

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112221\
 Data File : BG051169.D
 Acq On : 22 Nov 2021 14:06
 Operator : CG/JU
 Sample : M4783-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RBR-200033

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-BG111921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051169.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.262	294	302	309	rBV	40266	63565	4.46%	0.861%
2	5.744	377	384	397	rVB	339545	558846	39.24%	7.571%
3	7.359	651	659	676	rBV	337118	609579	42.80%	8.259%
4	8.205	797	803	810	rBV	89567	149730	10.51%	2.029%
5	9.380	995	1003	1011	rBV	216911	390392	27.41%	5.289%
6	10.779	1235	1241	1252	rBV2	20153	39649	2.78%	0.537%
7	11.031	1276	1284	1293	rBV	123016	223844	15.72%	3.033%
8	13.458	1689	1697	1705	rBV	554751	850334	59.71%	11.520%
9	14.839	1925	1932	1939	rVB	216754	335771	23.58%	4.549%
10	16.325	2179	2185	2198	rBV	445390	704886	49.50%	9.550%
11	17.588	2394	2400	2406	rBV	301762	466392	32.75%	6.319%
12	18.440	2539	2545	2553	rBV2	23001	38393	2.70%	0.520%
13	19.633	2744	2748	2753	rVB2	11326	17515	1.23%	0.237%
14	19.997	2806	2810	2815	rVB	10866	14393	1.01%	0.195%
15	20.180	2835	2841	2847	rBV	1071075	1424143	100.00%	19.294%
16	20.444	2880	2886	2891	rBV9	6381	15896	1.12%	0.215%
17	21.478	3057	3062	3075	rVB4	53783	110407	7.75%	1.496%
18	21.731	3101	3105	3111	rVB	59510	78042	5.48%	1.057%
19	21.889	3125	3132	3138	rBV	299077	500983	35.18%	6.787%
20	22.671	3262	3265	3269	rBV5	10870	17087	1.20%	0.231%
21	23.082	3330	3335	3340	rBV8	12502	29331	2.06%	0.397%
22	23.599	3417	3423	3430	rVB	117467	247014	17.34%	3.347%
23	25.291	3700	3711	3722	rVB2	154334	494966	34.76%	6.706%

