

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082622\
 Data File : BG054760.D
 Acq On : 26 Aug 2022 18:06
 Operator : CG/JU
 Sample : N4226-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B-1

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-BG082522.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054760.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.209	321	327	335	rBV	111558	173173	5.70%	1.183%
2	5.685	401	408	419	rBV	668948	1076976	35.42%	7.359%
3	7.295	674	682	693	rBV	696260	1212392	39.88%	8.284%
4	8.147	820	827	833	rBV	155032	274068	9.01%	1.873%
5	9.322	1017	1027	1039	rBV	432241	774177	25.46%	5.290%
6	10.973	1301	1308	1316	rBV	217157	399508	13.14%	2.730%
7	13.405	1715	1722	1736	rBV	1210834	1943853	63.93%	13.282%
8	14.780	1950	1956	1964	rBV	376601	585372	19.25%	4.000%
9	16.267	2202	2209	2223	rBV	826274	1272647	41.86%	8.696%
10	17.524	2416	2423	2429	rBV	459119	733801	24.14%	5.014%
11	17.565	2429	2430	2437	rVB	27906	31839	1.05%	0.218%
12	19.575	2766	2772	2778	rBV	65370	94246	3.10%	0.644%
13	19.933	2829	2833	2840	rVB	61891	90035	2.96%	0.615%
14	20.127	2860	2866	2880	rVB	2323592	3040393	100.00%	20.774%
15	20.415	2907	2915	2920	rBV6	16186	35546	1.17%	0.243%
16	20.803	2972	2981	2988	rBV	265412	366886	12.07%	2.507%
17	20.873	2988	2993	2997	rVB	168841	199970	6.58%	1.366%
18	21.431	3083	3088	3095	rBV	122227	196675	6.47%	1.344%
19	21.819	3146	3154	3160	rBV	470778	871018	28.65%	5.951%
20	22.659	3290	3297	3305	rVB6	12790	35325	1.16%	0.241%
21	23.570	3446	3452	3458	rVB3	18481	41999	1.38%	0.287%
22	24.105	3536	3543	3552	rBV4	23069	81294	2.67%	0.555%
