

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121621\
 Data File : BF126210.D
 Acq On : 16 Dec 2021 14:14
 Operator : JU/CG
 Sample : M5022-29
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP12

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-BF121521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126210.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.904	132	139	145	rBV	27527	49196	1.14%	0.150%
2	5.022	490	499	505	rBV	919373	1171489	27.16%	3.570%
3	5.428	562	568	571	rBV	3978256	4178383	96.87%	12.733%
4	5.828	633	636	640	rVB	128088	109740	2.54%	0.334%
5	6.434	734	739	742	rBV	3860659	4313488	100.00%	13.144%
6	6.816	800	804	807	rBV	1468850	1189660	27.58%	3.625%
7	7.375	894	899	902	rBV	2995077	2807843	65.09%	8.556%
8	7.586	931	935	939	rVB	51648	48161	1.12%	0.147%
9	7.998	1001	1005	1009	rBV	251297	194275	4.50%	0.592%
10	8.098	1017	1022	1025	rBV	1893985	1695015	39.30%	5.165%
11	9.175	1200	1205	1208	rBV	4730392	4210648	97.62%	12.831%
12	9.263	1216	1220	1223	rBV2	105010	88853	2.06%	0.271%
13	9.657	1282	1287	1294	rBV	104709	107907	2.50%	0.329%
14	9.851	1316	1320	1323	rBV	2189970	1796527	41.65%	5.475%
15	10.269	1387	1391	1393	rBV2	69186	67543	1.57%	0.206%
16	10.633	1449	1453	1457	rBV	2655301	2500666	57.97%	7.620%
17	11.304	1562	1567	1569	rBV2	70165	63805	1.48%	0.194%
18	11.333	1569	1572	1575	rVV	2147869	1757573	40.75%	5.356%
19	11.404	1579	1584	1587	rBV4	50452	67140	1.56%	0.205%
