

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051119\
 Data File : BM020276.D
 Acq On : 11 May 2019 17:19
 Operator : JU/SJ
 Sample : K2765-06
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P026-SS003-1218-01

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.351	396	402	414	rBV	908525	1355390	62.41%	8.688%
2	6.934	664	671	684	rBV	875153	1413212	65.07%	9.059%
3	7.298	725	733	746	rBV	940365	1497200	68.94%	9.597%
4	7.769	807	813	819	rBV	177764	292839	13.48%	1.877%
5	8.081	860	866	882	rBV	664648	1105318	50.90%	7.085%
6	8.934	1003	1011	1029	rBV	513548	887436	40.86%	5.689%
7	10.557	1281	1287	1297	rBV	180495	329169	15.16%	2.110%
8	13.027	1701	1707	1730	rBV	983537	1519116	69.95%	9.738%
9	13.869	1845	1850	1858	rBV	126030	177556	8.18%	1.138%
10	14.410	1936	1942	1959	rVB2	275821	446870	20.58%	2.865%
11	15.904	2190	2196	2208	rBV	864857	1333122	61.39%	8.546%
12	17.163	2403	2410	2420	rBV2	366167	556171	25.61%	3.565%
13	18.045	2555	2560	2570	rBV	88582	138582	6.38%	0.888%
14	19.327	2773	2778	2785	rBV4	28935	50381	2.32%	0.323%
15	19.792	2851	2857	2868	rBV	1687460	2171671	100.00%	13.921%
16	21.045	3066	3070	3075	rBV	76251	104465	4.81%	0.670%
17	21.350	3117	3122	3131	rBV	582168	759871	34.99%	4.871%
18	21.921	3217	3219	3222	rBV2	32458	37435	1.72%	0.240%
19	22.521	3318	3321	3327	rVB	91208	122220	5.63%	0.783%
20	22.909	3384	3387	3391	rVB	81099	107316	4.94%	0.688%
21	23.639	3505	3511	3520	rVB	398824	783338	36.07%	5.021%
22	24.150	3592	3598	3606	rVB2	213686	411456	18.95%	2.638%

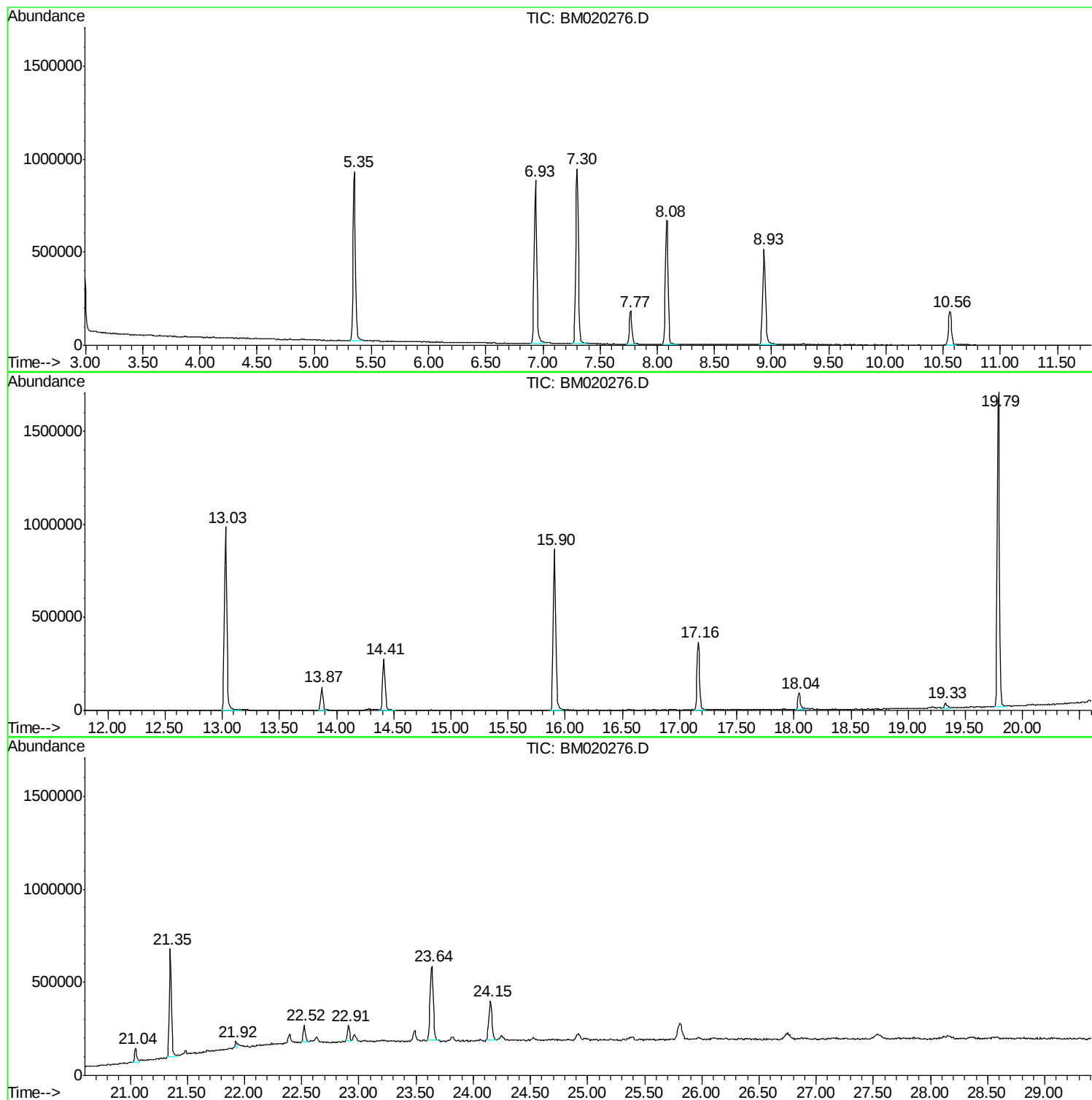
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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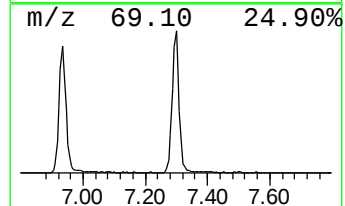
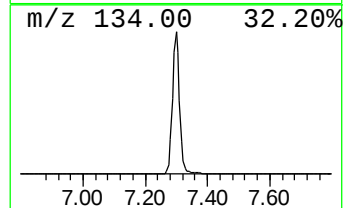
