

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
 Data File : BM018614.D
 Acq On : 17 Jan 2019 15:11
 Operator : JU/SJ
 Sample : K1139-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 S-2

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-BM010919.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	4.881	301	305	313	rVB	179695	242766	2.79%	0.272%
2	5.328	375	381	389	rBV	3009415	4240725	48.70%	4.747%
3	6.916	643	651	662	rVB	2844096	4583079	52.63%	5.130%
4	7.275	703	712	720	rBV	3209932	4968862	57.06%	5.562%
5	7.740	784	791	797	rBV	1368105	2114349	24.28%	2.367%
6	8.057	837	845	853	rVB	3008614	4693166	53.90%	5.253%
7	8.904	981	989	1000	rBV	2306946	3841801	44.12%	4.300%
8	10.528	1258	1265	1272	rBV	1665943	2779439	31.92%	3.111%
9	13.004	1679	1686	1697	rBV	4935649	7211992	82.82%	8.072%
10	13.845	1823	1829	1842	rBV	987282	1408506	16.18%	1.577%
11	14.263	1894	1900	1908	rVB4	55524	130515	1.50%	0.146%
12	14.386	1912	1921	1929	rBV2	2244884	3444797	39.56%	3.856%
13	14.792	1981	1990	1997	rBV9	36473	90552	1.04%	0.101%
14	15.880	2169	2175	2188	rBV	2506233	3488434	40.06%	3.905%
15	16.110	2206	2214	2219	rBV5	42719	96941	1.11%	0.109%
16	17.139	2382	2389	2394	rBV	2557372	3681944	42.28%	4.121%
17	17.180	2394	2396	2401	rVB	79855	93349	1.07%	0.104%
18	18.027	2533	2540	2551	rBV2	1086166	1843278	21.17%	2.063%
19	18.933	2690	2694	2700	rBV3	74935	137141	1.57%	0.154%
20	19.198	2735	2739	2744	rVB	195858	273870	3.15%	0.307%
21	19.251	2744	2748	2753	rBV3	85060	121456	1.39%	0.136%
