

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110520\
 Data File : BG047237.D
 Acq On : 6 Nov 2020 3:05
 Operator : CG/JU
 Sample : L4641-12
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P0122-CAS001-0406-01

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_G\METHODS\8270-BG110420.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG047237.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.562	371	378	387	rBV	889365	1365635	40.24%	7.355%
2	7.166	641	651	664	rBV	928933	1578146	46.50%	8.500%
3	8.006	785	794	806	rBV	237233	395788	11.66%	2.132%
4	9.169	984	992	1000	rBV	577404	1016210	29.94%	5.473%
5	10.227	1165	1172	1178	rBV2	53984	92228	2.72%	0.497%
6	10.815	1262	1272	1282	rBV	345711	602156	17.74%	3.243%
7	13.265	1682	1689	1697	rBV	1659697	2487639	73.30%	13.398%
8	13.464	1716	1723	1729	rVV2	23035	37834	1.11%	0.204%
9	13.529	1729	1734	1740	rVB2	56847	91978	2.71%	0.495%
10	14.087	1823	1829	1838	rVB	59508	97304	2.87%	0.524%
11	14.640	1914	1923	1933	rVV	571093	913360	26.91%	4.919%
12	16.132	2169	2177	2184	rBV	1443332	2114646	62.31%	11.390%
13	17.389	2384	2391	2396	rBV	694630	1053065	31.03%	5.672%
14	18.271	2536	2541	2549	rBV2	246311	382717	11.28%	2.061%
15	18.341	2549	2553	2557	rVB	69190	93564	2.76%	0.504%
16	18.611	2595	2599	2602	rBV2	28523	43996	1.30%	0.237%
17	19.540	2754	2757	2761	rBV4	84832	109765	3.23%	0.591%
18	19.998	2829	2835	2841	rBV	2618017	3393610	100.00%	18.278%
19	21.291	3051	3055	3066	rBV2	216654	414952	12.23%	2.235%
20	21.531	3092	3096	3102	rVB	135252	180979	5.33%	0.975%
21	21.649	3110	3116	3122	rBV	605900	988906	29.14%	5.326%
