

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060222\
 Data File : BF128663.D
 Acq On : 03 Jun 2022 03:38
 Operator : CG\JU
 Sample : N2989-05
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P015-SS007-0006-01

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-BF060222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128663.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.057	468	471	478	rVB	36534	45381	1.56%	0.211%
2	5.481	539	543	550	rBV	2636416	2858182	98.52%	13.301%
3	6.487	710	714	725	rBV	2997997	2901236	100.00%	13.501%
4	6.822	767	771	774	rBV	1016561	776230	26.76%	3.612%
5	7.387	861	867	870	rBV	1957862	1997153	68.84%	9.294%
6	8.104	984	989	993	rBV	1122234	969899	33.43%	4.513%
7	9.186	1166	1173	1176	rBV	3187307	2857873	98.51%	13.299%
8	9.863	1280	1288	1291	rBV	1272957	1050694	36.22%	4.889%
9	10.657	1415	1423	1426	rBV	2303922	2019861	69.62%	9.400%
10	10.992	1474	1480	1482	rBV3	26584	46655	1.61%	0.217%
11	11.022	1482	1485	1490	rVB3	63095	84788	2.92%	0.395%
12	11.104	1496	1499	1505	rVB	29789	32109	1.11%	0.149%
13	11.351	1536	1541	1544	rBV	1120374	939966	32.40%	4.374%
14	11.886	1628	1632	1643	rBV	567224	515128	17.76%	2.397%
15	12.669	1761	1765	1771	rBV	183745	171819	5.92%	0.800%
16	12.939	1807	1811	1814	rVB	2284384	1837175	63.32%	8.549%
17	13.798	1948	1957	1960	rBV	20905	32193	1.11%	0.150%
18	13.904	1967	1975	1984	rBV4	53636	183790	6.33%	0.855%
19	13.980	1984	1988	1993	rVB2	790396	1191590	41.07%	5.545%
