

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM030119\
 Data File : BM018996.D
 Acq On : 01 Mar 2019 20:44
 Operator : JU/SJ
 Sample : K1665-05
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 200053

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-BM021119.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	5.281	366	373	389	rBV	6230412	9171846	64.96%	8.725%
2	6.863	634	642	663	rBV	6468951	10368006	73.43%	9.863%
3	7.216	695	702	716	rBV	6513486	10453007	74.03%	9.944%
4	7.681	774	781	789	rBV	1093002	1687053	11.95%	1.605%
5	7.998	826	835	848	rBV	4491314	6940885	49.16%	6.603%
6	8.851	972	980	997	rBV	3747318	6109778	43.27%	5.812%
7	10.469	1247	1255	1269	rBV	1338421	2326230	16.48%	2.213%
8	12.951	1669	1677	1690	rBV	8386303	12326826	87.31%	11.727%
9	13.798	1815	1821	1831	rBV	511606	760415	5.39%	0.723%
10	14.333	1901	1912	1919	rBV2	2022189	3039708	21.53%	2.892%
11	14.398	1919	1923	1931	rVB	137455	209617	1.48%	0.199%
12	14.739	1973	1981	1990	rBV	94197	166935	1.18%	0.159%
13	15.386	2086	2091	2101	rVB	151228	237130	1.68%	0.226%
14	15.833	2160	2167	2186	rBV	7239450	10393406	73.61%	9.887%
15	17.086	2374	2380	2384	rBV2	2340269	3305382	23.41%	3.144%
16	17.127	2384	2387	2396	rVV	624321	888525	6.29%	0.845%
17	17.974	2525	2531	2535	rBV2	497867	710649	5.03%	0.676%
18	18.157	2557	2562	2566	rBV2	85369	142400	1.01%	0.135%
19	19.151	2723	2731	2739	rBV	660545	911044	6.45%	0.867%
20	19.262	2745	2750	2759	rBV	151794	243234	1.72%	0.231%
21	19.515	2789	2793	2802	rVB	523266	752726	5.33%	0.716%
22	19.721	2822	2828	2834	rBV	11608870	14119248	100.00%	13.432%
23	20.015	2869	2878	2882	rVB2	101338	202400	1.43%	0.193%
24	20.980	3038	3042	3052	rBV3	522493	715263	5.07%	0.680%
25	21.280	3087	3093	3097	rBV	2462927	3255418	23.06%	3.097%
26	21.315	3097	3099	3108	rVB	265386	321953	2.28%	0.306%
27	21.415	3113	3116	3123	rBV2	177675	242726	1.72%	0.231%
28	21.850	3187	3190	3194	rVB	238592	252195	1.79%	0.240%
