

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051119\
 Data File : BM020275.D
 Acq On : 11 May 2019 16:43
 Operator : JU/SJ
 Sample : K2765-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P026-SS003-0612-01

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_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	395	402	415	rBV	1060077	1591144	53.63%	8.309%
2	6.934	664	671	691	rBV	1033830	1688127	56.90%	8.816%
3	7.298	726	733	745	rBV	1112619	1764162	59.46%	9.213%
4	7.769	806	813	818	rBV	190030	314334	10.60%	1.642%
5	8.081	859	866	877	rBV	789705	1301259	43.86%	6.796%
6	8.934	1003	1011	1029	rBV	601595	1051331	35.44%	5.490%
7	10.557	1278	1287	1299	rBV	207781	370071	12.47%	1.933%
8	13.027	1701	1707	1718	rBV	1358542	2034649	68.58%	10.626%
9	13.869	1844	1850	1859	rBV	189134	266713	8.99%	1.393%
10	14.416	1936	1943	1957	rVB2	315439	500439	16.87%	2.613%
11	15.904	2190	2196	2211	rBV	1151173	1740007	58.65%	9.087%
12	17.162	2404	2410	2421	rBV2	424393	610456	20.58%	3.188%
13	18.045	2554	2560	2569	rBV	190304	289257	9.75%	1.511%
