

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM042319\
 Data File : BM020045.D
 Acq On : 23 Apr 2019 20:19
 Operator : JU/SJ
 Sample : K2516-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P041919

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-BM041519.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	5.110	356	361	381	rBV	556408	1086130	19.25%	3.539%
2	6.698	624	631	652	rBV	315151	718503	12.74%	2.341%
3	7.028	681	687	696	rBV2	1331669	2514459	44.57%	8.193%
4	7.098	696	699	719	rVB	130740	279769	4.96%	0.912%
5	7.304	728	734	754	rBV3	162935	353299	6.26%	1.151%
6	7.492	760	766	774	rBV	356921	568419	10.08%	1.852%
7	7.804	811	819	832	rBV	1249493	2059627	36.51%	6.711%
8	8.669	959	966	989	rBV	736204	1558190	27.62%	5.077%
9	10.269	1224	1238	1252	rBV	344211	729575	12.93%	2.377%
10	12.016	1530	1535	1546	rBV4	20602	70261	1.25%	0.229%
11	12.763	1655	1662	1686	rBV	2245811	3599093	63.80%	11.727%
12	13.645	1804	1812	1819	rBV	103358	179577	3.18%	0.585%
13	14.068	1876	1884	1891	rBV3	53862	100543	1.78%	0.328%
14	14.163	1891	1900	1909	rVV2	583882	949443	16.83%	3.093%
15	14.551	1960	1966	1974	rBV8	34604	60052	1.06%	0.196%
16	15.551	2130	2136	2140	rBV	50021	74017	1.31%	0.241%
17	15.674	2150	2157	2173	rBV	1745017	2894841	51.31%	9.432%
18	16.021	2212	2216	2226	rBV2	34064	68208	1.21%	0.222%
19	16.415	2276	2283	2289	rBV2	77982	118972	2.11%	0.388%
20	16.486	2289	2295	2303	rVB5	51775	100744	1.79%	0.328%
21	16.927	2364	2370	2380	rBV2	684349	1084211	19.22%	3.533%
22	17.821	2516	2522	2531	rBV	388507	666128	11.81%	2.170%
23	17.892	2532	2534	2539	rVB	51353	68846	1.22%	0.224%
24	18.345	2606	2611	2616	rBV2	64926	101895	1.81%	0.332%
25	18.409	2618	2622	2632	rVB2	64096	93281	1.65%	0.304%
26	18.592	2649	2653	2662	rVB3	42566	70647	1.25%	0.230%