20	14.086	1999	2006	2012	rBV	169653	200902	6.92%	0.935%
21	14.563	2077	2087	2096	rBV	29658	97267	3.35%	0.453%
22	15.457	2234	2239	2243	rBV	440984	539071	18.58%	2.509%
23	16.721	2451	2454	2464	rVB6	27586	54781	1.89%	0.255%
24	18.062	2678	2682	2691	rVB6	14137	33717	1.16%	0.157%
25	18.521	2754	2760	2771	rVB6	17657	51410	1.77%	0.239%

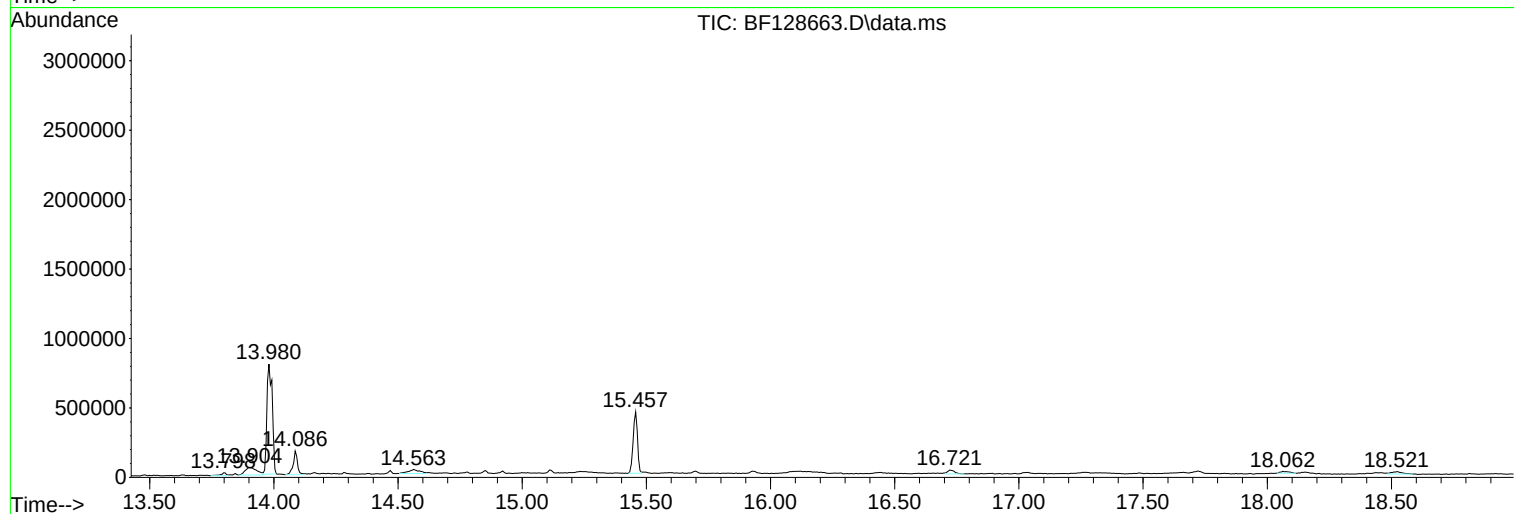
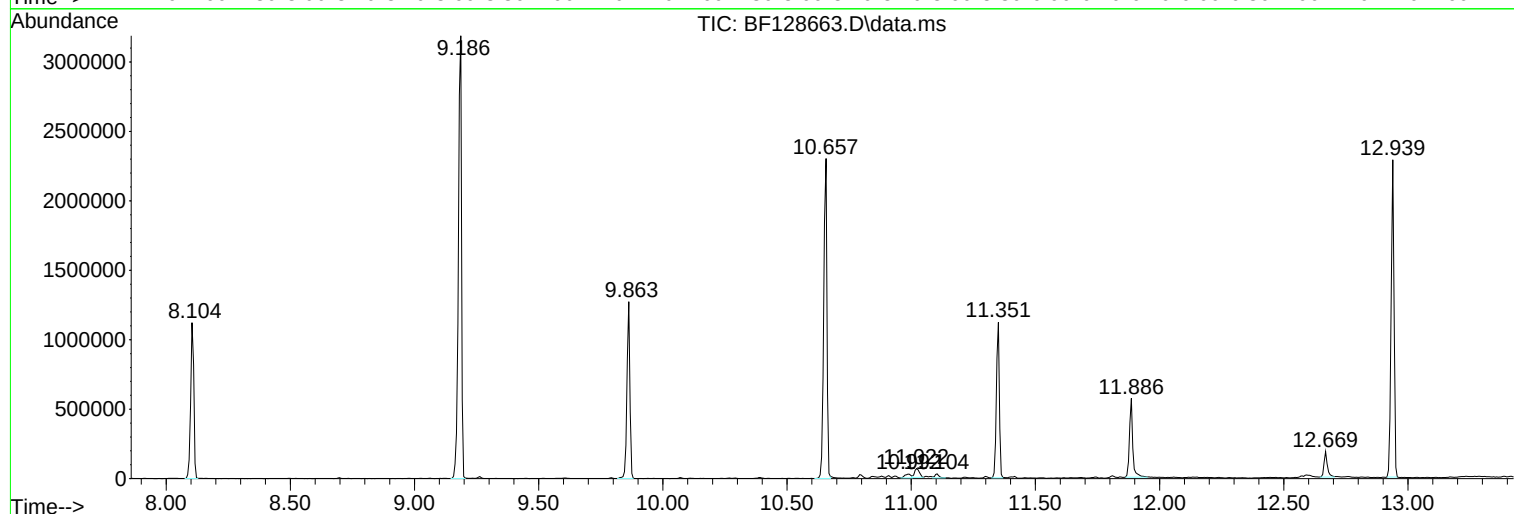
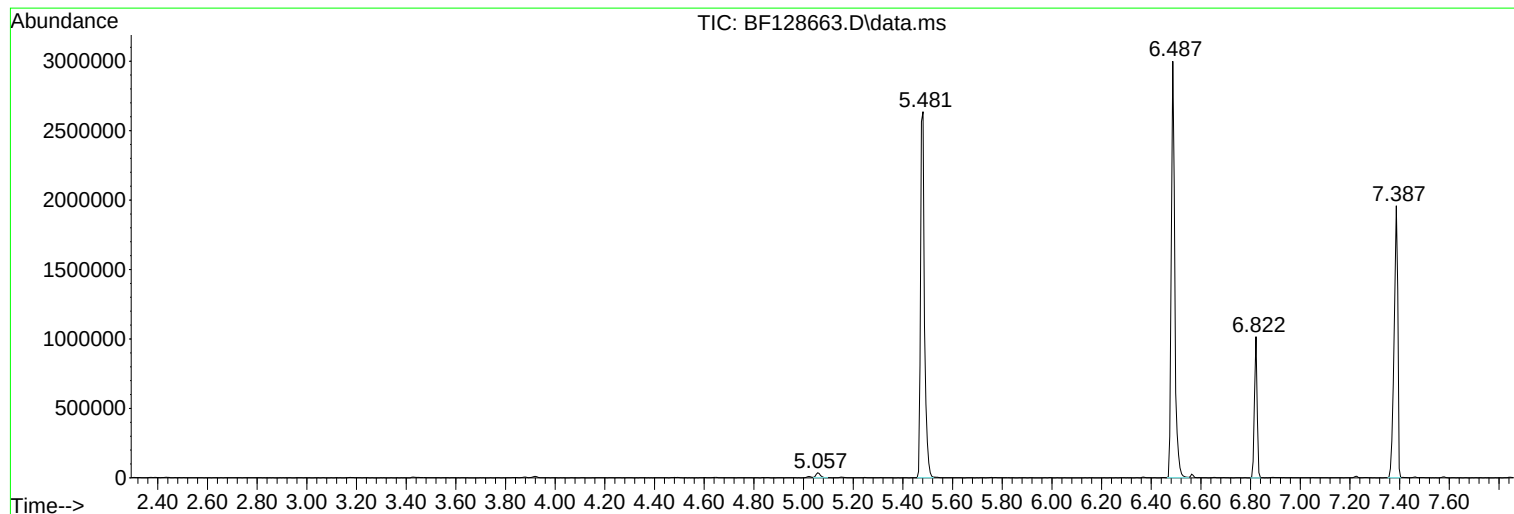
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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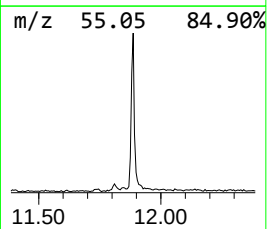
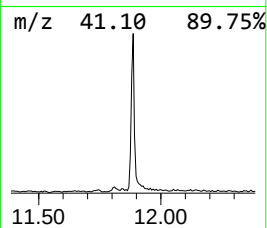
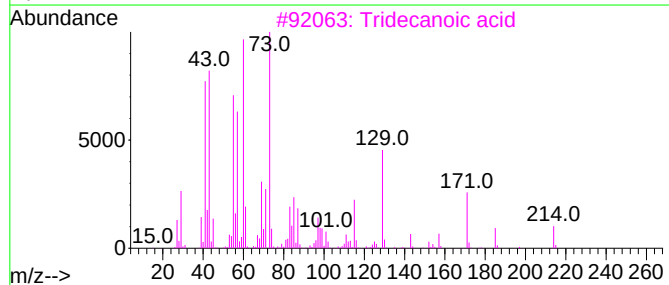
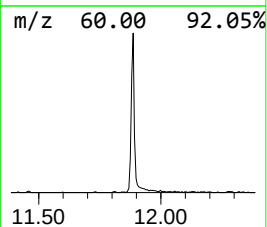
