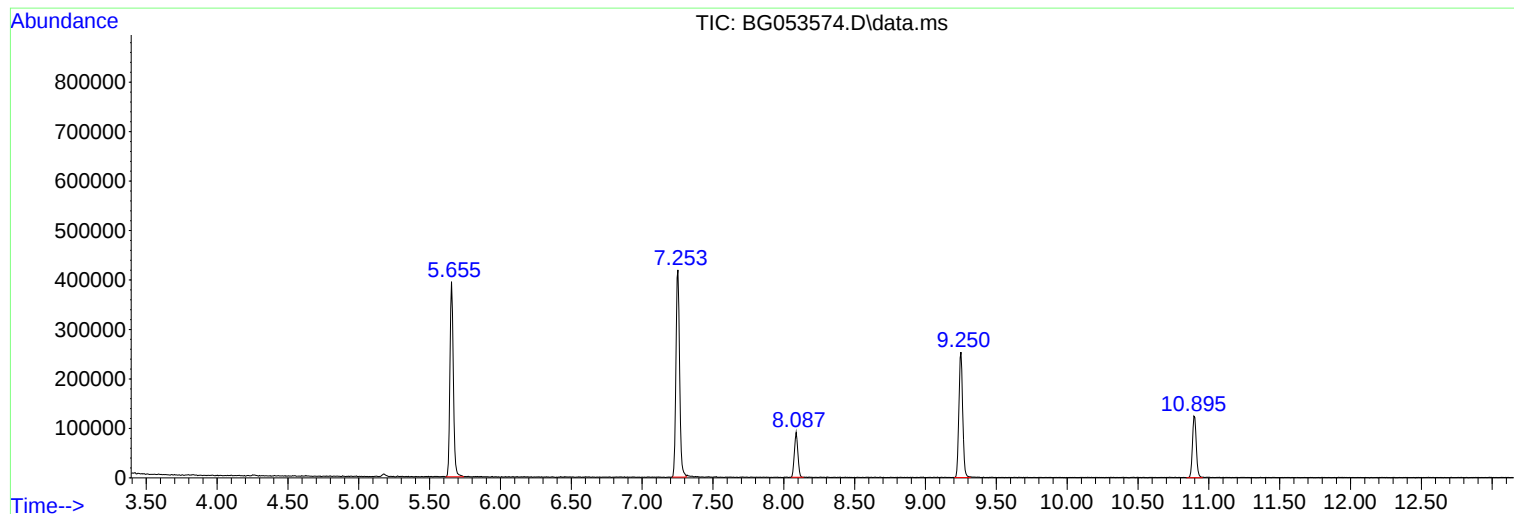
Sum of corrected areas: 7806141

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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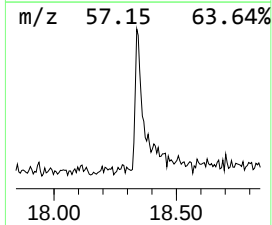
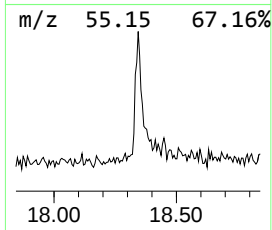
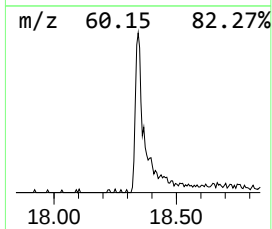
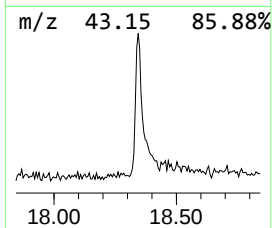
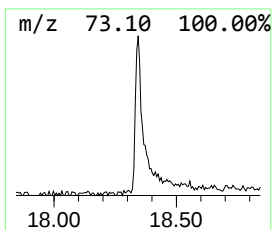
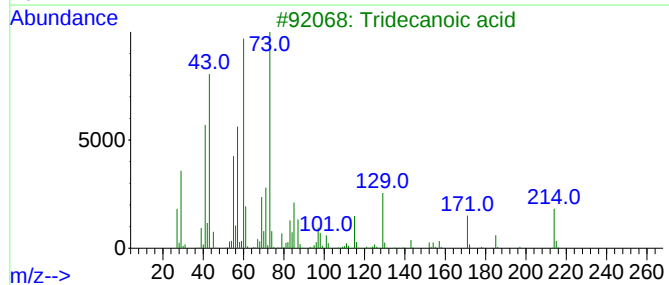
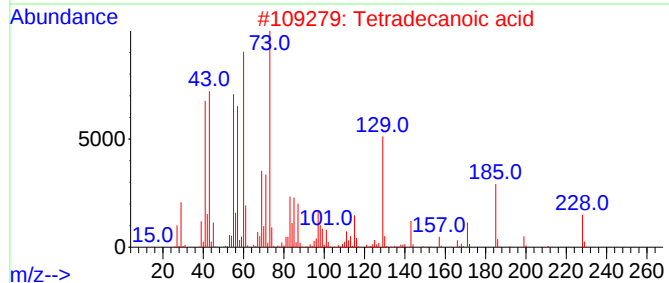
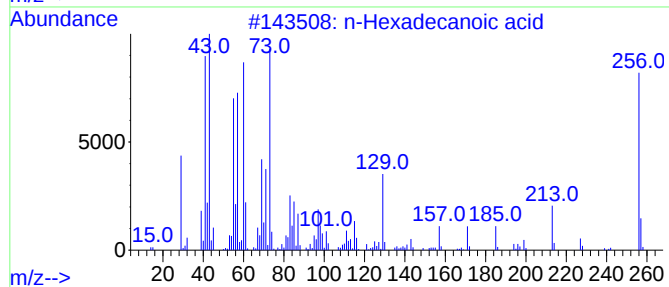
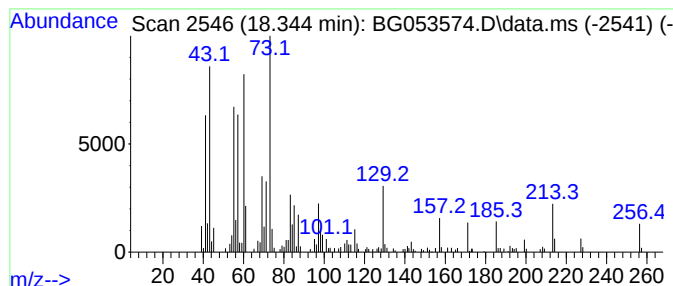
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.344	11.70 ng	254700	Phenanthrene-d10	17.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Dodecanoic acid	200	C12H24O2	000143-07-7	64
