

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110520\
 Data File : BG047236.D
 Acq On : 6 Nov 2020 2:25
 Operator : CG/JU
 Sample : L4641-11
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P0122-CAS001-0204-01

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: BG047236.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.559	371	378	389	rBV	813979	1299892	37.68%	6.579%
2	7.163	643	651	664	rBV	883116	1509865	43.77%	7.641%
3	8.004	785	794	802	rBV	220798	372932	10.81%	1.887%
4	9.167	985	992	1001	rBV	546467	961282	27.87%	4.865%
5	10.224	1165	1172	1180	rVB2	108167	189941	5.51%	0.961%
6	10.818	1263	1273	1282	rBV	314283	571685	16.57%	2.893%
7	13.268	1682	1690	1697	rBV	1563565	2392612	69.36%	12.109%
8	13.532	1729	1735	1742	rVB	89054	138660	4.02%	0.702%
9	14.085	1822	1829	1839	rBV	105242	165646	4.80%	0.838%
10	14.643	1910	1924	1933	rBV	573928	898532	26.05%	4.547%
11	16.129	2170	2177	2193	rBV	1477352	2169751	62.90%	10.981%
12	17.387	2385	2391	2397	rBV	724666	1053355	30.54%	5.331%
13	18.268	2536	2541	2550	rBV	318607	506310	14.68%	2.562%
14	18.344	2550	2554	2558	rVB	165263	210371	6.10%	1.065%
15	18.609	2595	2599	2602	rBV2	30847	50727	1.47%	0.257%
16	19.537	2754	2757	2764	rBV4	119406	171909	4.98%	0.870%
17	19.995	2830	2835	2841	rBV	2766266	3449513	100.00%	17.458%
18	21.288	3051	3055	3067	rBV	229263	470149	13.63%	2.379%
19	21.529	3092	3096	3102	rVB	647730	840714	24.37%	4.255%
20	21.646	3110	3116	3128	rVB	686533	1143853	33.16%	5.789%
21	24.848	3653	3661	3673	rVB2	414175	1191183	34.53%	6.029%