20	11.863	1659	1662	1666	rBV2	102106	88004	2.04%	0.268%
21	12.751	1810	1813	1815	rBV	50631	46305	1.07%	0.141%
22	12.921	1837	1842	1845	rBV	3816058	3399917	78.82%	10.360%
23	13.821	1990	1995	2003	rBV	272497	290711	6.74%	0.886%
24	13.962	2015	2019	2023	rBV	1056900	1030622	23.89%	3.141%
25	14.457	2099	2103	2117	rBV2	78482	107163	2.48%	0.327%
26	15.092	2207	2211	2214	rBV2	40592	56288	1.30%	0.172%
27	15.409	2260	2265	2271	rBV	984935	1151625	26.70%	3.509%
28	15.468	2271	2275	2282	rVB2	36769	50246	1.16%	0.153%
29	15.898	2344	2348	2352	rBV2	43703	68993	1.60%	0.210%
30	16.398	2429	2433	2440	rVB4	26778	46446	1.08%	0.142%
31	17.439	2604	2610	2617	rVB8	27741	61940	1.44%	0.189%

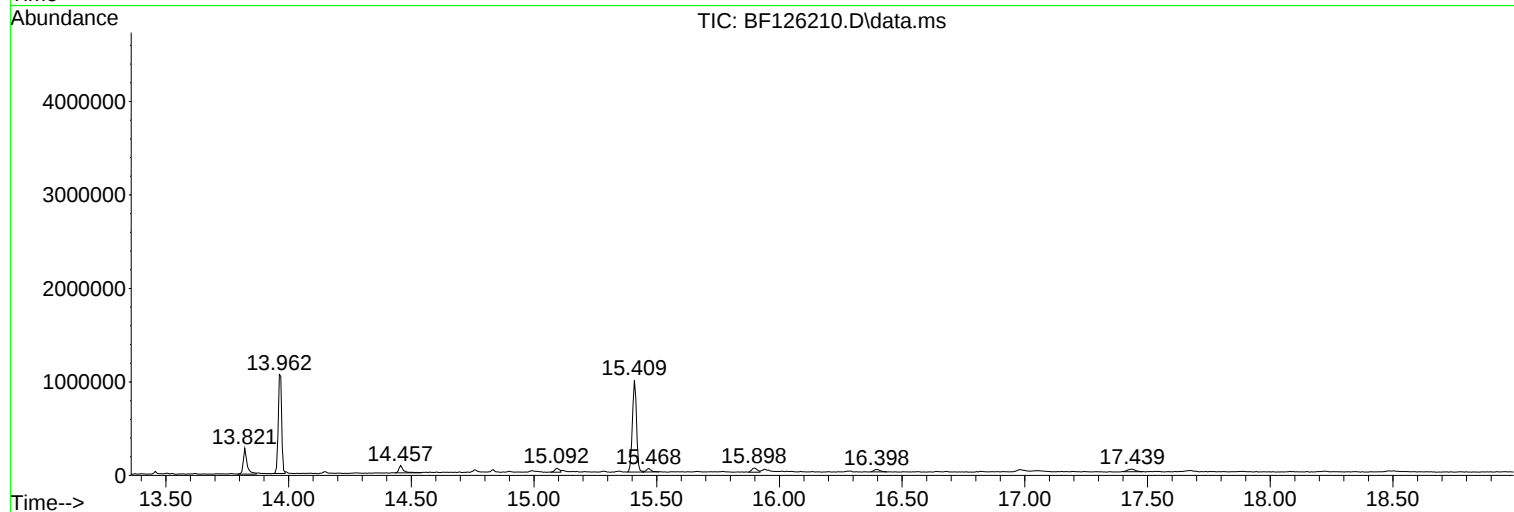
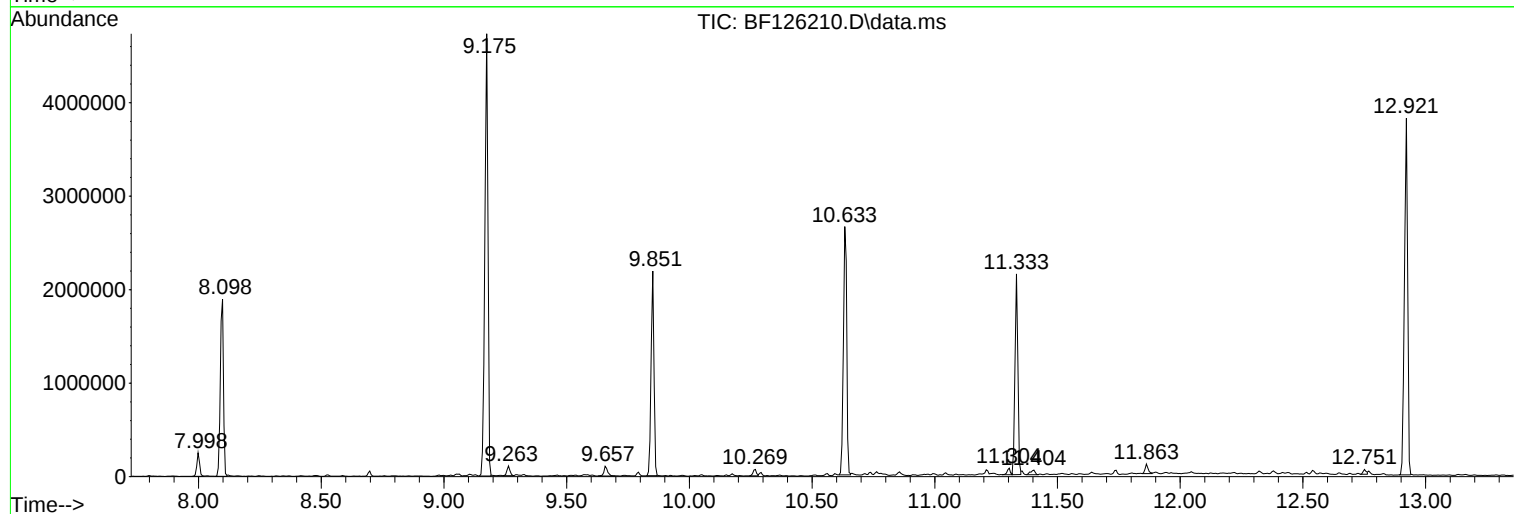