14	19.327	2774	2778	2789	rBV3	54736	84608	2.85%	0.442%
15	19.792	2851	2857	2870	rBV	2430517	2966726	100.00%	15.493%
16	21.045	3066	3070	3083	rBV	274710	373718	12.60%	1.952%
17	21.350	3117	3122	3128	rBV	593866	786002	26.49%	4.105%
18	21.486	3142	3145	3150	rVB2	42167	45046	1.52%	0.235%
19	21.927	3216	3220	3221	rBV2	64199	78536	2.65%	0.410%
20	22.392	3296	3299	3306	rVB3	80618	105352	3.55%	0.550%
21	22.521	3317	3321	3327	rBV	174490	251403	8.47%	1.313%
22	22.909	3383	3387	3392	rVB	96610	123764	4.17%	0.646%
23	23.638	3504	3511	3521	rBV	403506	811616	27.36%	4.238%

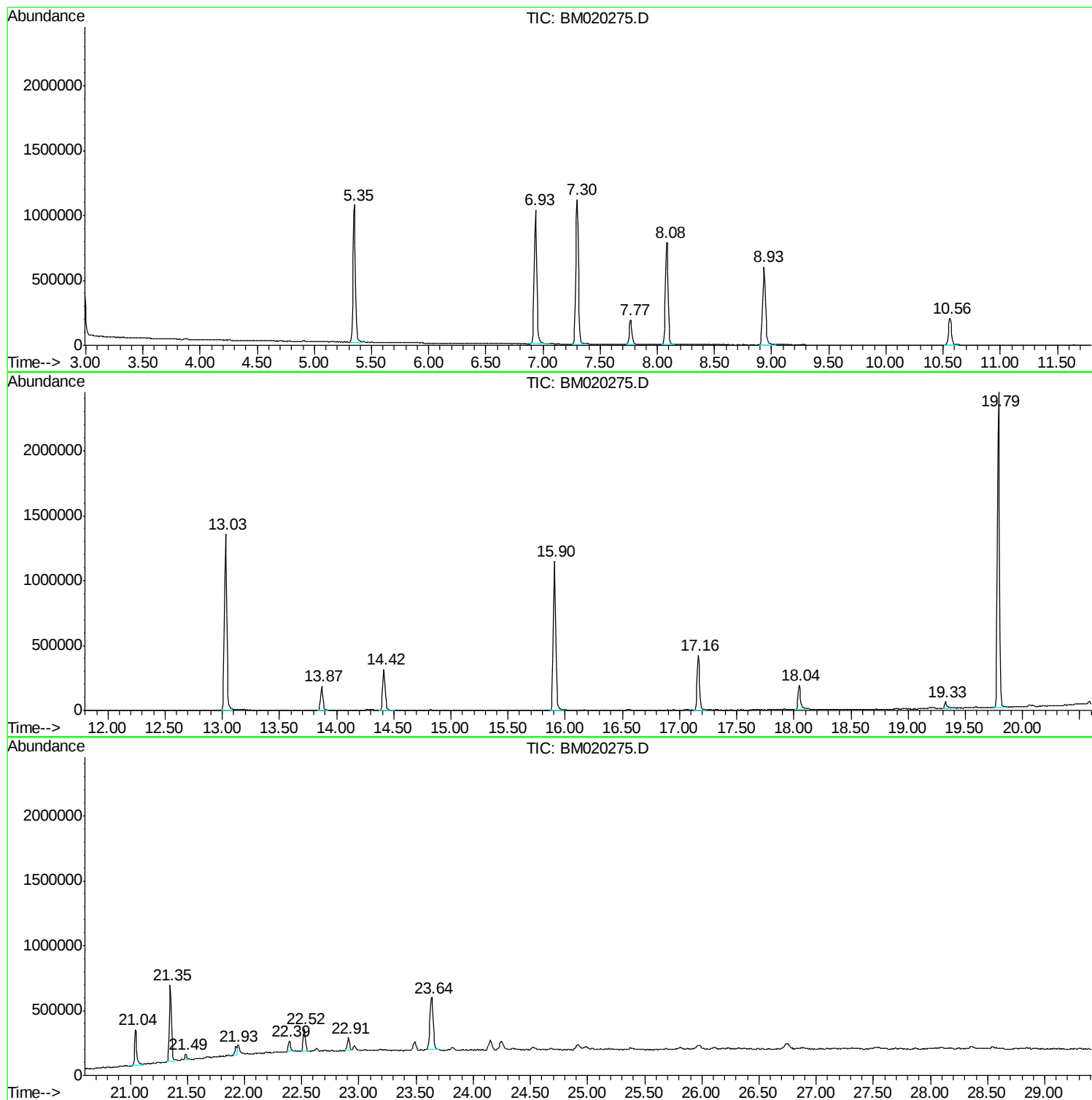
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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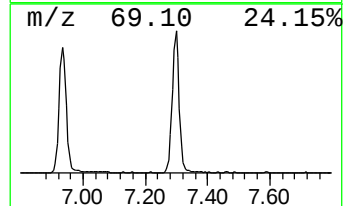
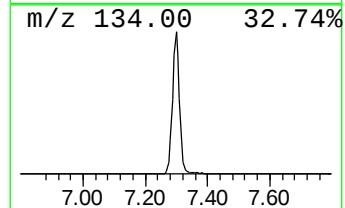
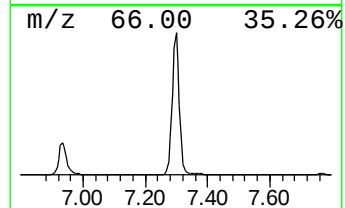
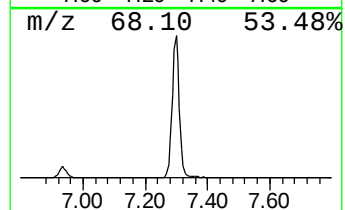
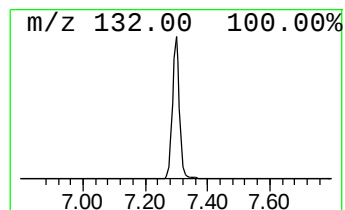
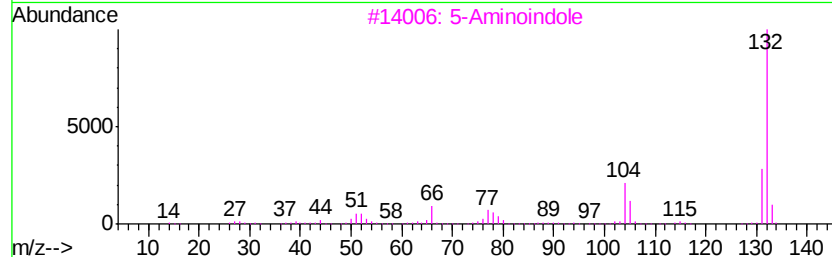
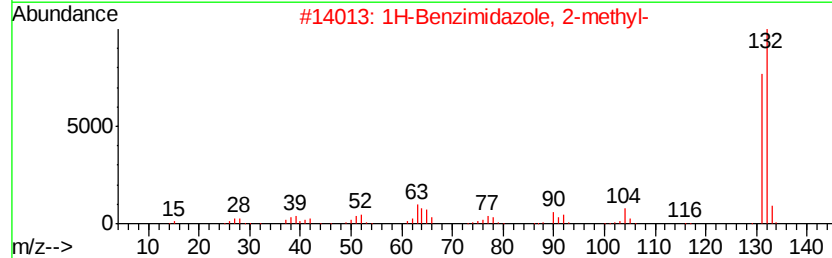
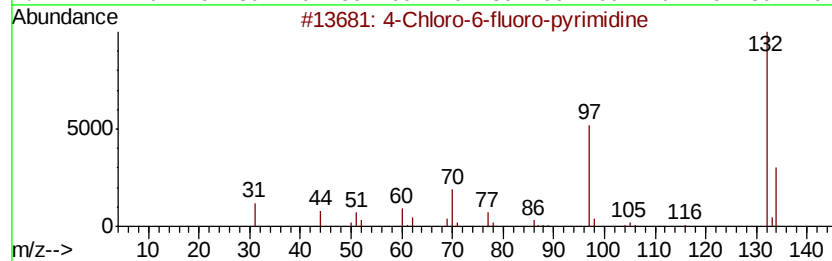