27	19.115	2737	2742	2752	rBV	280145	488266	8.65%	1.591%
28	19.574	2814	2820	2835	rVB	4731759	5641592	100.00%	18.382%
29	20.844	3031	3036	3044	rBV	345618	554958	9.84%	1.808%
30	21.150	3083	3088	3098	rBV	887444	1377275	24.41%	4.487%
31	21.692	3177	3180	3183	rVB	109127	109019	1.93%	0.355%
32	22.133	3252	3255	3258	rBV	125419	162135	2.87%	0.528%
33	22.262	3273	3277	3284	rVB3	80588	123648	2.19%	0.403%
34	22.615	3333	3337	3341	rVB	148507	196513	3.48%	0.640%

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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

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35	23.150	3424	3428	3435	rVB	143494	215279	3.82%	0.701%
36	23.327	3452	3458	3471	rBV	693352	1452930	25.75%	4.734%
37	23.762	3528	3532	3540	rVB2	116599	201279	3.57%	0.656%

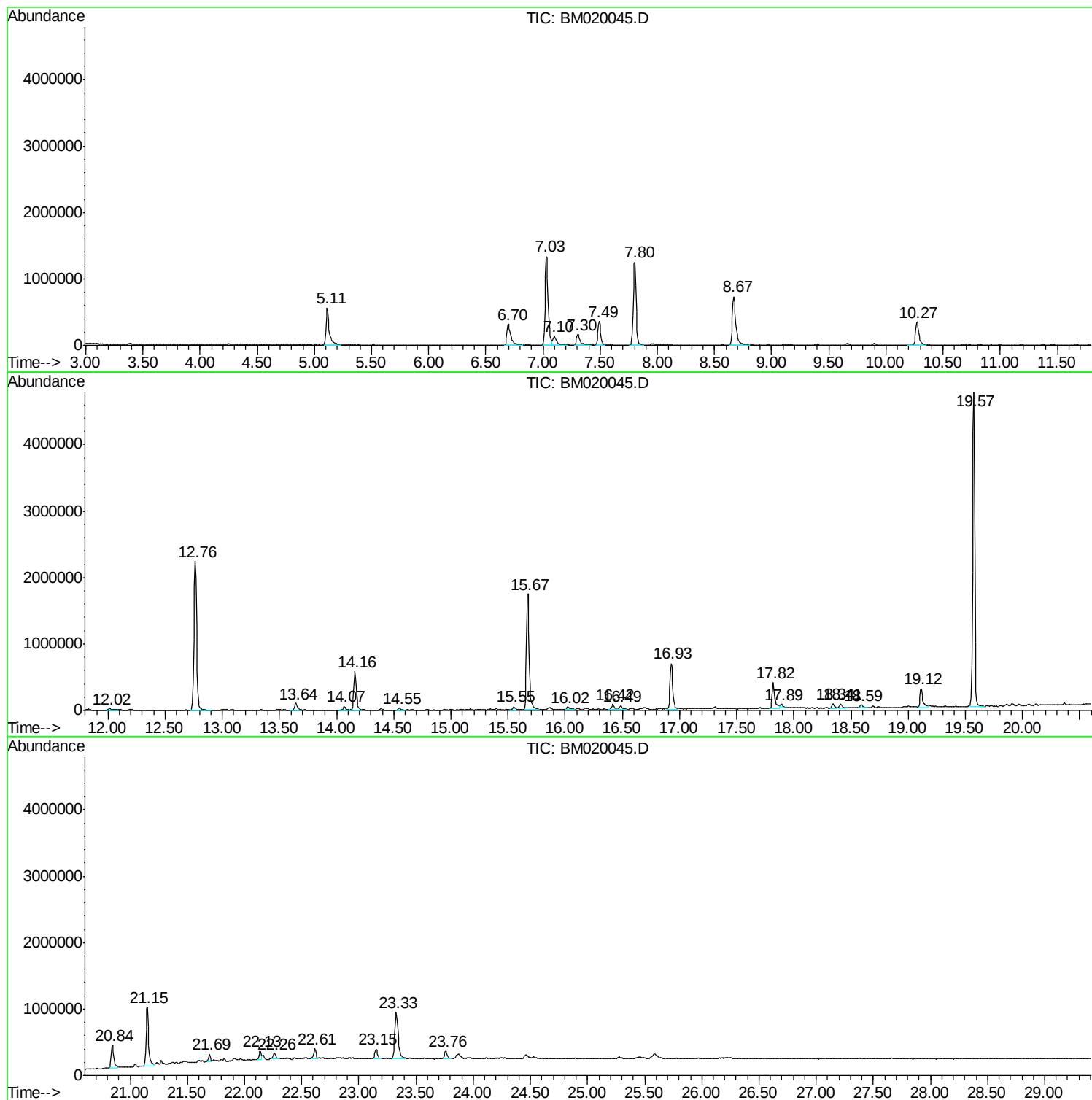
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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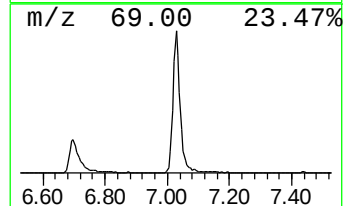
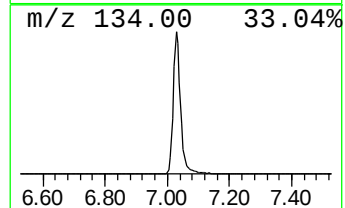
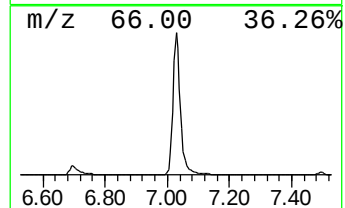
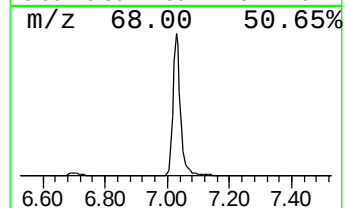
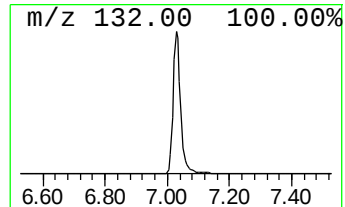
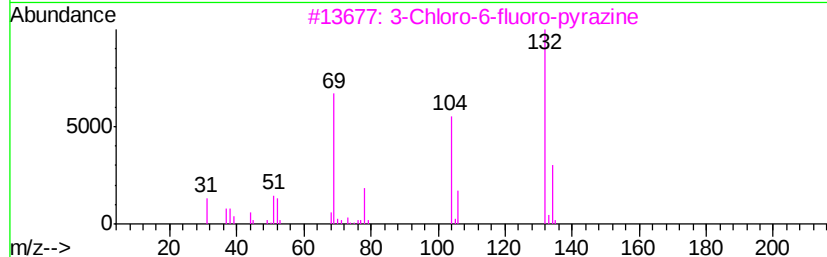
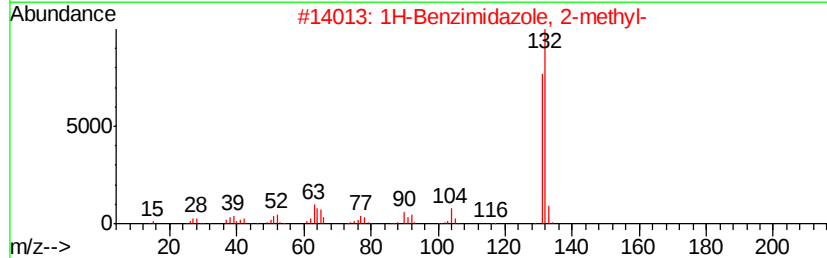
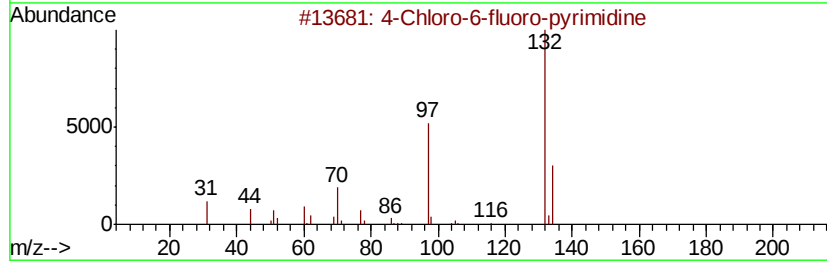
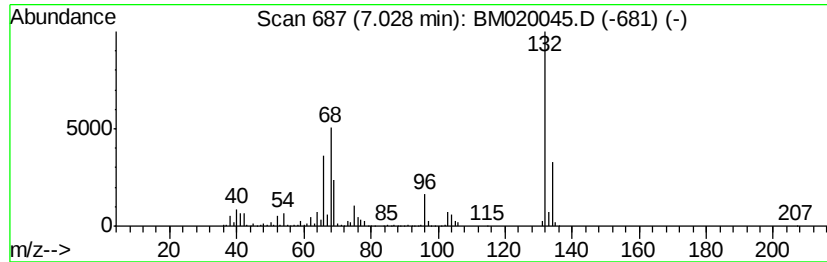
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.03 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	88.47 ng	2514460	1,4-Dichlorobenzene-d4	7.49

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		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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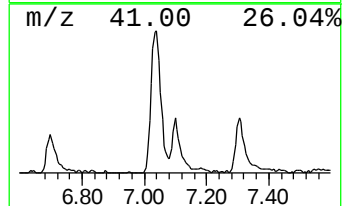
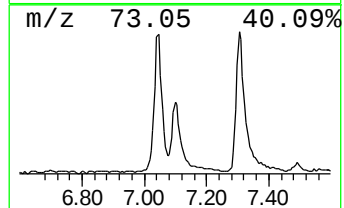
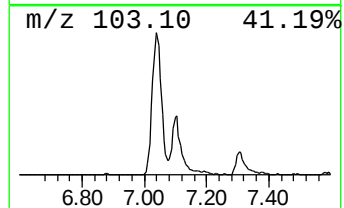
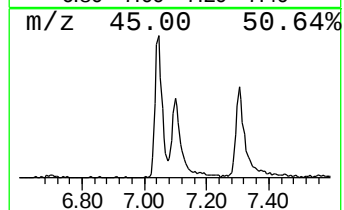