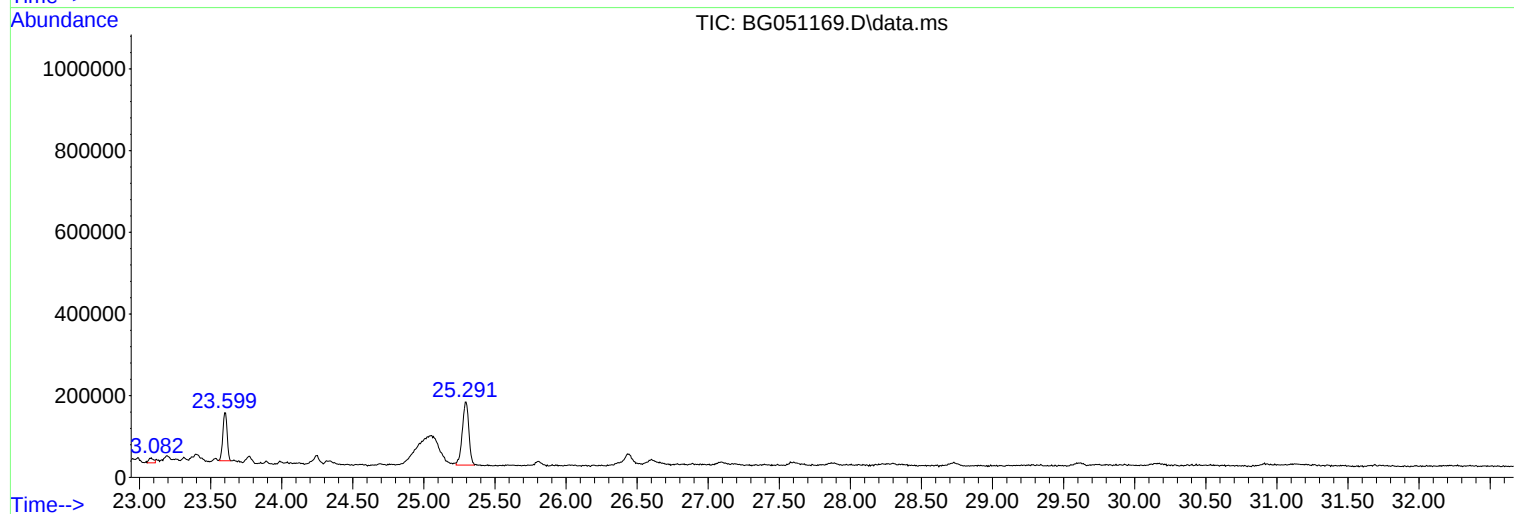
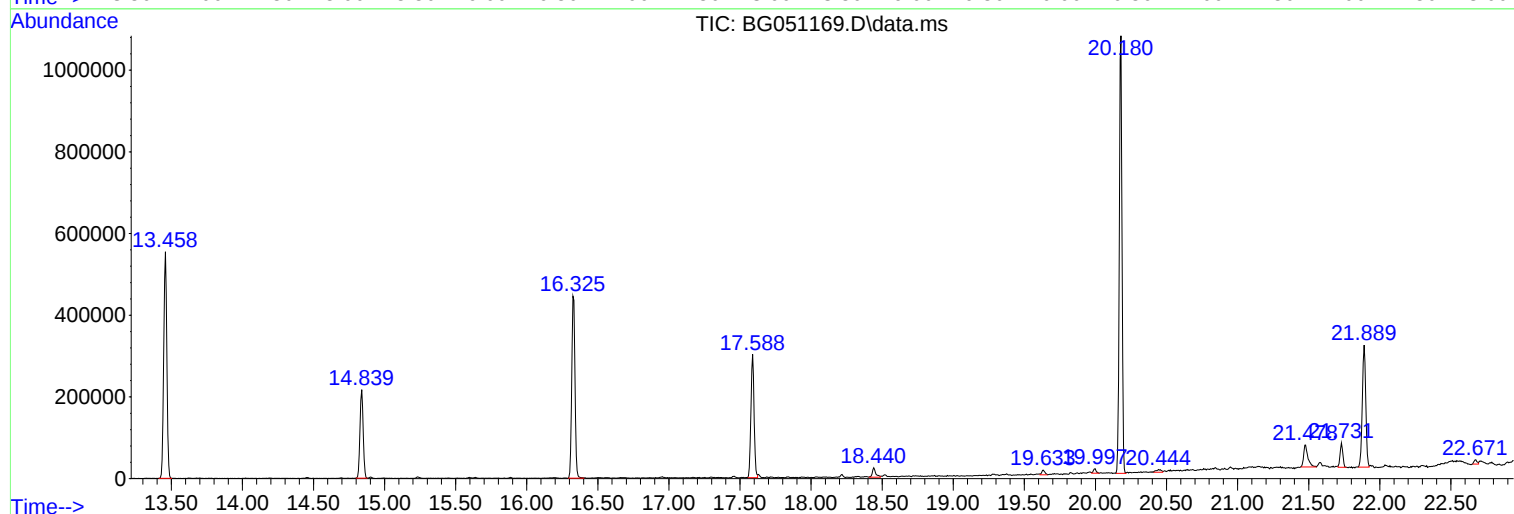
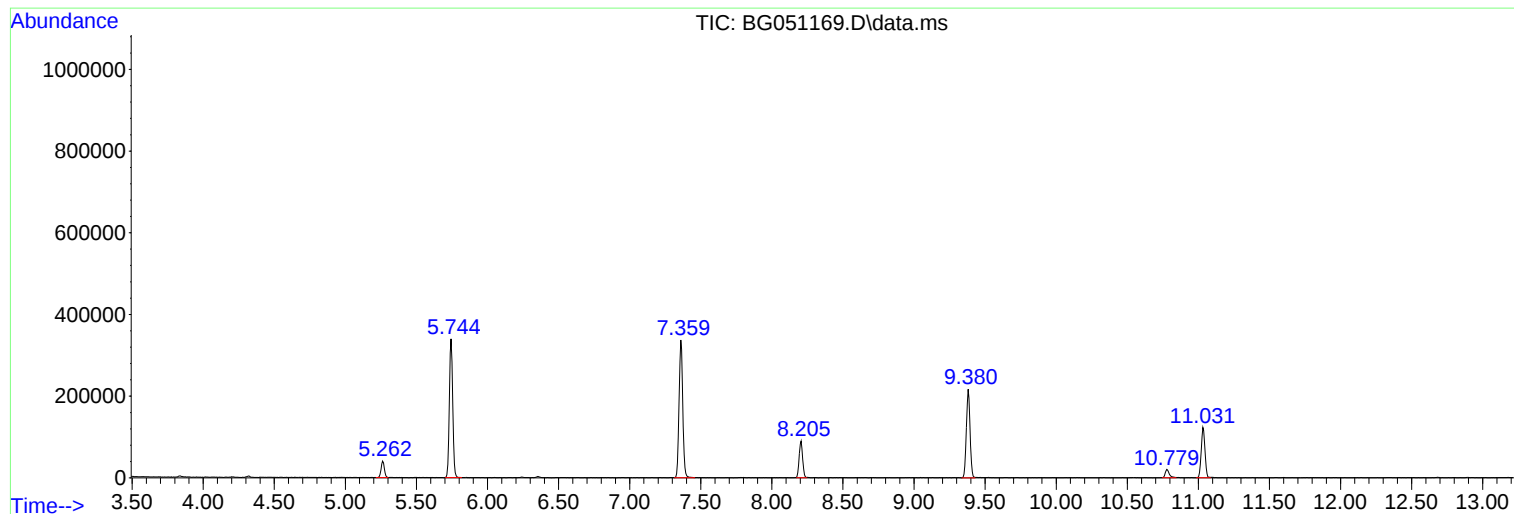
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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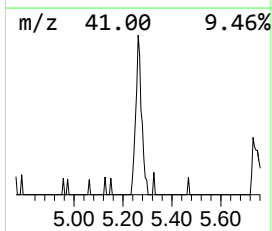
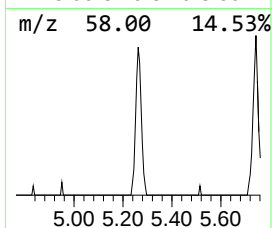
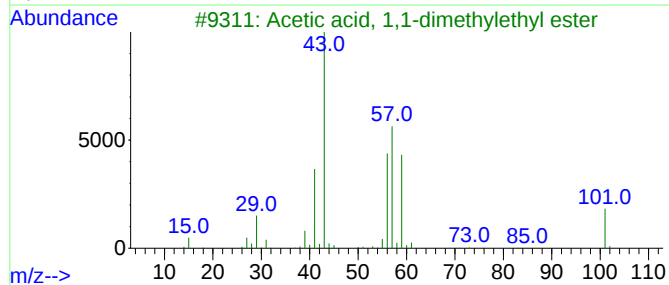
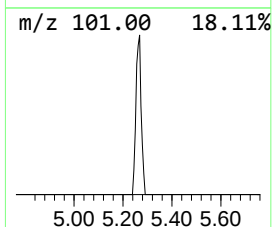
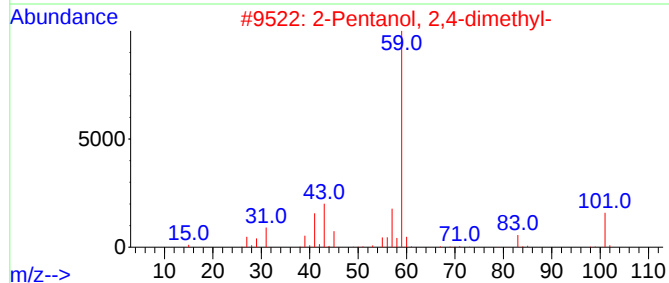
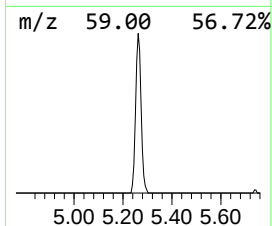
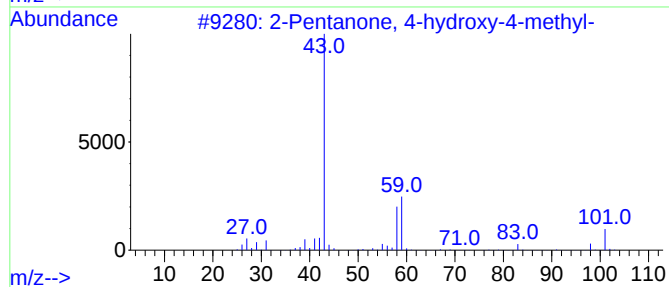
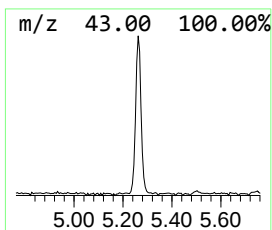
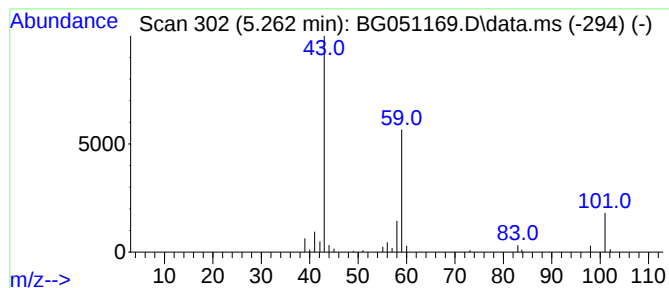
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.262	8.49 ng	63565	1,4-Dichlorobenzene-d4	8.205

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	40	
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38	