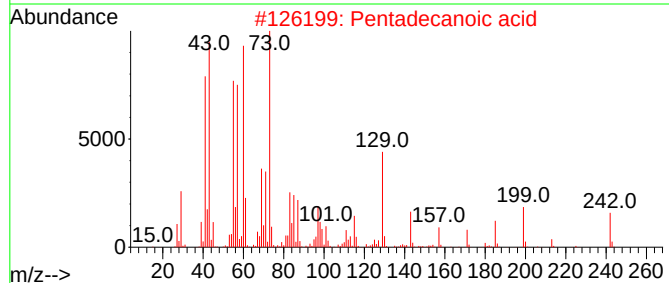
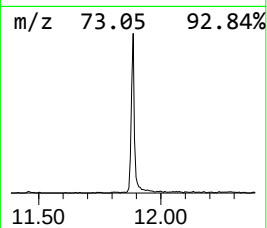
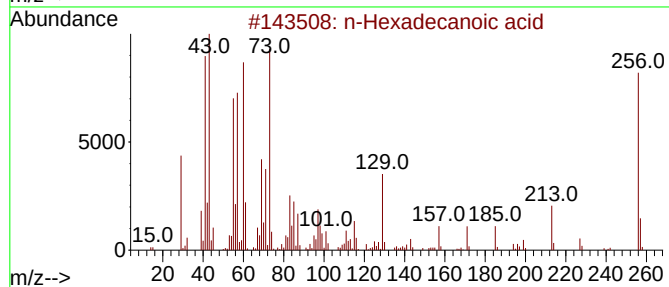
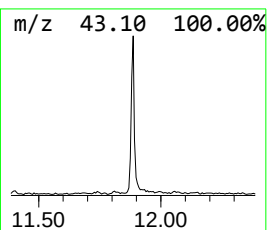
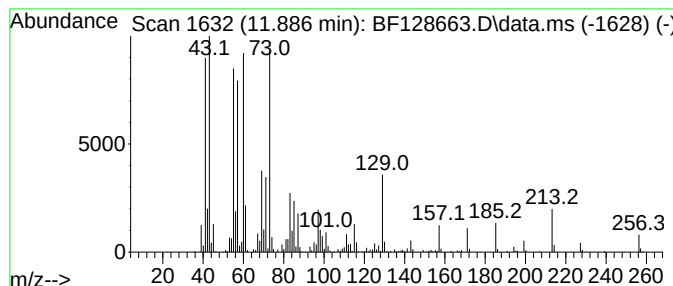
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	10.96 ng	515128	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	55



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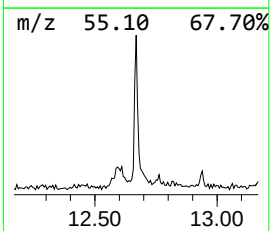
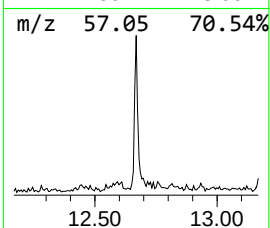
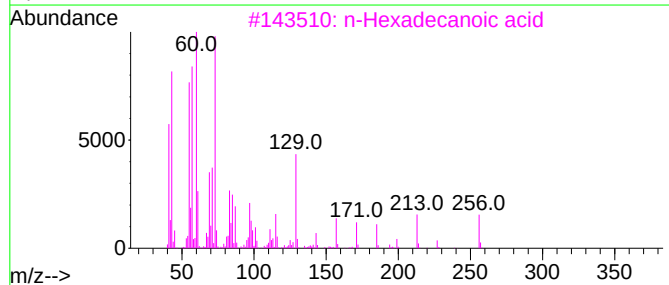
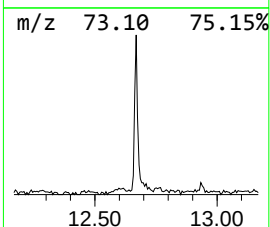
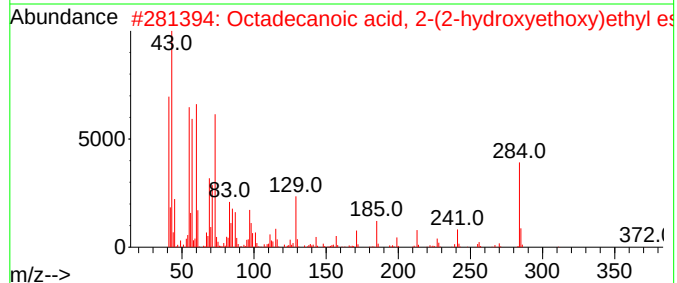
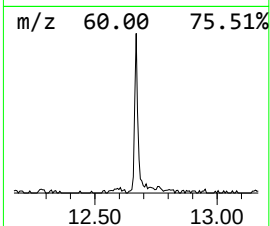
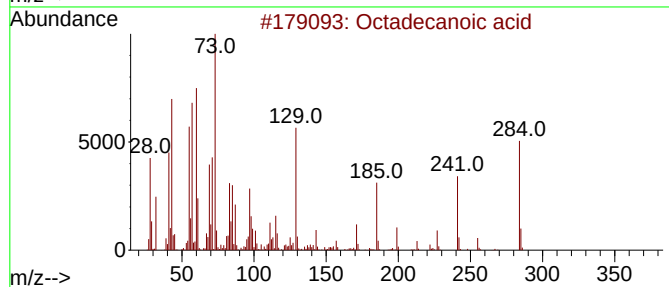
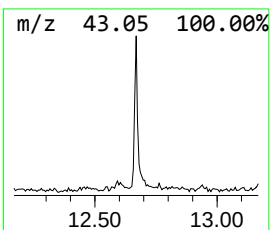