22	19.309	2753	2758	2770	rBV2	667644	1063396	12.21%	1.190%
23	19.568	2798	2802	2810	rVB	187387	309628	3.56%	0.347%
24	19.768	2831	2836	2846	rBV	6998550	8707853	100.00%	9.747%
25	21.027	3047	3050	3058	rBV	673635	775263	8.90%	0.868%
26	21.333	3096	3102	3106	rBV	2900182	3982638	45.74%	4.458%
27	21.468	3122	3125	3129	rVB	448143	476920	5.48%	0.534%
28	21.909	3196	3200	3208	rVB	1236445	1529604	17.57%	1.712%
29	22.374	3275	3279	3290	rVB	2332524	3281892	37.69%	3.673%
30	22.509	3298	3302	3305	rVB	253288	343453	3.94%	0.384%
31	22.891	3361	3367	3376	rBV	2954312	4792981	55.04%	5.365%
32	23.468	3459	3465	3479	rVB	2835025	5181425	59.50%	5.800%
33	23.603	3482	3488	3496	rVV	1753091	3324561	38.18%	3.721%
34	24.121	3570	3576	3587	rBV	2092757	3931786	45.15%	4.401%

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Instrument :
BNA_M
ClientSampleId :
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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	24.880	3699	3705	3713	rBV	981565	2153984	24.74%	2.411%
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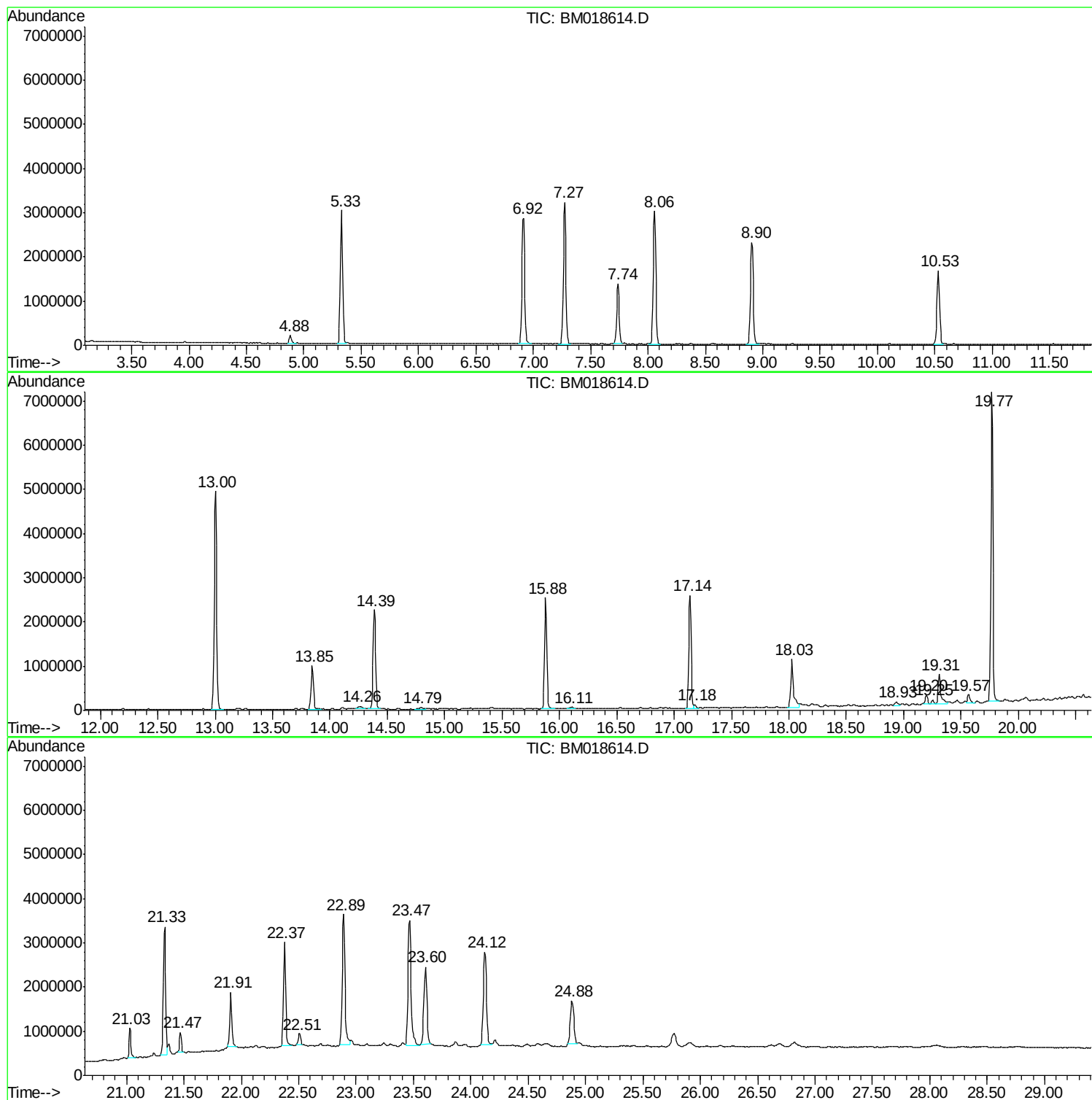
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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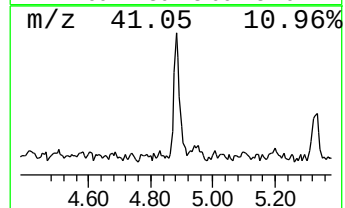
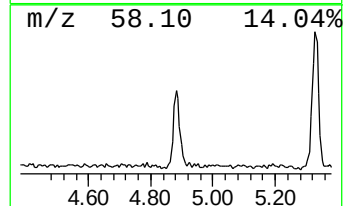
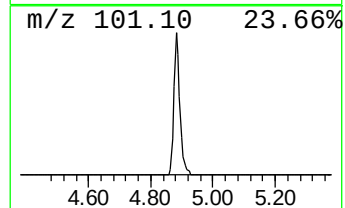
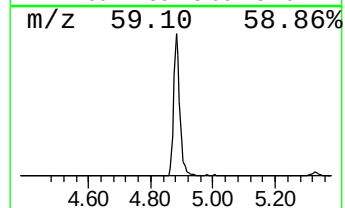
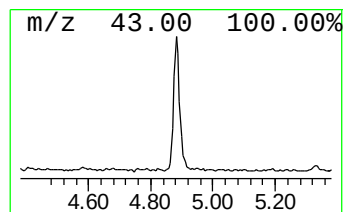
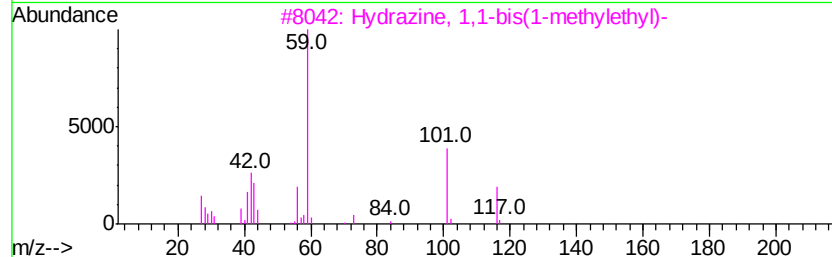
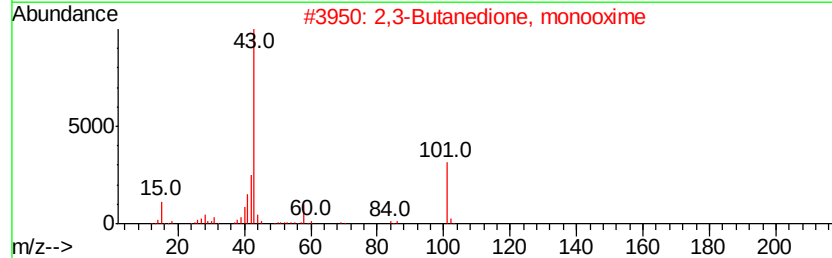