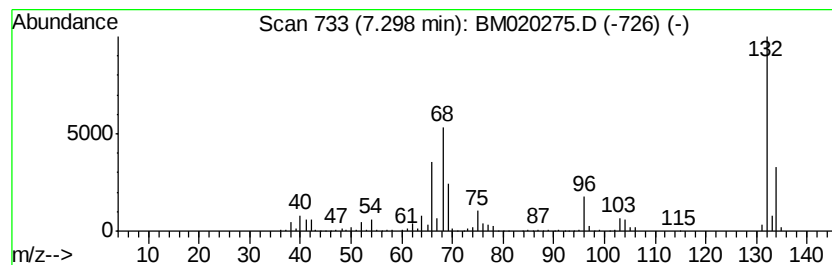
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	112.25 ng	1764160	1,4-Dichlorobenzene-d4	7.76

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		5-Aminoindole	132	C8H8N2	005192-03-0	22
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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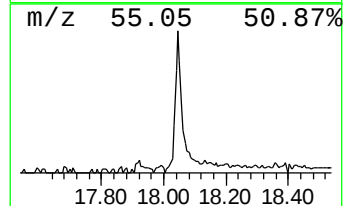
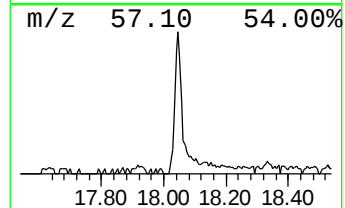
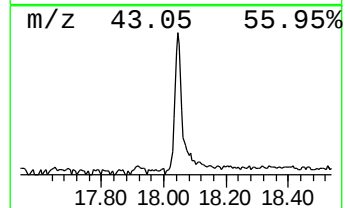
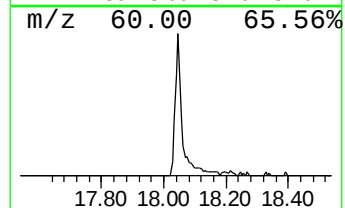
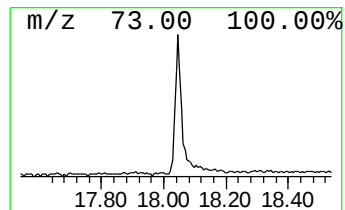
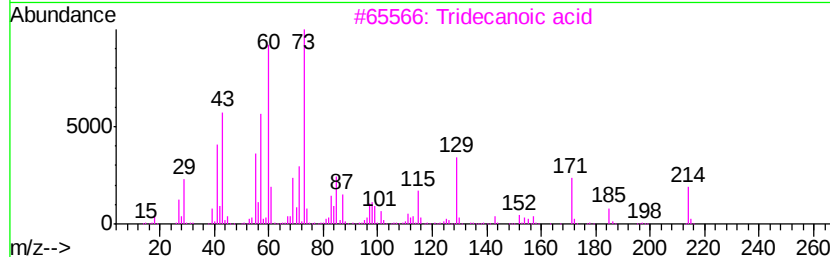
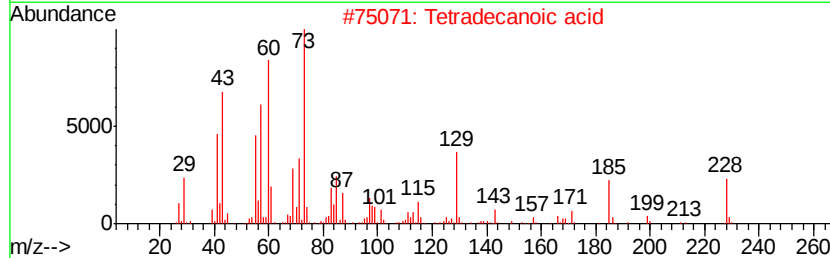
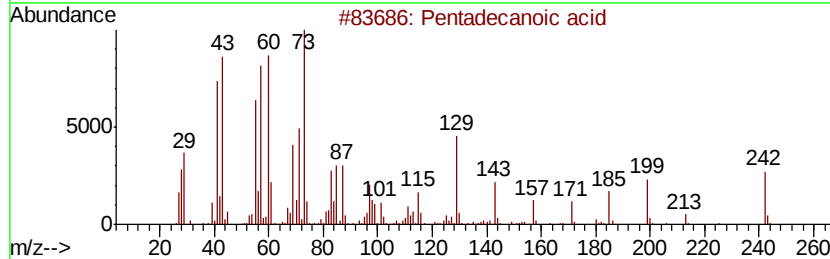
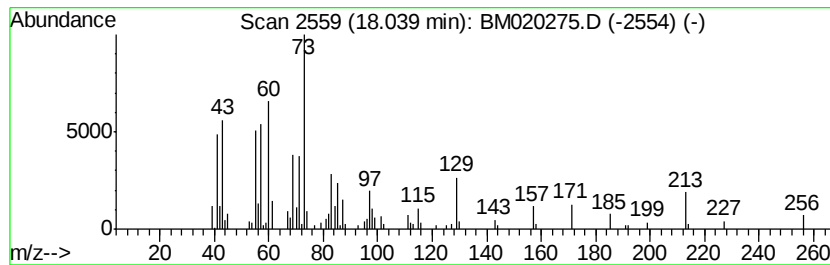
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Peak Number 3 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	9.48 ng	289257	Phenanthrene-d10	17.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	50
3		Tridecanoic acid	214	C13H26O2	000638-53-9	40
4		.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	38