22	24.845	3653	3660	3670	rVB3	410650	1112138	32.77%	5.990%

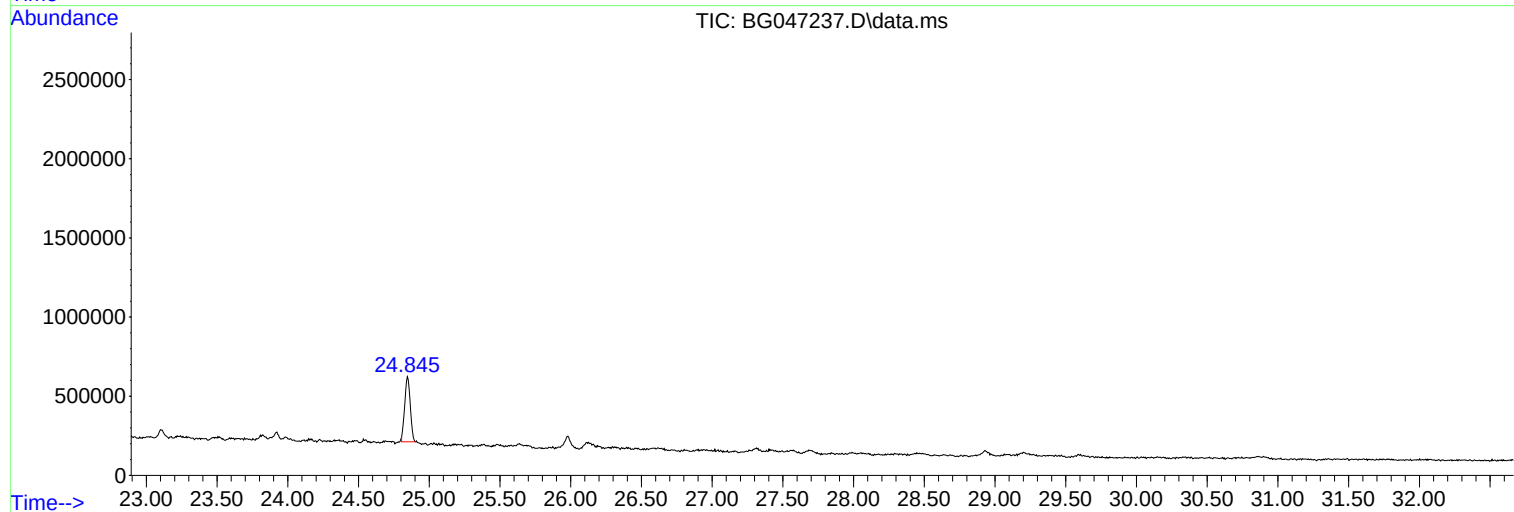
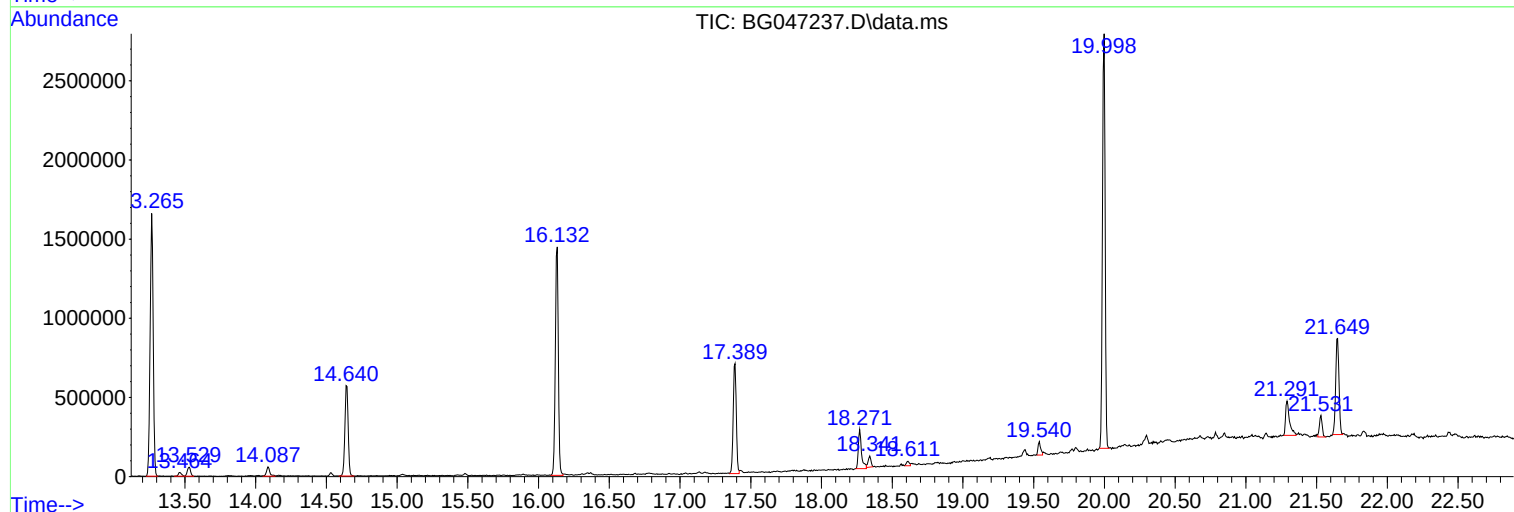
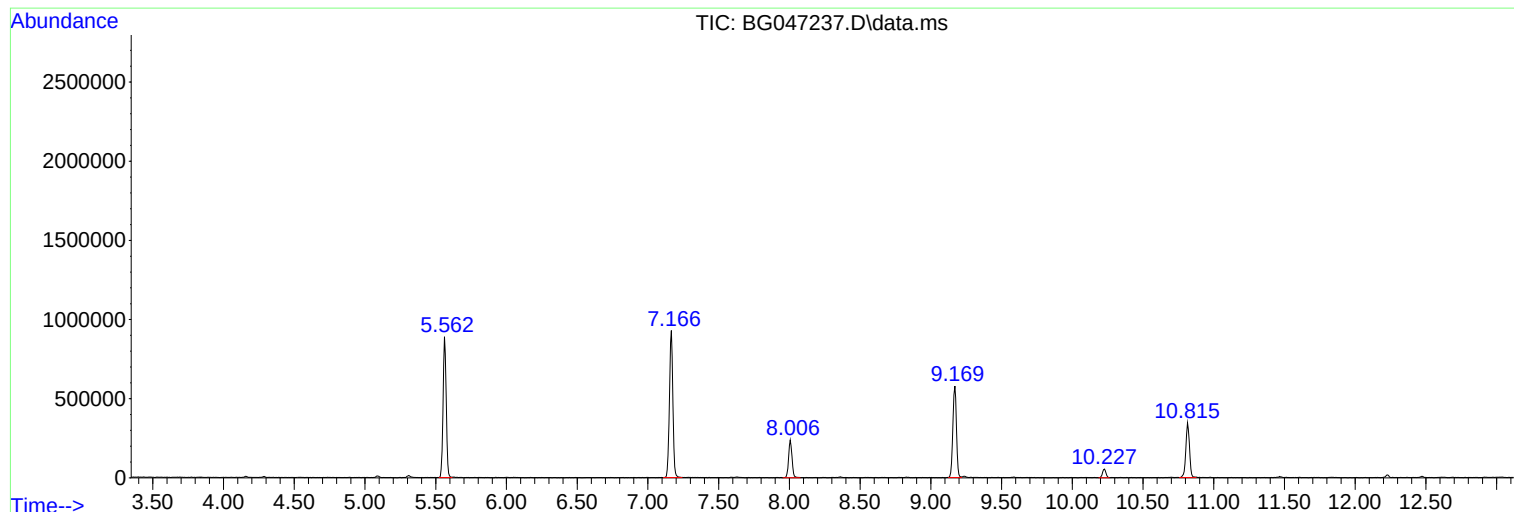
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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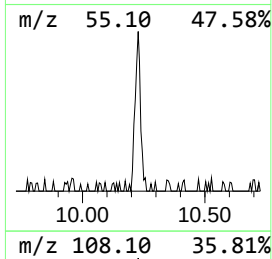
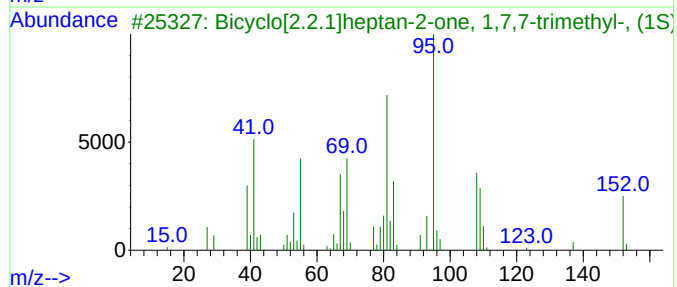
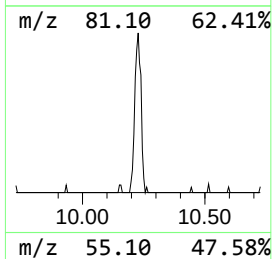
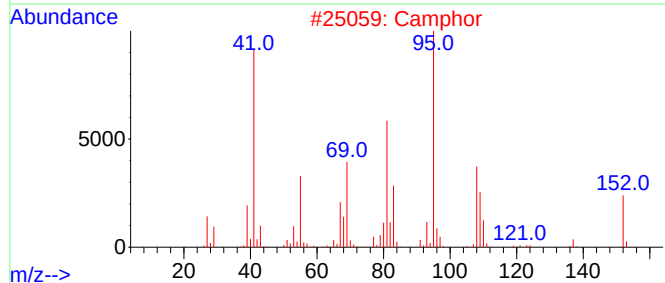
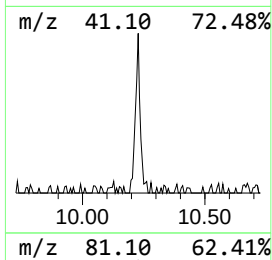
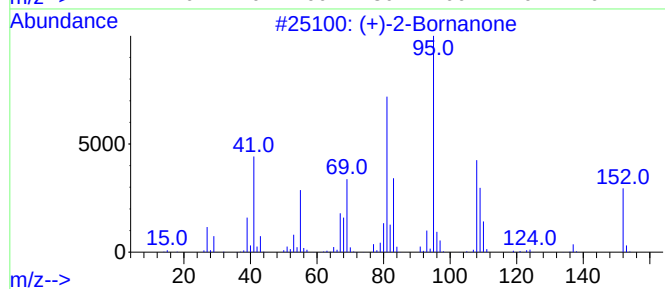
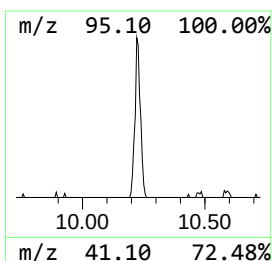
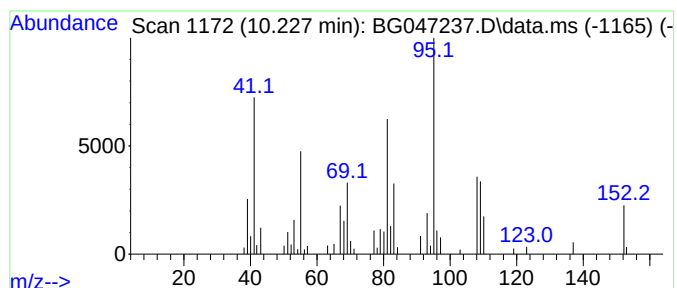
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TIC Integration Parameters: LSCINT.P