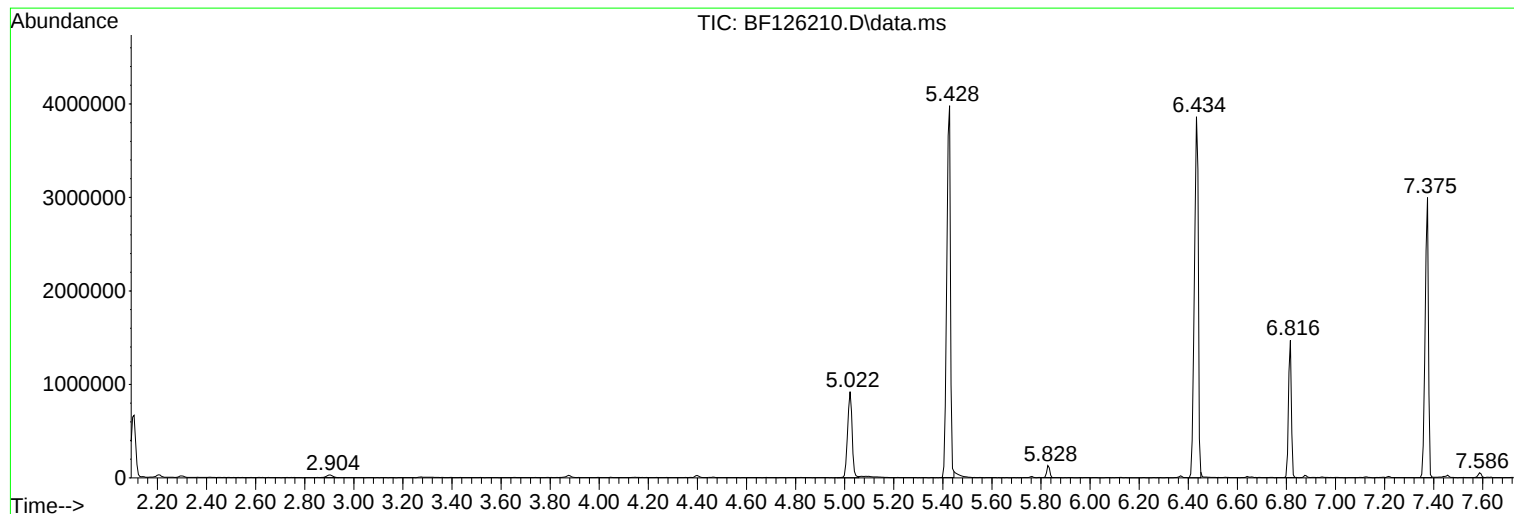
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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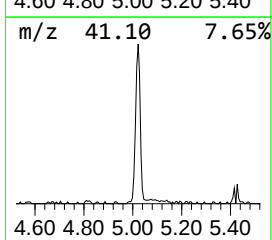
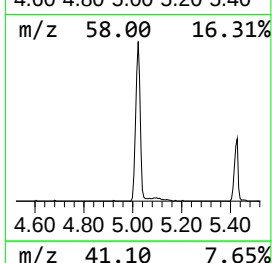
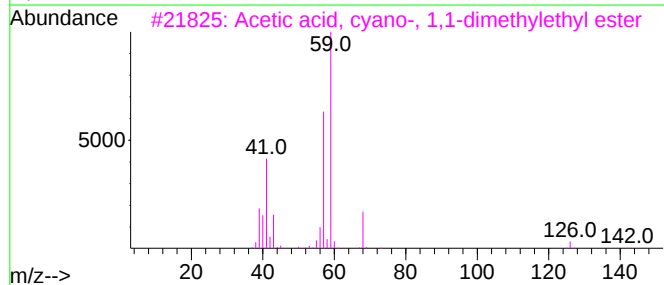
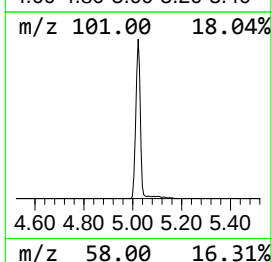
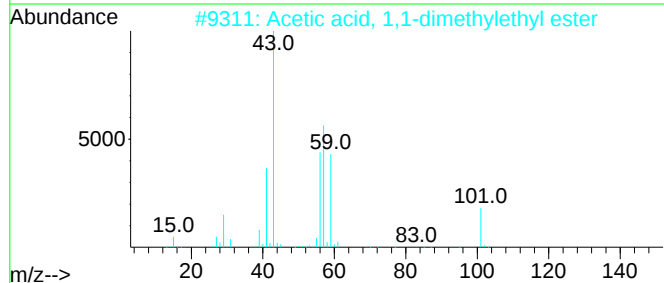
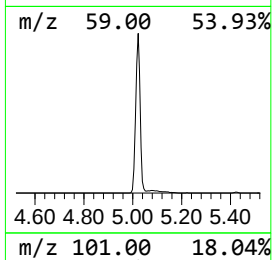
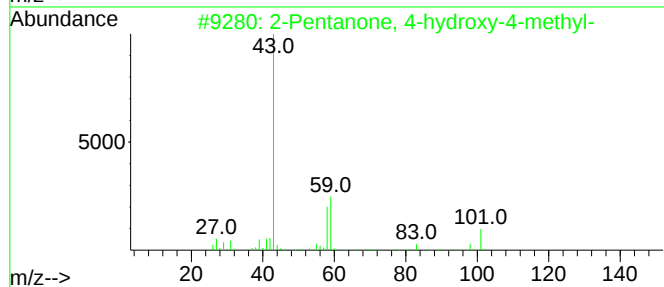
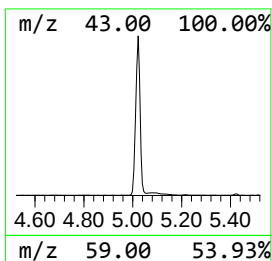
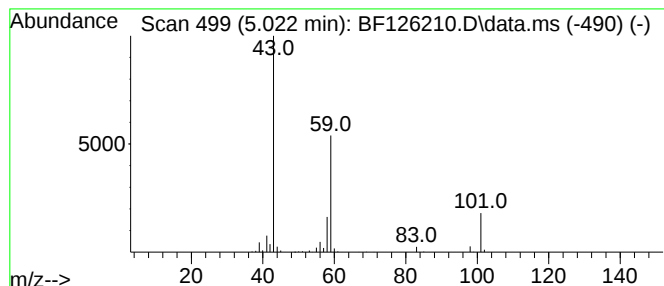
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	19.69 ng	1171490	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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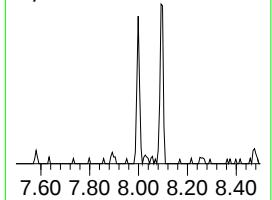