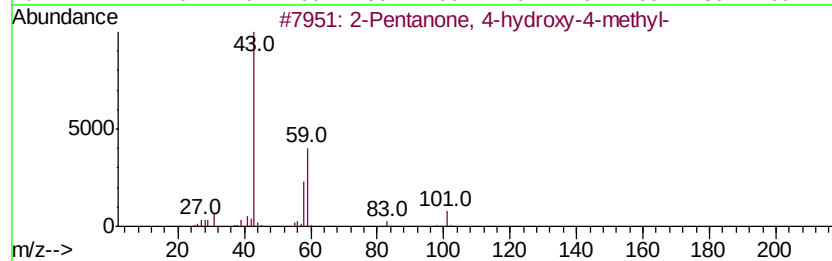
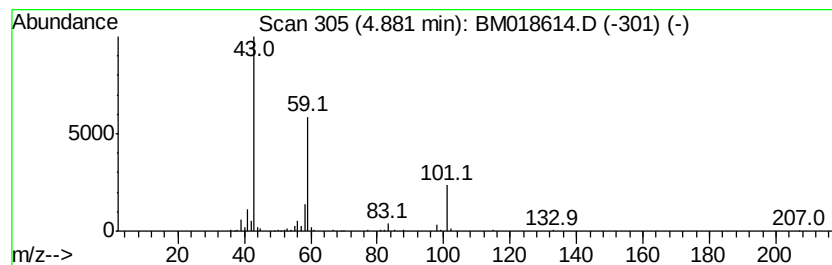
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	2.30 ng	242766	1,4-Dichlorobenzene-d4	7.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
3			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	23
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16



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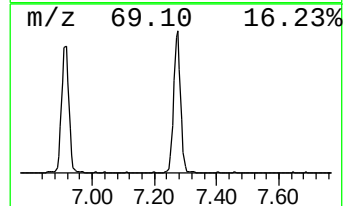
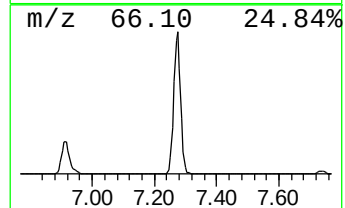
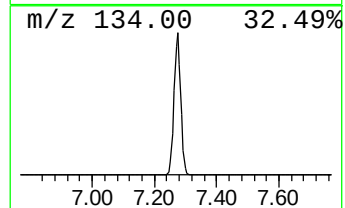
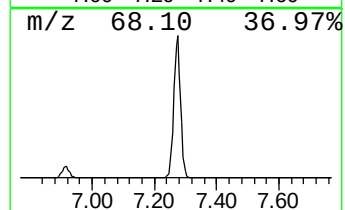
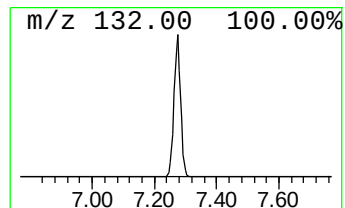
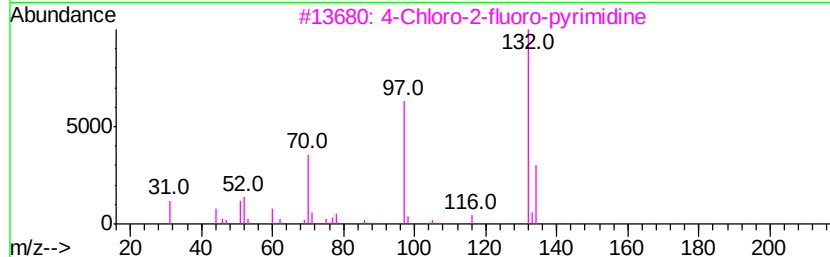
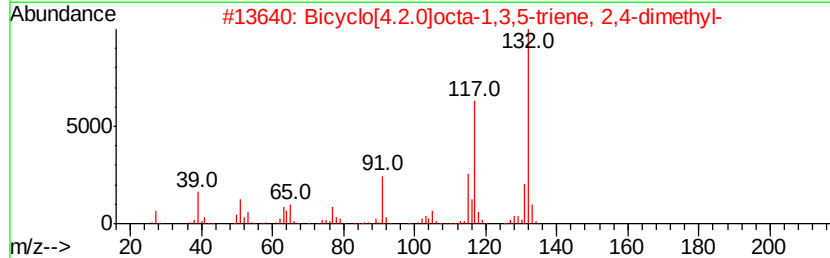
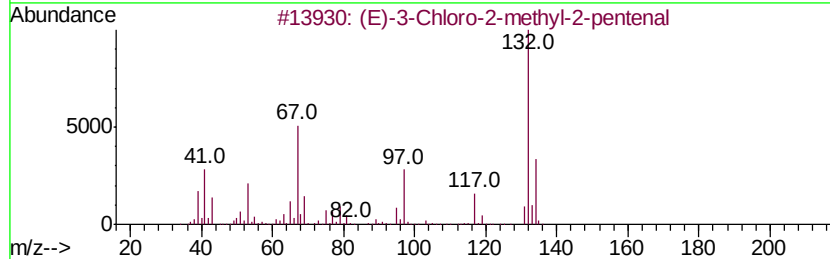
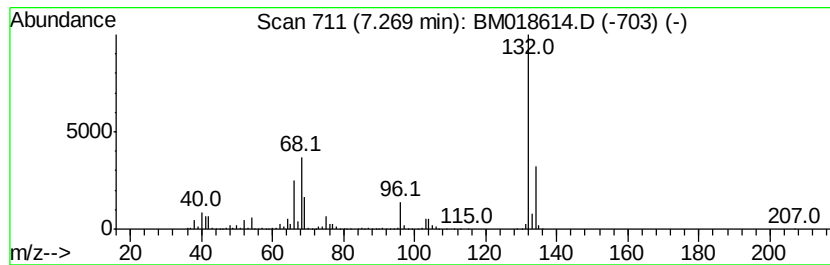
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.27	47.00 ng	4968860	1,4-Dichlorobenzene-d4	7.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		4-Chloro-2-fluoropyrimidine	132	C4H2ClFN2	051422-00-5	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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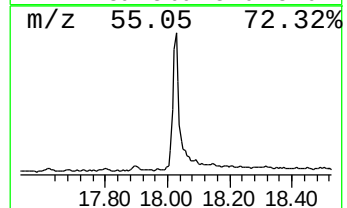
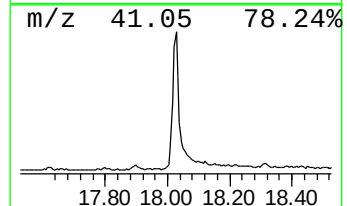
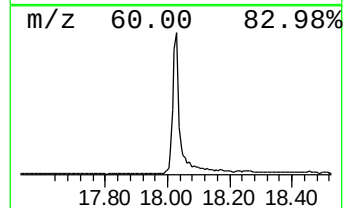
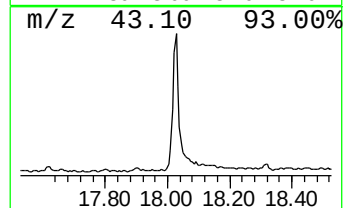
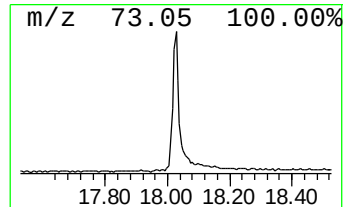
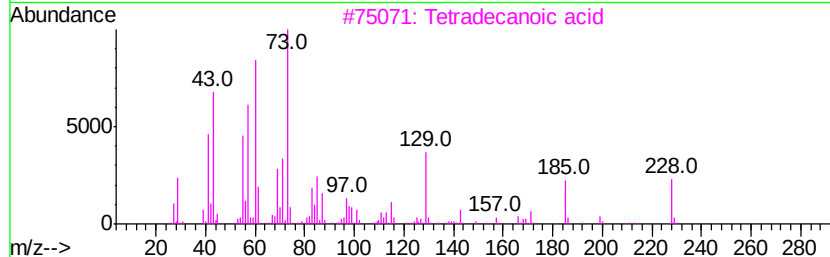
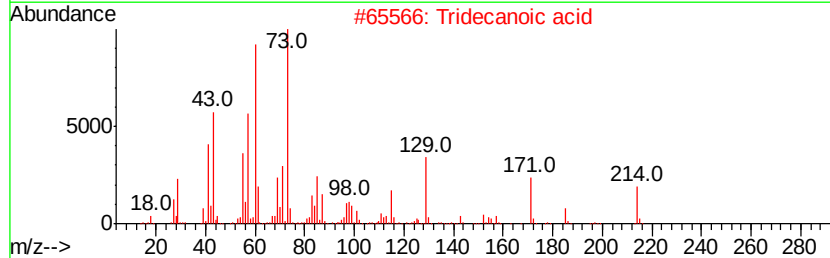
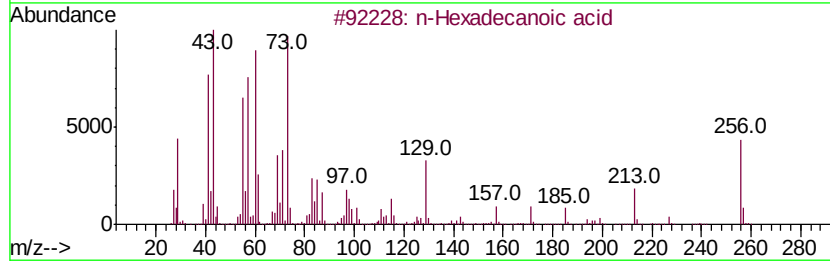
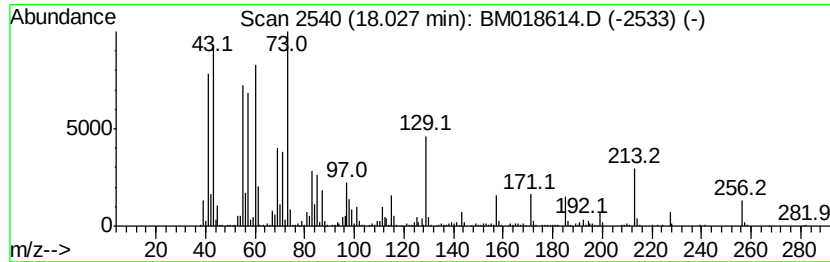