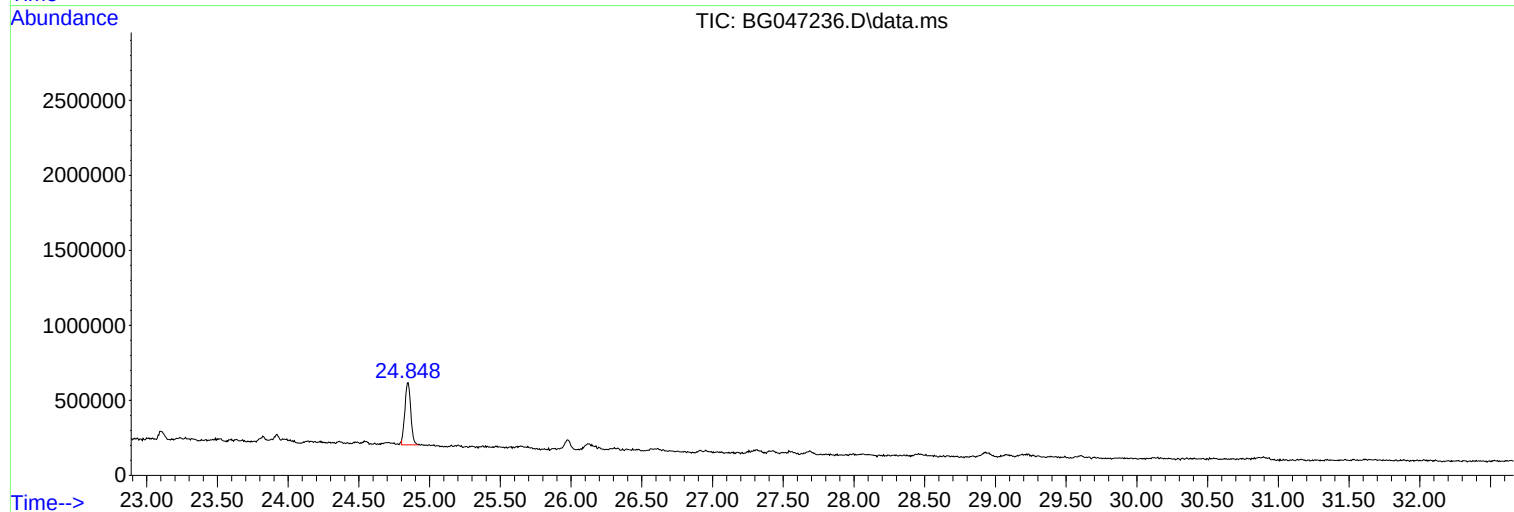
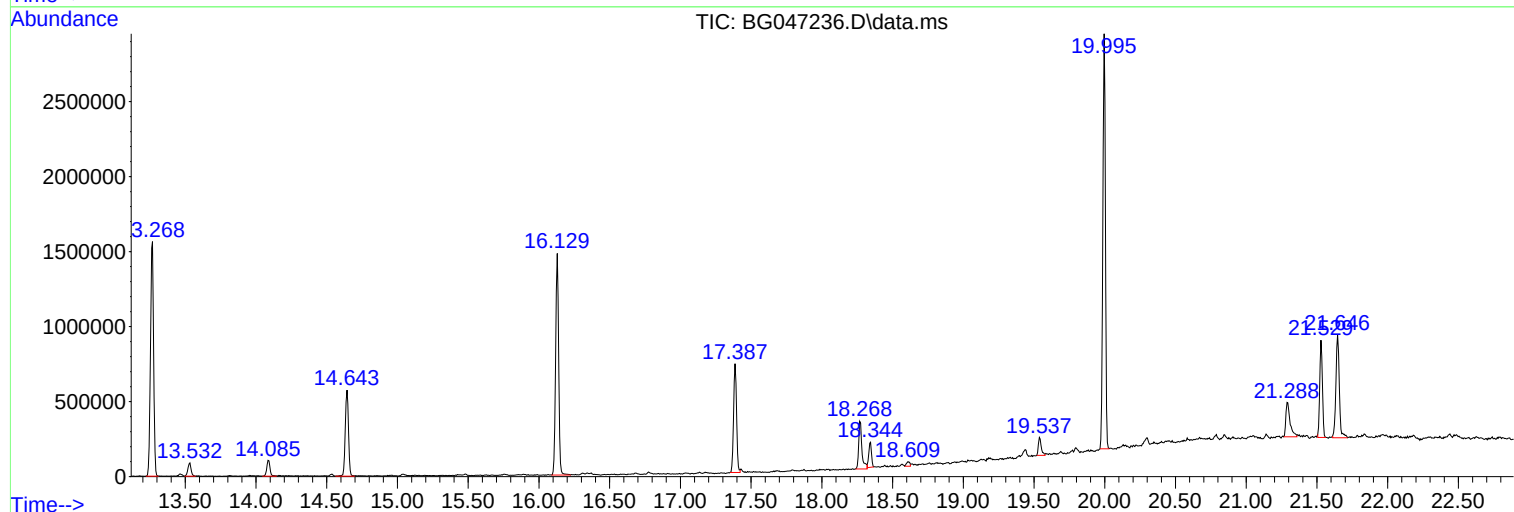
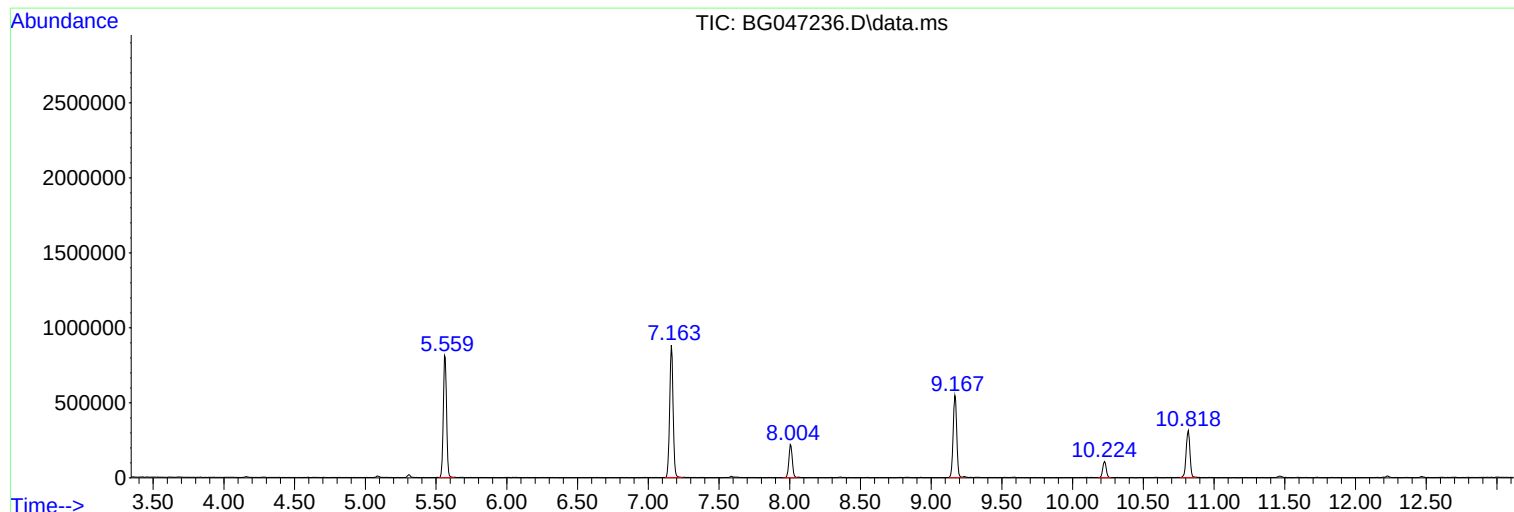
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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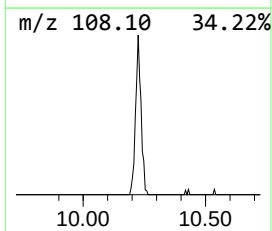
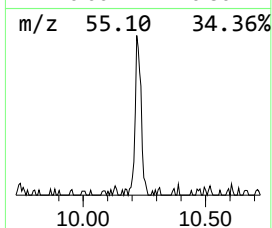
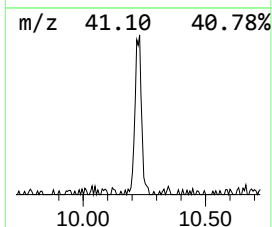
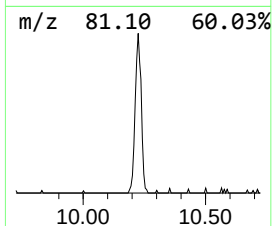
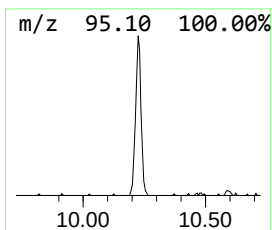
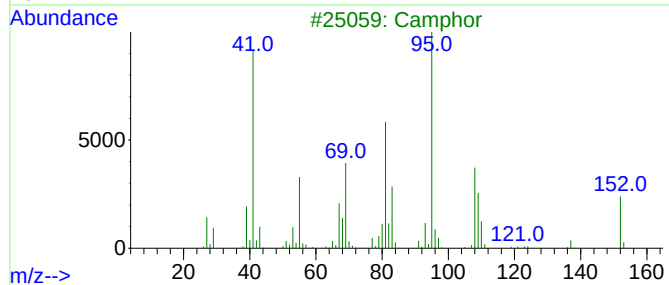
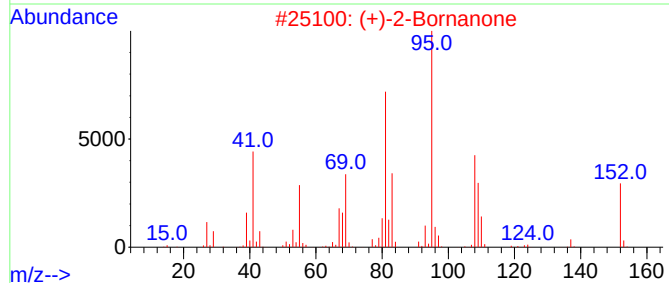
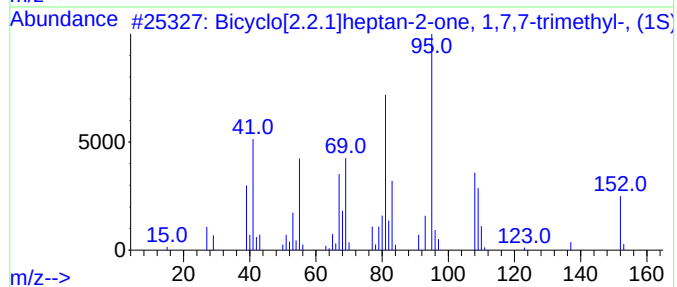
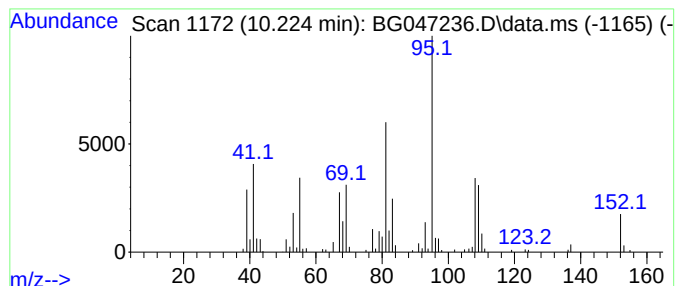
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.225	6.64 ng	189941	Naphthalene-d8	10.818

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	94