5		Dodecanoic acid	200	C12H24O2	000143-07-7	38



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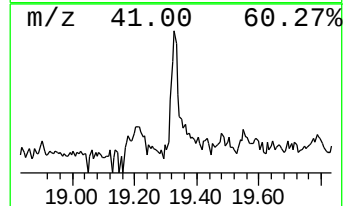
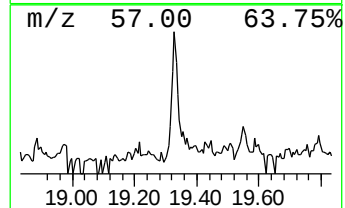
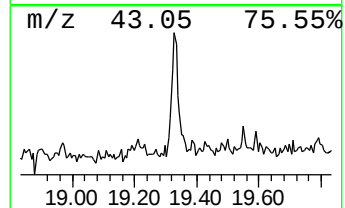
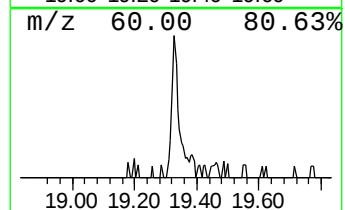
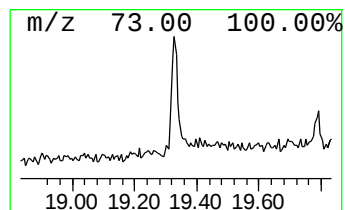
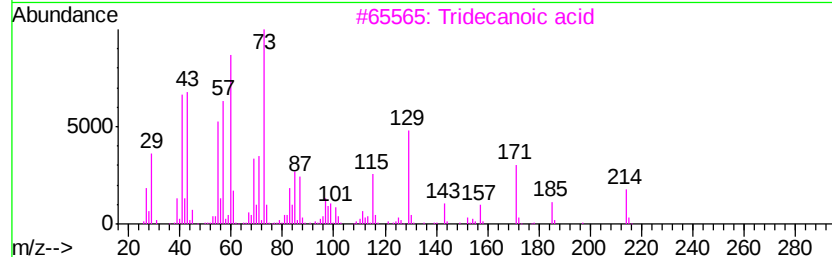
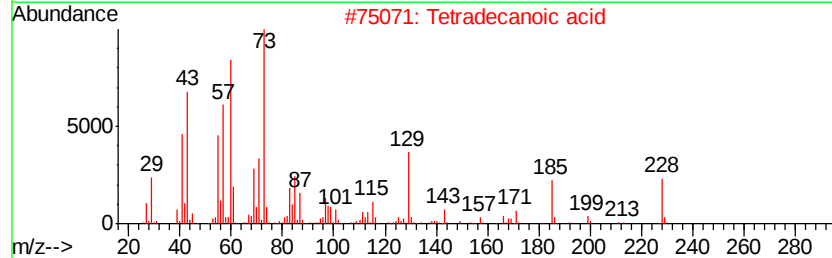
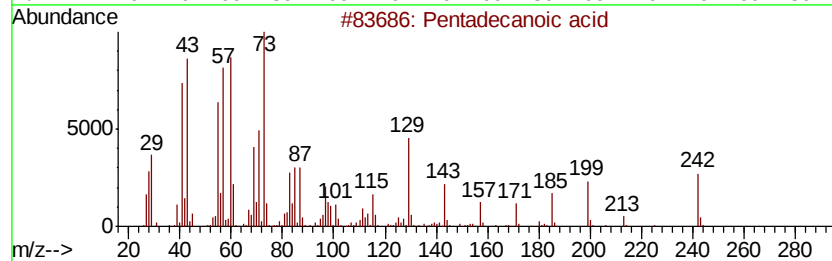
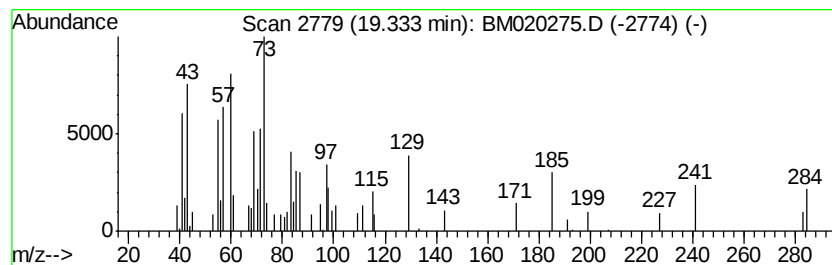
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Peak Number 4 Tetradecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.33	2.15 ng	84608	Chrysene-d12	21.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
3	Tridecanoic acid	214	C13H26O2	000638-53-9	53
4	n-Decanoic acid	172	C10H20O2	000334-48-5	38
5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	35



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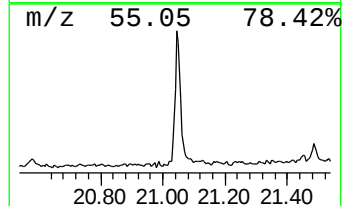
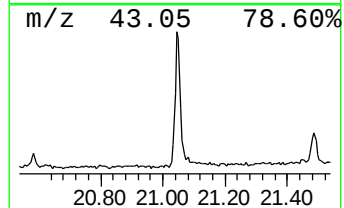
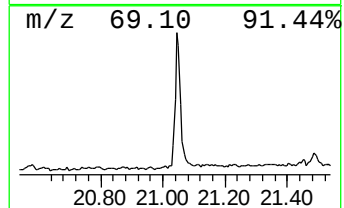