Peak Number 1 (+)-2-Bornanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.227	3.06 ng	92228	Naphthalene-d8	10.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(+)-2-Bornanone	152	C10H16O	000464-49-3	97
2			Camphor	152	C10H16O	000076-22-2	97
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	95
4			5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58
5			Tricyclo[2.2.1.0(2,6)]heptan-3-o...	152	C10H16O	062560-53-6	49



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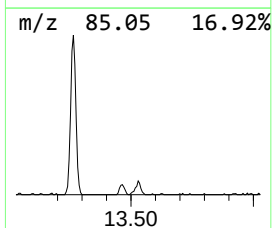
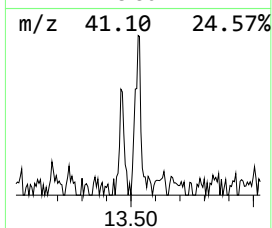
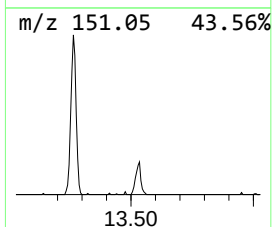
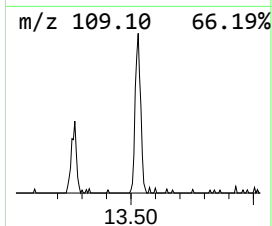
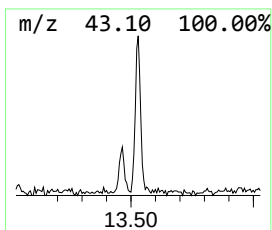
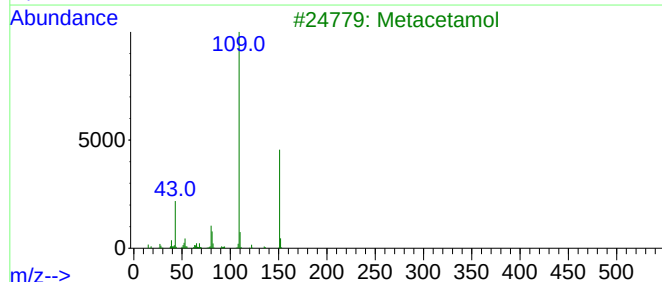
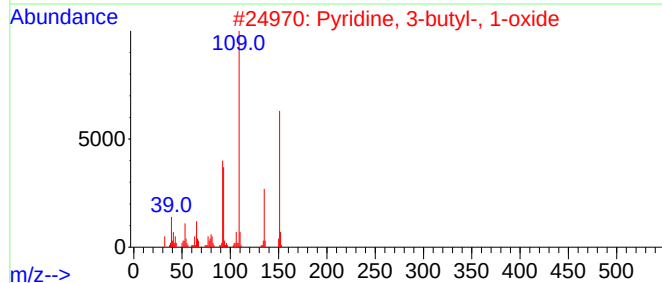
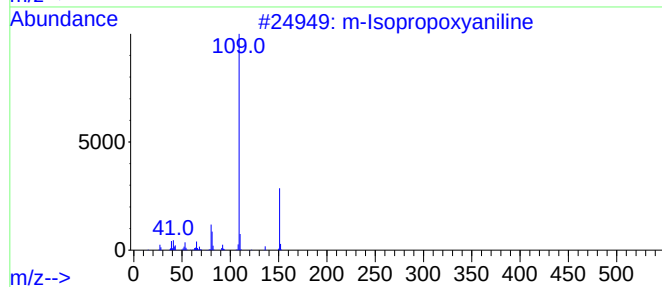
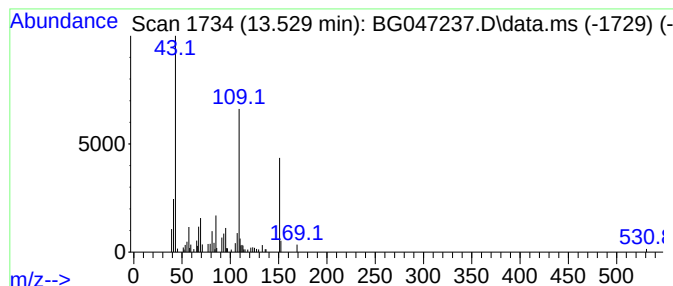