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.03	10.01 ng	1843280	Phenanthrene-d10	17.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2		Tridecanoic acid	214	C13H26O2	000638-53-9	76
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		n-Decanoic acid	172	C10H20O2	000334-48-5	70
5		Undecanoic acid	186	C11H22O2	000112-37-8	64



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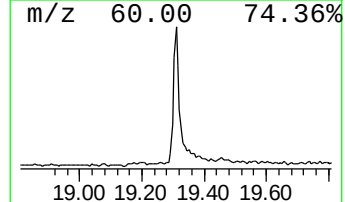
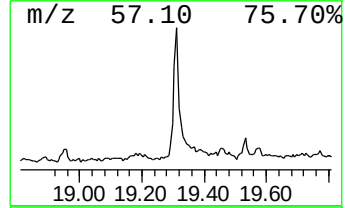
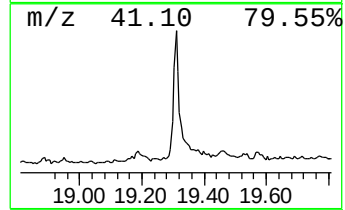
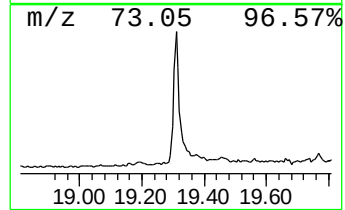
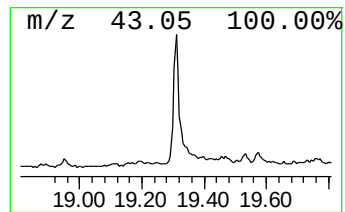
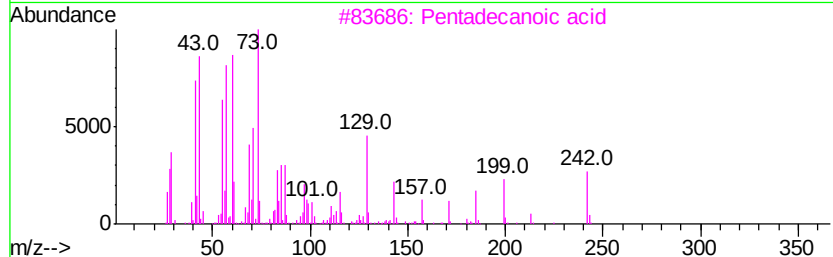
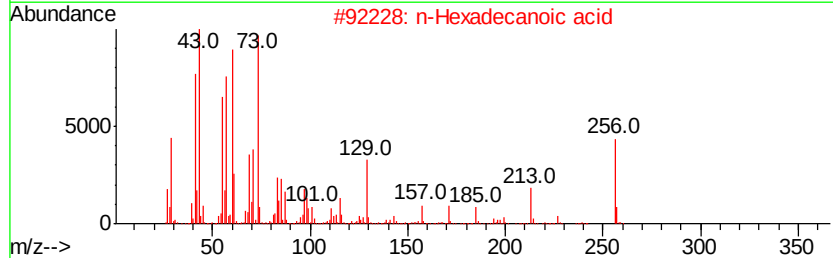
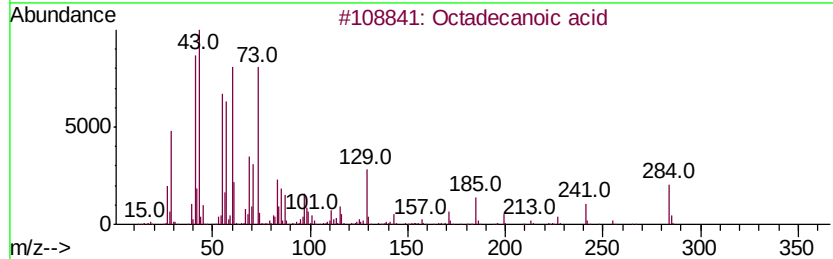
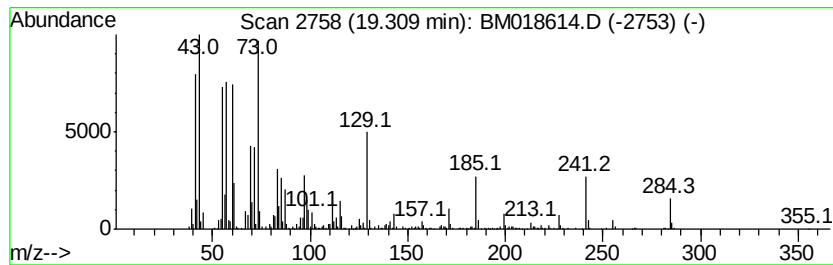
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.31	5.34 ng	1063400	Chrysene-d12		21.33
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74



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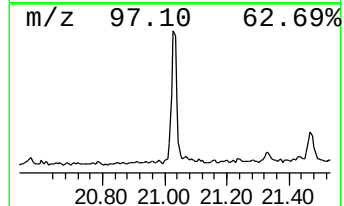
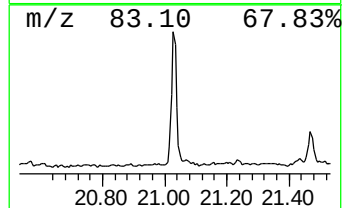
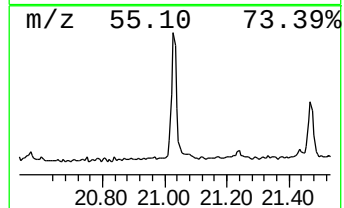
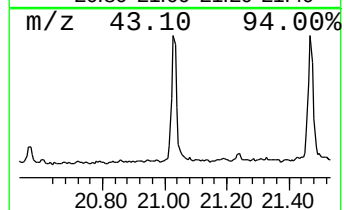
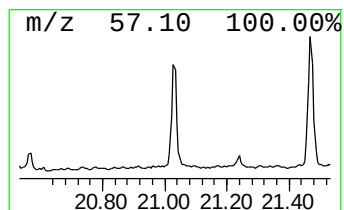
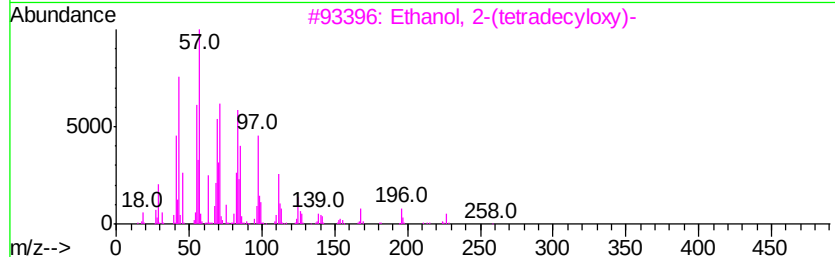
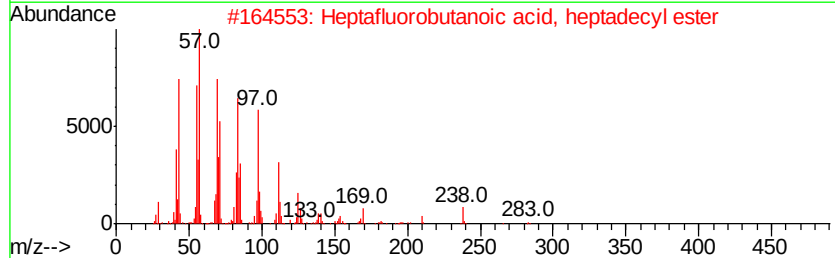
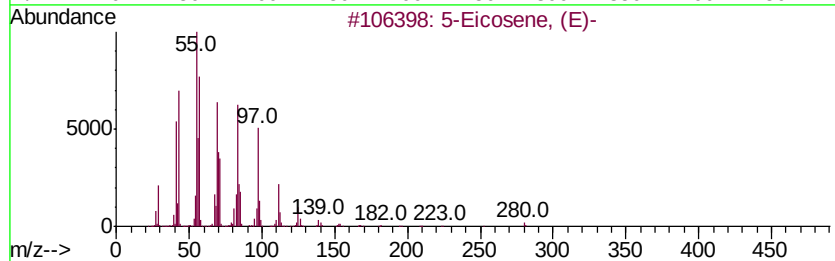
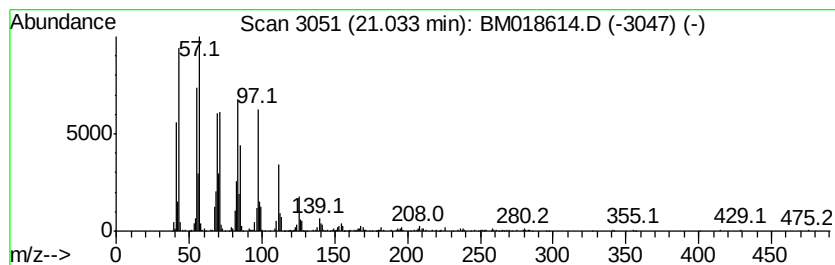
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 5-Eicosene, (E)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.03	3.89 ng	775263	Chrysene-d12	21.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	96