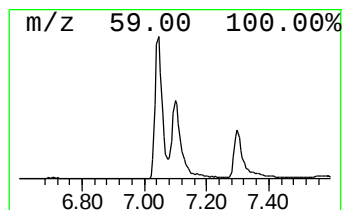
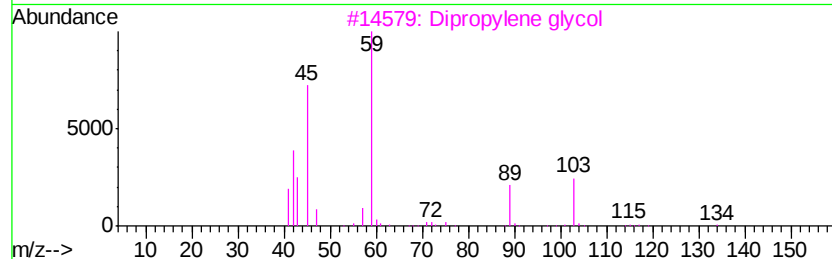
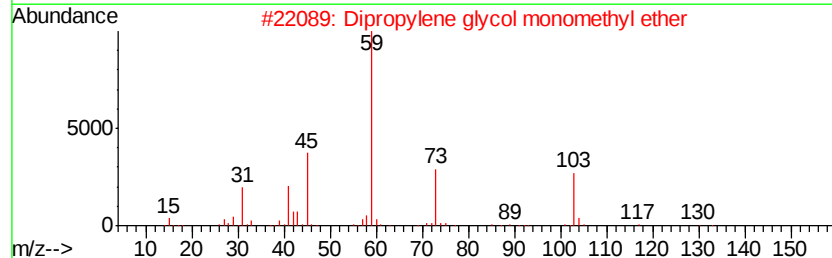
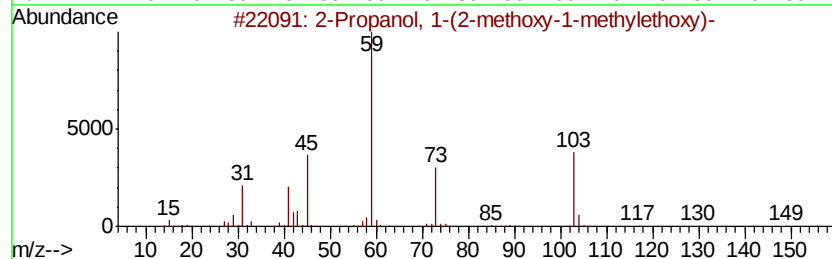
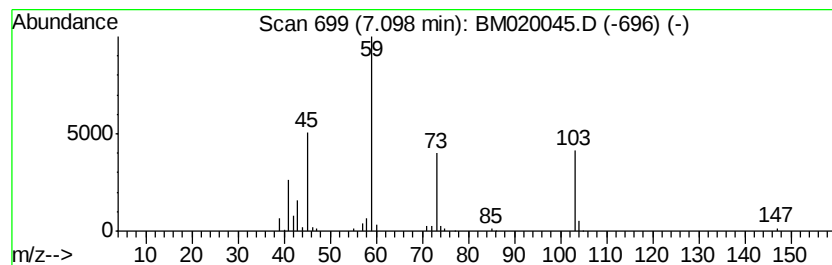
Instrument :
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM041519.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
7.10	9.84 ng	279769	1,4-Dichlorobenzene-d4	7.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methyl-...	148	C7H16O3	020324-32-7	72
2	Dipropylene glycol monomethyl ether	148	C7H16O3	034590-94-8	72
3	Dipropylene glycol	134	C6H14O3	025265-71-8	56
4	2-Butanol, 3,3'-oxybis-	162	C8H18O3	054305-61-2	56
5	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	53



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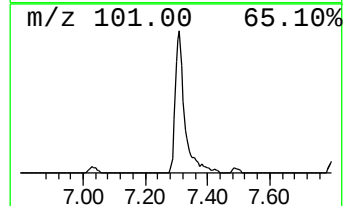
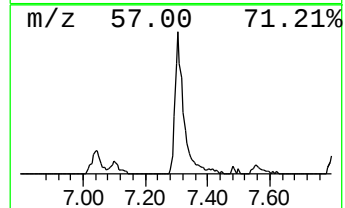
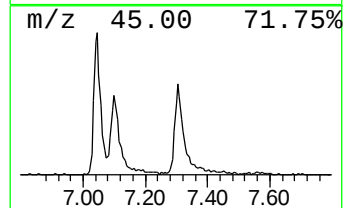
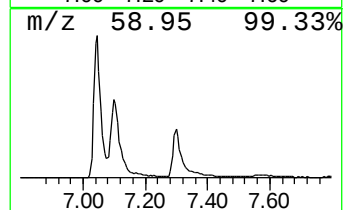
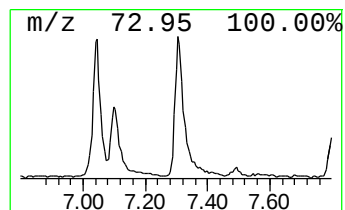
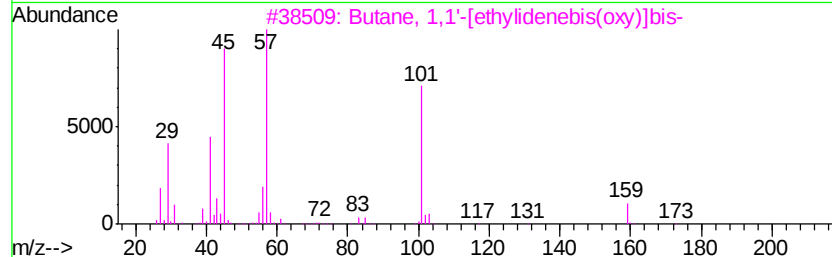
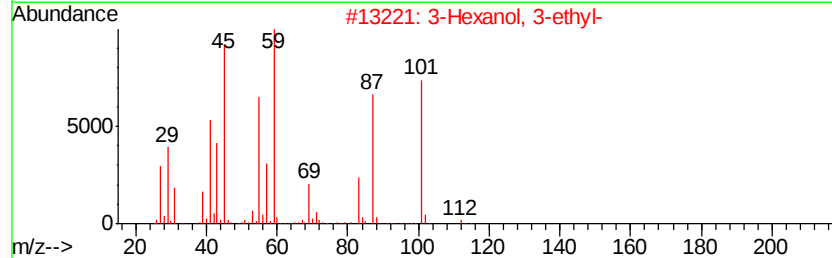
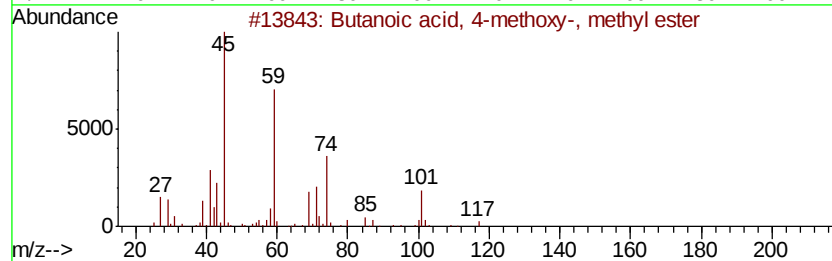
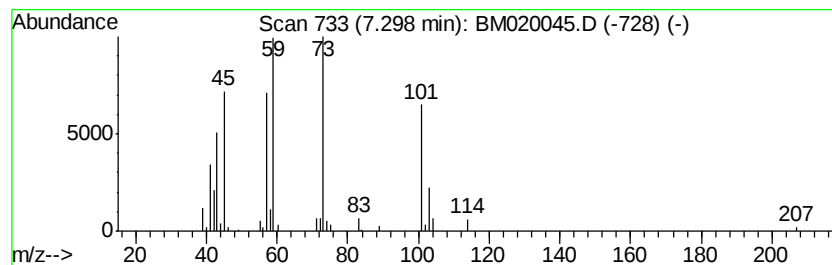
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanoic acid, 4-methoxy-, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.30	12.43 ng	353299	1,4-Dichlorobenzene-d4	7.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	53
2		3-Hexanol, 3-ethyl-	130	C8H18O	000597-76-2	50
3		Butane, 1,1'-[ethylidenebis(oxo)]...	174	C10H22O2	000871-22-7	38
4		1,3-Dioxolane, 2-ethyl-	102	C5H10O2	002568-96-9	35
5		Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	32



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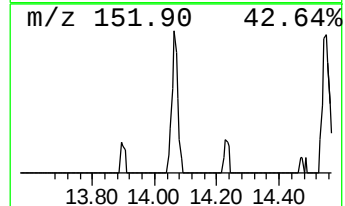
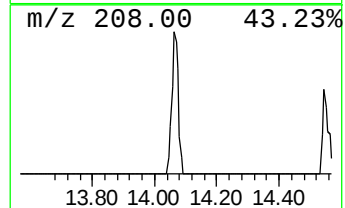
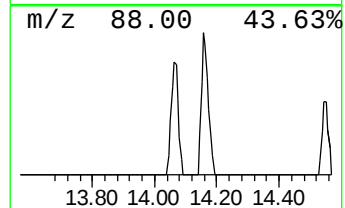
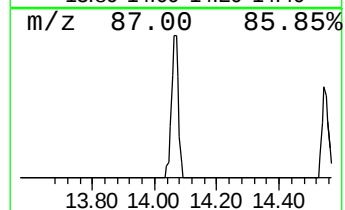