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	58



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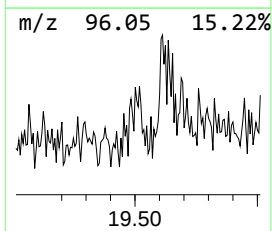
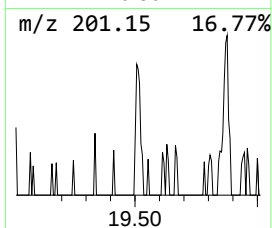
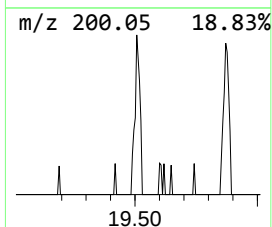
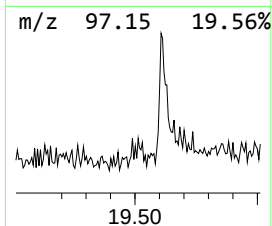
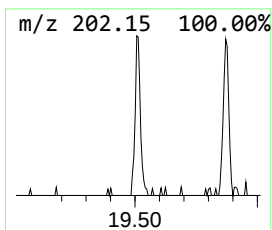
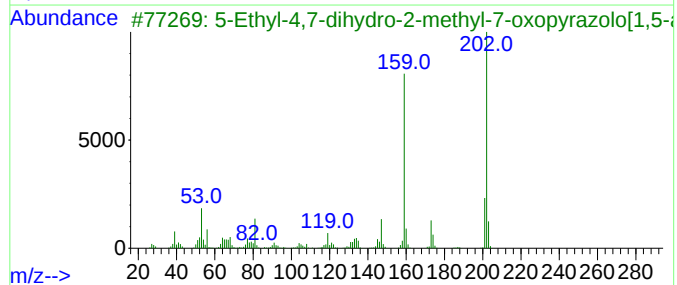
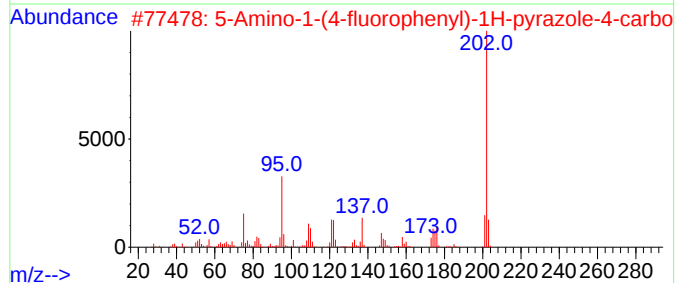
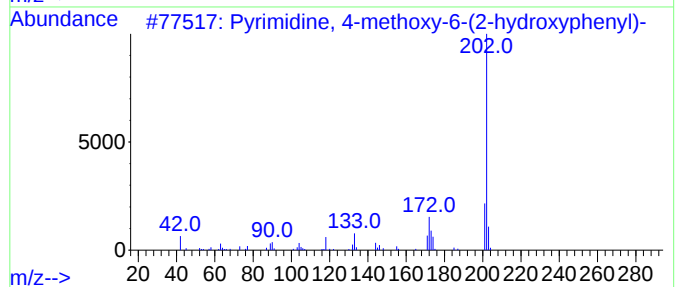
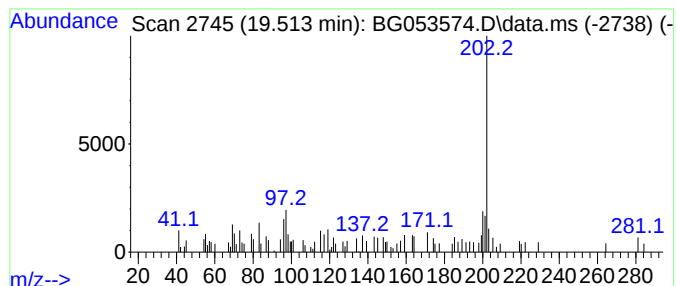
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Pyrimidine, 4-methoxy-6-(2-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.513	2.49 ng	54272	Phenanthrene-d10	17.