

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
 Data File : BF125240.D
 Acq On : 26 Aug 2021 23:30
 Operator : JU/CG
 Sample : M3545-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NCS-COMP-2

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125240.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	17	24	29	rVB	1024031	1362324	36.66%	4.794%
2	5.534	581	586	589	rBV	4171564	3716124	100.00%	13.076%
3	6.533	751	756	770	rBV	3487611	3602652	96.95%	12.677%
4	6.916	817	821	824	rBV	1211276	1052020	28.31%	3.702%
5	7.475	911	916	919	rBV	2646098	2273874	61.19%	8.001%
6	8.098	1018	1022	1035	rBV	133241	304809	8.20%	1.073%
7	8.192	1035	1038	1042	rBV	1376441	1225500	32.98%	4.312%
8	9.269	1217	1221	1224	rBV	3991863	3391404	91.26%	11.933%
9	9.951	1333	1337	1344	rVB	1343716	1230799	33.12%	4.331%
10	10.733	1467	1470	1484	rVB	2165646	2069084	55.68%	7.280%
11	11.433	1586	1589	1593	rBV	1235419	1130673	30.43%	3.978%
12	11.951	1674	1677	1682	rBV	178100	178803	4.81%	0.629%
13	12.651	1793	1796	1807	rBV	36334	51538	1.39%	0.181%
14	12.739	1807	1811	1816	rBV3	62744	80136	2.16%	0.282%
15	13.021	1855	1859	1862	rBV	3525645	3157585	84.97%	11.110%
16	13.980	2013	2022	2029	rBV4	84852	338948	9.12%	1.193%
17	14.074	2035	2038	2042	rVB	1389165	1205529	32.44%	4.242%
18	14.539	2115	2117	2122	rVB3	64745	64752	1.74%	0.228%
19	14.833	2164	2167	2174	rBV	584827	606062	16.31%	2.133%
20	15.574	2288	2293	2306	rVB2	1021143	1377278	37.06%	4.846%

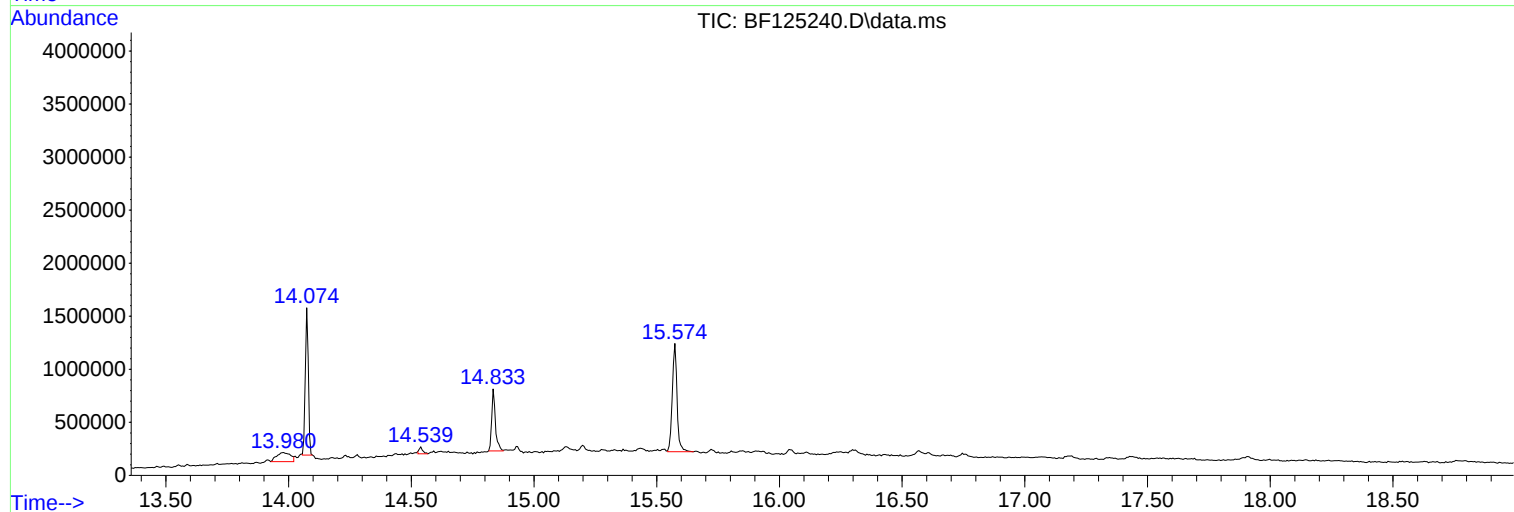
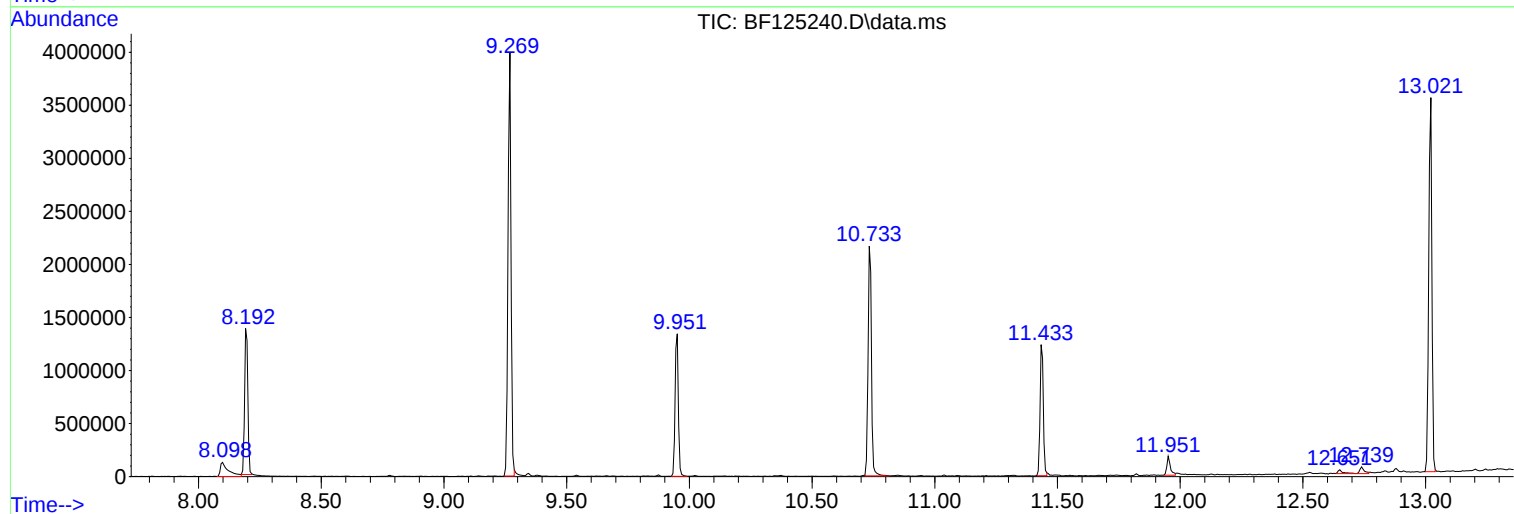