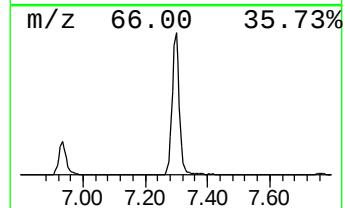
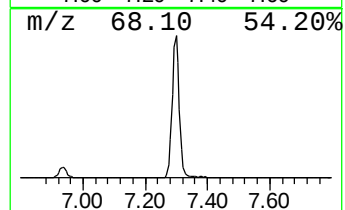
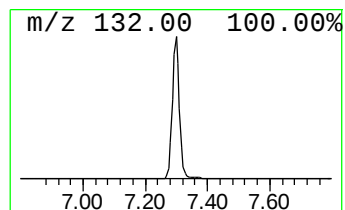
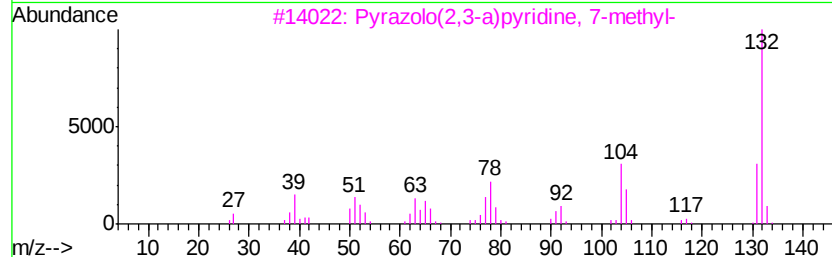
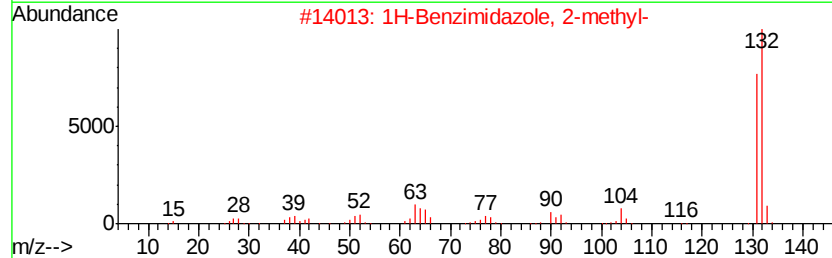
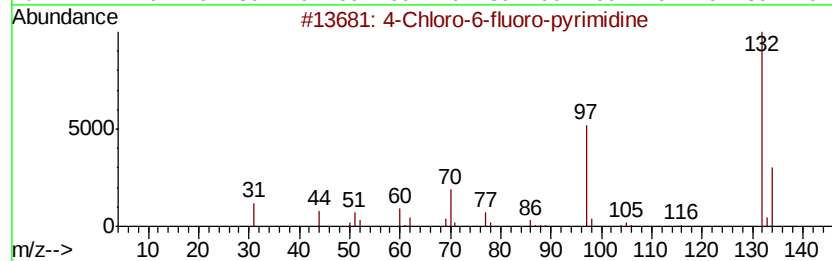
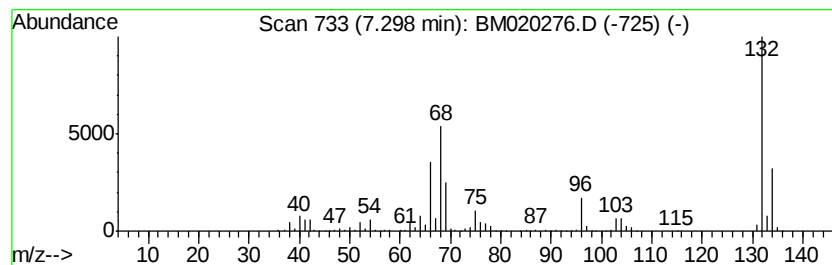
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.30 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.30	102.25 ng	1497200	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13



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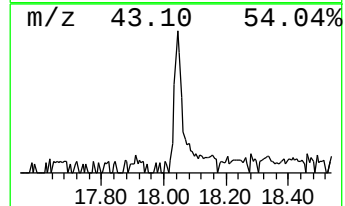
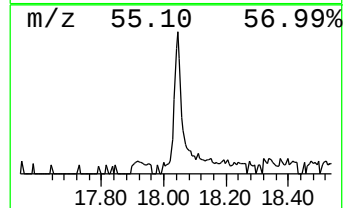
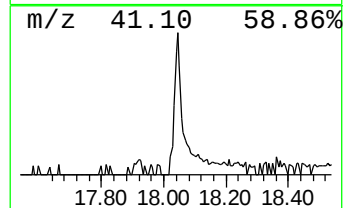
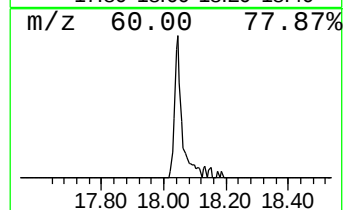
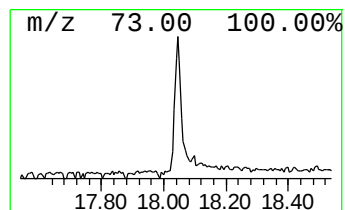
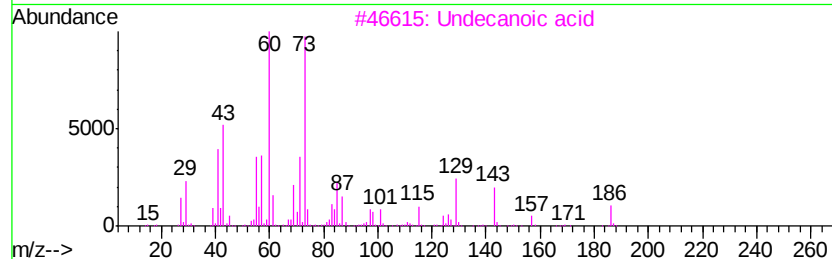
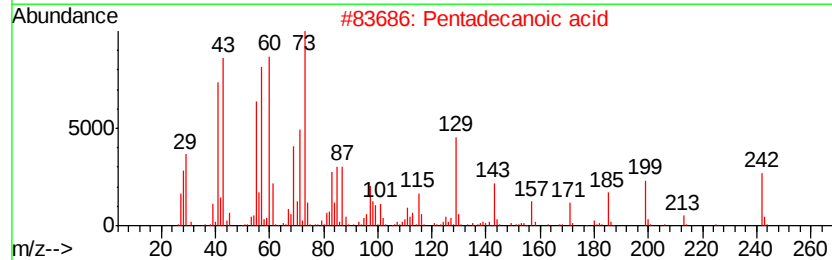
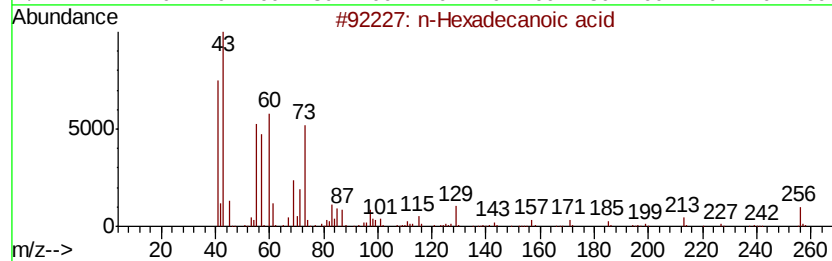