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrimidine, 4-methoxy-6-(2-hydro...	202	C11H10N2O2	097630-79-0	50
2			5-Amino-1-(4-fluorophenyl)-1H-py...	202	C10H7FN4	051516-70-2	50
3			5-Ethyl-4,7-dihydro-2-methyl-7-o...	202	C10H10N4O	903195-75-5	50
4			1,2,3-Thiadiazole, 4-(4-trifluor...	230	C9H5F3N2S	253122-65-5	50
5			Acetic acid, 1,2,3-trimethyl-4-p...	261	C16H23NO2	1000271-58-1	50



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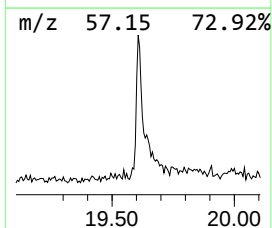
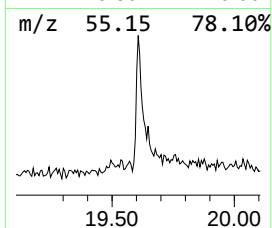
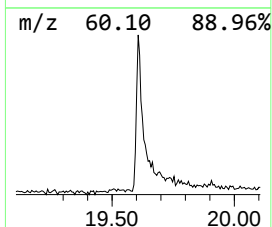
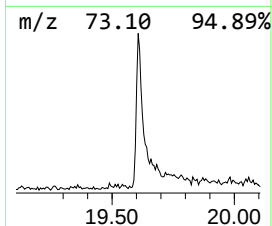
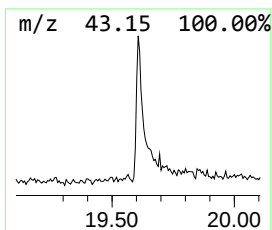
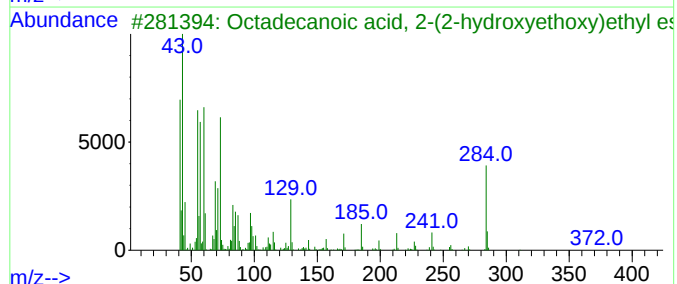