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 m-Isopropoxyaniline Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.529	2.01 ng	91978	Acenaphthene-d10	14.640

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			m-Isopropoxyaniline	151	C9H13NO	041406-00-2	58
2			Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	53
3			Metacetamol	151	C8H9NO2	000621-42-1	53
4			Tiocarlide	400	C23H32N2O2S	000910-86-1	53
5			2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	43



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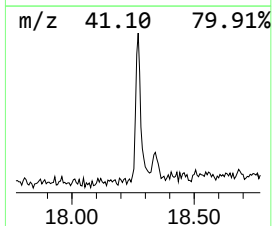
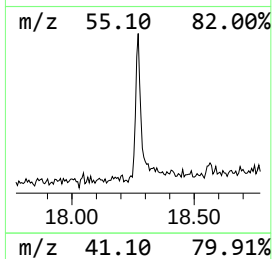
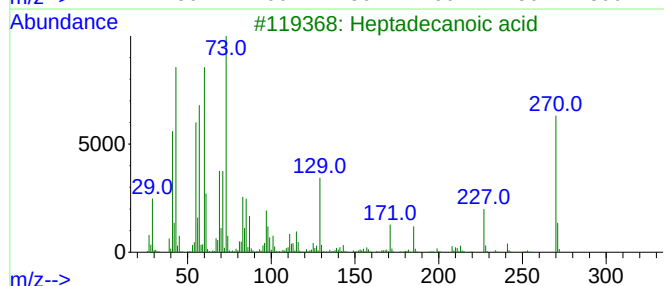
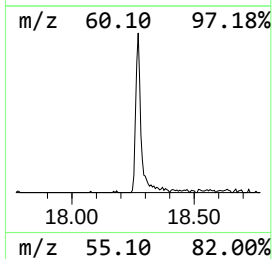
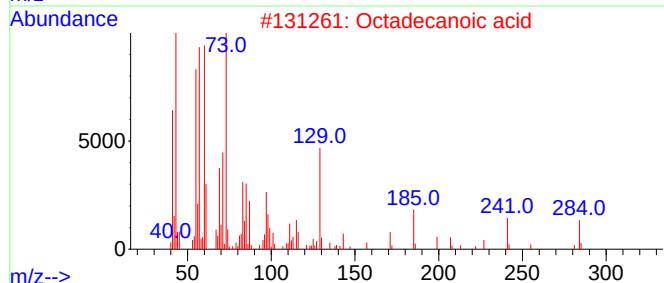
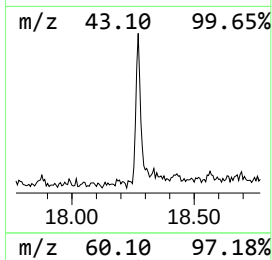