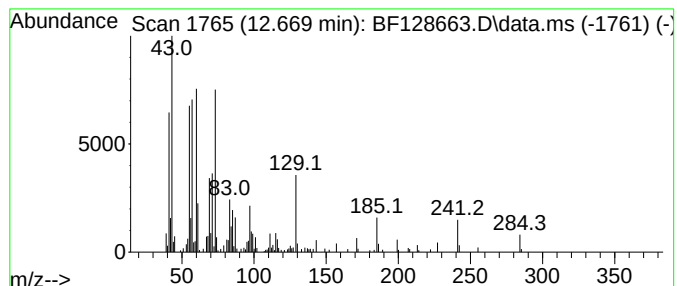
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.669	3.66 ng	171819	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	74



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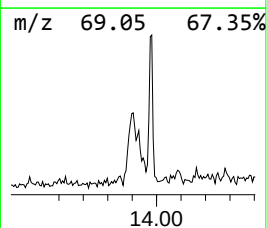
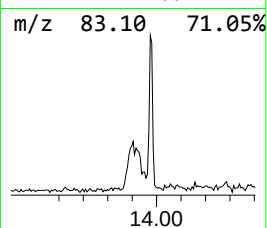
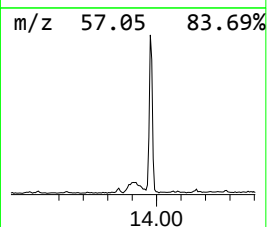
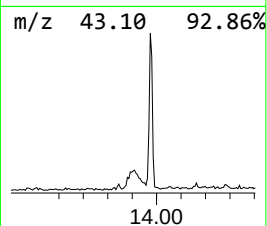
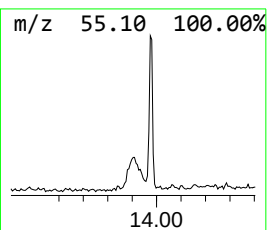
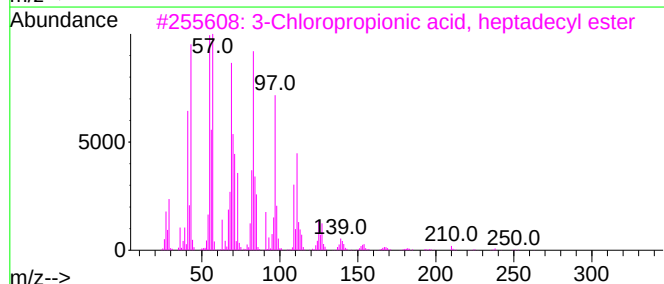
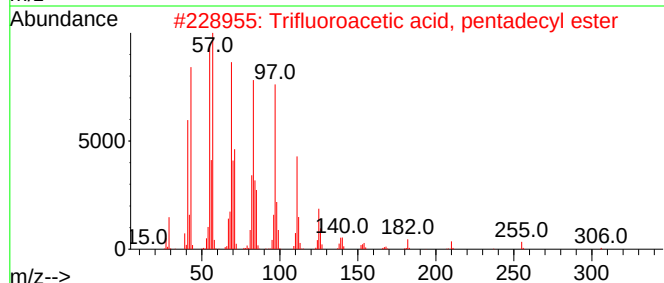
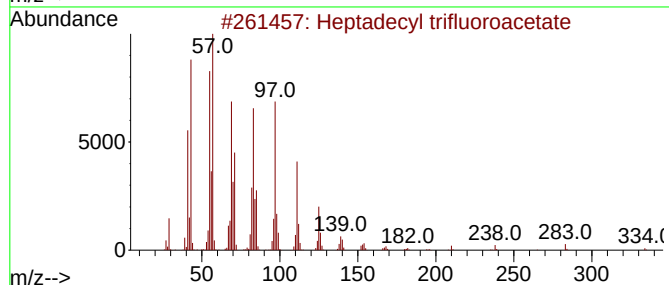
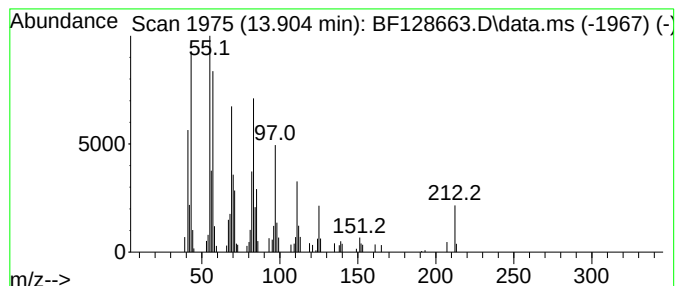
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	3.08 ng	183790	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	83