2			(+)-2-Bornanone	152	C10H16O	000464-49-3	64
3			Camphor	152	C10H16O	000076-22-2	64
4			5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58
5			Bicyclo[3.3.0]octan-3-one, 6-iod...	264	C9H13IO	1000150-13-4	50



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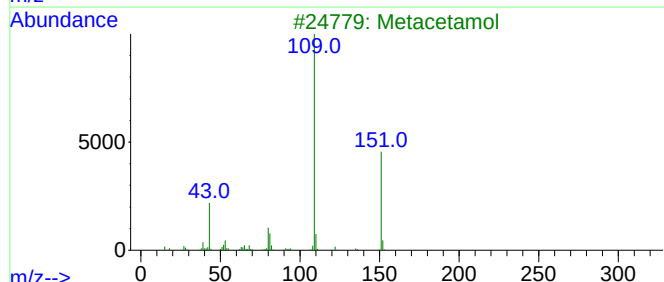
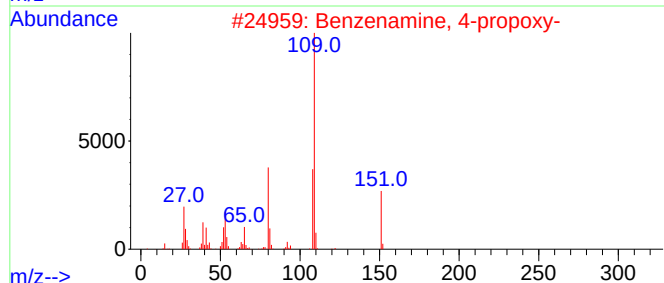
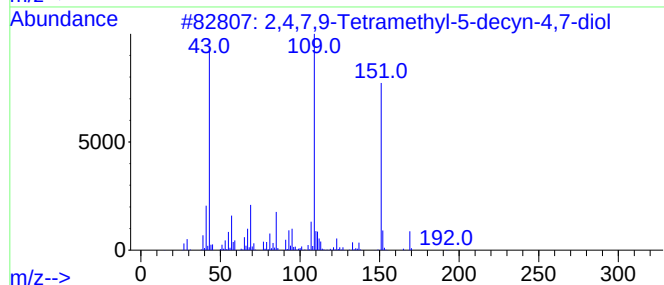
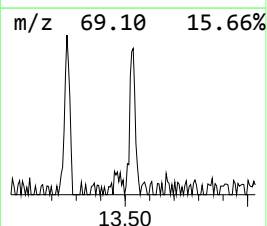
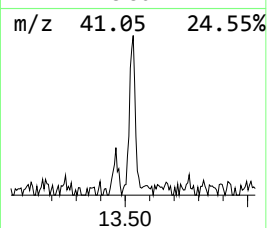
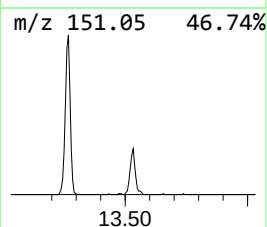
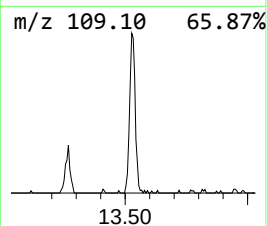
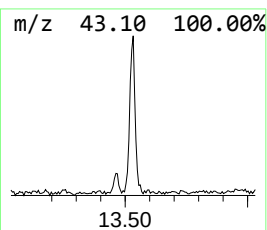
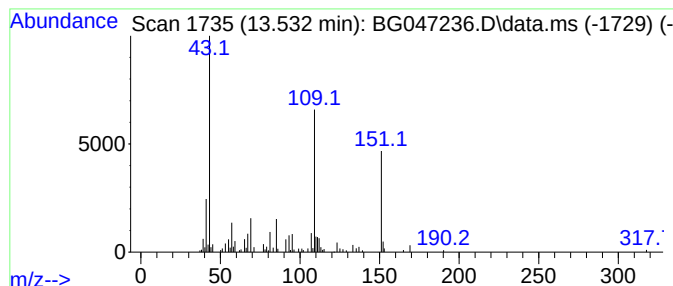
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.532	3.09 ng	138660	Acenaphthene-d10	14.643