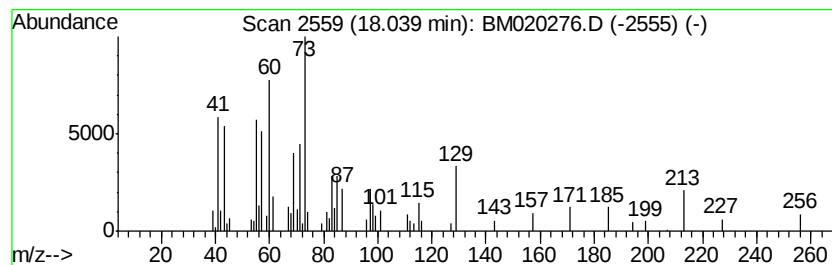
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.04	4.98 ng	138582	Phenanthrene-d10		17.16
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Undecanoic acid	186	C11H22O2	000112-37-8	47
4	Dodecanoic acid	200	C12H24O2	000143-07-7	43
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	22



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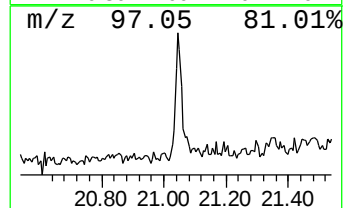
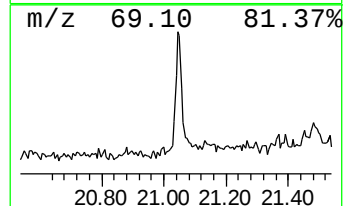
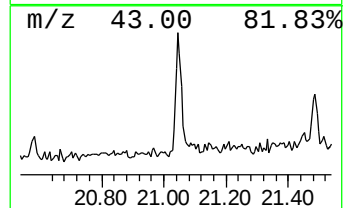
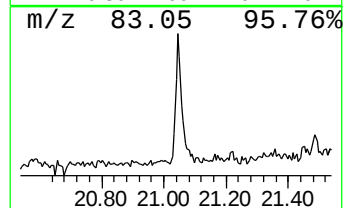
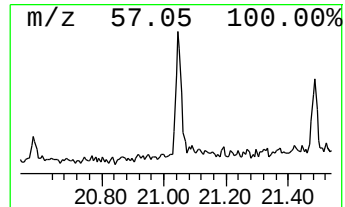
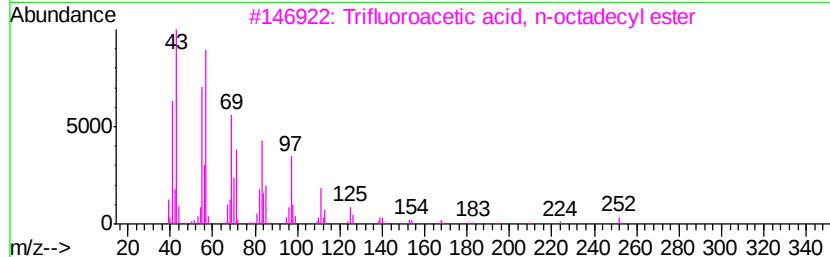
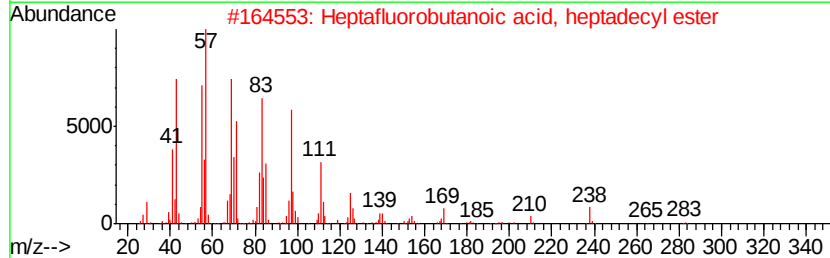
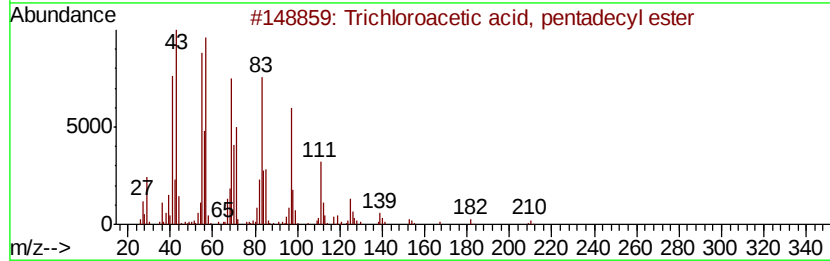
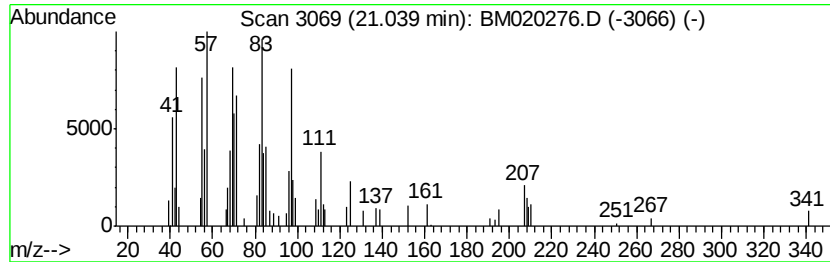