29	22.309	3265	3268	3274	rVB	353148	441371	3.13%	0.420%
30	22.815	3350	3354	3358	rBV	468292	673437	4.77%	0.641%
31	23.380	3446	3450	3455	rBV	260825	367234	2.60%	0.349%
32	23.527	3469	3475	3488	rVB2	1507906	2856841	20.23%	2.718%
33	24.027	3556	3560	3568	rVB	299809	524454	3.71%	0.499%

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ALS Vial : 13 Sample Multiplier: 1

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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-BM021119.M
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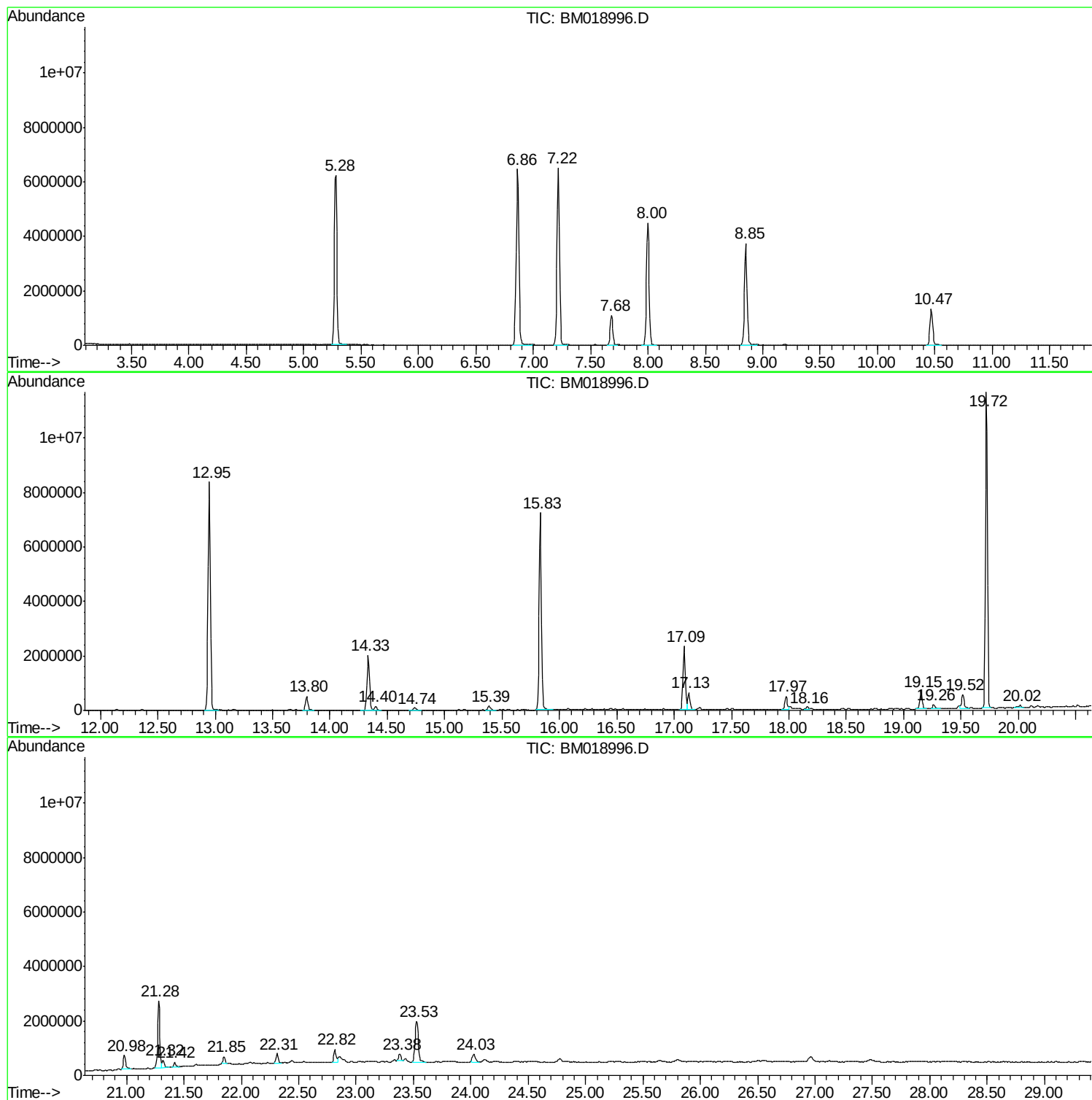
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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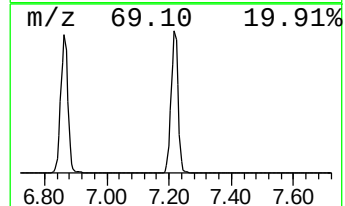
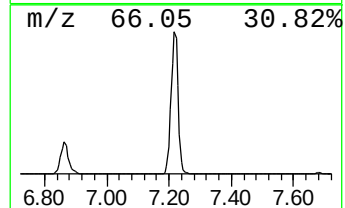
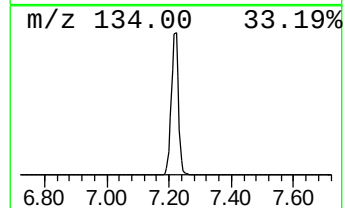
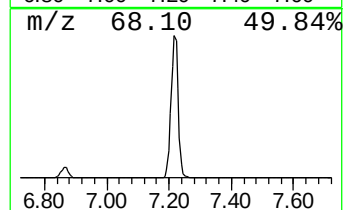
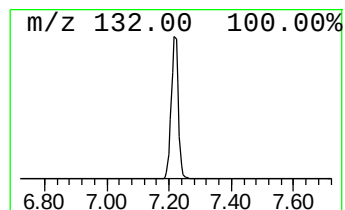
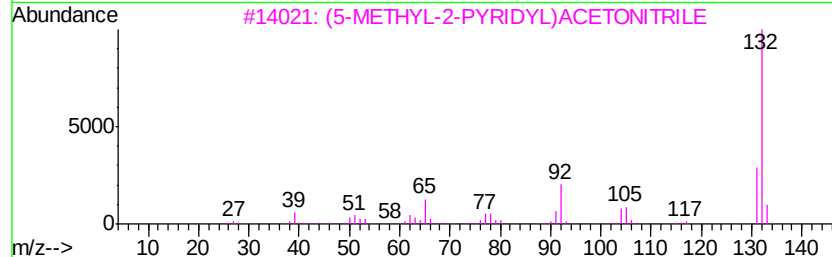