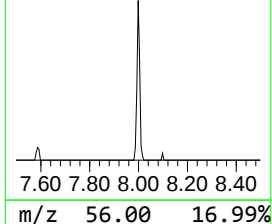
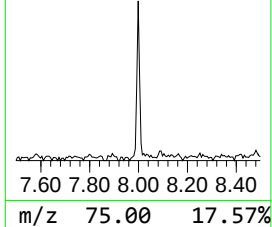
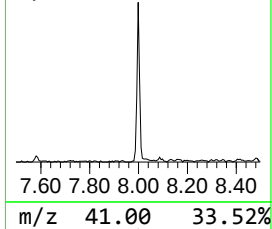
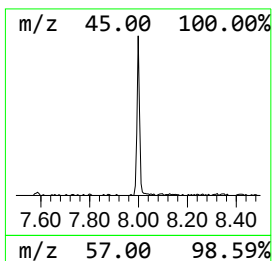
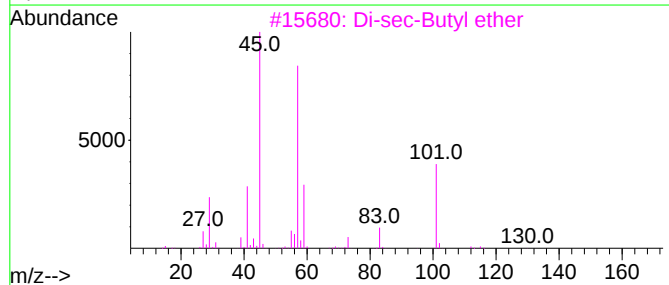
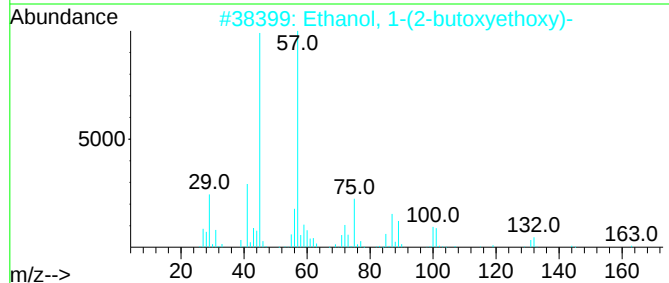
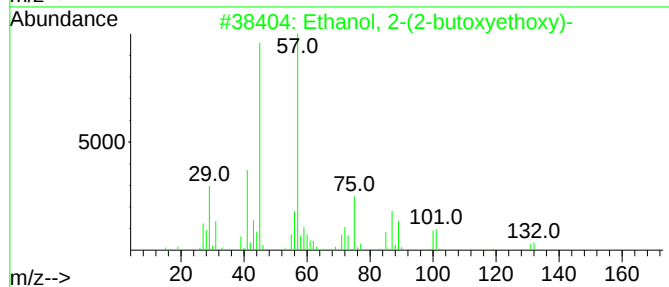
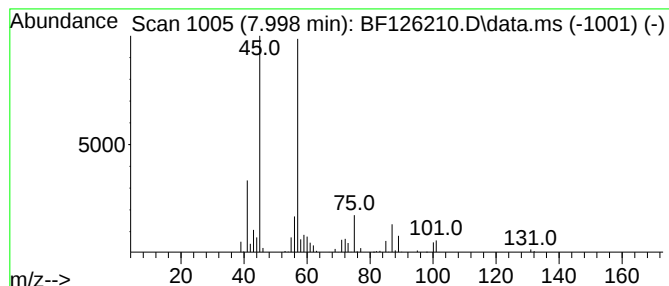
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.998	2.29 ng	194275	Naphthalene-d8	8.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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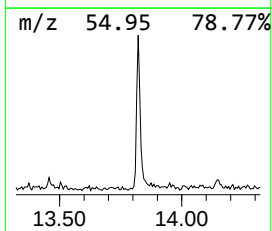
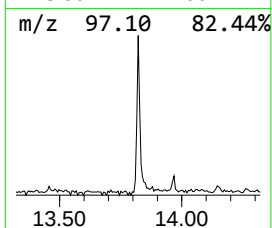
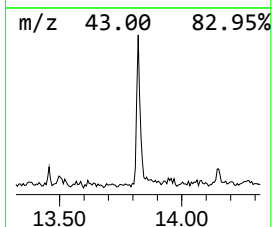
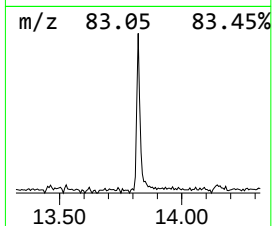
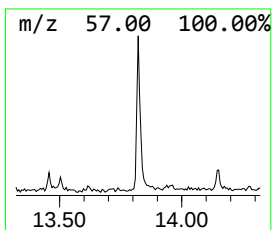