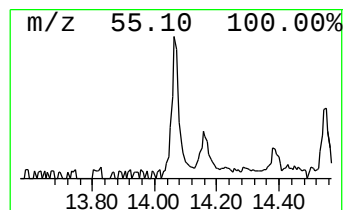
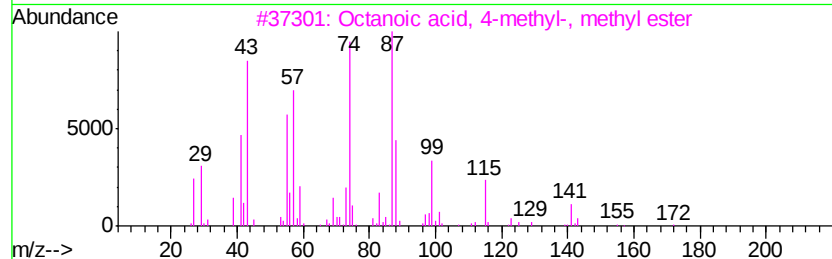
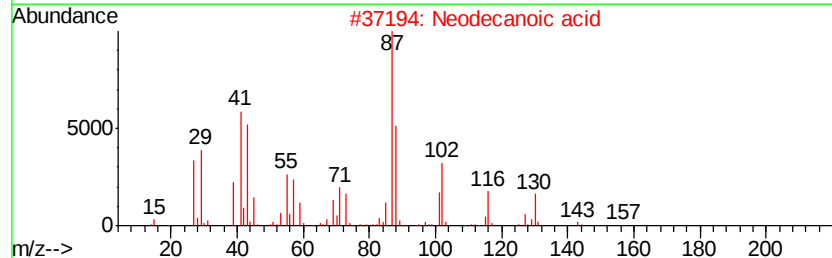
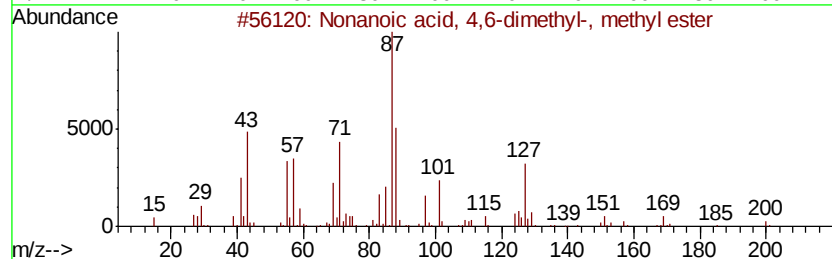
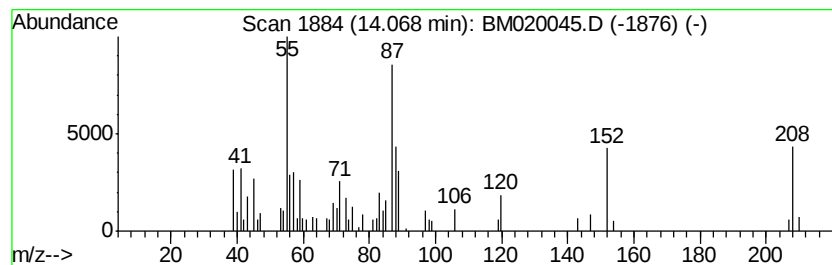
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 unknown14.07 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.07	2.12 ng	100543	Acenaphthene-d10	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanoic acid, 4,6-dimethyl-, me...	200	C12H24O2	055955-66-3	38
2		Neodecanoic acid	172	C10H20O2	026896-20-8	35
3		Octanoic acid, 4-methyl-, methyl...	172	C10H20O2	015870-07-2	32
4		4-Heptanol, 3,4-dimethyl-	144	C9H20O	005406-10-0	22
5		.alpha.-Methyl 4-O-methyl-D-mann...	208	C8H16O6	1000127-87-5	17



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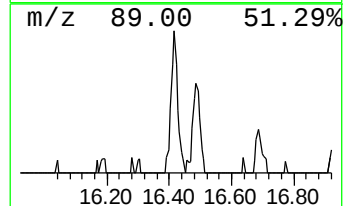
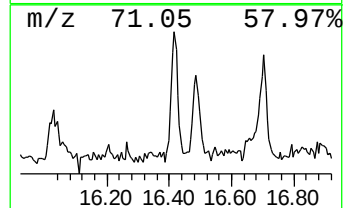
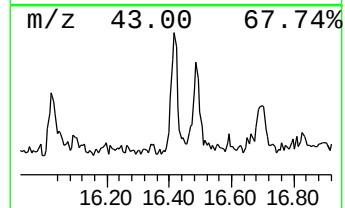
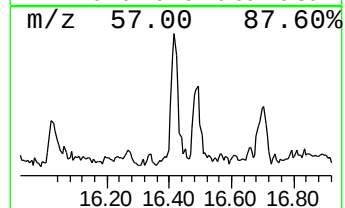
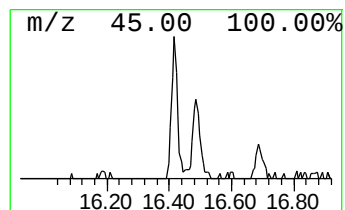
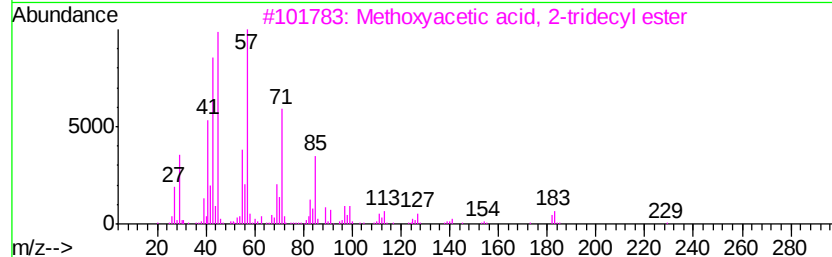
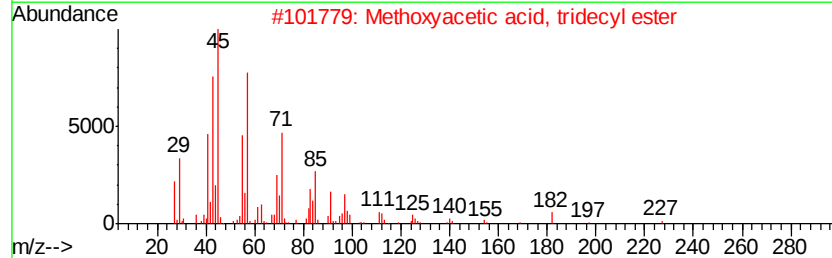
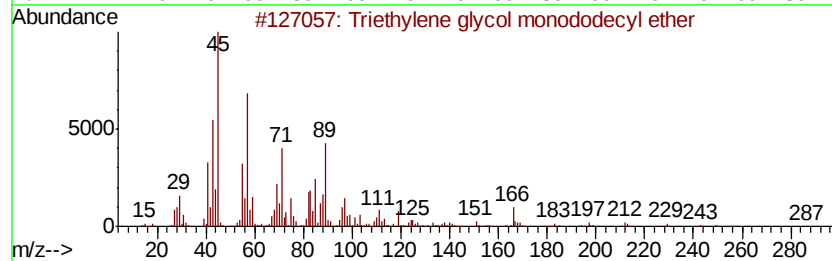
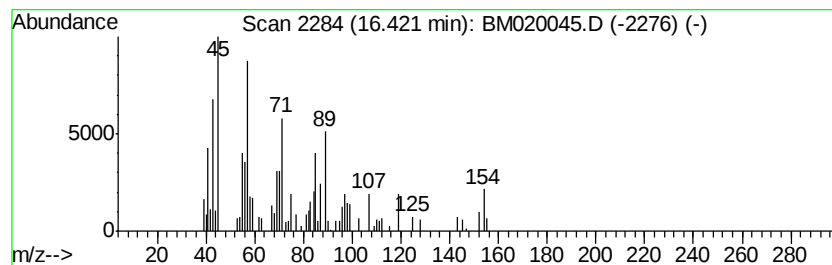
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Triethylene glycol monododecyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.42	2.19 ng	118972	Phenanthrene-d10		16.93	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triethylene glycol monododecyl e...	318	C18H38O4	003055-94-5	83
2		Methoxyacetic acid, tridecyl ester	272	C16H32O3	1000281-82-0	49
3		Methoxyacetic acid, 2-tridecyl e...	272	C16H32O3	1000282-04-5	35
4		Cyclooctane, (methoxymethoxy)-	172	C10H20O2	042604-11-5	27
5		Propanoic acid, 2-methyl-, decyl...	228	C14H28O2	005454-22-8	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM042319\