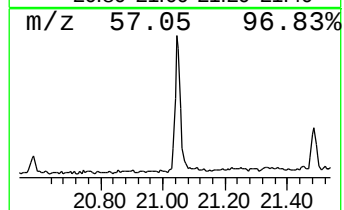
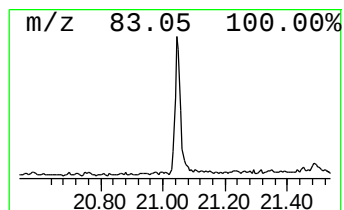
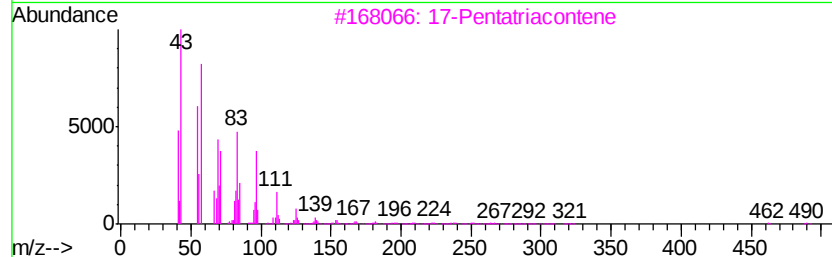
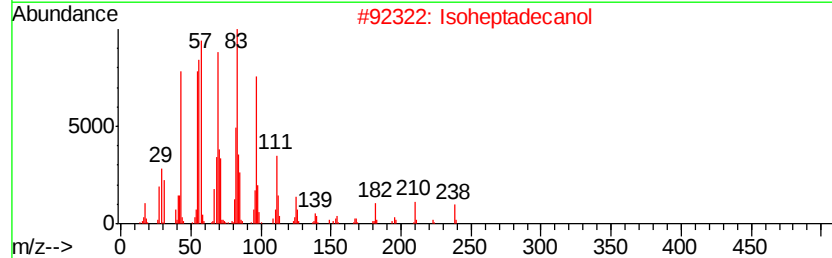
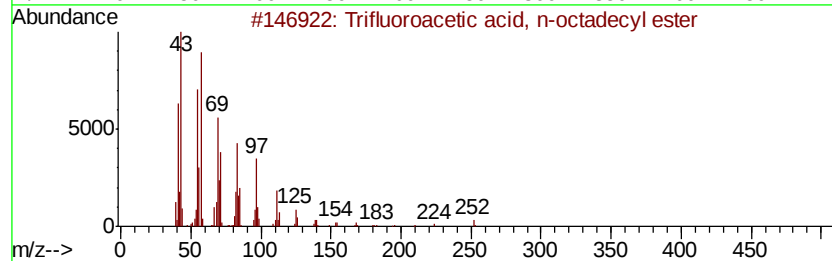
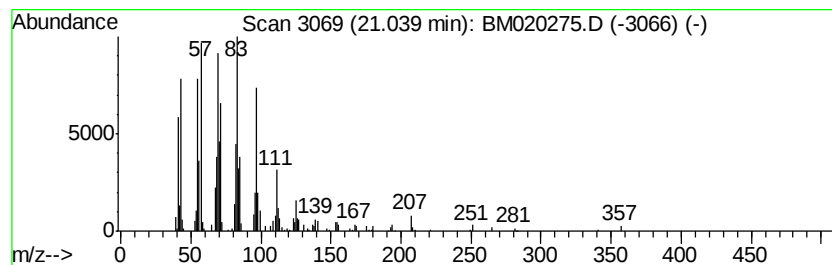
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Peak Number 5 Trifluoroacetic acid, n-oct... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.04	9.51 ng	373718	Chrysene-d12	21.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetic acid, n-octadecv...	366	C20H37F3O2	079392-43-1	91
2		Isoheptadecanol	256	C17H36O	057289-07-3	91
3		17-Pentatriacontene	491	C35H70	006971-40-0	91
4		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	87



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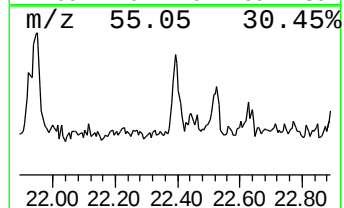
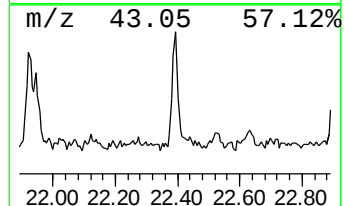
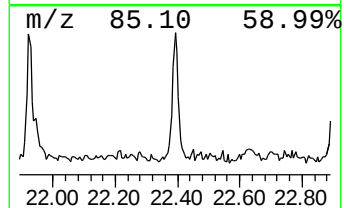
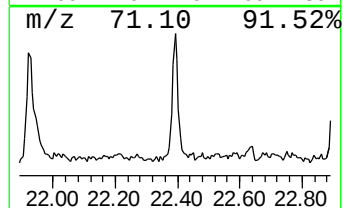
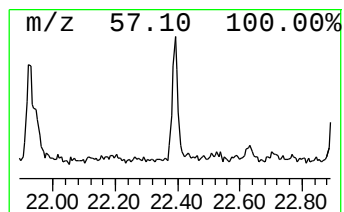
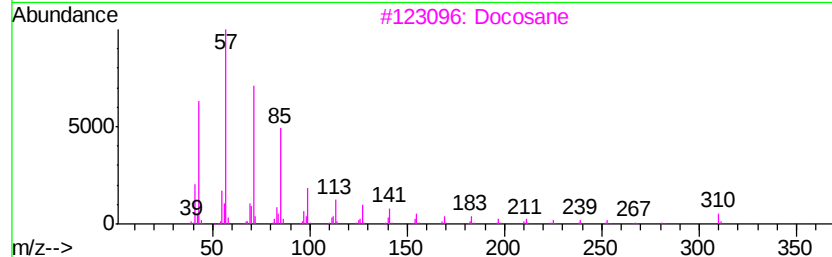
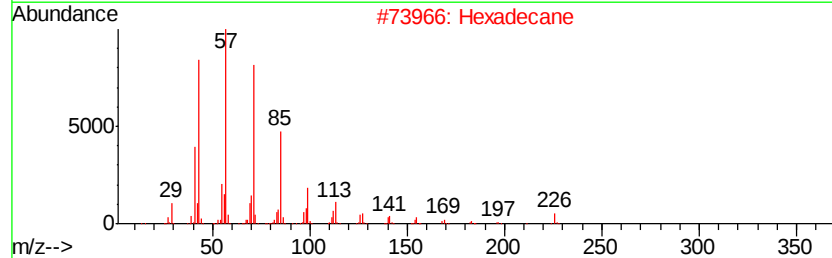