23	24.210	3558	3561	3569	rVB5	18320	34543	1.14%	0.236%
24	24.868	3666	3673	3683	rVB2	15396	47313	1.56%	0.323%
25	25.015	3692	3698	3708	rBV2	17752	52210	1.72%	0.357%
26	25.186	3716	3727	3749	rVB2	273093	880413	28.96%	6.016%
27	26.420	3927	3937	3949	rBV4	26899	89982	2.96%	0.615%

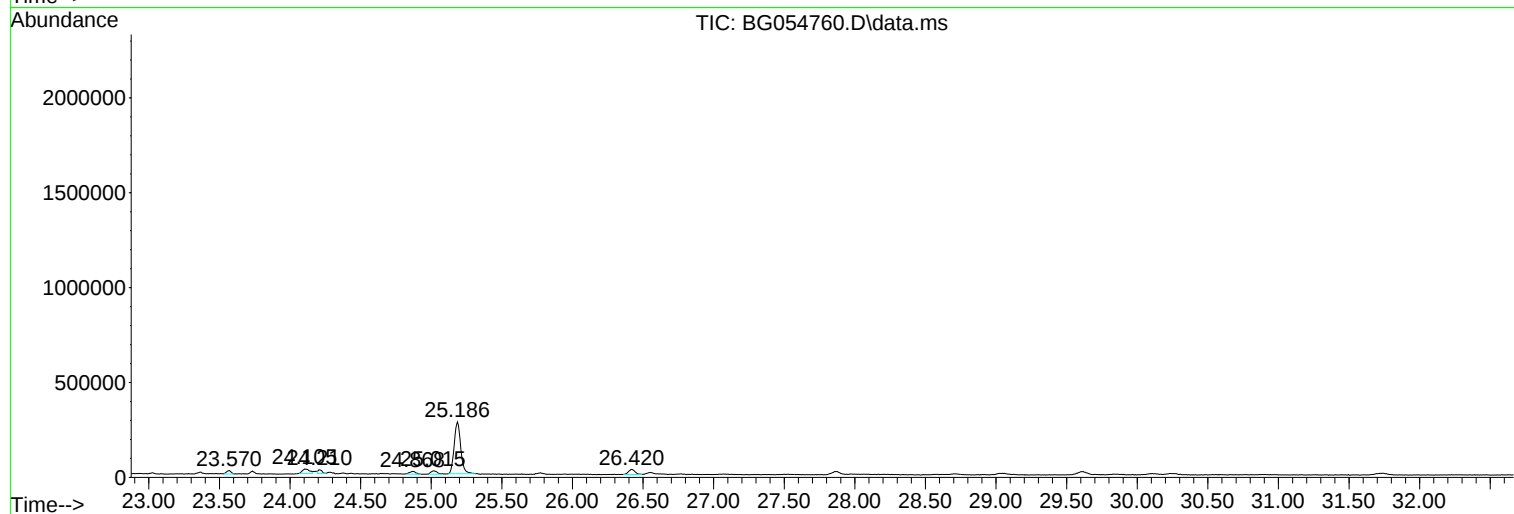
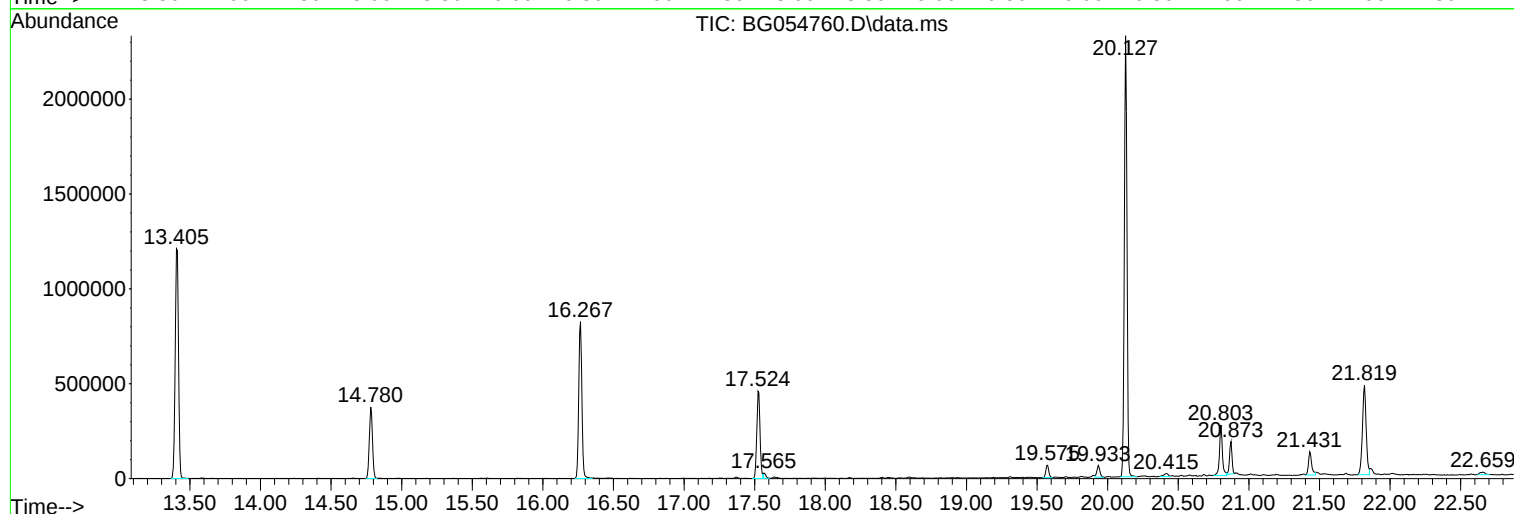
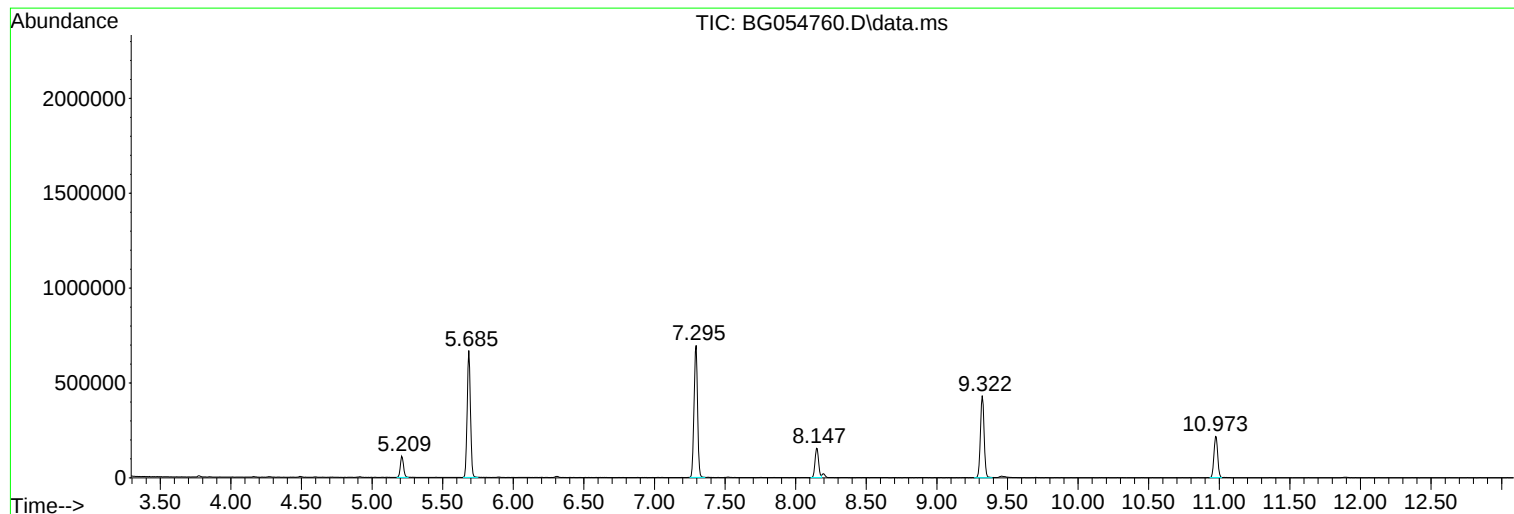
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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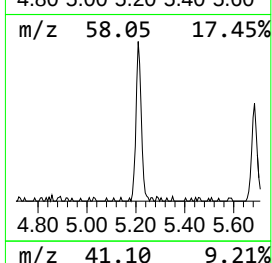
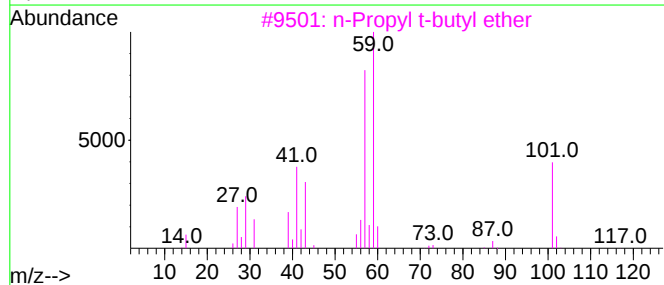
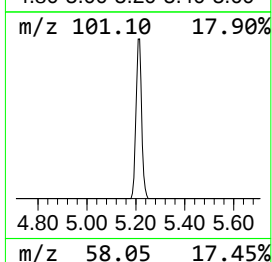
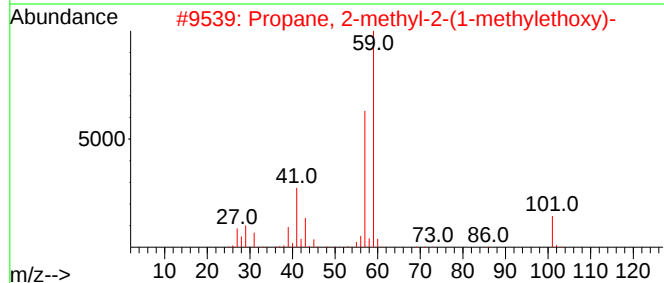
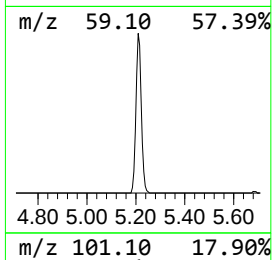
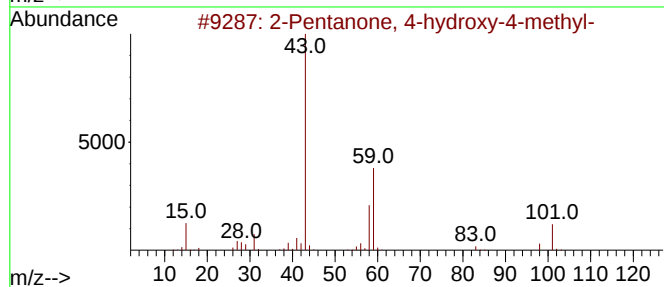
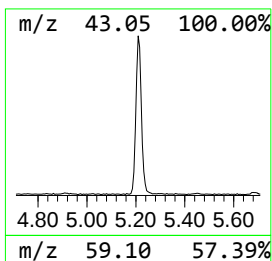