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Peak Number 4 Trichloroacetic acid, penta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.04	2.75 ng	104465	Chrysene-d12	21.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	83
2	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	83
3	Trifluoroacetic acid, n-octadecv...	366	C20H37F3O2	079392-43-1	83
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	80
5	1-Hexacosanol	382	C26H54O	000506-52-5	74



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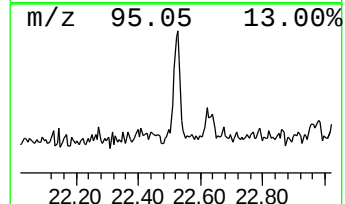
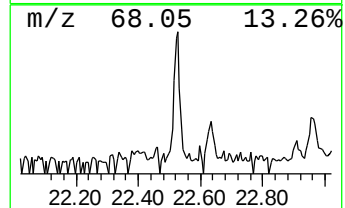
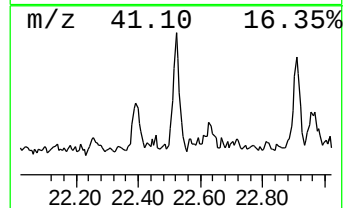
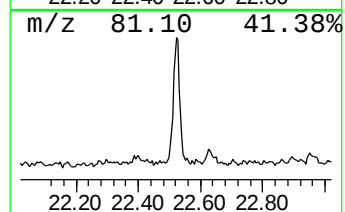
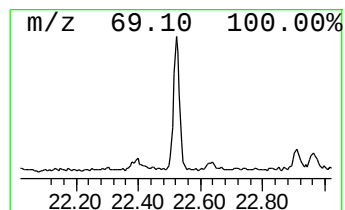
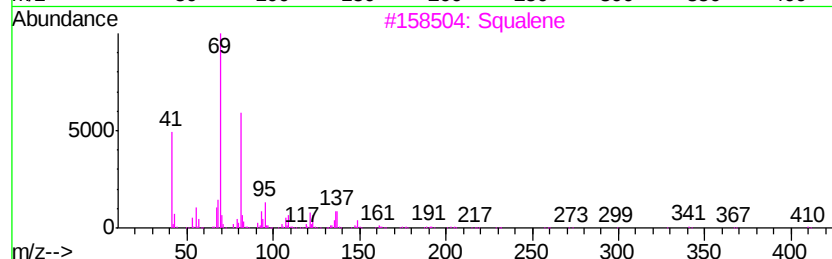
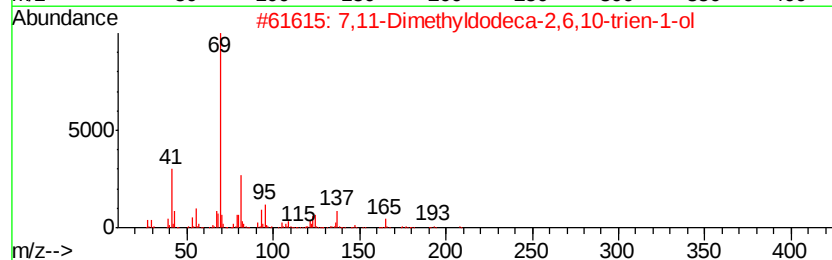
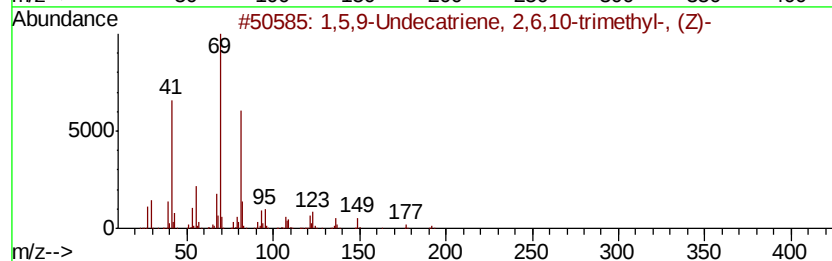
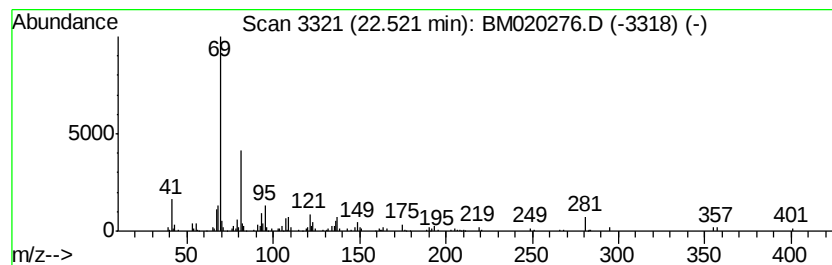