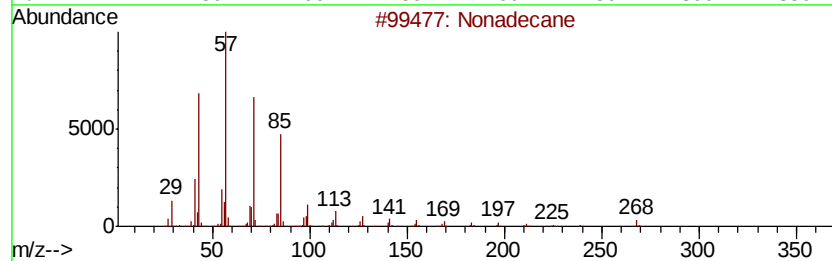
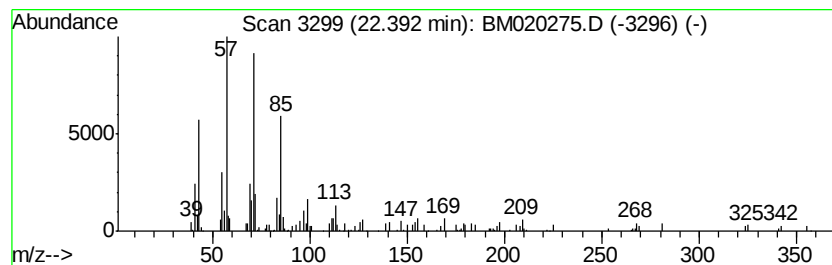
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Peak Number 6 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
22.39	2.68 ng	105352	Chrysene-d12		21.35
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Hexadecane	226	C16H34	000544-76-3	80
3	Docosane	310	C22H46	000629-97-0	80
4	Triacontane	422	C30H62	000638-68-6	80
5	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	80



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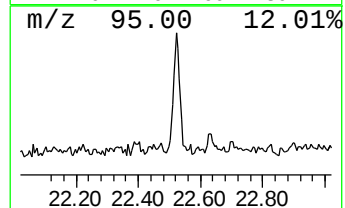
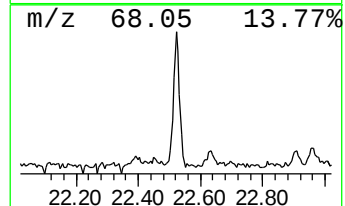
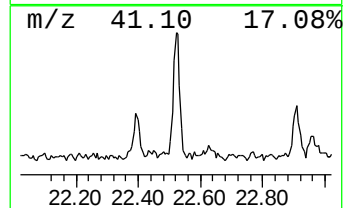
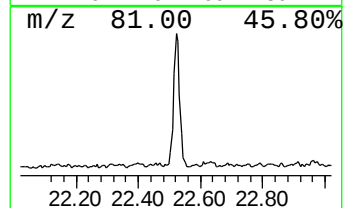
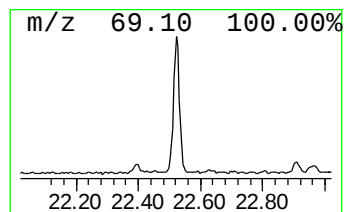
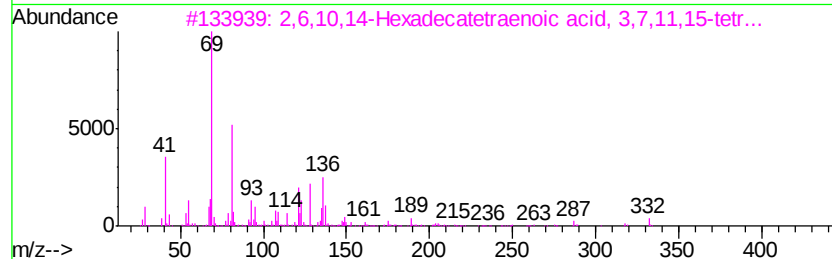
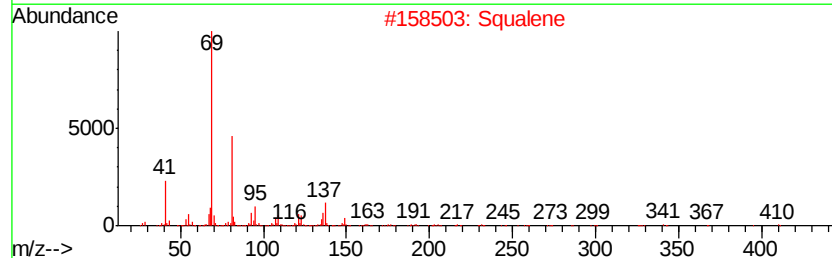
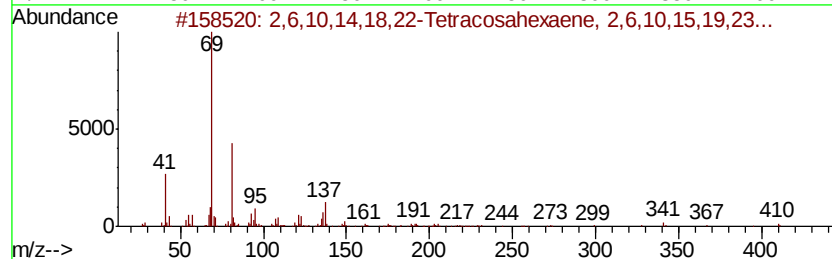
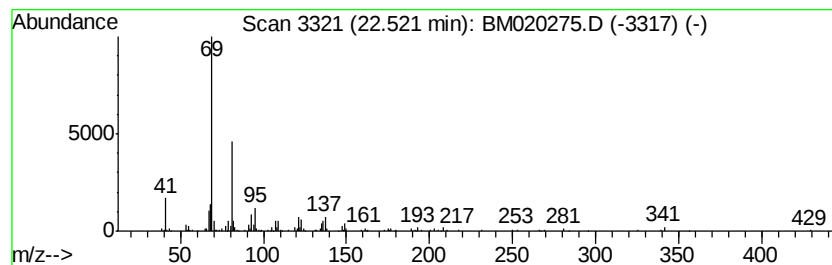
Instrument :
BNA_M
ClientSampleId :
P026-SS003-0612-01

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