4	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	28	
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25	



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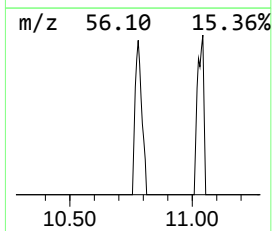
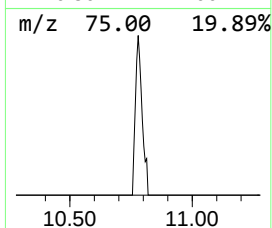
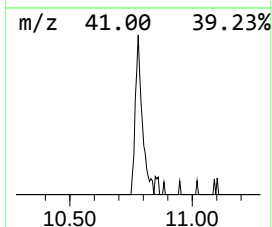
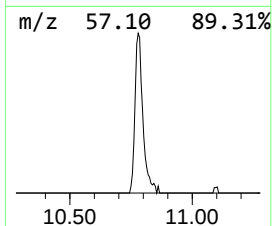
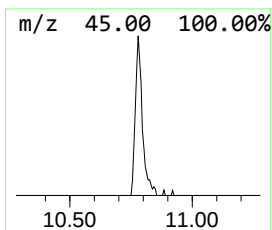
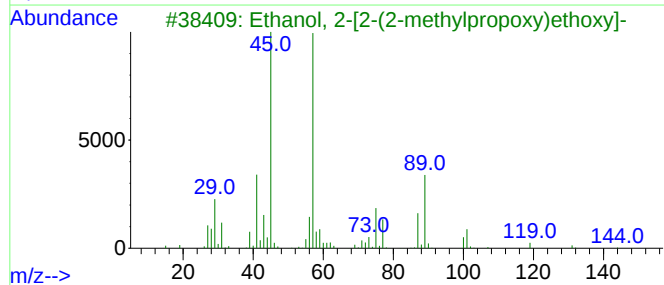
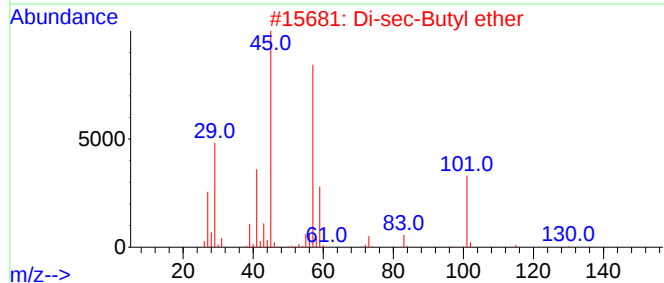
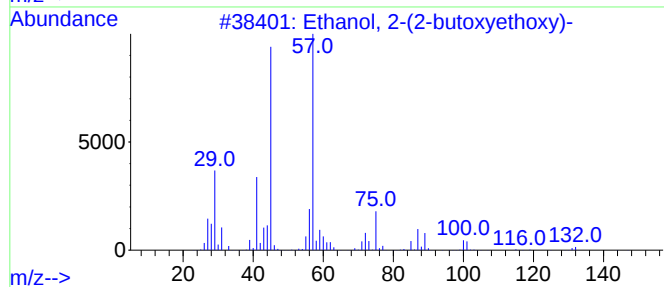
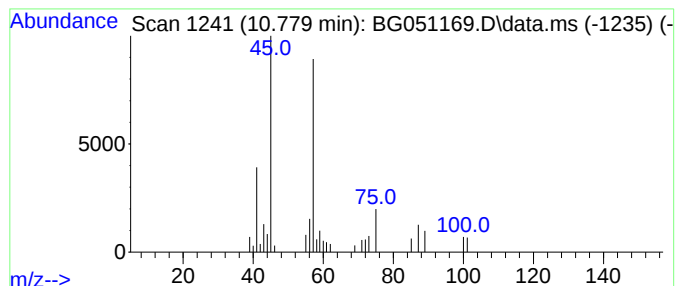
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.779	3.54 ng	39649	Naphthalene-d8	11.031

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	45
4			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	45
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	43