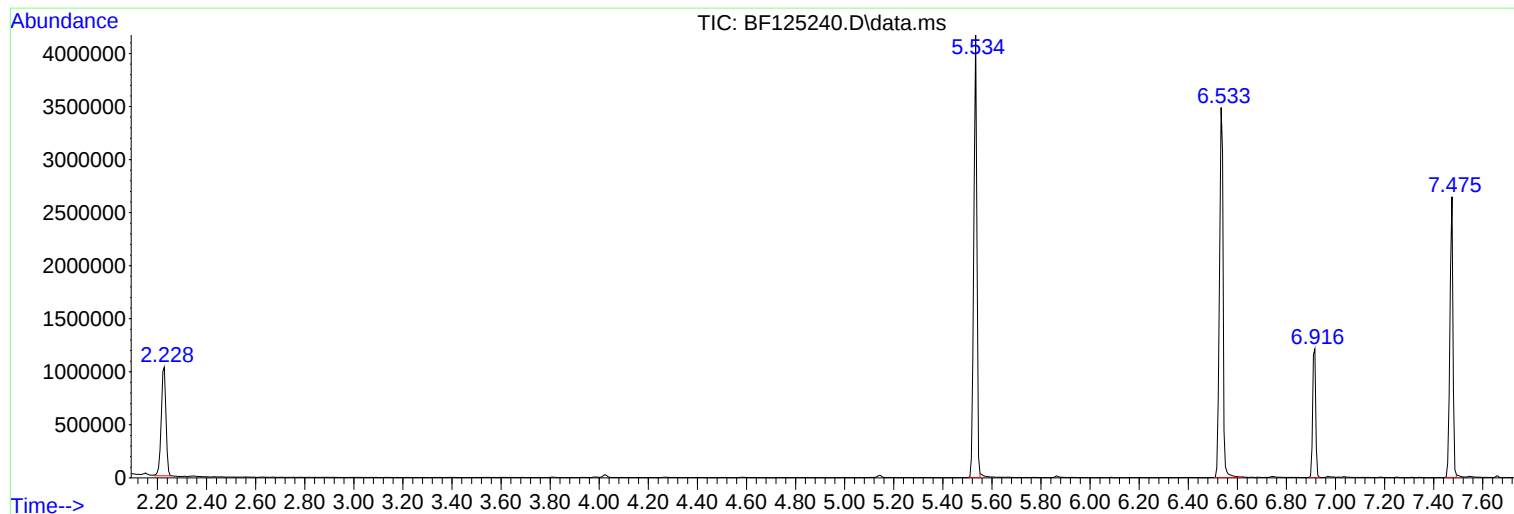
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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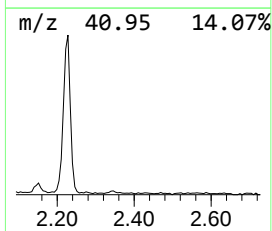
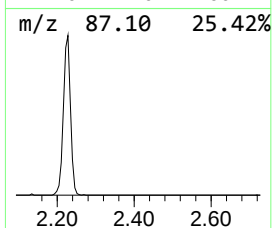
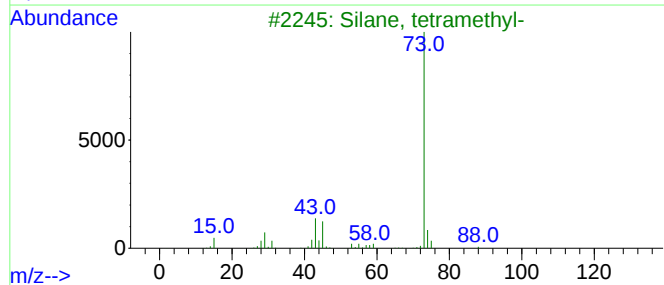
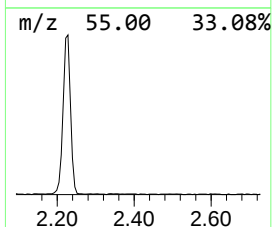
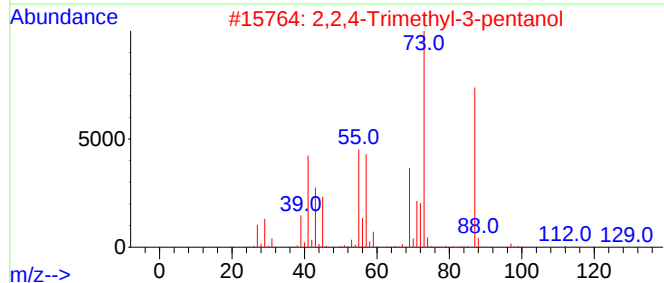
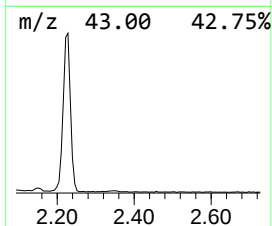
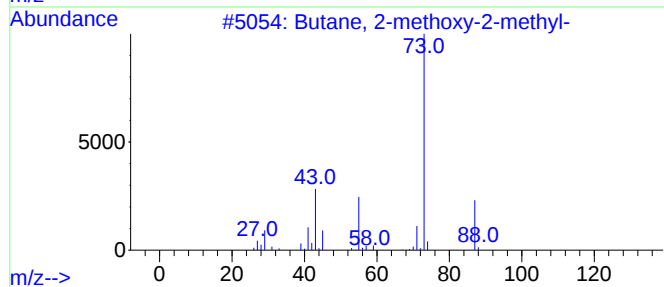
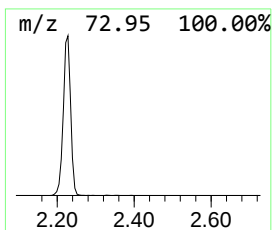
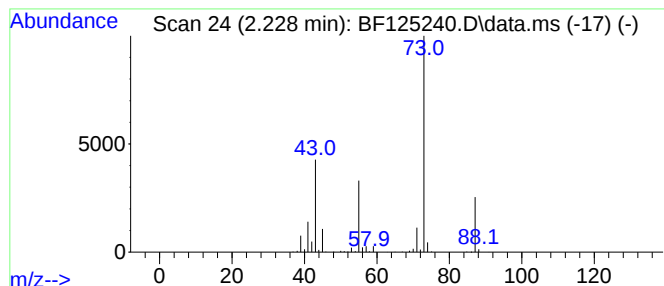
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	25.90 ng	1362320	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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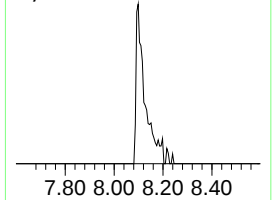
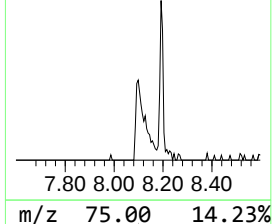