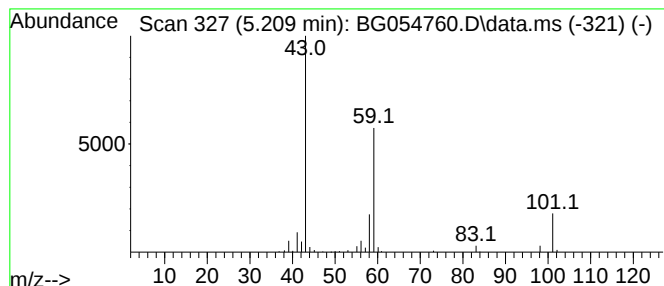
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.209	12.64 ng	173173	1,4-Dichlorobenzene-d4	8.153

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33		
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		



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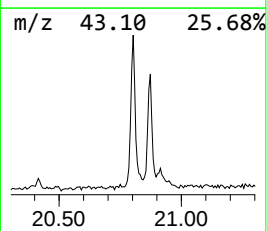
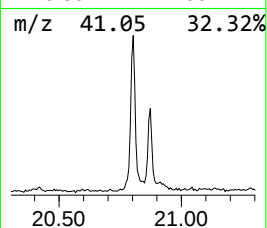
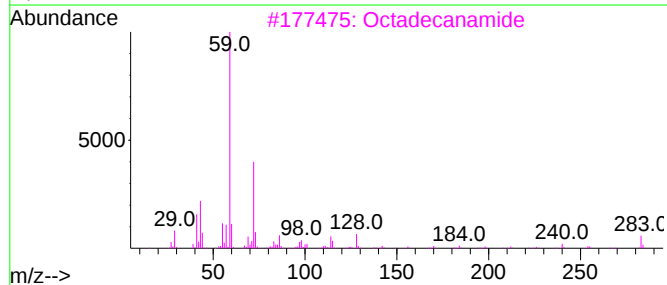
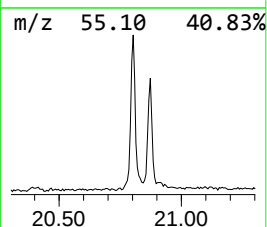
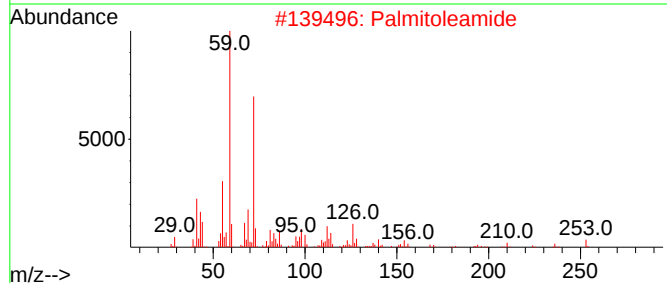
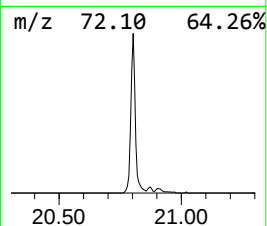
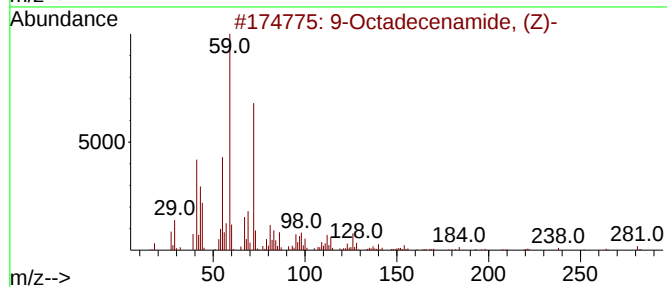
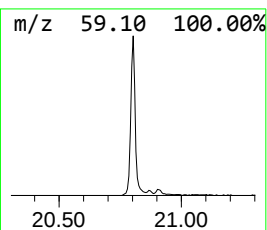
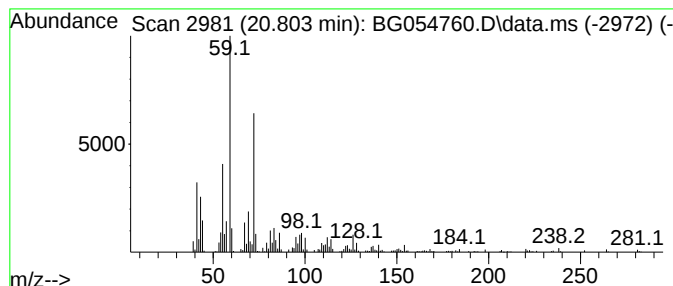