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	81
3			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	76
4			1-Octadecanol	270	C18H38O	000112-92-5	74
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	74



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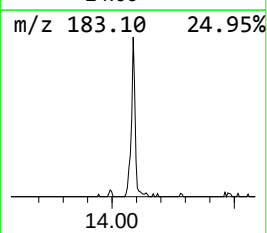
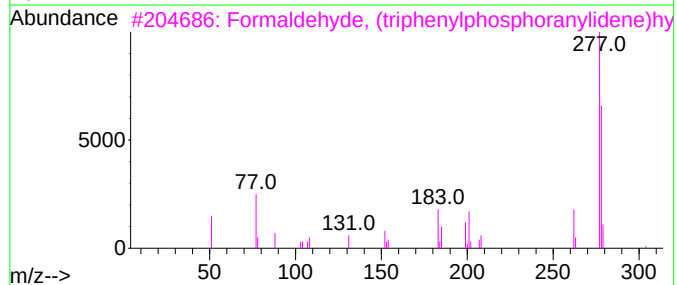
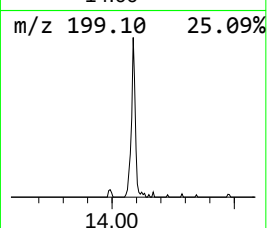
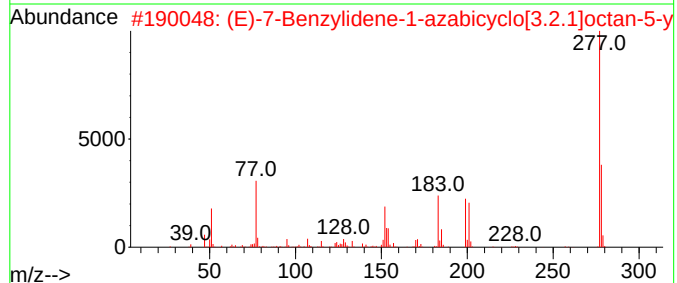
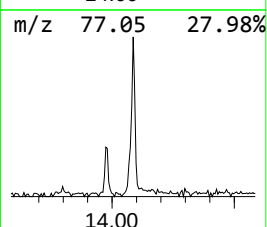
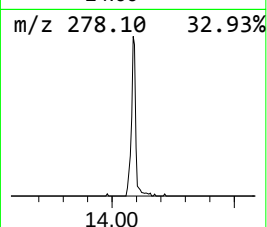
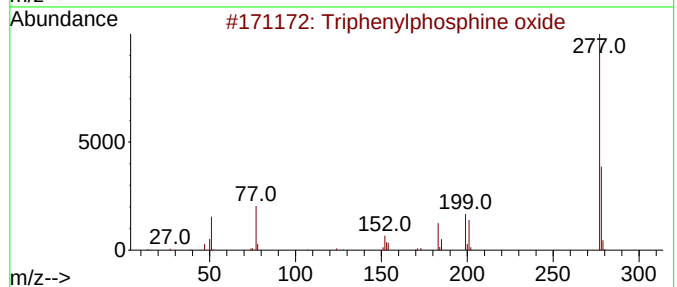
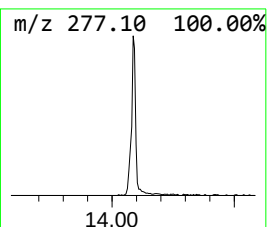
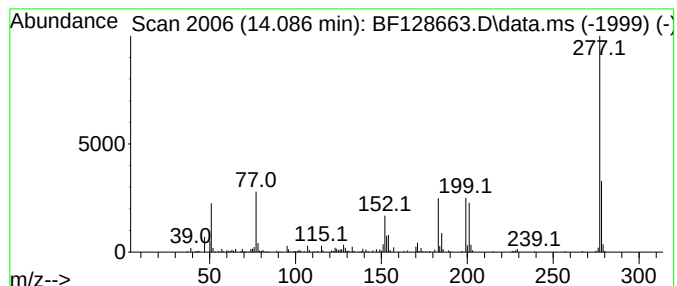
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	3.37 ng	200902	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	74