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Acq On : 23 Apr 2019 20:19
Operator : JU/SJ
Sample : K2516-01
Misc :
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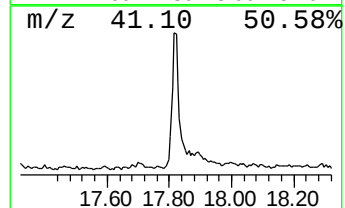
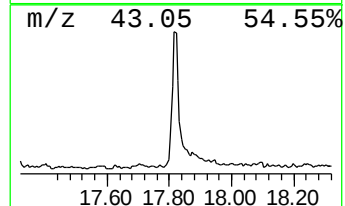
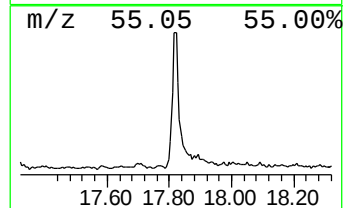
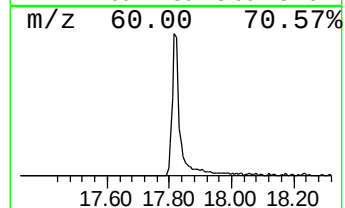
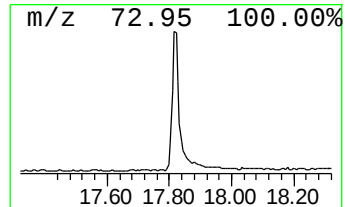
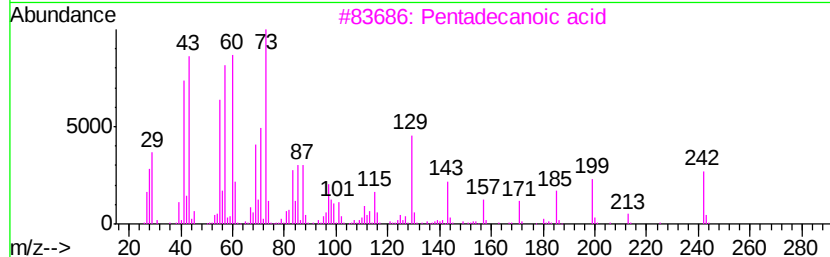
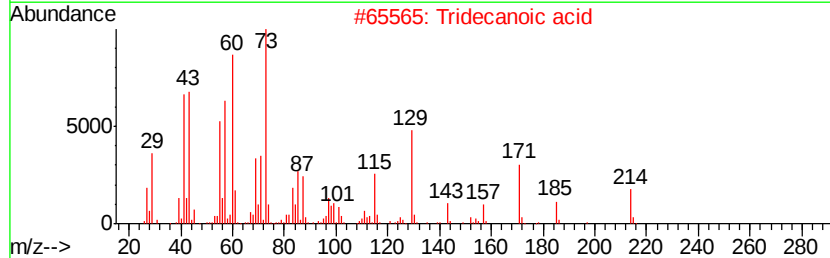
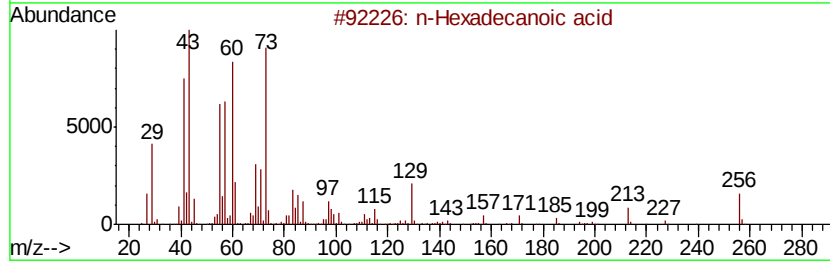
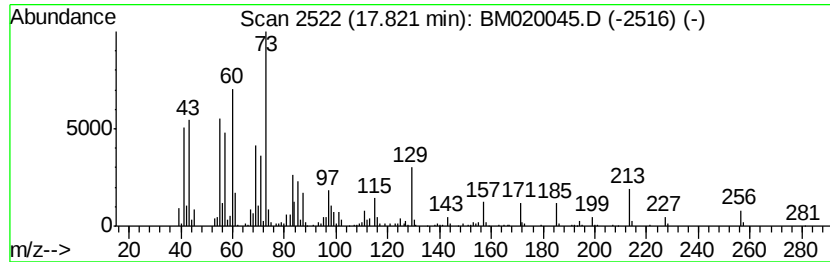
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.82	12.29 ng	666128	Phenanthrene-d10	16.93		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	97
2	Tridecanoic acid		214	C13H26O2	000638-53-9	92
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	53
5	n-Decanoic acid		172	C10H20O2	000334-48-5	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM042319\
Data File : BM020045.D
Acq On : 23 Apr 2019 20:19
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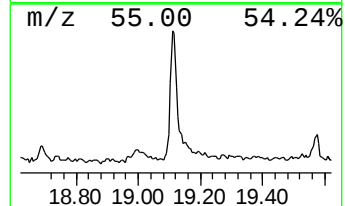
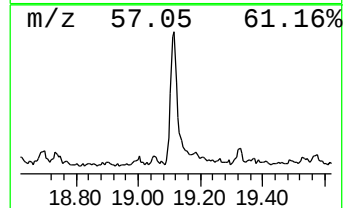
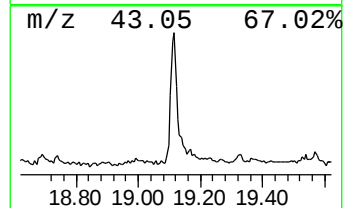
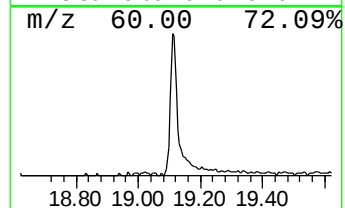
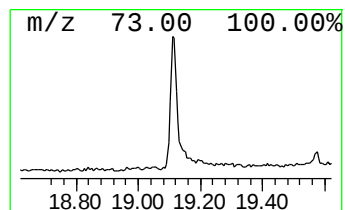
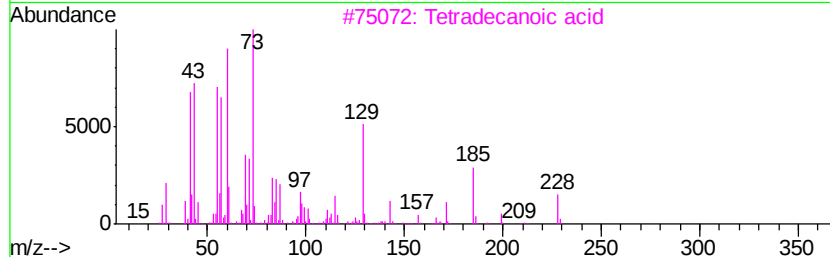
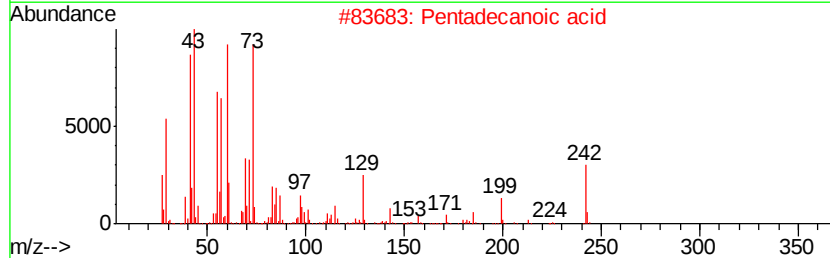
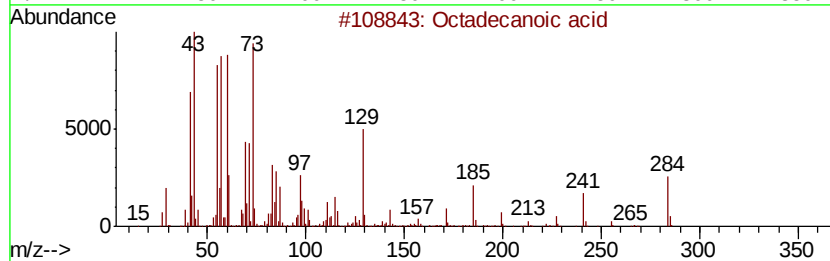
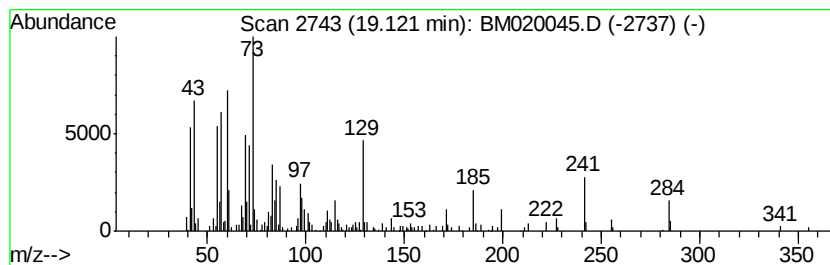
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.12	7.09 ng	488266	Chrysene-d12	21.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
5		n-Decanoic acid	172	C10H20O2	000334-48-5	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM042319\
Data File : BM020045.D
Acq On : 23 Apr 2019 20:19
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Sample : K2516-01
Misc :