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87	
2	Benzenamine, 4-propoxy-	151	C9H13NO	004469-80-1	59	
3	Metacetamol	151	C8H9NO2	000621-42-1	59	
4	1H-Pyrazole, 4-[4-(3-chloropheno...	278	C15H19ClN2O	1000302-33-9	50	
5	Diacetamate	193	C10H11NO3	002623-33-8	45	



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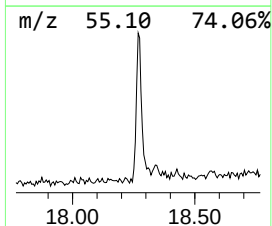
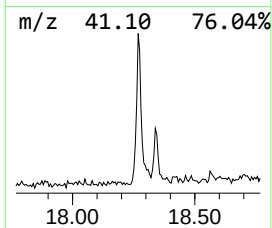
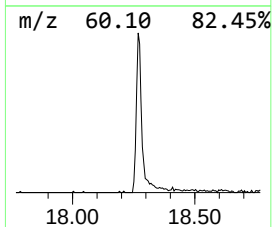
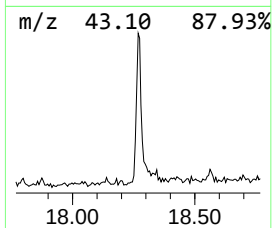
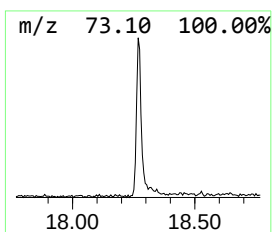
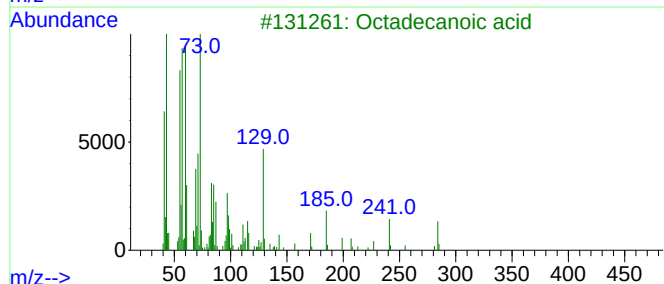
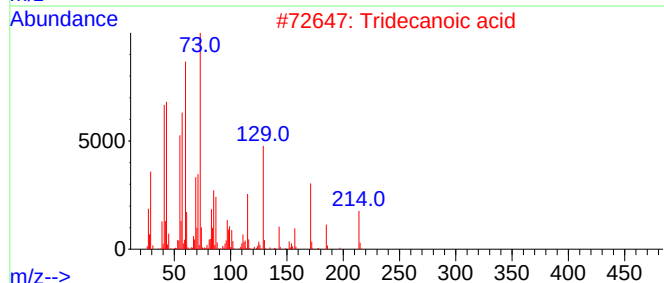
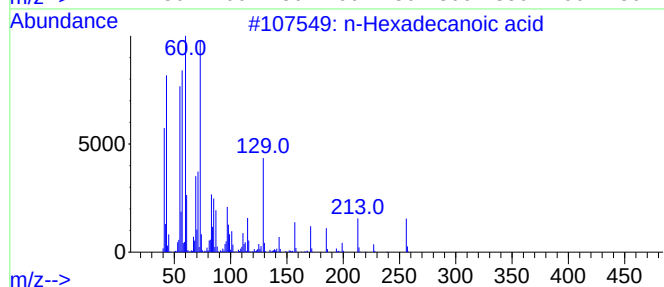
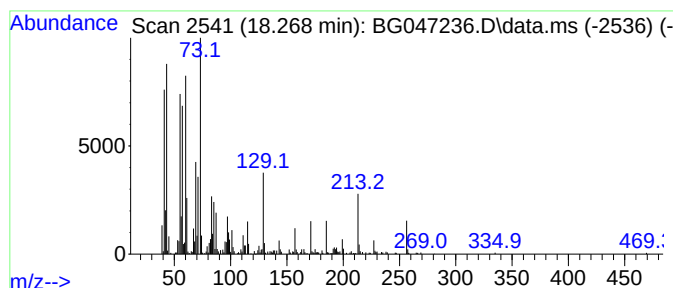
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.268	9.61 ng	506310	Phenanthrene-d10	17.387