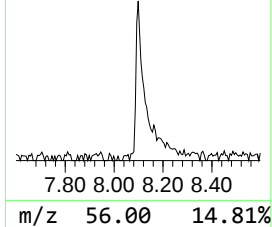
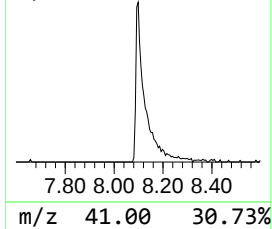
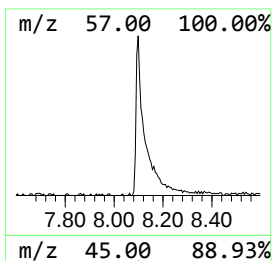
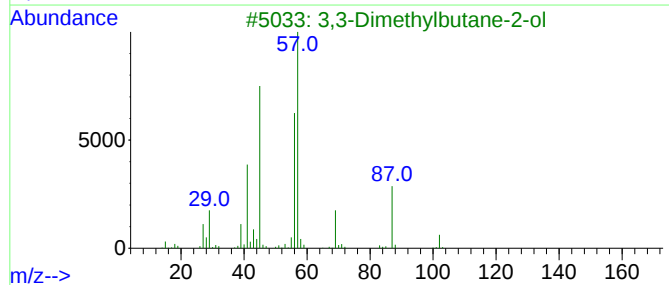
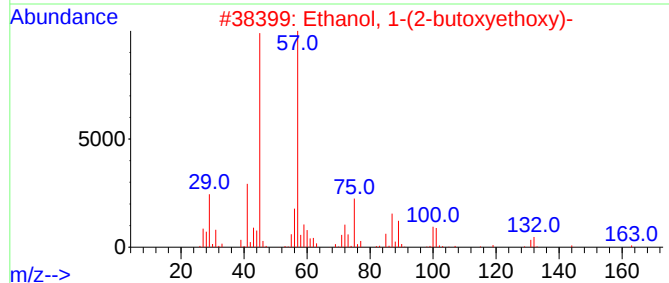
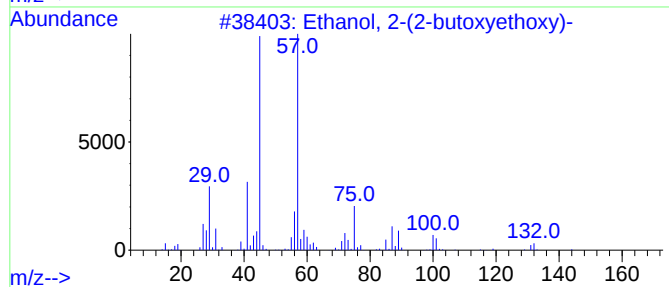
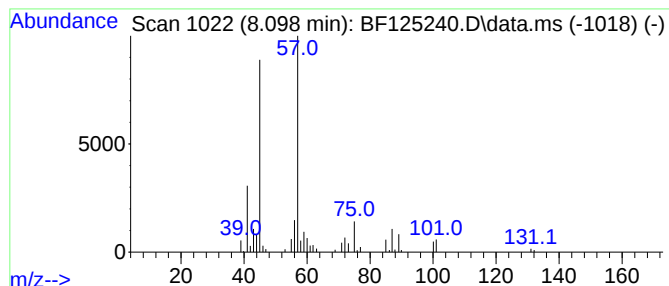
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	4.97 ng	304809	Naphthalene-d8	8.192

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	83
3			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
4			DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	50
5			Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	50



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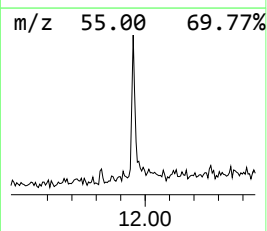
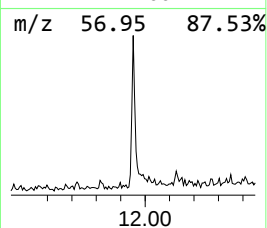