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ClientSampleId :
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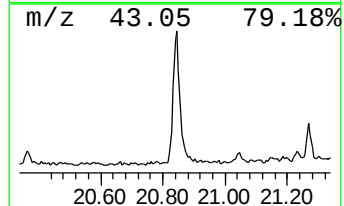
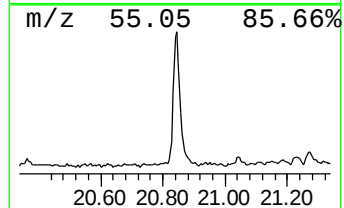
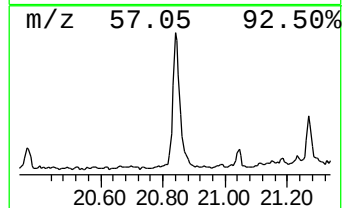
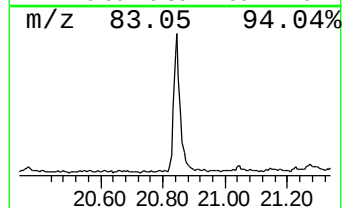
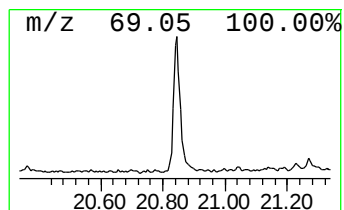
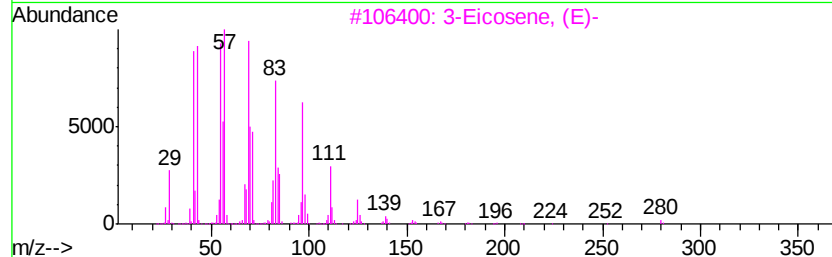
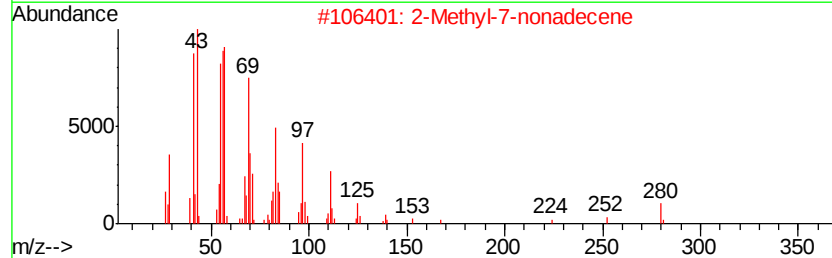
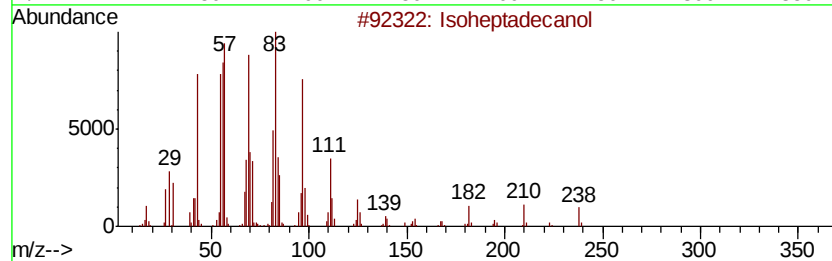
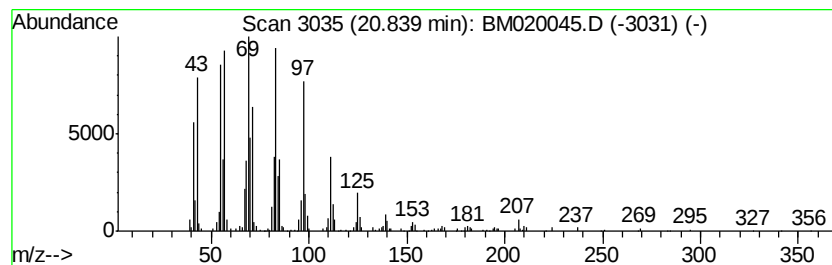
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Isoheptadecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.84	8.06 ng	554958	Chrysene-d12	21.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isoheptadecanol	256	C17H36O	057289-07-3	91
2		2-Methyl-7-nonadecene	280	C20H40	219750-68-2	90
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	90
4		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	90
5		Cyclotetracosane	336	C24H48	000297-03-0	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM042319\
Data File : BM020045.D
Acq On : 23 Apr 2019 20:19
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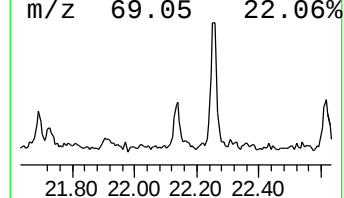
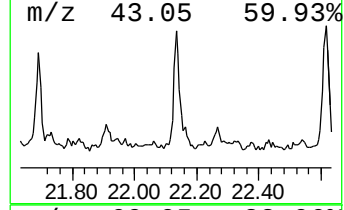
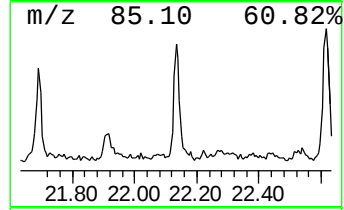
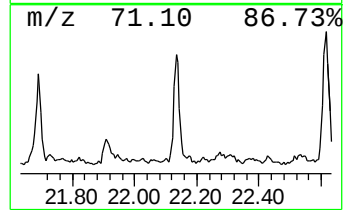
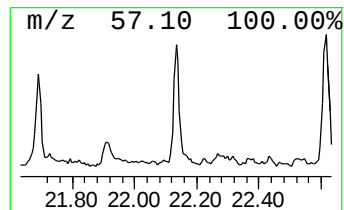
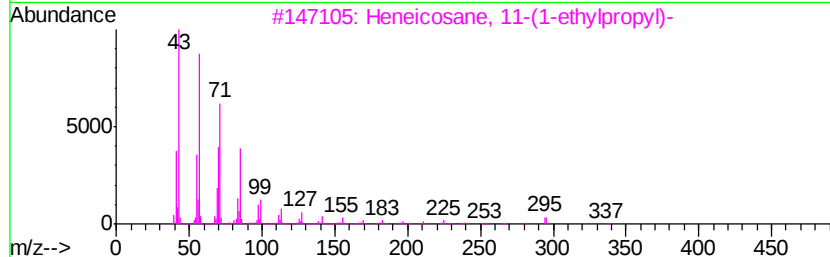
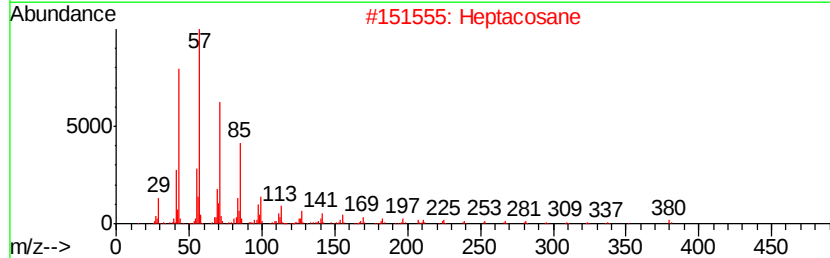
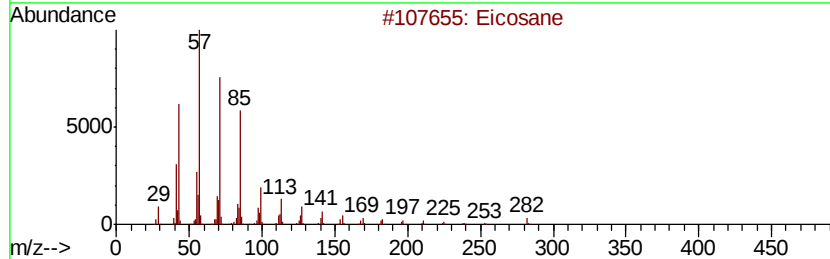
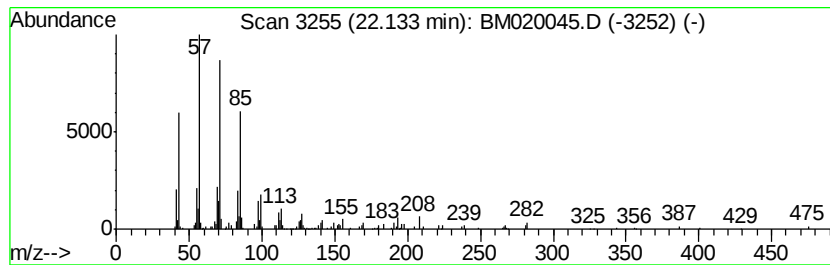
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.13	2.35 ng	162135	Chrysene-d12	21.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Heptacosane	380	C27H56	000593-49-7	87
3		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
4		Heneicosane	296	C21H44	000629-94-7	83