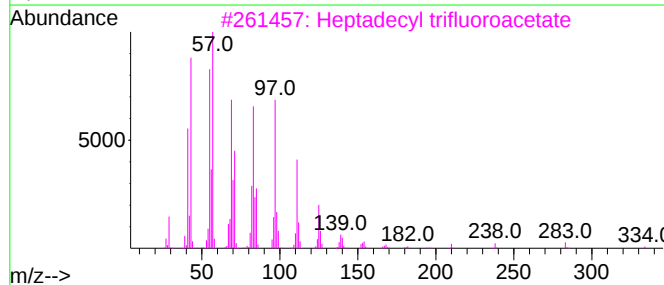
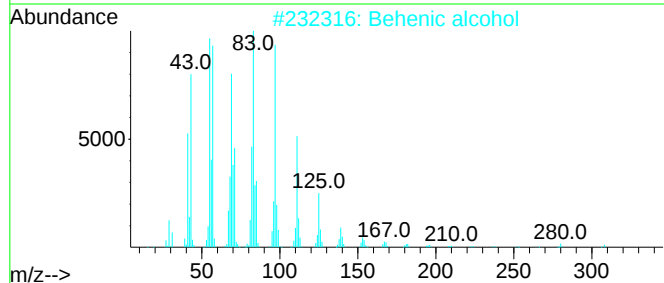
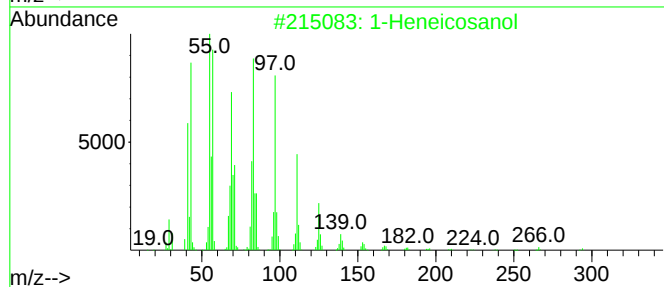
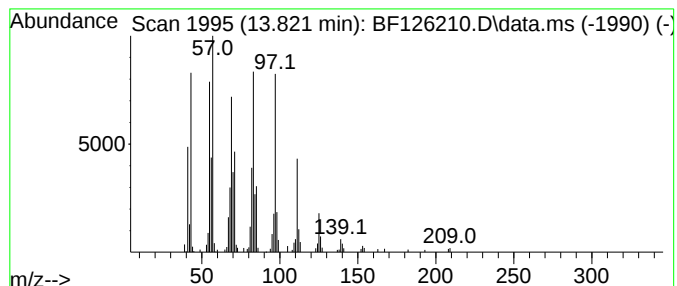
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Peak Number 3 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.821	5.64 ng	290711	Chrysene-d12	13.968	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	93
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	91



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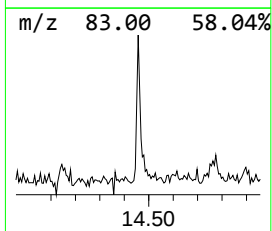
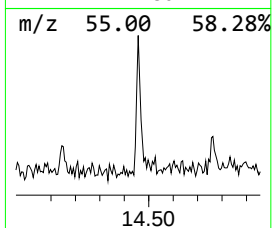
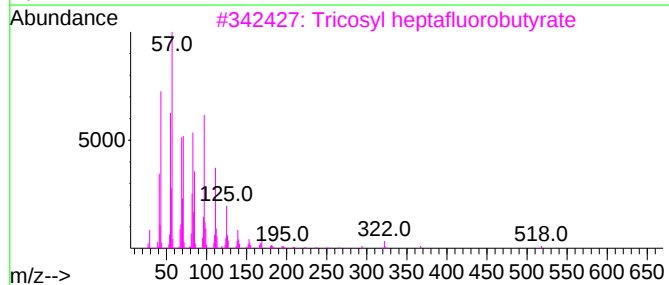
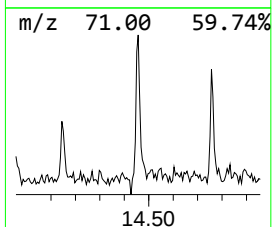
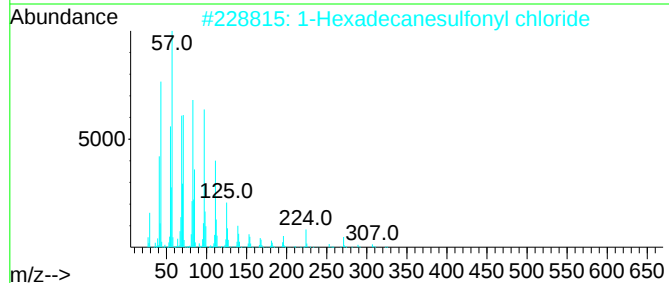