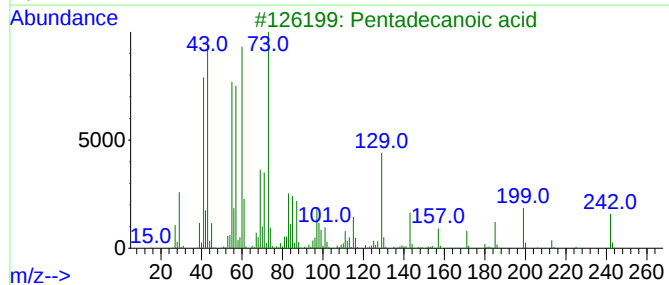
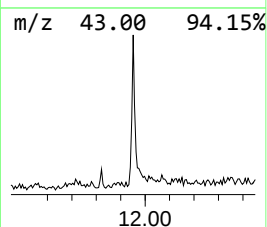
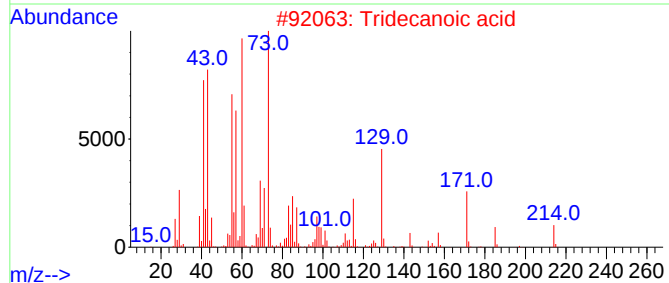
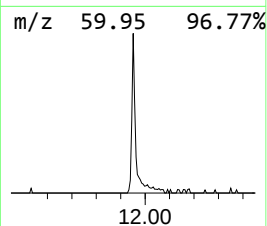
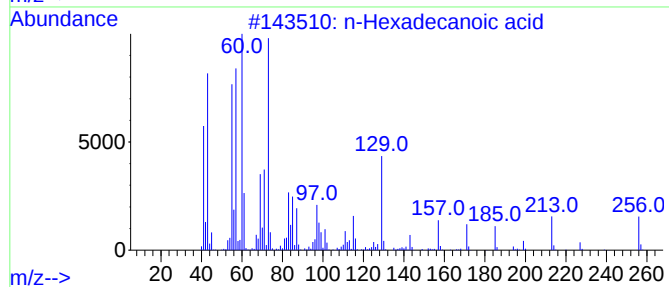
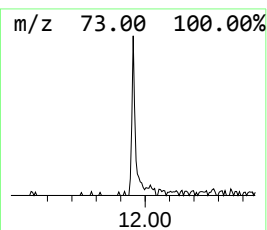
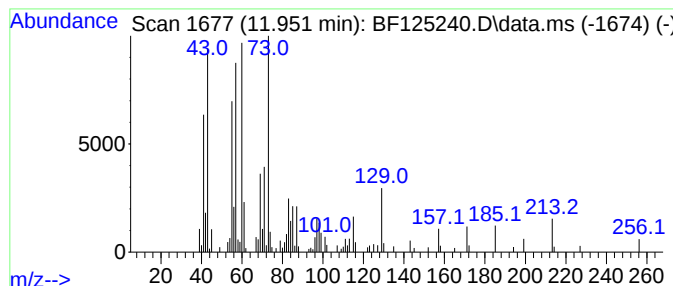
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	3.16 ng	178803	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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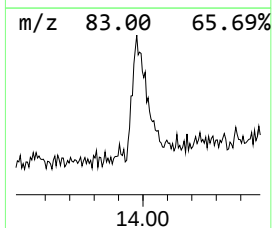
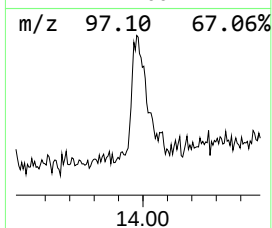
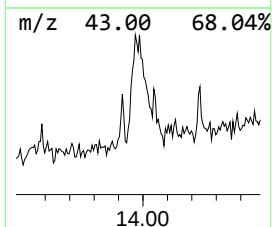
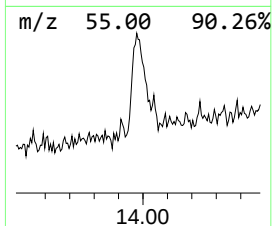
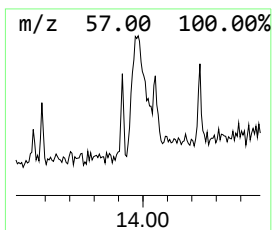
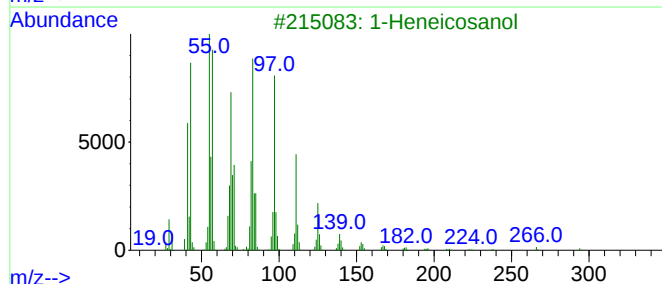
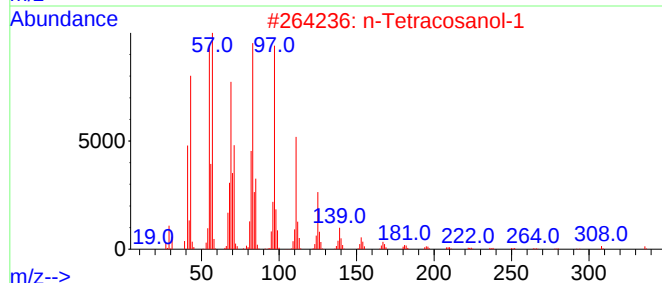
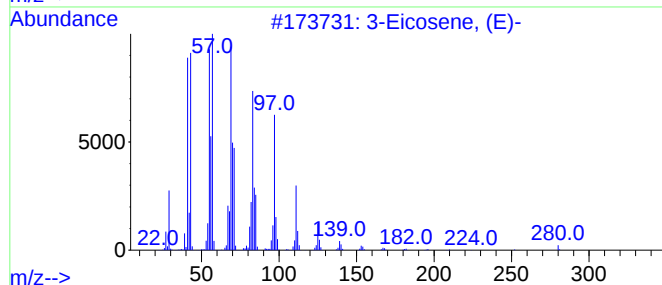