2	Heptafluorobutanoic acid, heptadecanoic acid				



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ClientSampleId :
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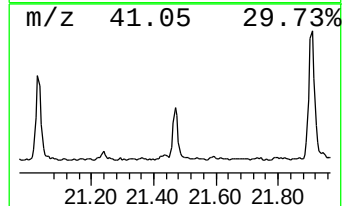
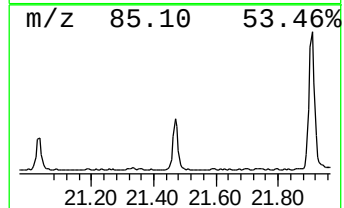
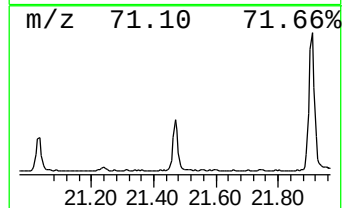
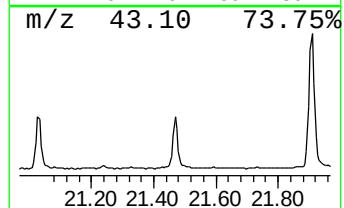
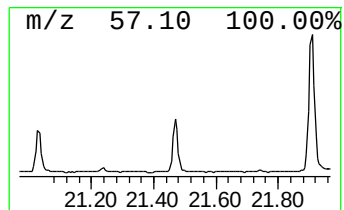
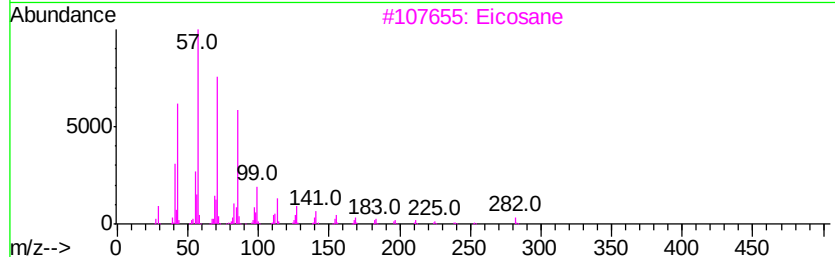
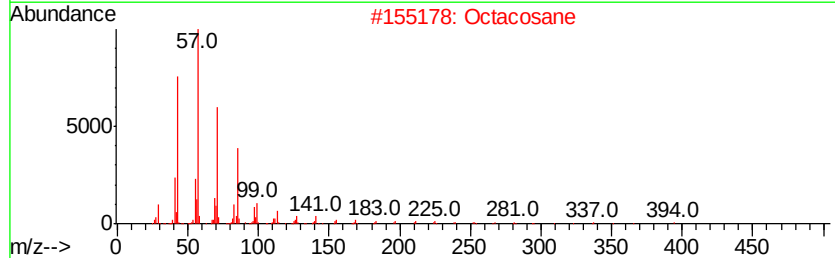
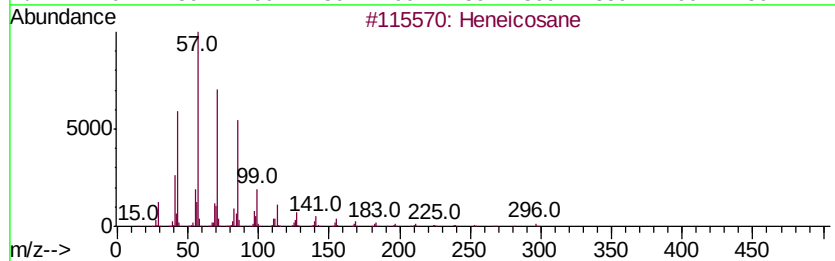
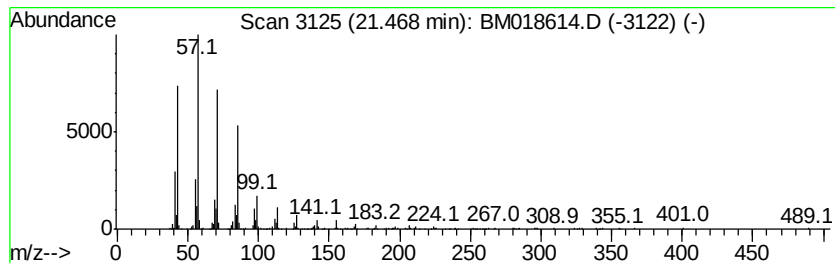
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.47	2.40 ng	476920	Chrysene-d12	21.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	97
2	Octacosane		394	C28H58	000630-02-4	91
3	Eicosane		282	C20H42	000112-95-8	91
4	Pentadecane, 8-heptyl-		310	C22H46	071005-15-7	91
5	Tridecane, 6-propyl-		226	C16H34	055045-10-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
 Data File : BM018614.D
 Acq On : 17 Jan 2019 15:11
 Operator : JU/SJ
 Sample : K1139-03
 Misc :
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Instrument :
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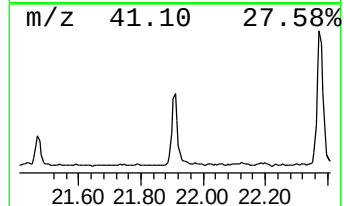
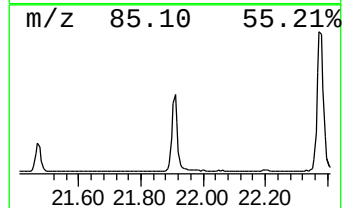
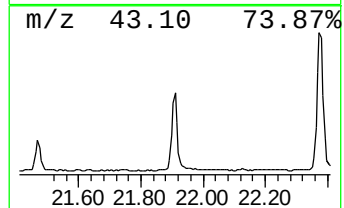
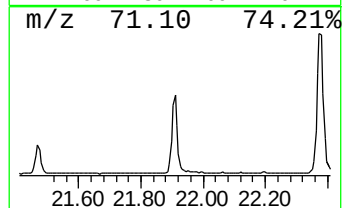
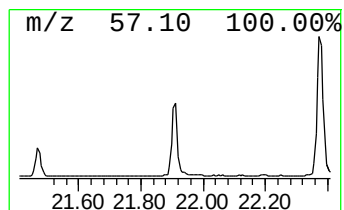
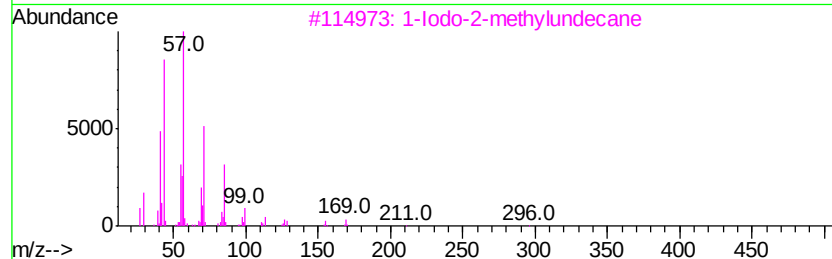
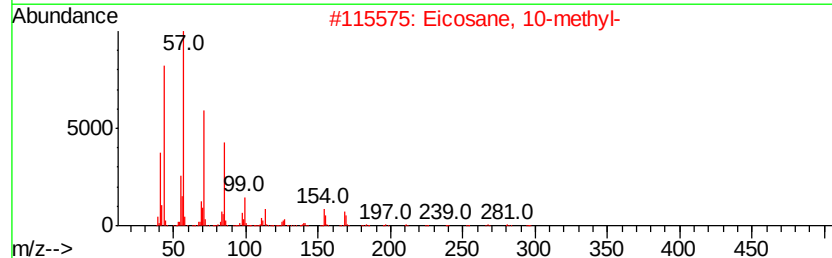
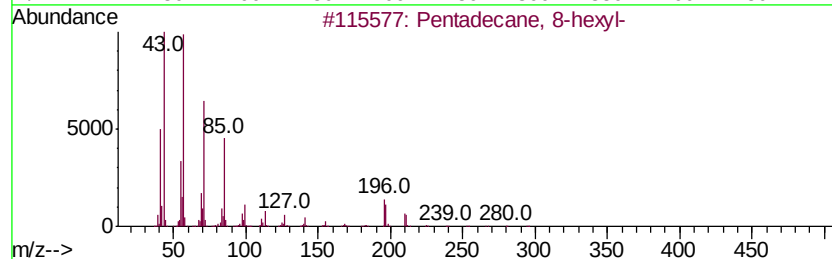