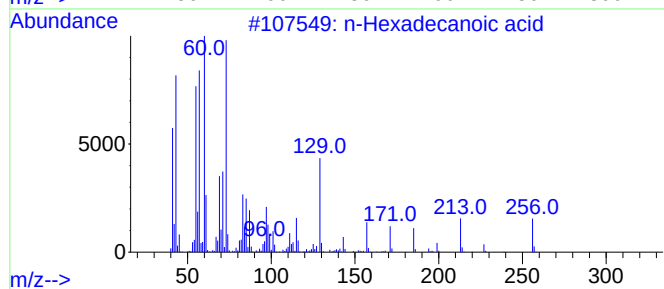
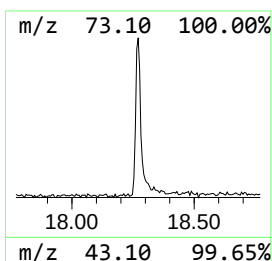
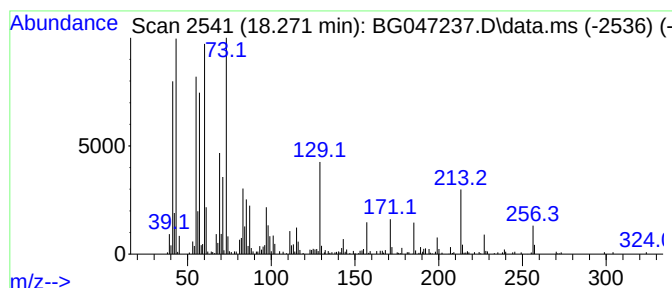
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.270	7.27 ng	382717	Phenanthrene-d10	17.389

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	93
3			Heptadecanoic acid	270	C17H34O2	000506-12-7	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			Tridecanoic acid	214	C13H26O2	000638-53-9	90



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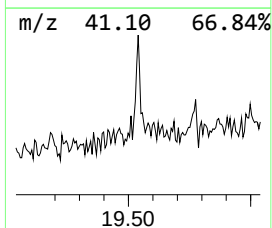
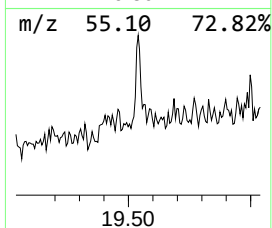
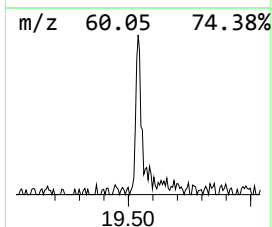
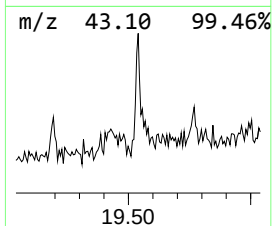
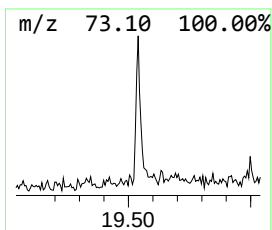
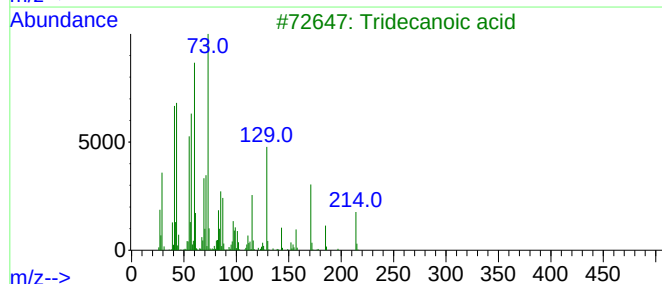
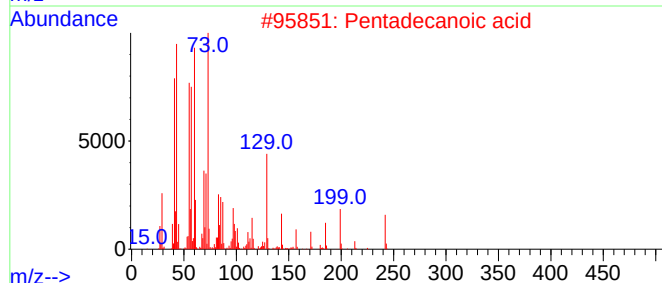