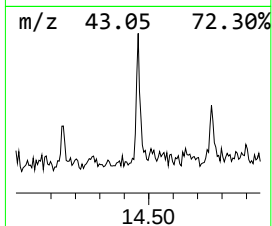
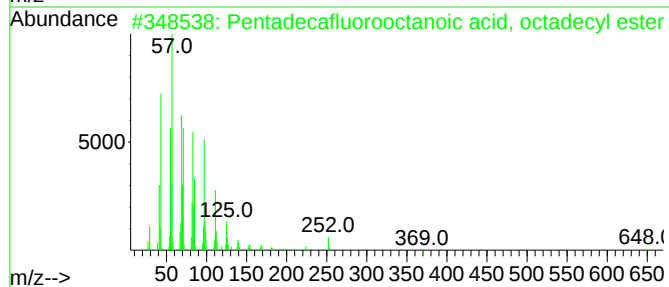
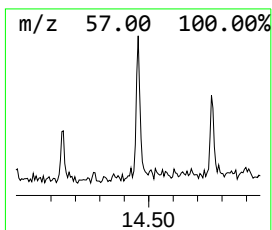
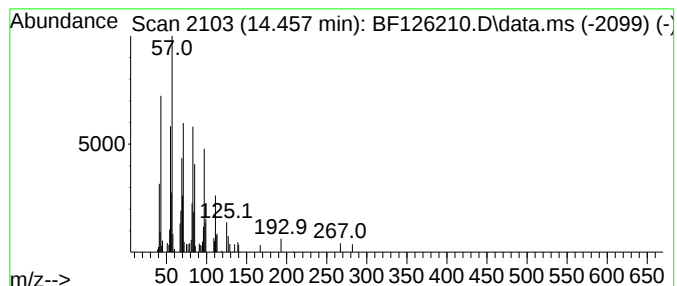
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Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.457	2.08 ng	107163	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
3			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
4			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
5			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.022	19.7	ng	1171490	1	6.816	1189660	20.0
Ethanol, 2-(2-b...	7.998	2.3	ng	194275	2	8.098	1695020	20.0
1-Heneicosanol	13.821	5.6	ng	290711	5	13.968	1030620	20.0
Pentadecafluoro...	14.457	2.1	ng	107163	5	13.968	1030620	20.0