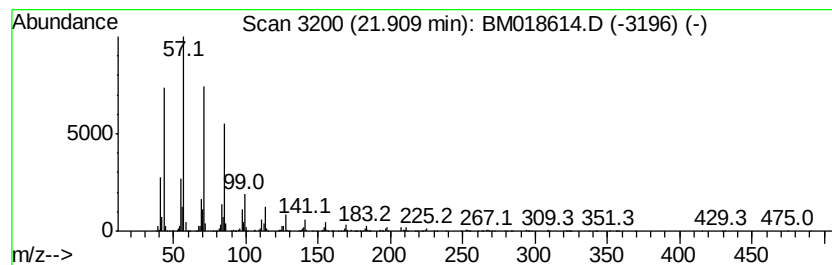
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TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 8 Pentadecane, 8-hexyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.91	7.68 ng	1529600	Chrysene-d12	21.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
2		Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
3		1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	93
4		Tetratriacontane	479	C34H70	014167-59-0	91
5		Heptacosane	380	C27H56	000593-49-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
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Instrument :
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 ClientSampleId :
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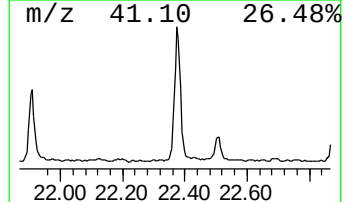
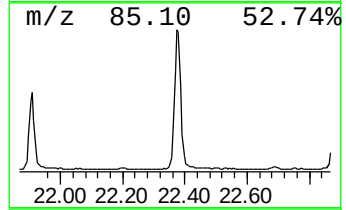
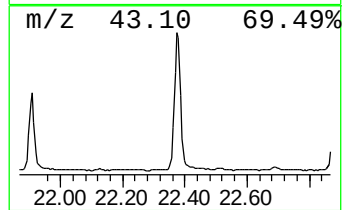
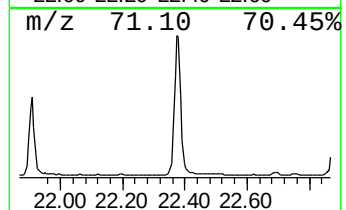
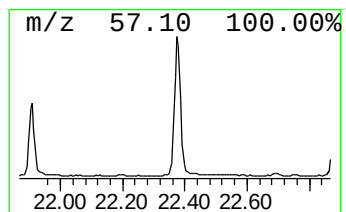
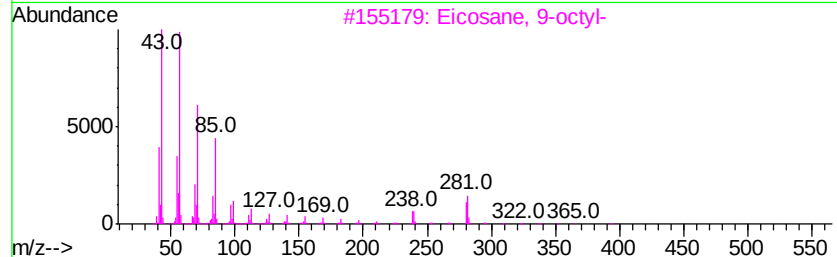
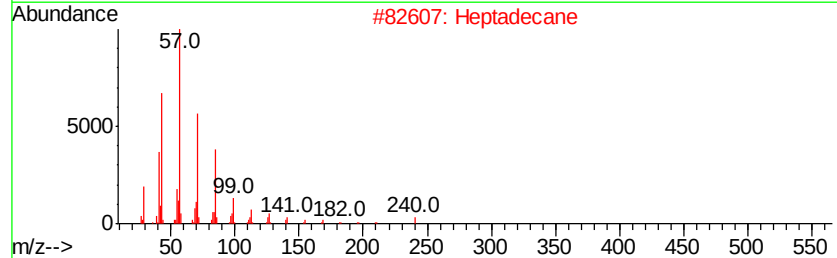
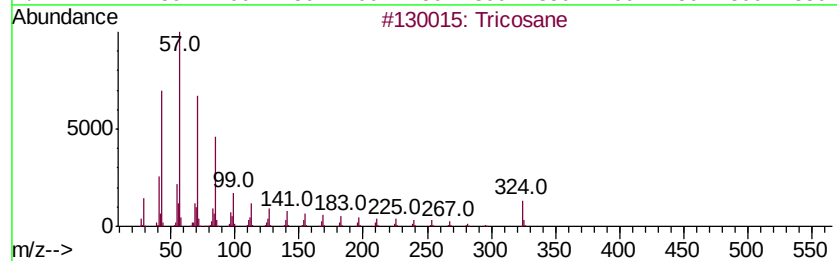
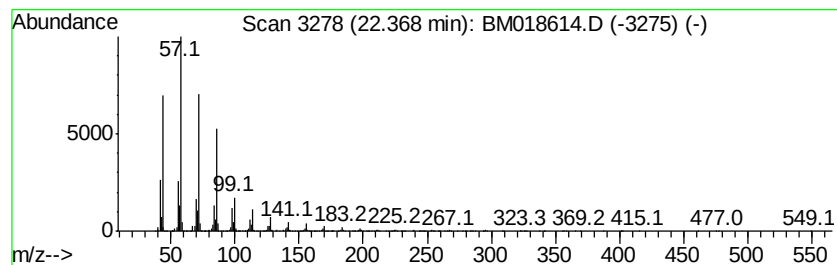
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Tricosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.37	16.48 ng	3281890	Chrysene-d12	21.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane		324	C23H48	000638-67-5	95
2	Heptadecane		240	C17H36	000629-78-7	94
3	Eicosane, 9-octyl-		394	C28H58	013475-77-9	94
4	Heptadecane, 9-hexyl-		324	C23H48	055124-79-3	93