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Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.803	8.42 ng	366886	Chrysene-d12	21.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2			Palmitoleamide	253	C16H31NO	106010-22-4	80
3			Octadecanamide	283	C18H37NO	000124-26-5	78
4			Octanamide	143	C8H17NO	000629-01-6	59
5			Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50



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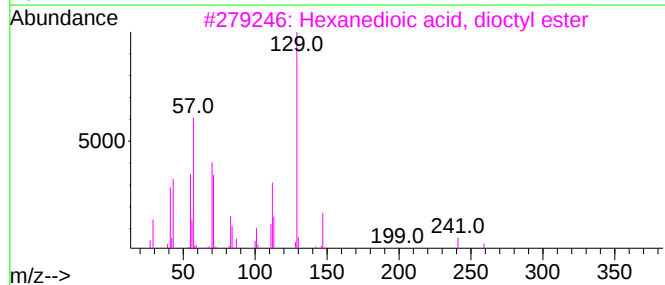
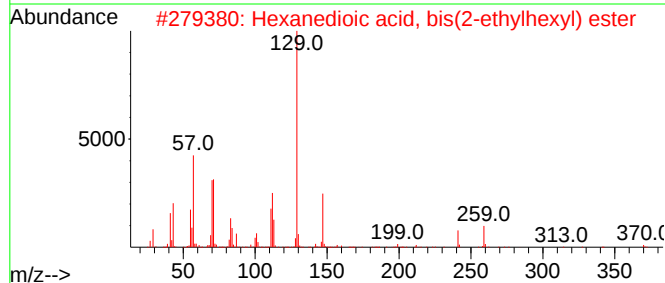
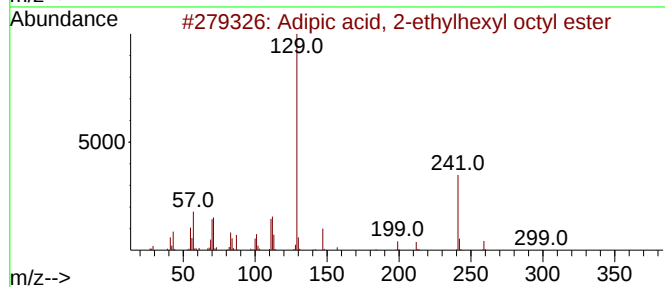
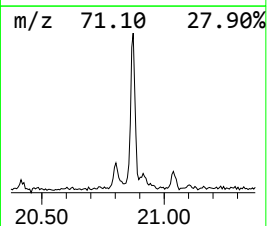
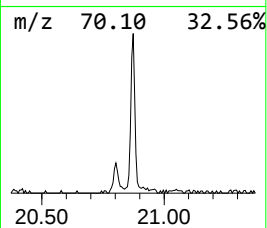
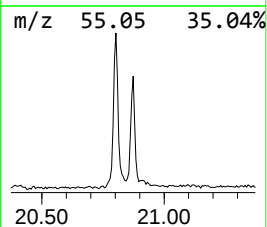
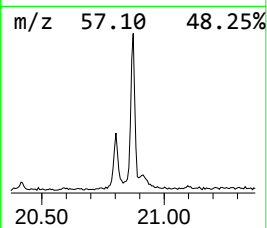
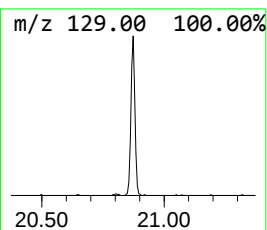
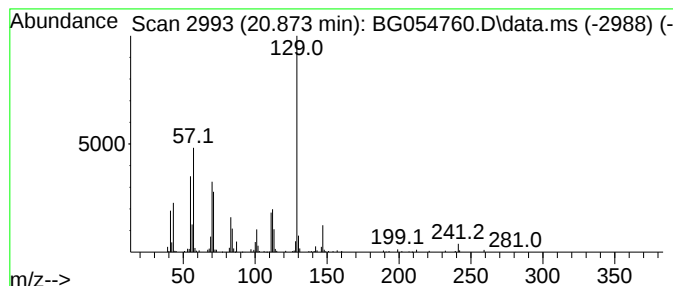