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Octadecanoic acid	284	C18H36O2	000057-11-4	81
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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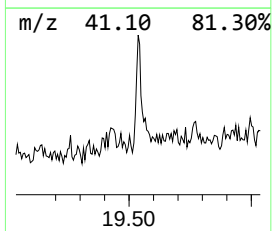
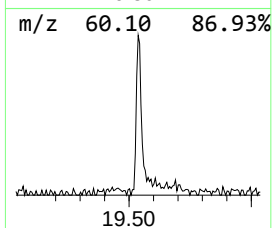
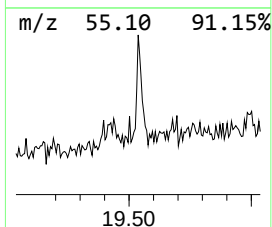
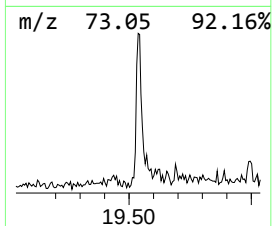
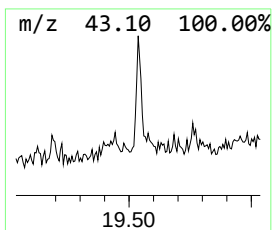
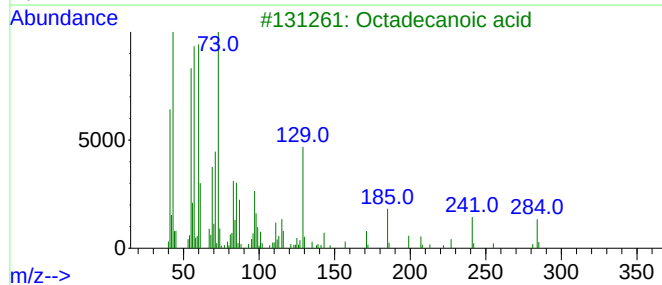
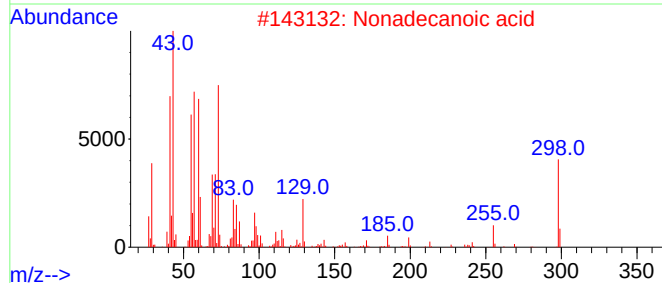
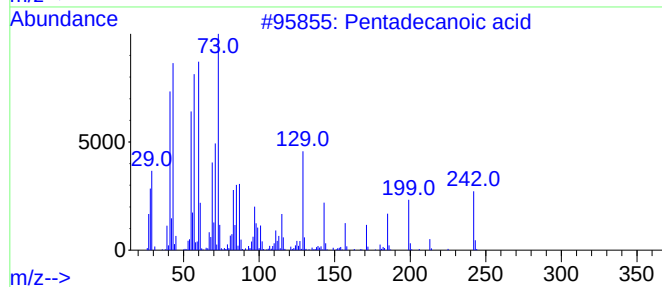
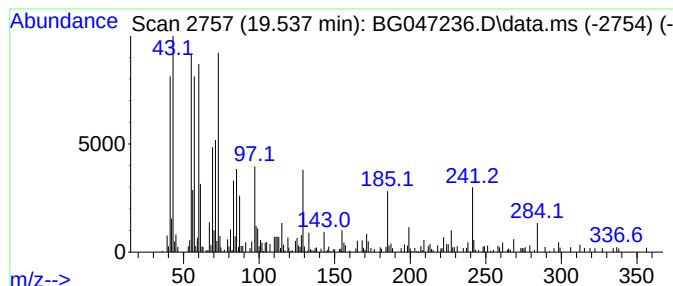
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Peak Number 4 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.537	3.01 ng	171909	Chrysene-d12	21.646