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
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Operator : JU/SJ
Sample : K1139-03
Misc :
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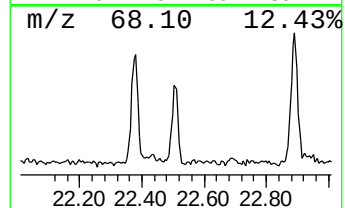
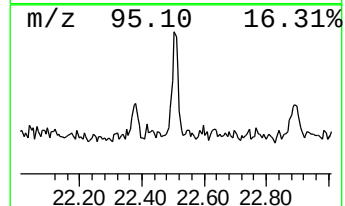
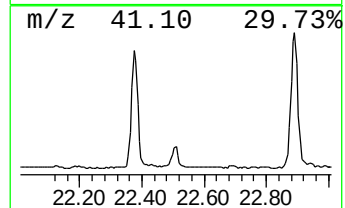
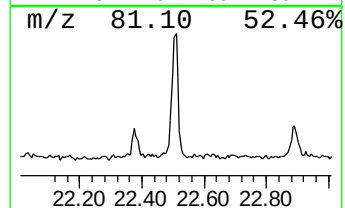
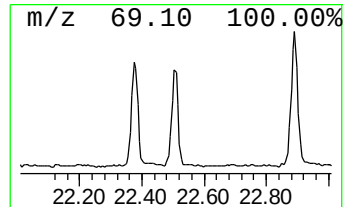
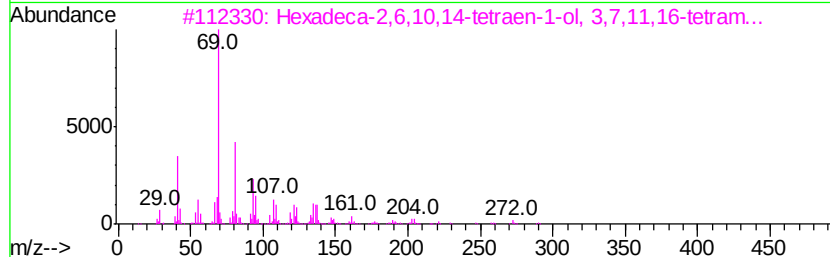
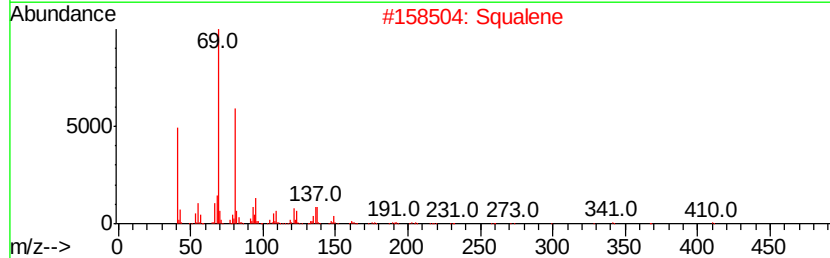
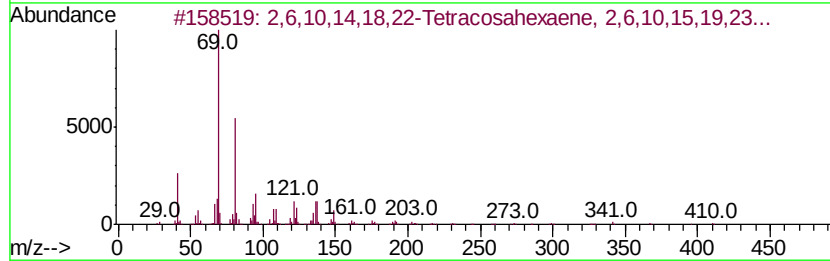
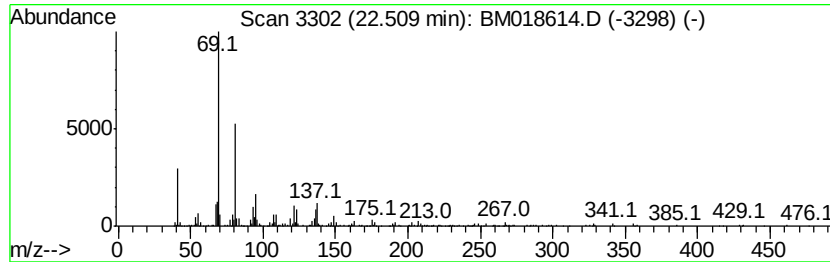
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.51	2.07 ng	343453	Perylene-d12	23.60	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
2	Squalene	410	C30H50	007683-64-9	87
3	Hexadeca-2,6,10,14-tetraen-1-ol, ...	290	C20H34O	007614-21-3	72
4	Farnesol isomer a	222	C15H26O	1000108-92-4	72
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
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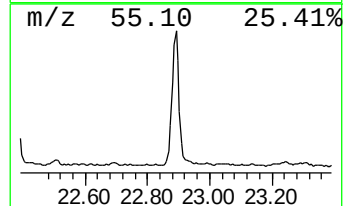
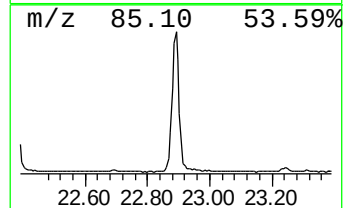
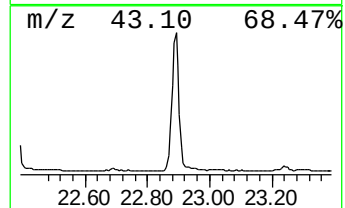
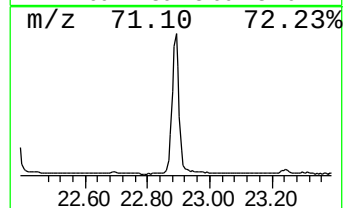
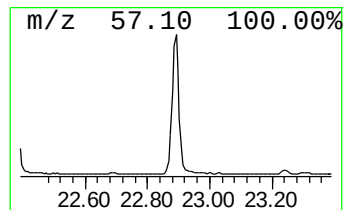
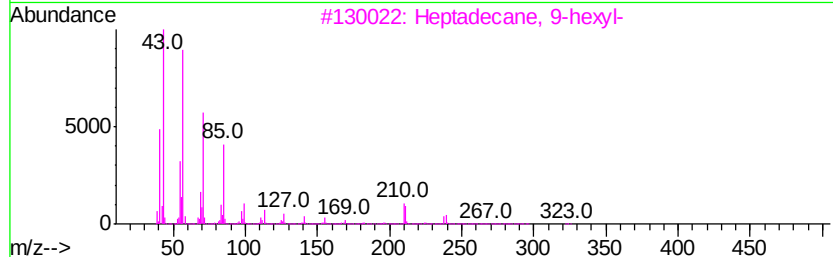
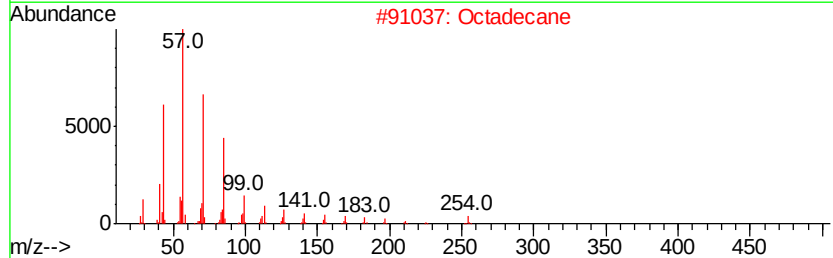
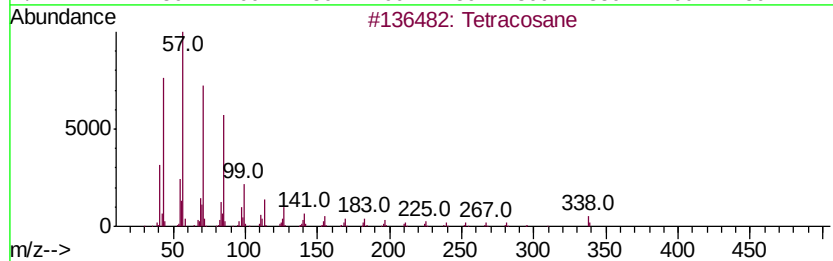
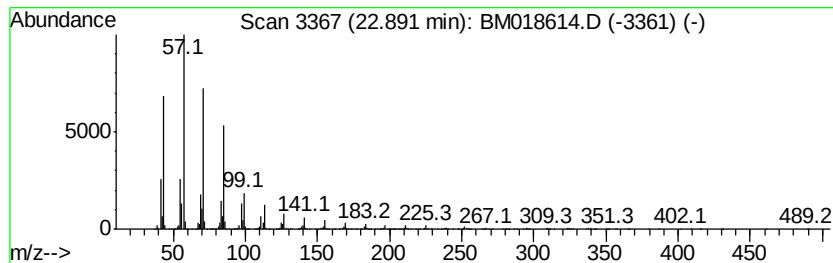
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.89	28.83 ng	4792980	Perylene-d12	23.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	95