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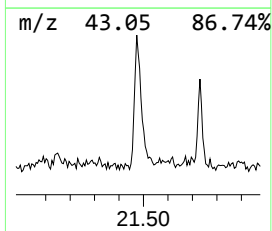
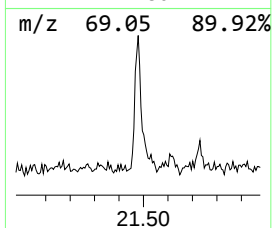
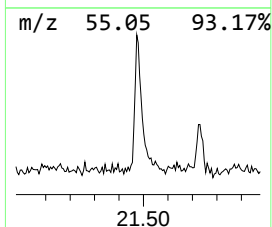
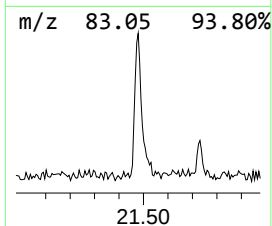
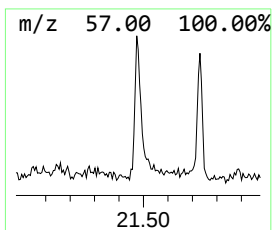
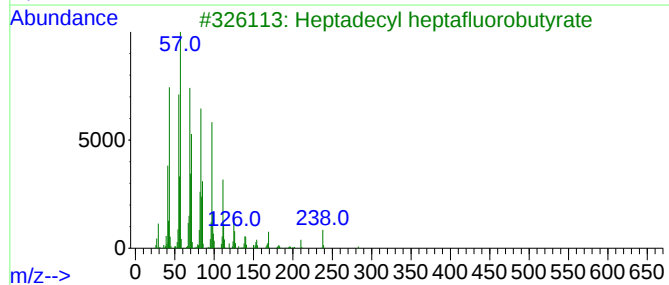
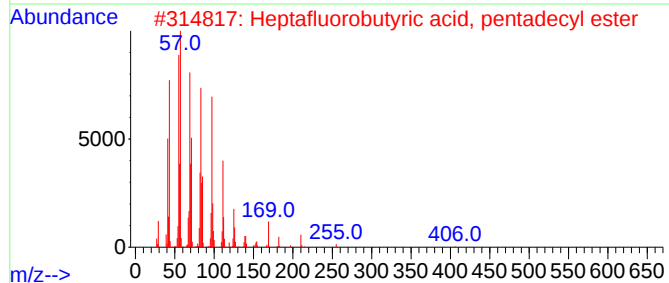
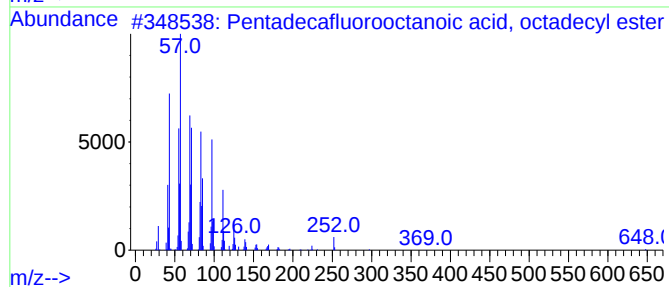
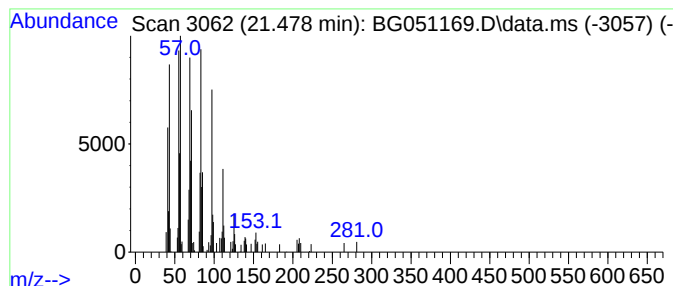
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Peak Number 3 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.478	4.41 ng	110407	Chrysene-d12	21.889

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	93



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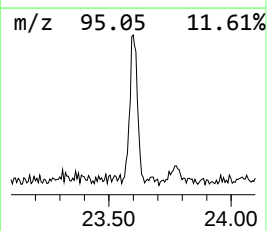
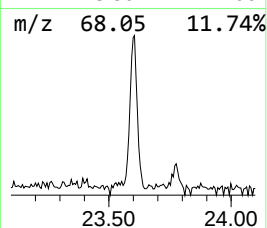
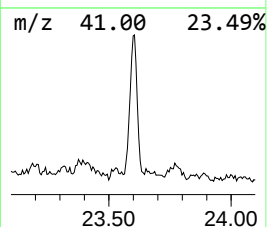
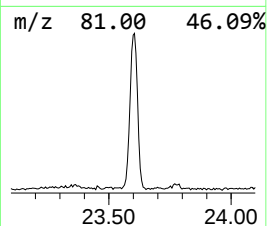