5		Hexadecane	226	C16H34	000544-76-3	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM042319\
Data File : BM020045.D
Acq On : 23 Apr 2019 20:19
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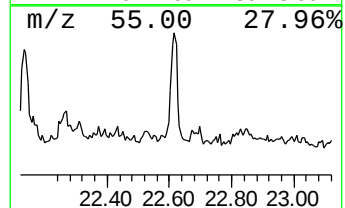
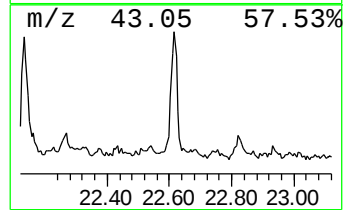
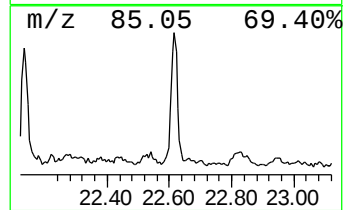
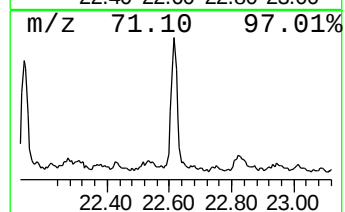
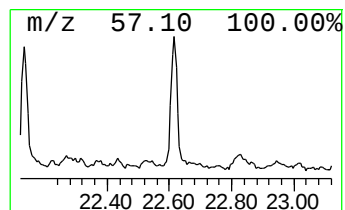
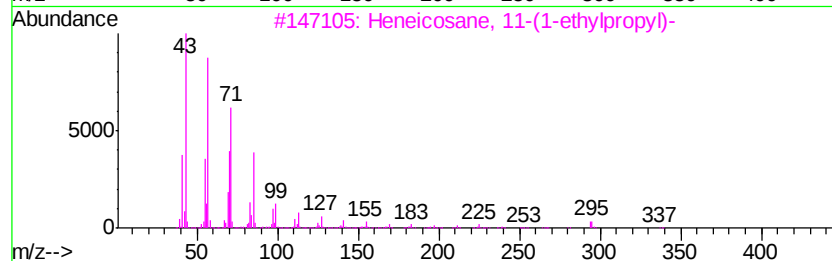
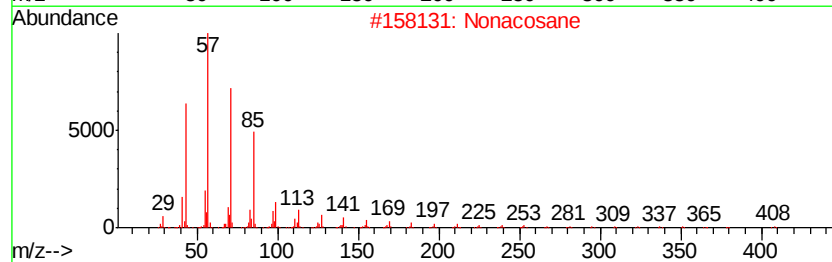
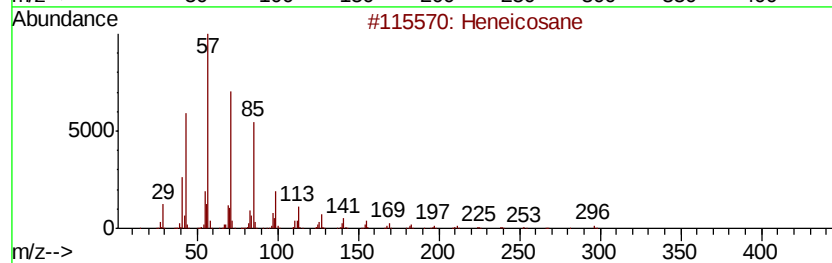
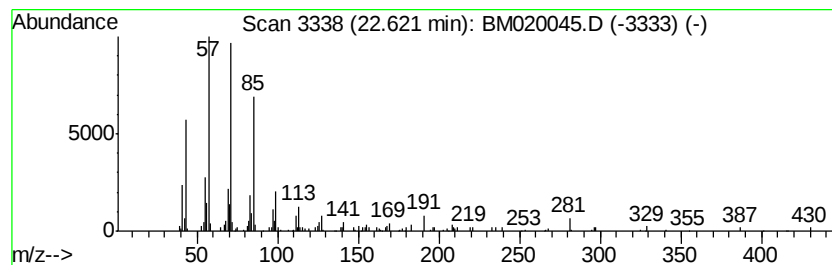
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.62	2.71 ng	196513	Perylene-d12	23.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	87
2		Nonacosane	408	C29H60	000630-03-5	87
3		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
4		Octacosane	394	C28H58	000630-02-4	81
5		Eicosane	282	C20H42	000112-95-8	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM042319\
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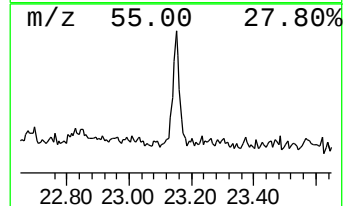
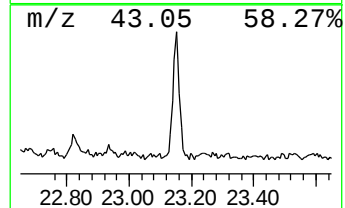
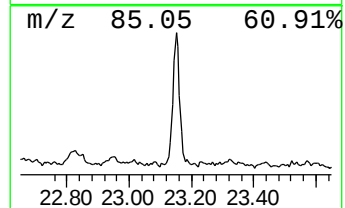
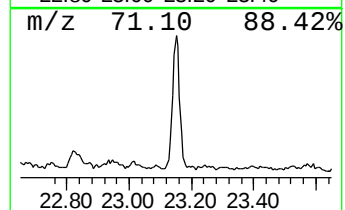
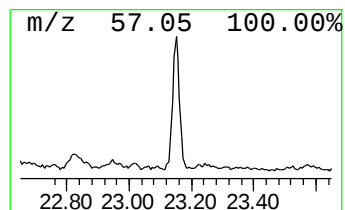
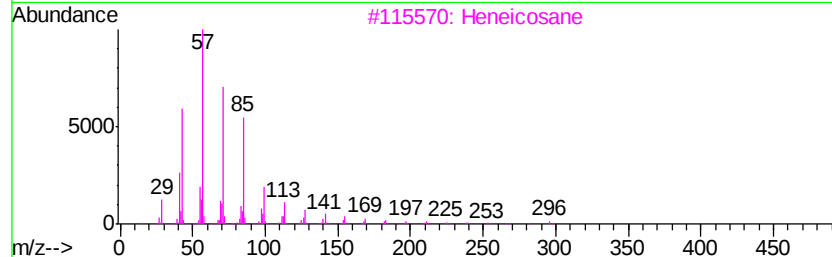
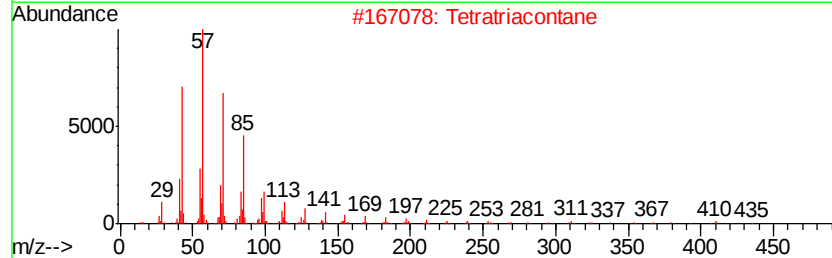
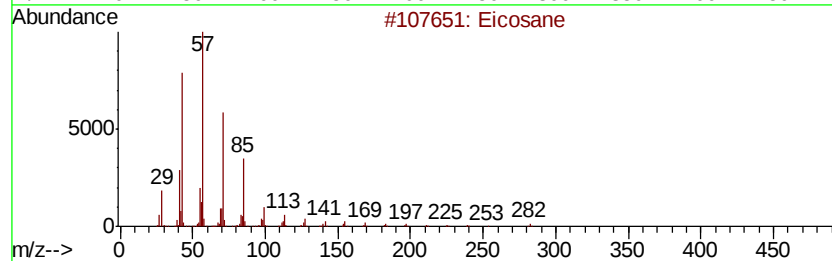
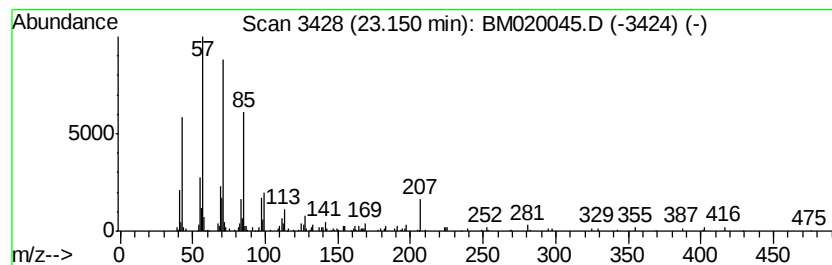
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Docosane, 9-butyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.15	2.96 ng	215279	Perylene-d12	23.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	91
2		Tetratriacontane	479	C34H70	014167-59-0	87
3		Heneicosane	296	C21H44	000629-94-7	87
4		Docosane, 9-butyl-	366	C26H54	055282-14-9	86
5		Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM042319\