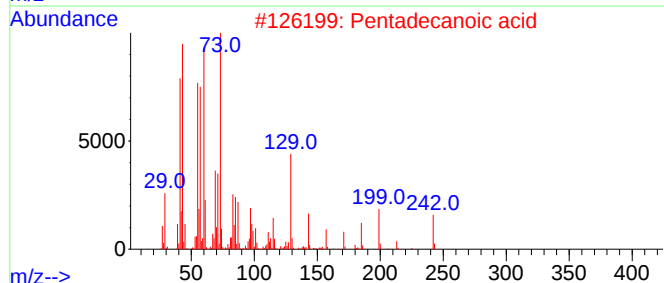
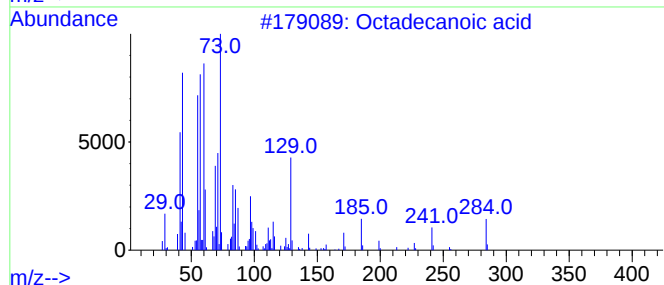
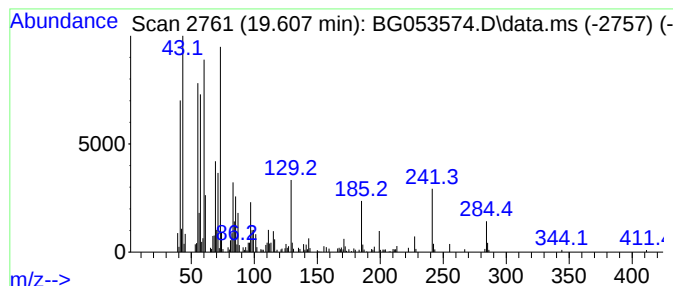
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Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.607	16.02 ng	365971	Chrysene-d12	21.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			Dodecanoic acid	200	C12H24O2	000143-07-7	58



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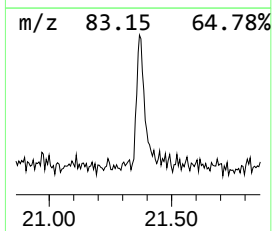
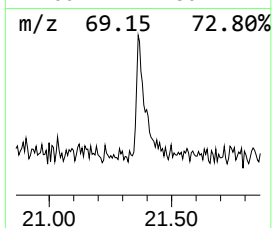
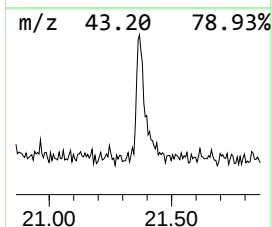
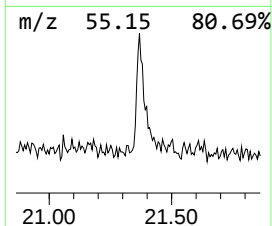
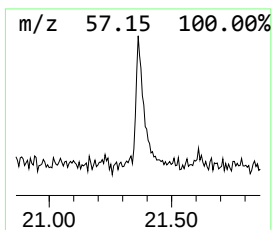
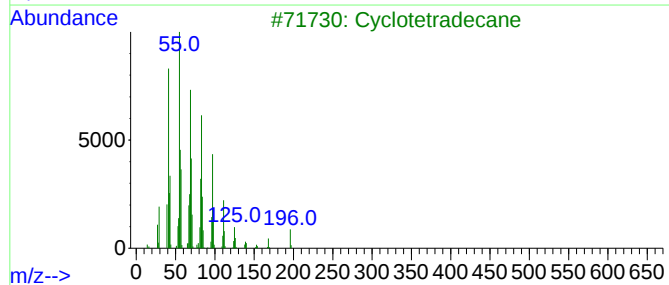