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Peak Number 4 Adipic acid, 2-ethylhexyl o... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.873	4.59 ng	199970	Chrysene-d12	21.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	90
2			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	86
3			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	76
4			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	64
5			Diisooctyl adipate	370	C22H42O4	001330-86-5	58



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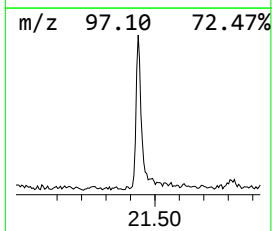
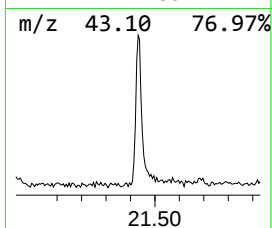
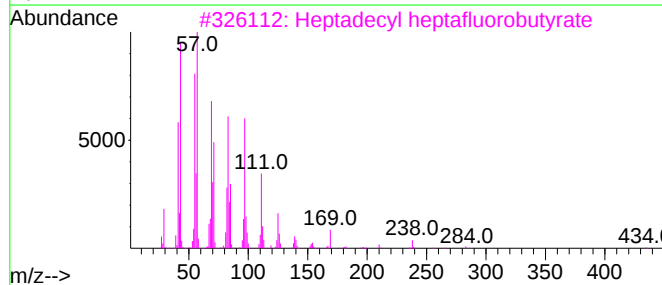
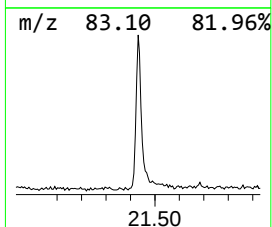
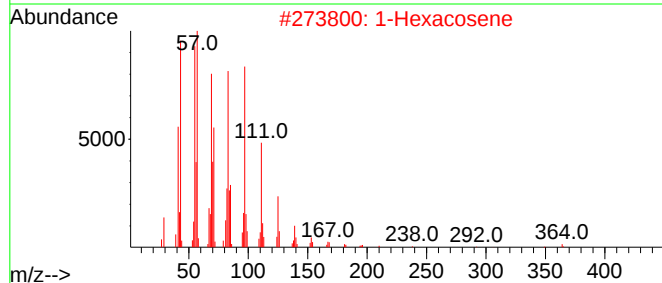
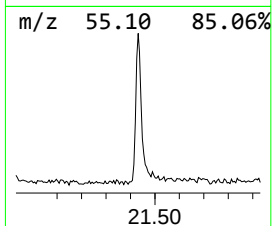
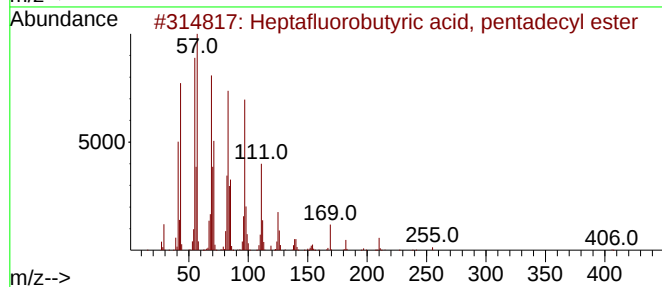
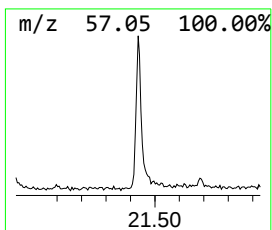
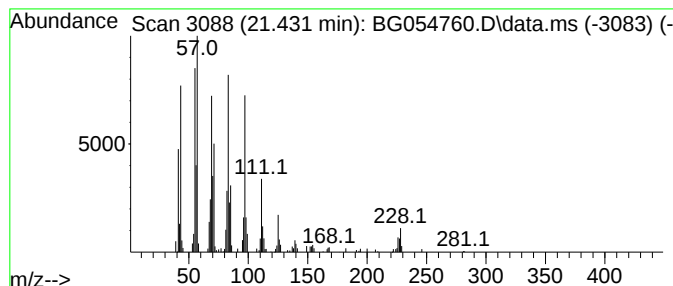