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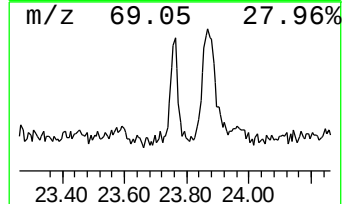
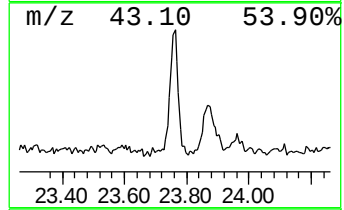
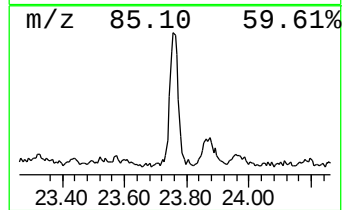
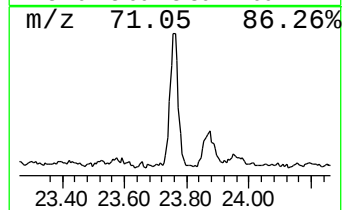
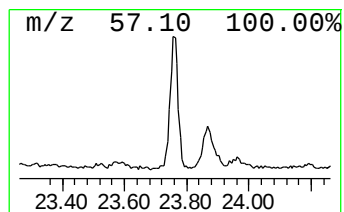
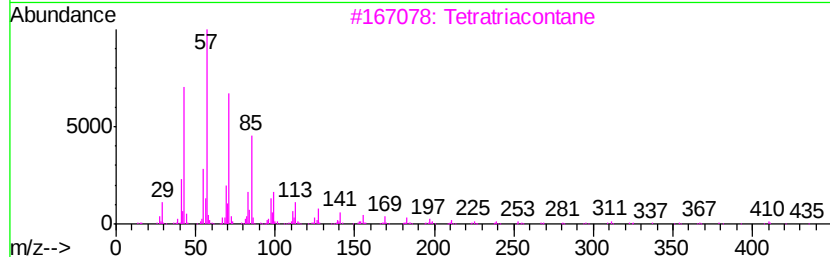
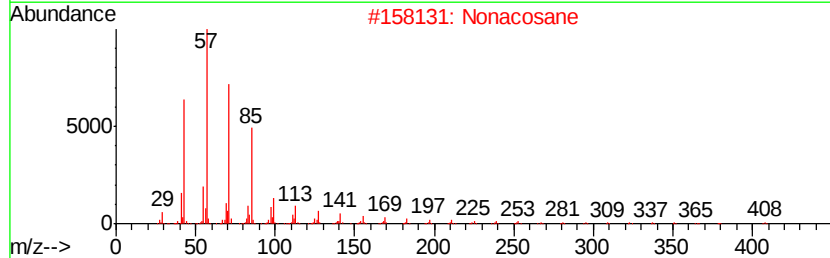
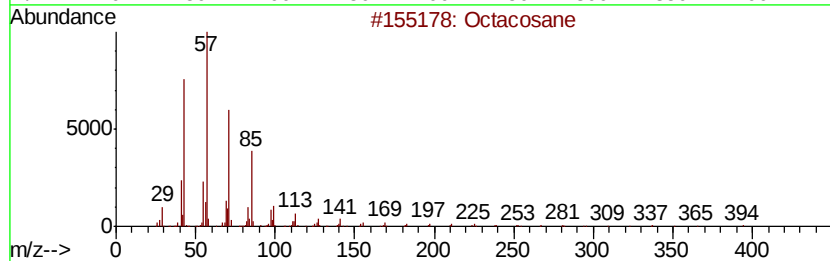
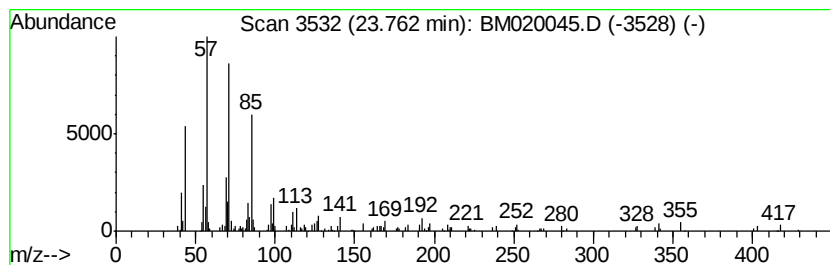
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Tetratriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.76	2.77 ng	201279	Perylene-d12	23.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	74
2		Nonacosane	408	C29H60	000630-03-5	74
3		Tetratriacontane	479	C34H70	014167-59-0	74
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	74
5		Docosane	310	C22H46	000629-97-0	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM042319\
Data File : BM020045.D
Acq On : 23 Apr 2019 20:19
Operator : JU/SJ
Sample : K2516-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P041919

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.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
unknown7.03	7.03	88.5	ng	2514460	1	7.49	568419	20.0
2-Propanol, 1-(2-...	7.10	9.8	ng	279769	1	7.49	568419	20.0
Butanoic acid, 4-...	7.30	12.4	ng	353299	1	7.49	568419	20.0
unknown14.07	14.07	2.1	ng	100543	3	14.16	949443	20.0
Triethylene glyco...	16.42	2.2	ng	118972	4	16.93	1084210	20.0
n-Hexadecanoic acid	17.82	12.3	ng	666128	4	16.93	1084210	20.0
Octadecanoic acid	19.12	7.1	ng	488266	5	21.15	1377280	20.0
Isoheptadecanol	20.84	8.1	ng	554958	5	21.15	1377280	20.0
Eicosane	22.13	2.4	ng	162135	5	21.15	1377280	20.0
Heneicosane	22.62	2.7	ng	196513	6	23.33	1452930	20.0
Docosane, 9-butyl-	23.15	3.0	ng	215279	6	23.33	1452930	20.0
Tetratriacontane	23.76	2.8	ng	201279	6	23.33	1452930	20.0