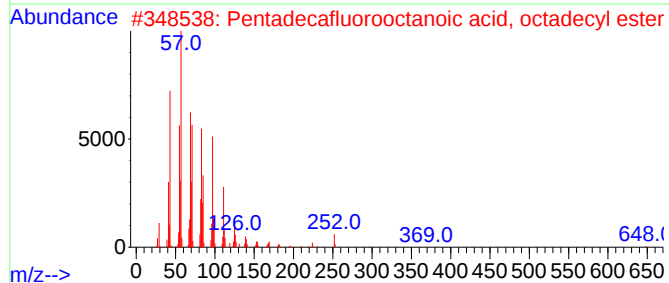
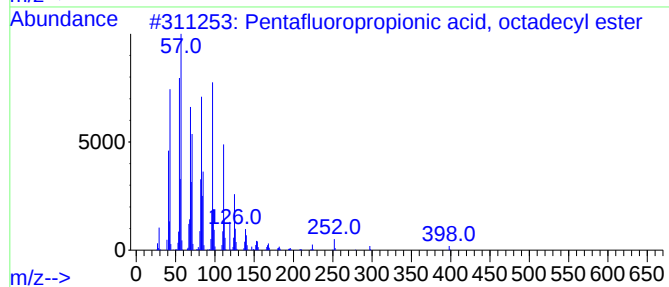
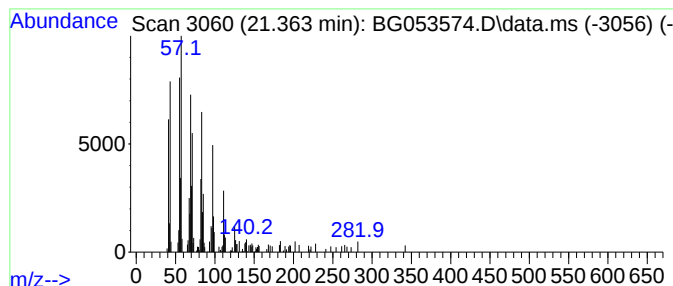
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Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.363	6.12 ng	139868	Chrysene-d12	21.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
3			Cyclotetradecane	196	C14H28	000295-17-0	90
4			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	90
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.344	11.7	ng	254700	4	17.457	435499	20.0
Pyrimidine, 4-m...	19.513	2.5	ng	54272	4	17.457	435499	20.0
Octadecanoic acid	19.607	16.0	ng	365971	5	21.739	456940	20.0
Pentafluoroprop...	21.363	6.1	ng	139868	5	21.739	456940	20.0