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Heptafluorobutyric acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.431	4.52 ng	196675	Chrysene-d12		21.819	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...		424	C19H31F7O2	959261-23-5	94
2	1-Hexacosene		364	C26H52	018835-33-1	94
3	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	94
4	Trichloroacetic acid, hexadecyl ...		386	C18H33Cl3O2	074339-54-1	94
5	1-Heneicosanol		312	C21H44O	015594-90-8	93



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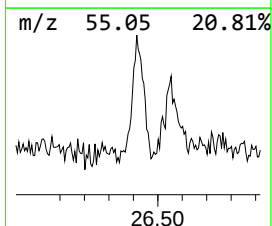
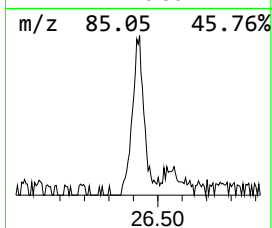
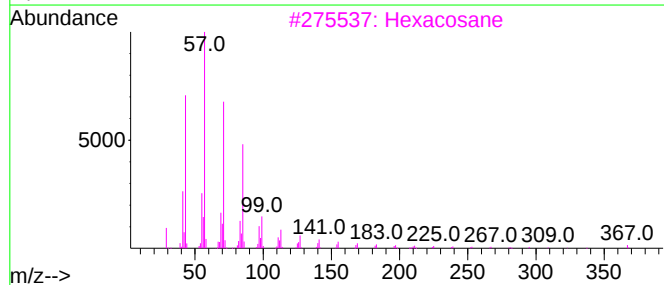
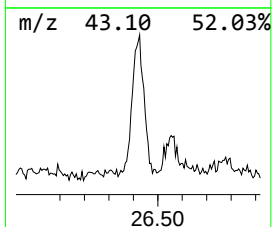
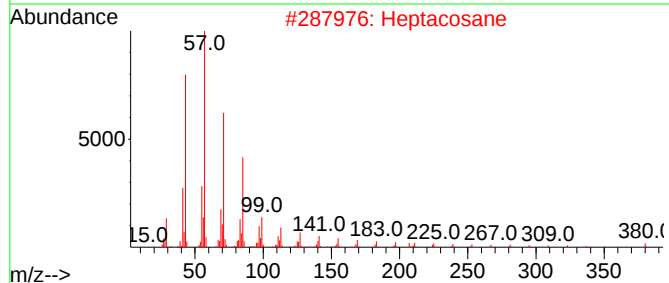
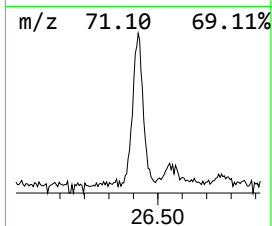
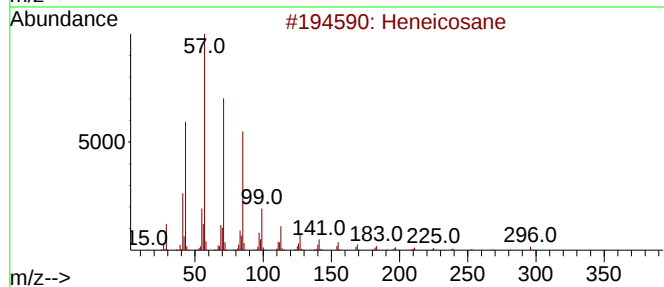