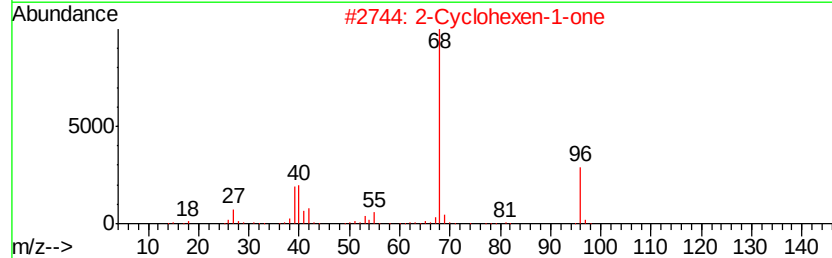
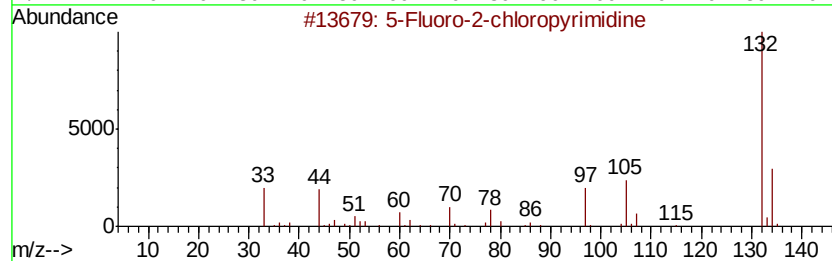
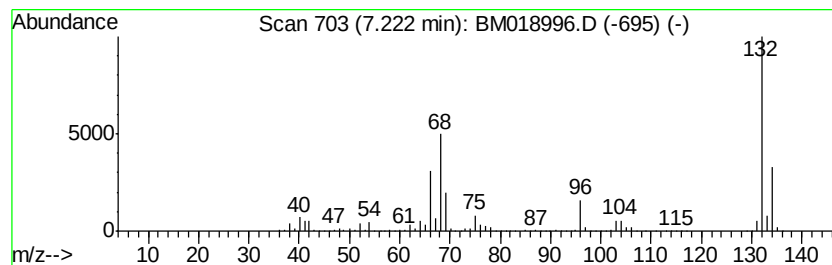
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.22 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	123.92 ng	10453000	1,4-Dichlorobenzene-d4	7.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
3		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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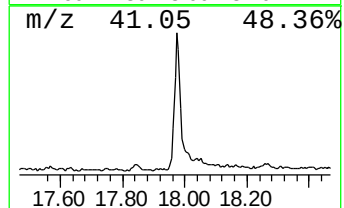
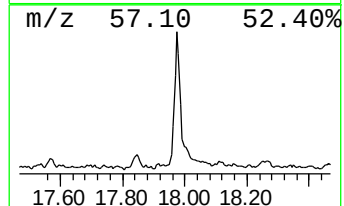
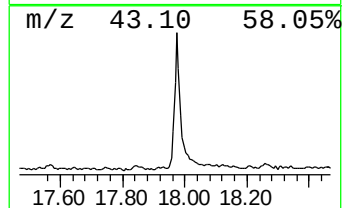
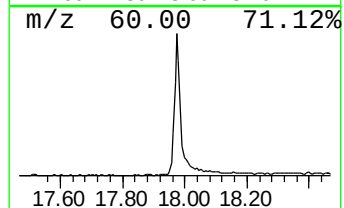
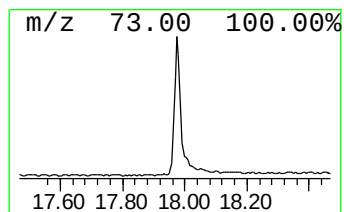
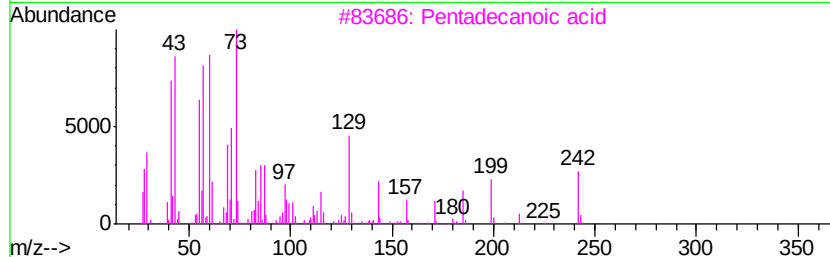
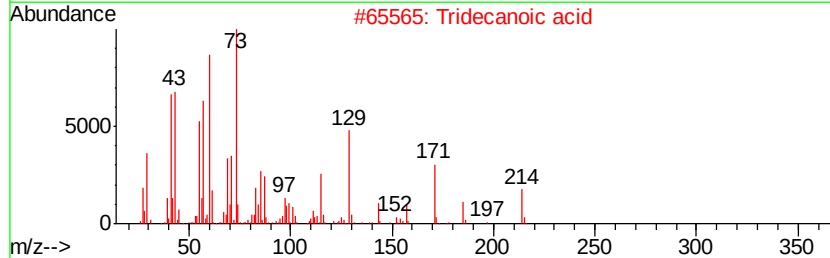
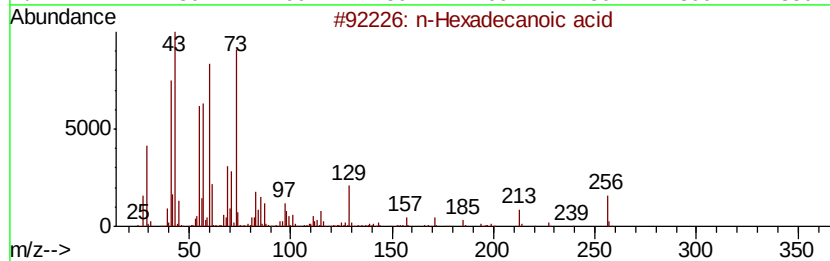
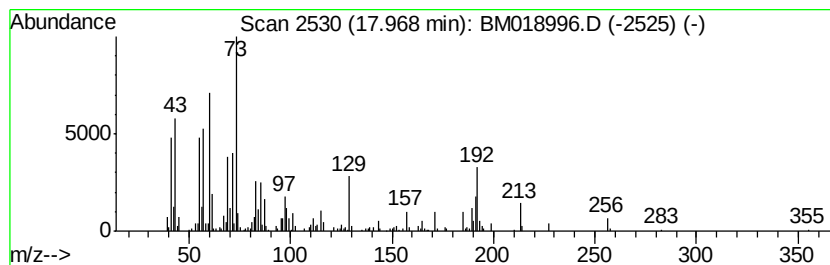
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.97	4.30 ng	710649	Phenanthrene-d10	17.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4		n-Decanoic acid	172	C10H20O2	000334-48-5	59