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	50
4			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	38
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	38



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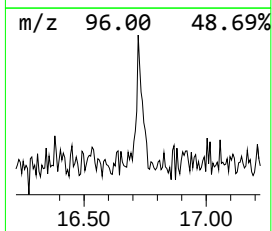
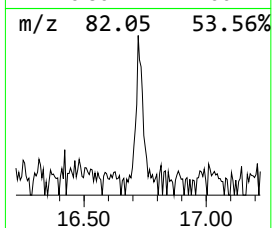
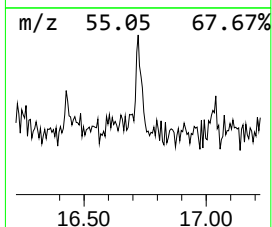
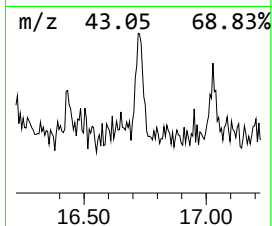
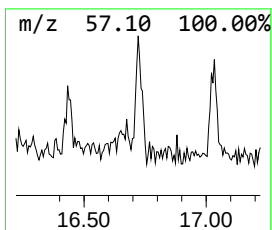
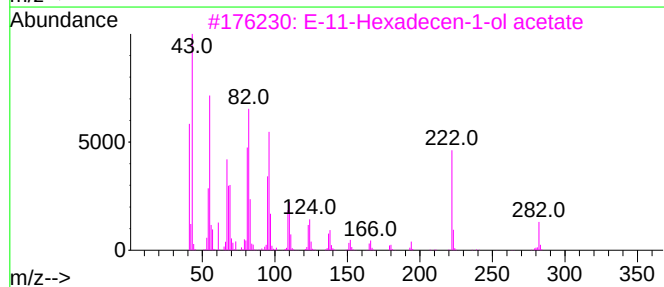
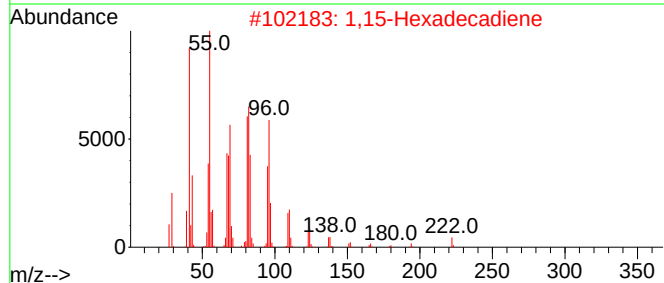
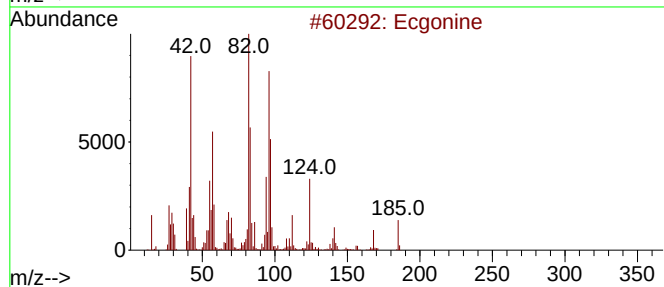
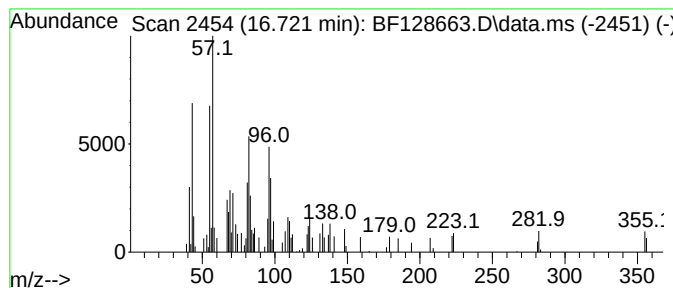
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ecgonine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.721	2.03 ng	54781	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ecgonine	185	C9H15NO3	000481-37-8	92
2			1,15-Hexadecadiene	222	C16H30	021964-51-2	58
3			E-11-Hexadecen-1-ol acetate	282	C18H34O2	1000130-88-1	58
4			7-Azabicyclo[4.1.0]heptane, 1-me...	111	C7H13N	025022-25-7	49
5			1-Dodecen-1-ol, acetate	226	C14H26O2	056438-08-5	49



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.886	11.0	ng	515128	4	11.351	939966	20.0
Octadecanoic acid	12.669	3.7	ng	171819	4	11.351	939966	20.0
Heptadecyl trif...	13.904	3.1	ng	183790	5	13.992	1191590	20.0
Triphenylphosph...	14.086	3.4	ng	200902	5	13.992	1191590	20.0
Ecgonine	16.721	2.0	ng	54781	6	15.457	539071	20.0