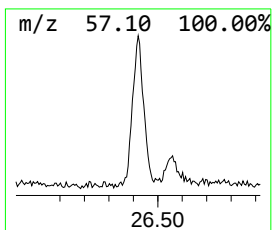
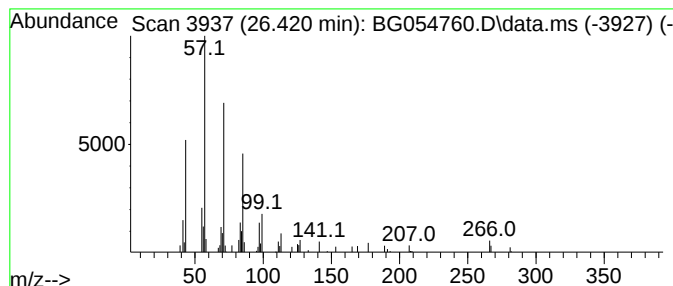
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Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.420	2.04 ng	89982	Perylene-d12	25.186

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	87
2		Heptacosane	380	C27H56	000593-49-7	86
3		Hexacosane	366	C26H54	000630-01-3	83
4		Pentacosane	352	C25H52	000629-99-2	83
5		Octadecane	254	C18H38	000593-45-3	80



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.209	12.6	ng	173173	1	8.153	274068	20.0
9-Octadecenamid...	20.803	8.4	ng	366886	5	21.819	871018	20.0
Adipic acid, 2-...	20.873	4.6	ng	199970	5	21.819	871018	20.0
Heptafluorobuty...	21.431	4.5	ng	196675	5	21.819	871018	20.0
Heneicosane	26.420	2.0	ng	89982	6	25.186	880413	20.0