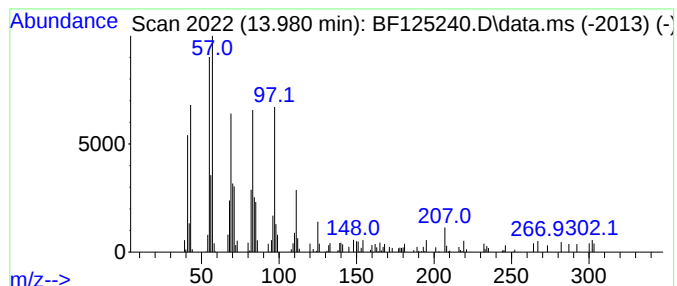
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Peak Number 4 3-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	5.62 ng	338948	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	83
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	76
3			1-Heneicosanol	312	C21H44O	015594-90-8	76
4			1-Heptacosanol	396	C27H56O	002004-39-9	76
5			1-Tricosene	322	C23H46	018835-32-0	76



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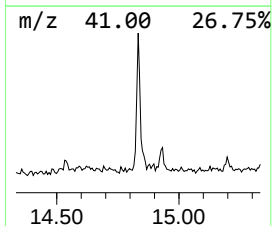
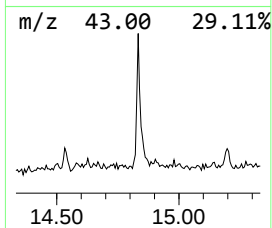
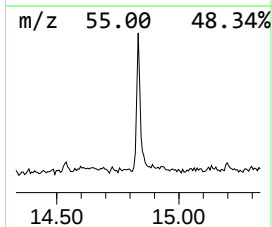
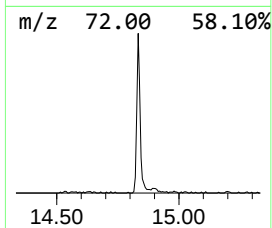
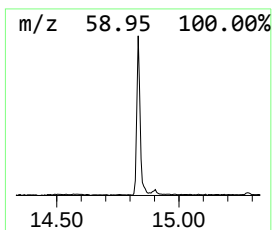
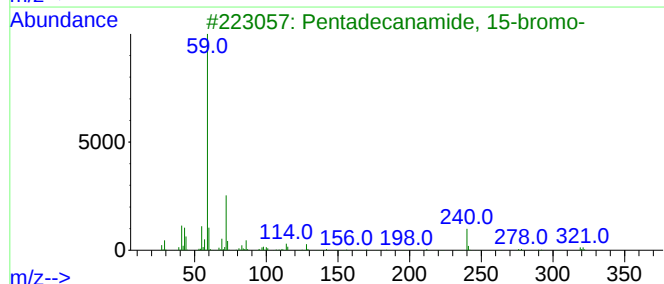
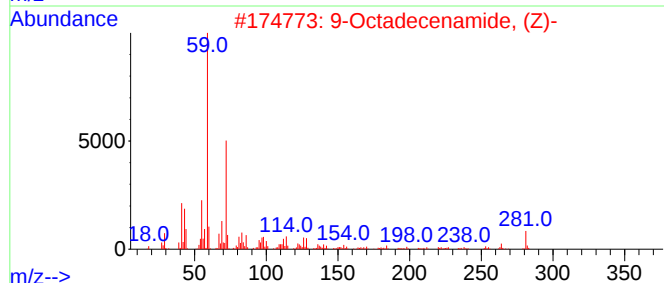