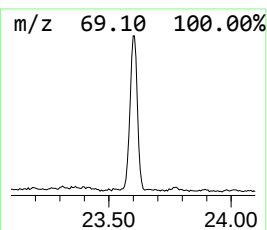
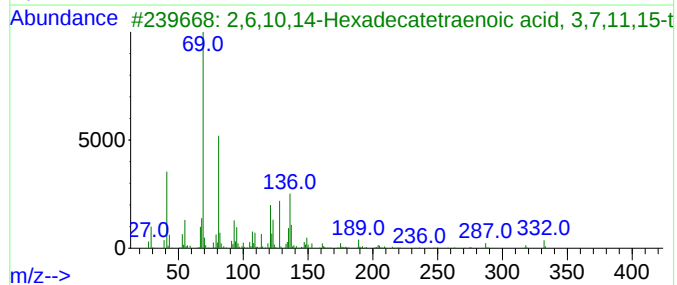
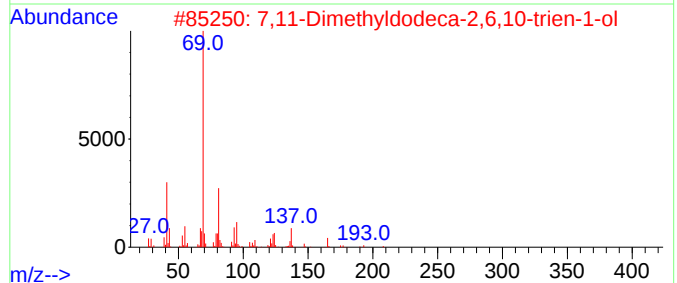
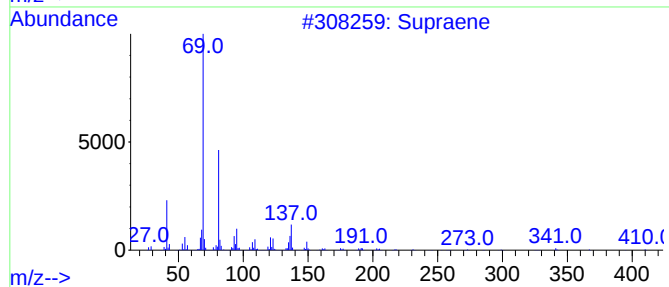
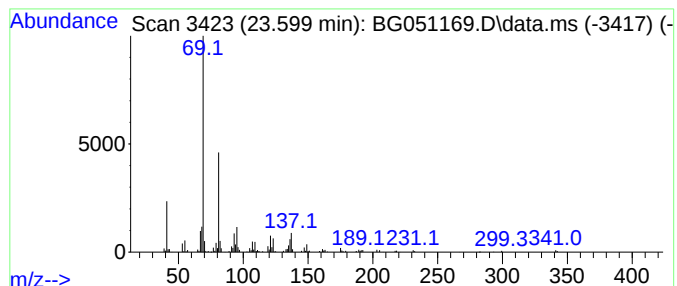
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Peak Number 4 Supraene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.599	9.98 ng	247014	Perylene-d12	25.291

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	78
3			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78
4			2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	72
5			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.262	8.5	ng	63565	1	8.205	149730	20.0
Ethanol, 2-(2-b...	10.779	3.5	ng	39649	2	11.031	223844	20.0
Pentadecafluoro...	21.478	4.4	ng	110407	5	21.889	500983	20.0
Supraene	23.599	10.0	ng	247014	6	25.291	494966	20.0