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Peak Number 5 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.52	3.12 ng	122220	Perylene-d12	23.64	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
3	Squalene	410	C30H50	007683-64-9	59
4	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	59
5	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	59



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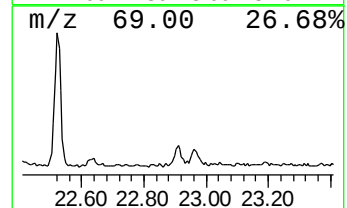
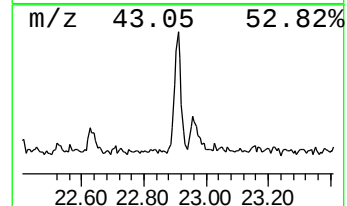
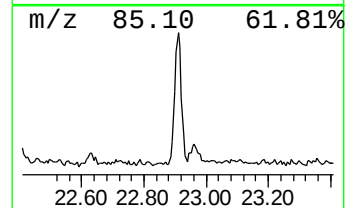
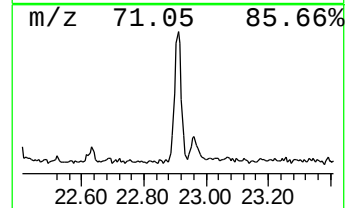
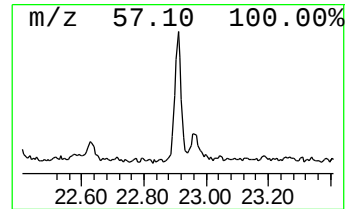
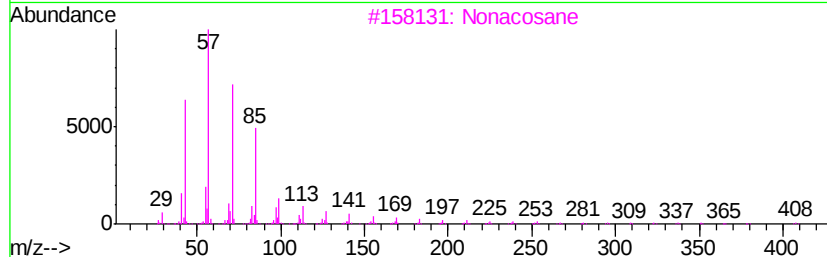
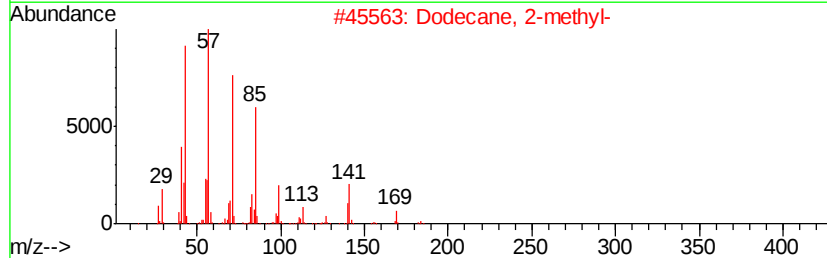
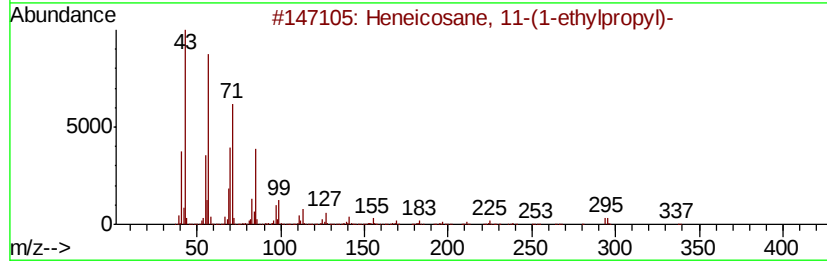
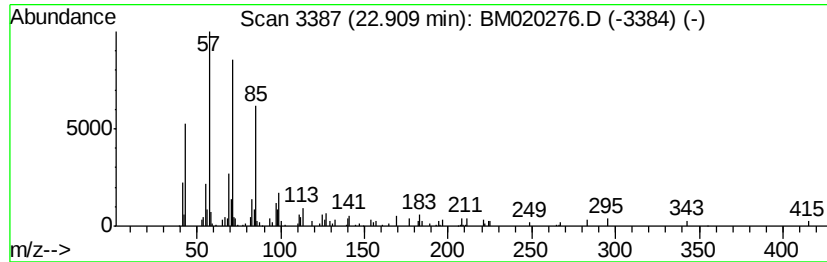
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Peak Number 6 Heneicosane, 11-(1-ethylpro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.91	2.74 ng	107316	Perylene-d12	23.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91	