5		Undecanoic acid	186	C11H22O2	000112-37-8	38



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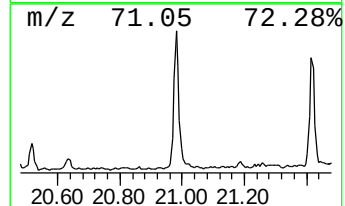
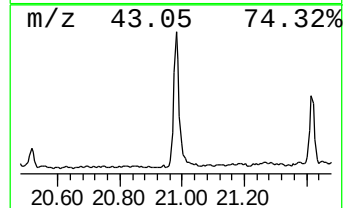
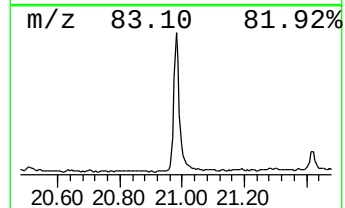
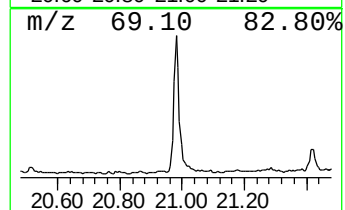
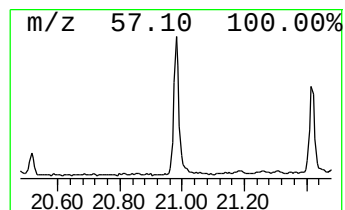
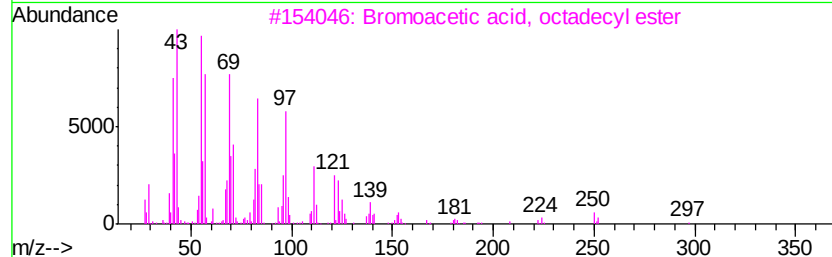
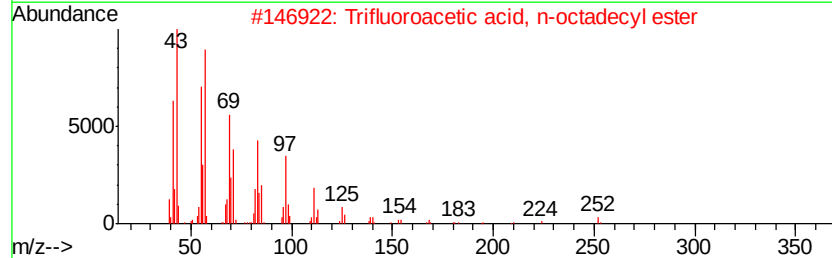
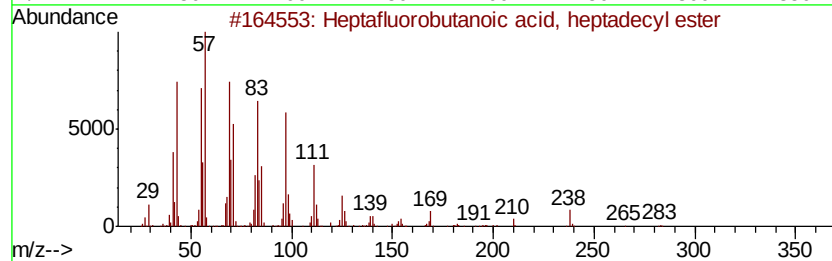
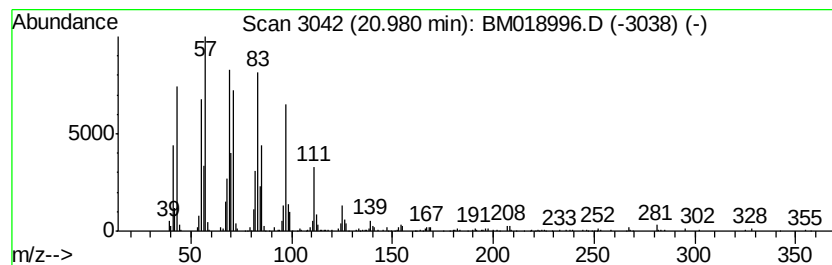
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptafluorobutanoic acid, h... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
20.98	4.39 ng	715263	Chrysene-d12	21.28		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
2		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
3		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	80



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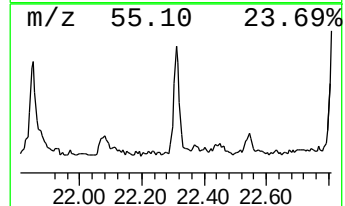