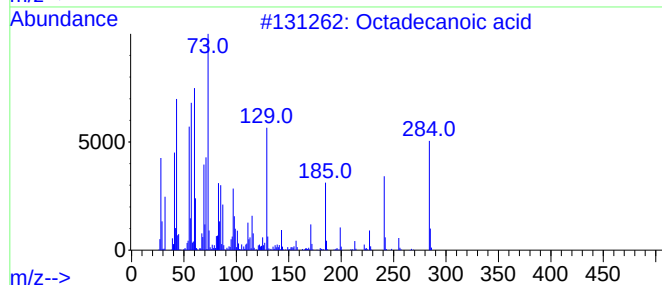
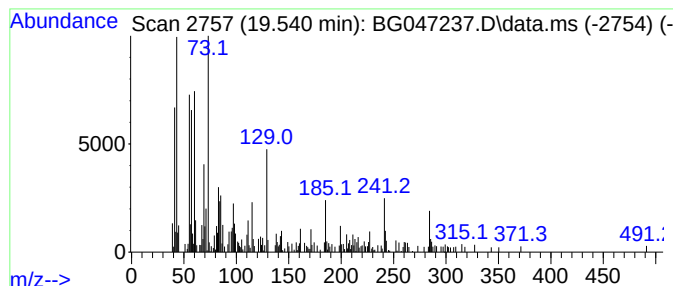
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.540	2.22 ng	109765	Chrysene-d12	21.649

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3			Tridecanoic acid	214	C13H26O2	000638-53-9	58
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	47



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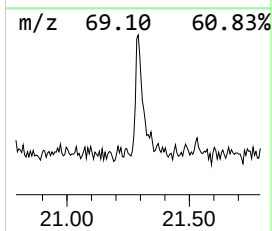
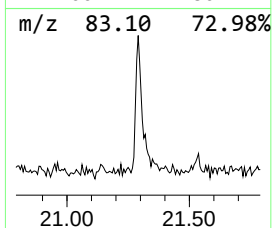
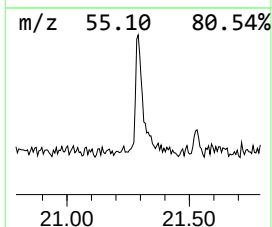
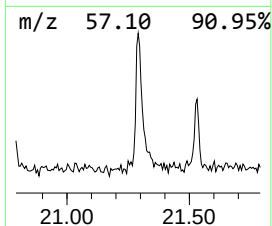
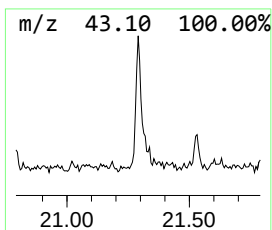
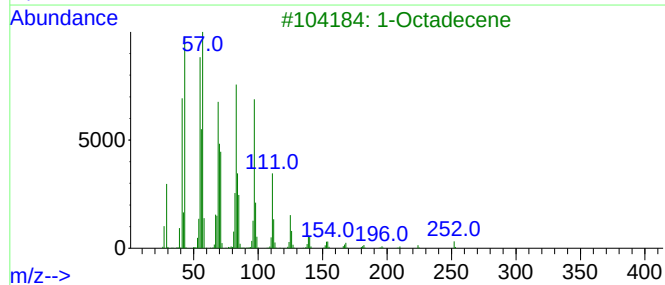
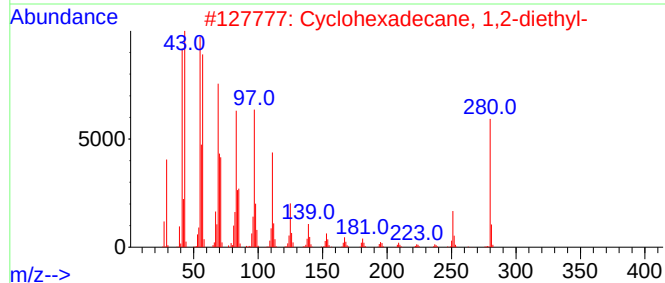
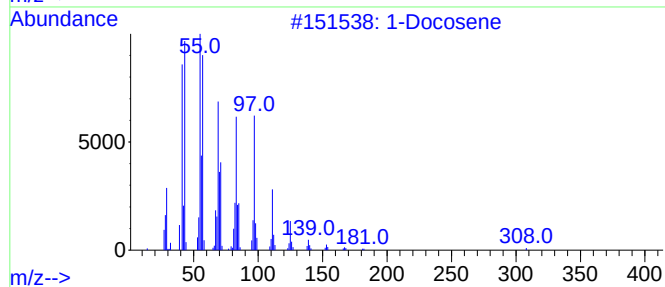
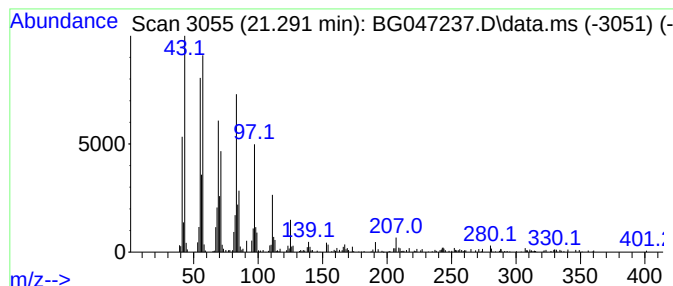
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Peak Number 5 1-Docosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.291	8.39 ng	414952	Chrysene-d12	21.649

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	98
2			Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	93
3			1-Octadecene	252	C18H36	000112-88-9	93
4			9-Tricosene, (Z)-	322	C23H46	027519-02-4	91
5			Cyclooctacosane	392	C28H56	000297-24-5	91



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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(+)-2-Bornanone	10.227	3.1	ng	92228	2	10.815	602156	20.0
m-Isopropoxyani...	13.529	2.0	ng	91978	3	14.640	913360	20.0
n-Hexadecanoic ...	18.270	7.3	ng	382717	4	17.389	1053070	20.0
Octadecanoic acid	19.540	2.2	ng	109765	5	21.649	988906	20.0
1-Docosene	21.291	8.4	ng	414952	5	21.649	988906	20.0