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
2			Nonadecanoic acid	298	C19H38O2	000646-30-0	86
3			Octadecanoic acid	284	C18H36O2	000057-11-4	81
4			Eicosanoic acid	312	C20H40O2	000506-30-9	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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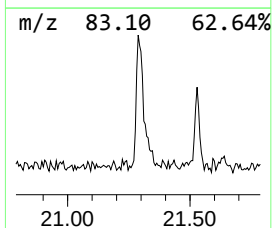
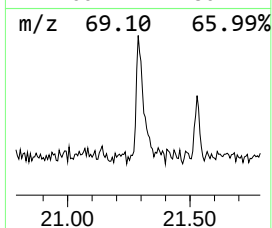
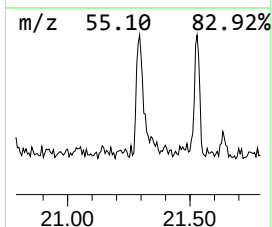
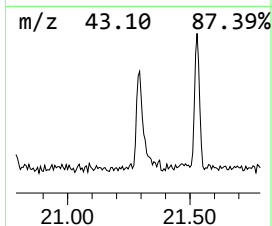
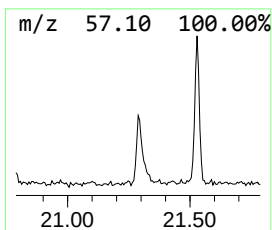
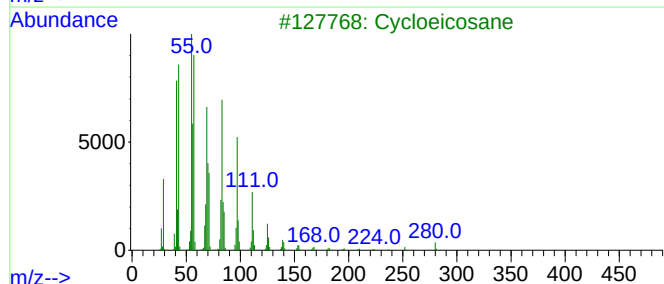
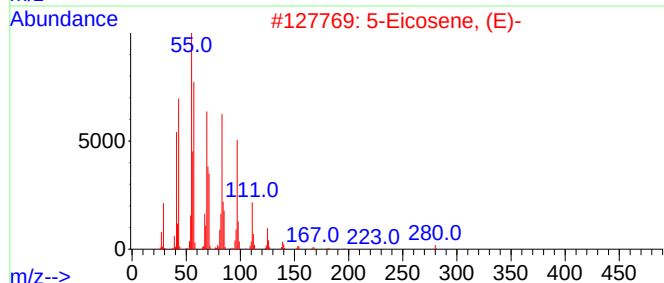
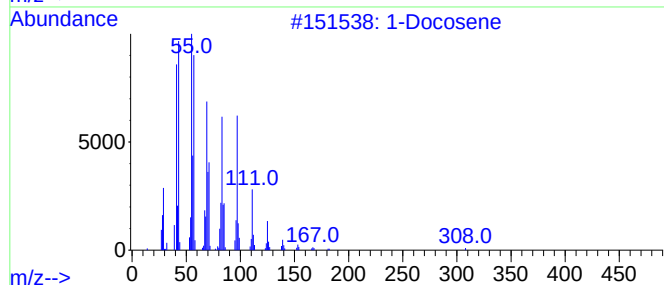
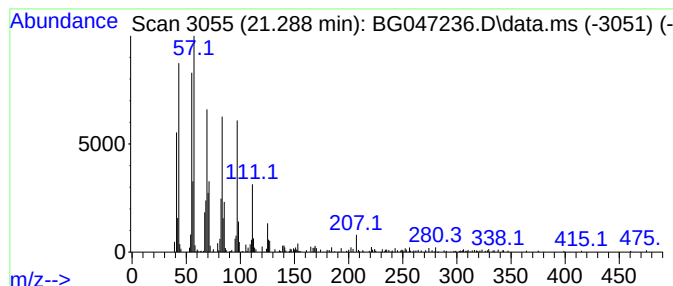
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Peak Number 5 1-Docosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.288	8.22 ng	470149	Chrysene-d12	21.646

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	96
2			5-Eicosene, (E)-	280	C20H40	074685-30-6	96
3			Cycloeicosane	280	C20H40	000296-56-0	95
4			9-Hexacosene	364	C26H52	071502-22-2	94
5			3-Eicosene, (E)-	280	C20H40	074685-33-9	93



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TIC Library : C:\Database\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Bicyclo[2.2.1]h...	10.225	6.6	ng	189941	2	10.818	571685	20.0
2,4,7,9-Tetrame...	13.532	3.1	ng	138660	3	14.643	898532	20.0
n-Hexadecanoic ...	18.268	9.6	ng	506310	4	17.387	1053360	20.0
Pentadecanoic acid	19.537	3.0	ng	171909	5	21.646	1143850	20.0
1-Docosene	21.288	8.2	ng	470149	5	21.646	1143850	20.0