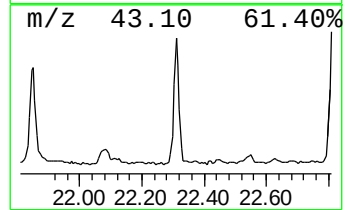
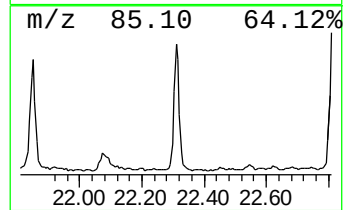
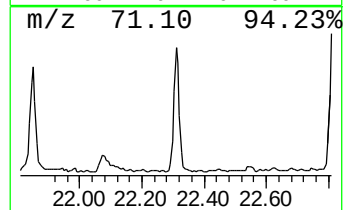
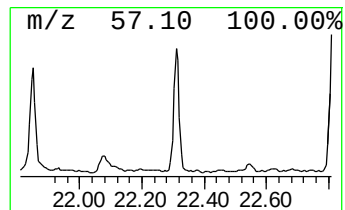
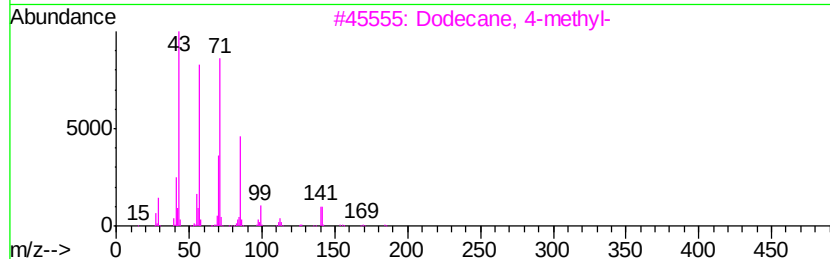
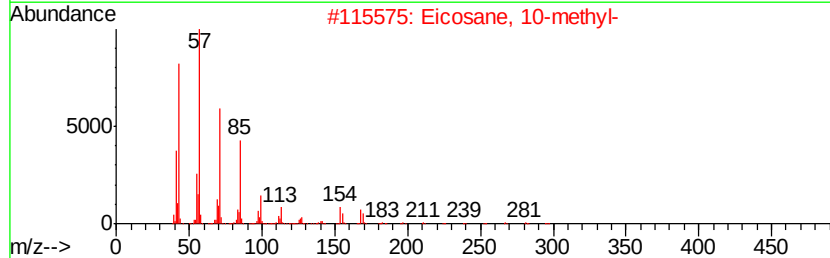
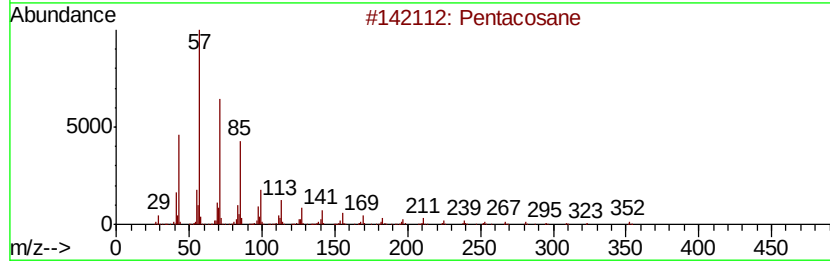
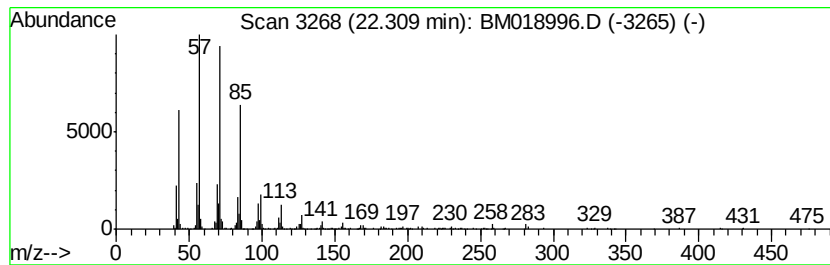
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.31	2.71 ng	441371	Chrysene-d12	21.28
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentacosane	352 C25H52	000629-99-2	90
2	Eicosane, 10-methyl-	296 C21H44	054833-23-7	90
3	Dodecane, 4-methyl-	184 C13H28	006117-97-1	83
4	Heptacosane	380 C27H56	000593-49-7	81
5	Heptadecane, 2,6,10,15-tetramethyl-	296 C21H44	054833-48-6	72



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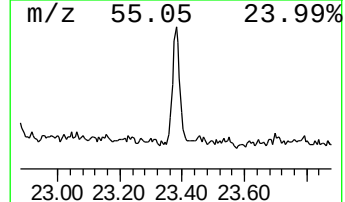
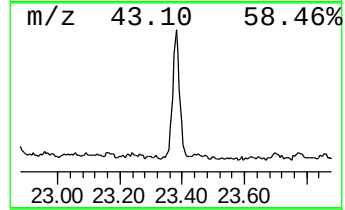
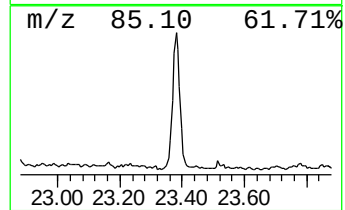
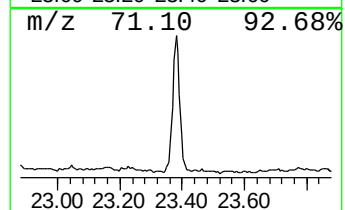