Peak Number 7 2,6,10,14,18,22-Tetracosahexaene... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.52	6.20 ng	251403	Perylene-d12	23.64	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	83
2	Squalene	410	C30H50	007683-64-9	72
3	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
4	Propanoic acid, 2,2-dimethyl-, [...	306	C20H34O2	1000164-38-8	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051119\
Data File : BM020275.D
Acq On : 11 May 2019 16:43
Operator : JU/SJ
Sample : K2765-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

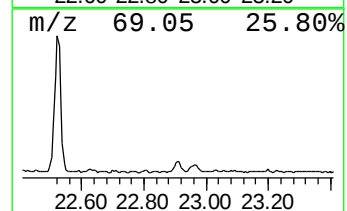
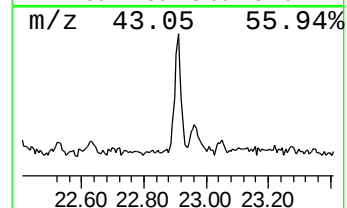
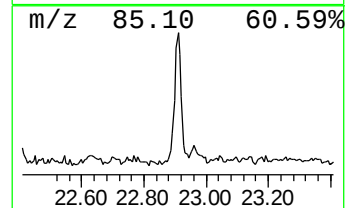
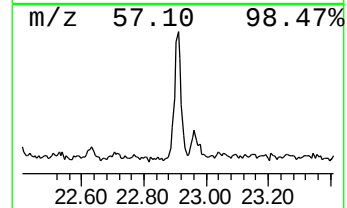
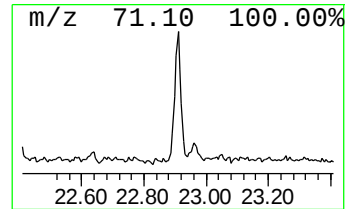
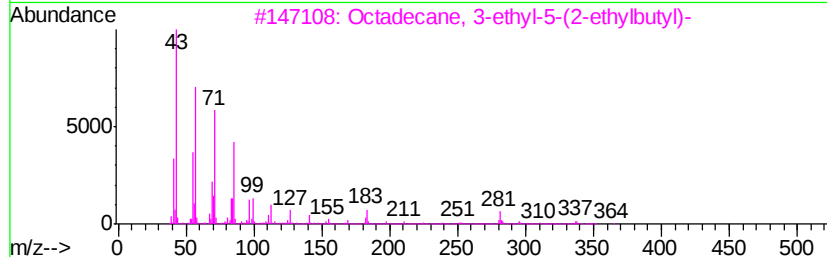
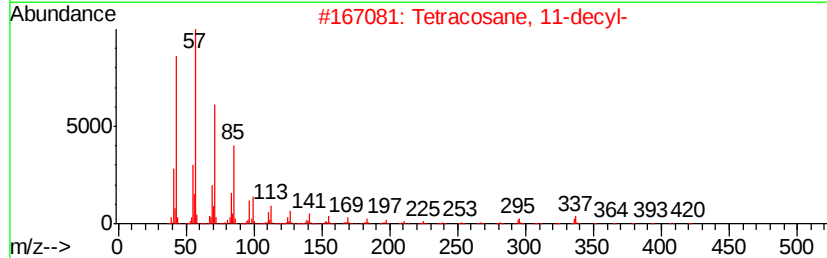
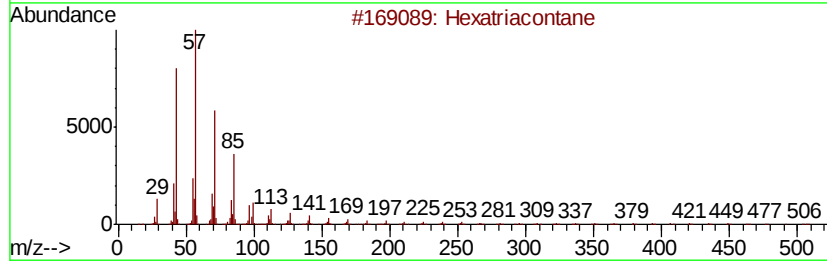
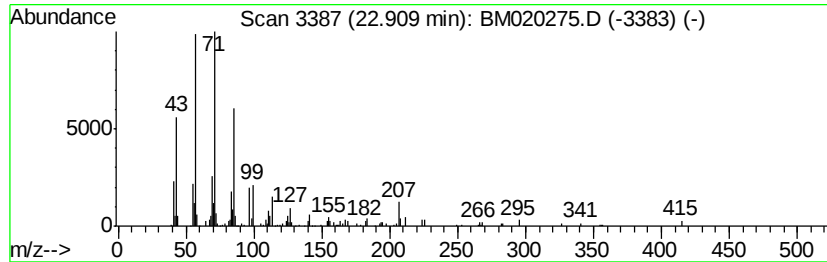
Instrument :
BNA_M
ClientSampleId :
P026-SS003-0612-01

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

Peak Number 8 Hexatriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.91	3.05 ng	123764	Perylene-d12	23.64	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontane	507	C36H74	000630-06-8	80
2	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	80
3	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	80
4	Tetratetracontane	619	C44H90	007098-22-8	80
5	Heneicosane	296	C21H44	000629-94-7	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM051119\
Data File : BM020275.D
Acq On : 11 May 2019 16:43
Operator : JU/SJ
Sample : K2765-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P026-SS003-0612-01

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	112.3	ng	1764160	1	7.76	314334	20.0
Pentadecanoic acid	18.04	9.5	ng	289257	4	17.16	610456	20.0
Tetradecanoic acid	19.33	2.1	ng	84608	5	21.35	786002	20.0
Trifluoroacetic a...	21.04	9.5	ng	373718	5	21.35	786002	20.0
Nonadecane	22.39	2.7	ng	105352	5	21.35	786002	20.0
2,6,10,14,18,22-T...	22.52	6.2	ng	251403	6	23.64	811616	20.0
Hexatriacontane	22.91	3.0	ng	123764	6	23.64	811616	20.0