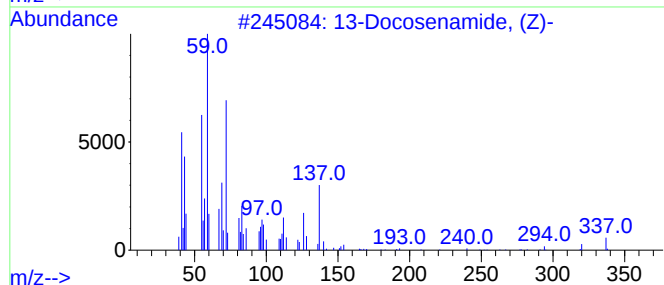
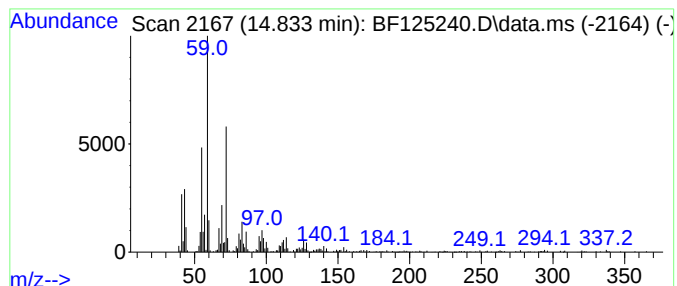
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	8.80 ng	606062	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	91
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
3			Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	59
4			Butanamide, 3-methyl-	101	C5H11NO	000541-46-8	38
5			Dodecanamide	199	C12H25NO	001120-16-7	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.228	25.9	ng	1362320	1	6.916	1052020	20.0
Ethanol, 2-(2-b...	8.098	5.0	ng	304809	2	8.192	1225500	20.0
n-Hexadecanoic ...	11.951	3.2	ng	178803	4	11.433	1130670	20.0
3-Eicosene, (E)-	13.980	5.6	ng	338948	5	14.074	1205530	20.0
13-Docosenamide...	14.833	8.8	ng	606062	6	15.574	1377280	20.0