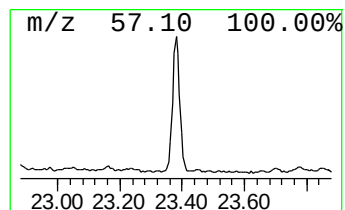
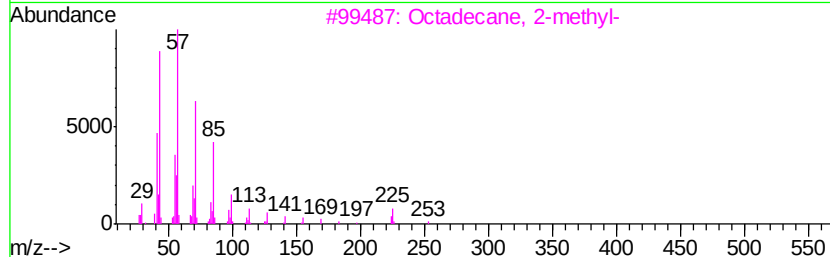
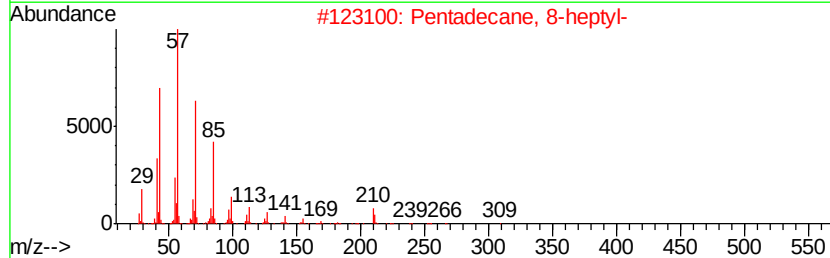
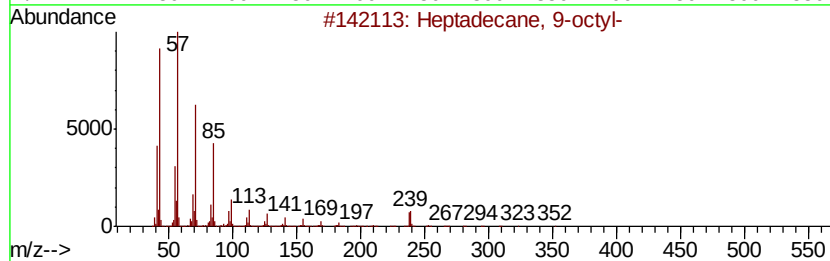
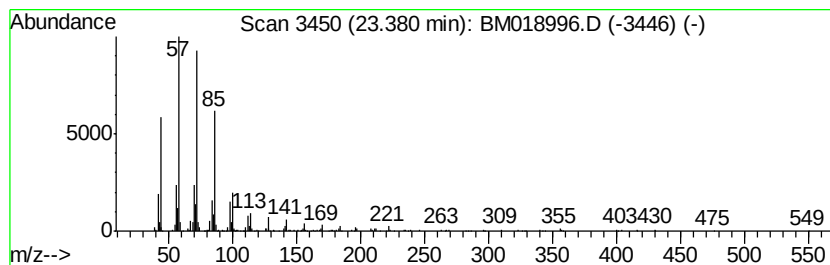
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.38	2.57 ng	367234	Perylene-d12	23.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
3		Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
4		Heneicosane	296	C21H44	000629-94-7	87
5		Hexadecane	226	C16H34	000544-76-3	86



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ClientSampleId :
200053

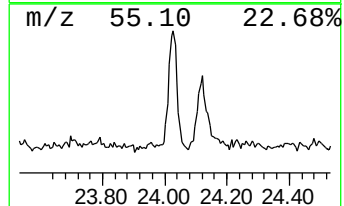
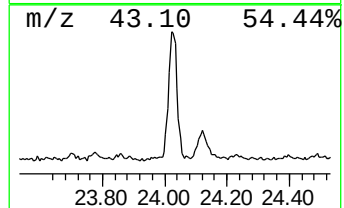
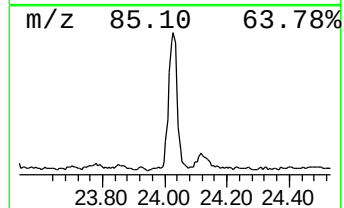
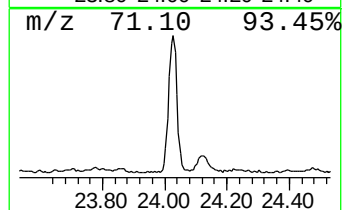
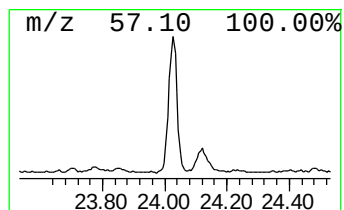
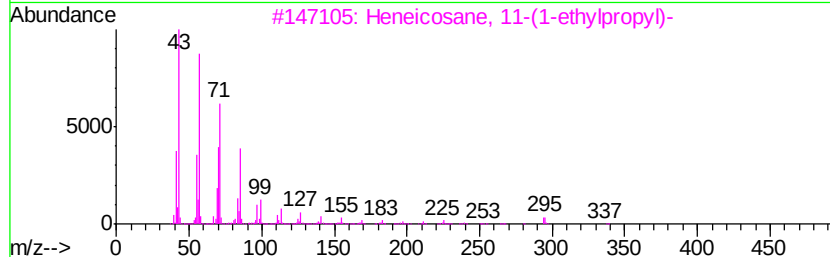
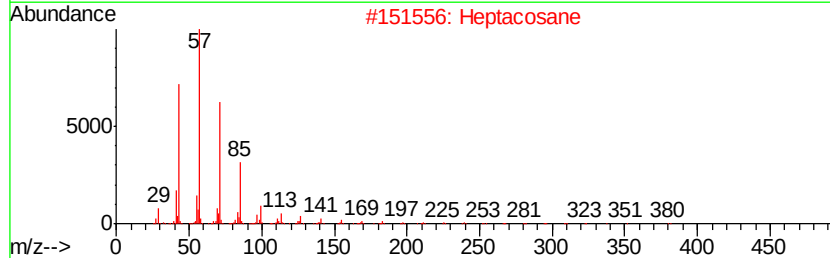
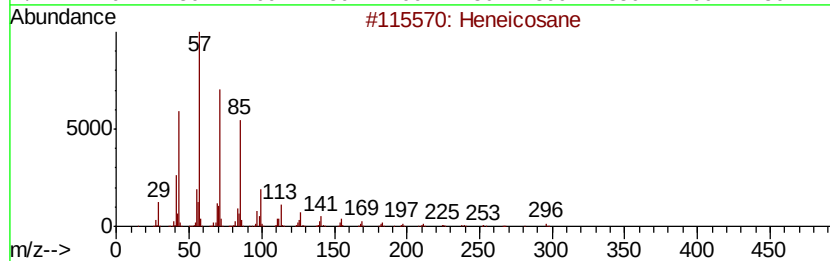
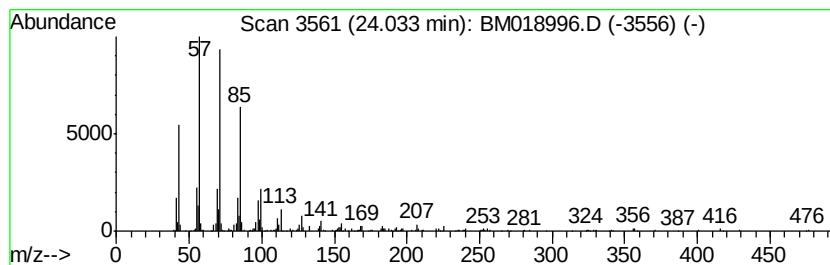
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.03	3.67 ng	524454	Perylene-d12	23.53

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Heptacosane		380	C27H56	000593-49-7	87
3	Heneicosane, 11-(1-ethylpropyl)-		366	C26H54	055282-11-6	83
4	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	80
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM030119\
Data File : BM018996.D
Acq On : 01 Mar 2019 20:44
Operator : JU/SJ
Sample : K1665-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
200053

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.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
unknown7.22	7.22	123.9	ng	10453000	1	7.68	1687050	20.0
n-Hexadecanoic acid	17.97	4.3	ng	710649	4	17.09	3305380	20.0
Heptafluorobutano...	20.98	4.4	ng	715263	5	21.28	3255420	20.0
Pentacosane	22.31	2.7	ng	441371	5	21.28	3255420	20.0
Heptadecane, 9-oc...	23.38	2.6	ng	367234	6	23.53	2856840	20.0
Heneicosane	24.03	3.7	ng	524454	6	23.53	2856840	20.0