2	Dodecane, 2-methyl-	184	C13H28	001560-97-0	87	
3	Nonacosane	408	C29H60	000630-03-5	86	
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	86	
5	Octadecane	254	C18H38	000593-45-3	86	



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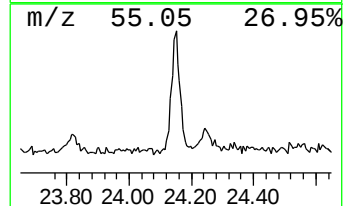
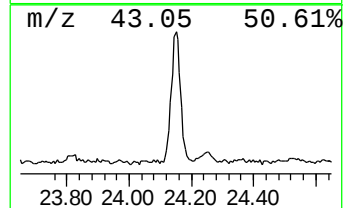
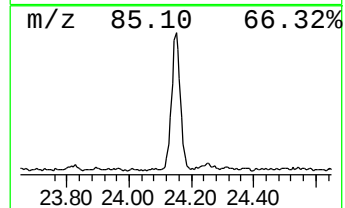
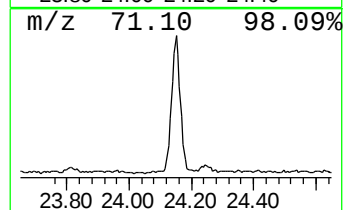
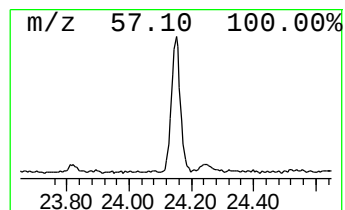
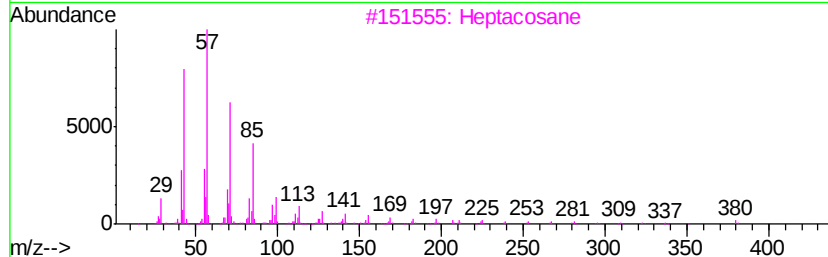
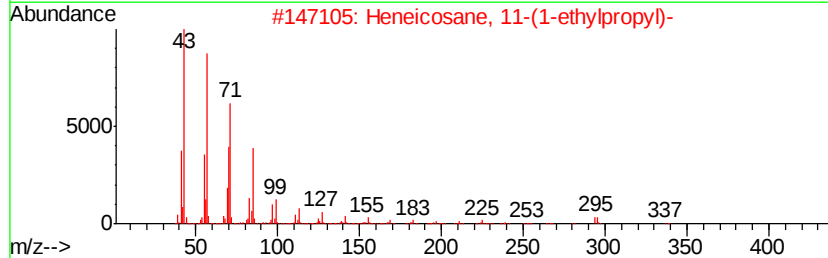
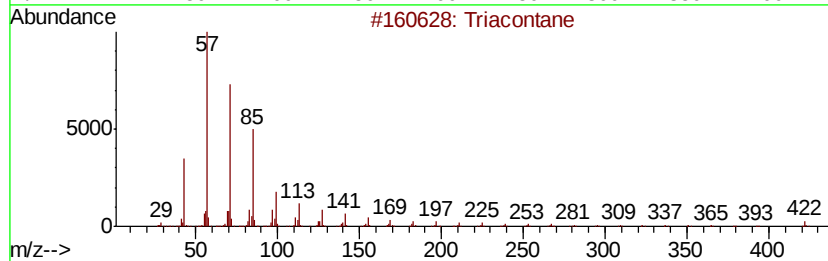
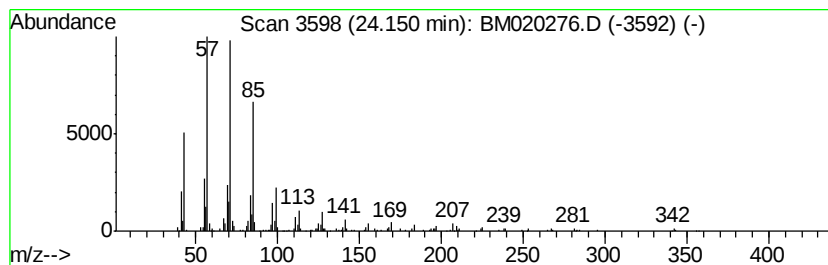
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Triacontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.15	10.51 ng	411456	Perylene-d12	23.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	91
2		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
3		Heptacosane	380	C27H56	000593-49-7	83
4		Octadecane, 2-methyl-	268	C19H40	001560-88-9	80
5		Tetracosane, 11-decyl-	479	C34H70	055429-84-0	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM051119\
Data File : BM020276.D
Acq On : 11 May 2019 17:19
Operator : JU/SJ
Sample : K2765-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P026-SS003-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.30	7.30	102.3	ng	1497200	1	7.77	292839	20.0
n-Hexadecanoic acid	18.04	5.0	ng	138582	4	17.16	556171	20.0
Trichloroacetic a...	21.04	2.8	ng	104465	5	21.35	759871	20.0
1,5,9-Undecatrien...	22.52	3.1	ng	122220	6	23.64	783338	20.0
Heneicosane, 11-(...	22.91	2.7	ng	107316	6	23.64	783338	20.0
Triacontane	24.15	10.5	ng	411456	6	23.64	783338	20.0