2		Octadecane	254	C18H38	000593-45-3	94
3		Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	93
4		Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018614.D
Acq On : 17 Jan 2019 15:11
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Sample : K1139-03
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ALS Vial : 7 Sample Multiplier: 1

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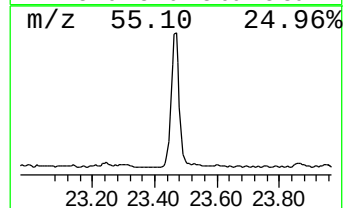
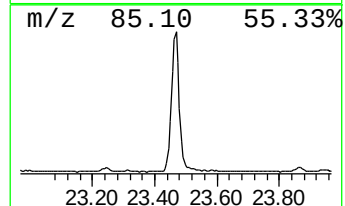
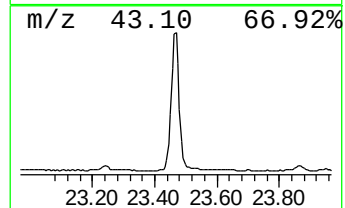
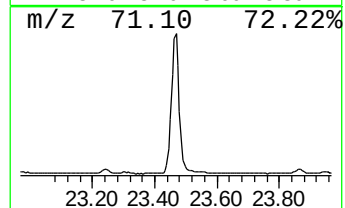
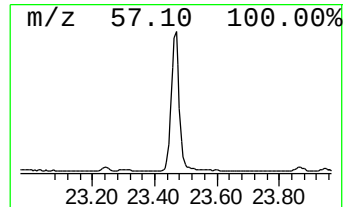
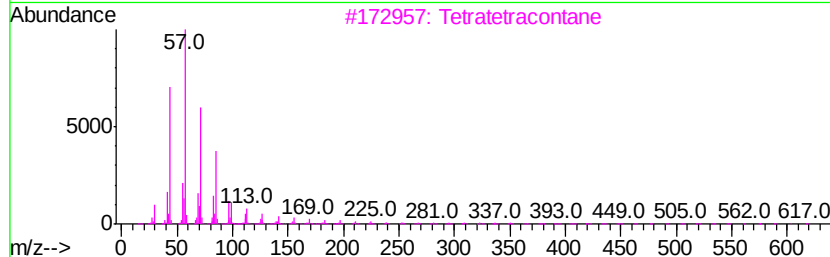
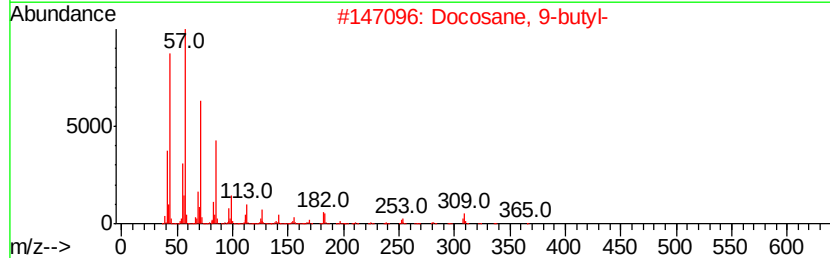
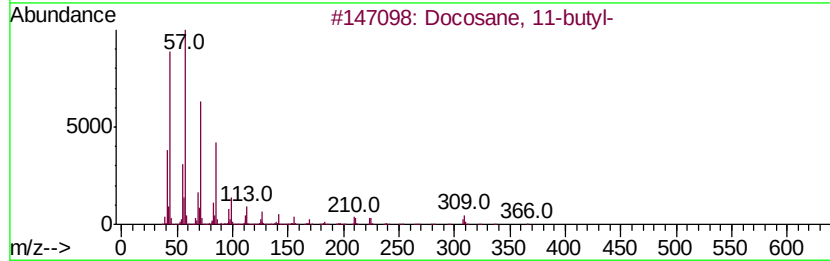
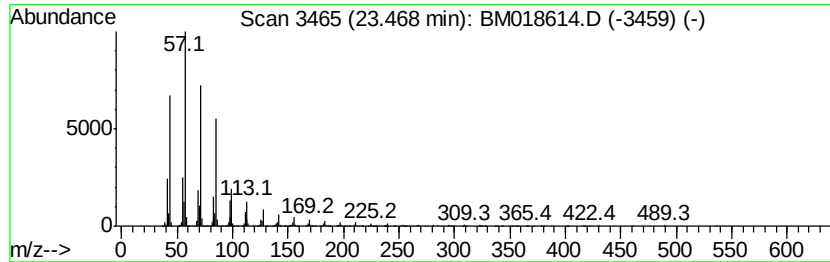
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Docosane, 11-butyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.47	31.17 ng	5181430	Perylene-d12	23.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 11-butyl-	366	C26H54	013475-76-8	93
2		Docosane, 9-butyl-	366	C26H54	055282-14-9	93
3		Tetratetracontane	619	C44H90	007098-22-8	91
4		Tetratriacontane	479	C34H70	014167-59-0	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
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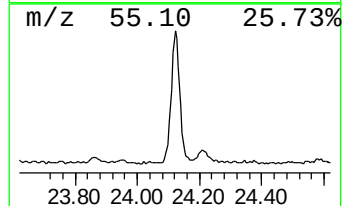
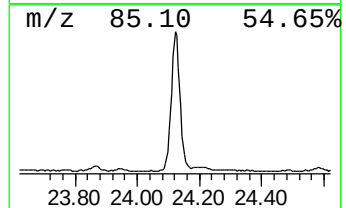
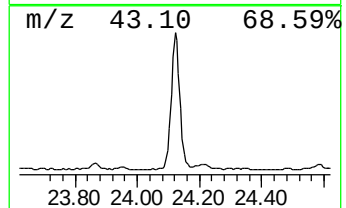
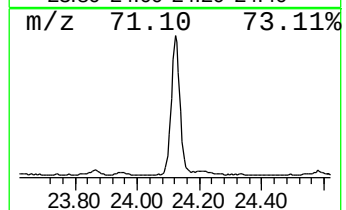
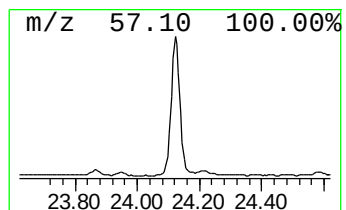
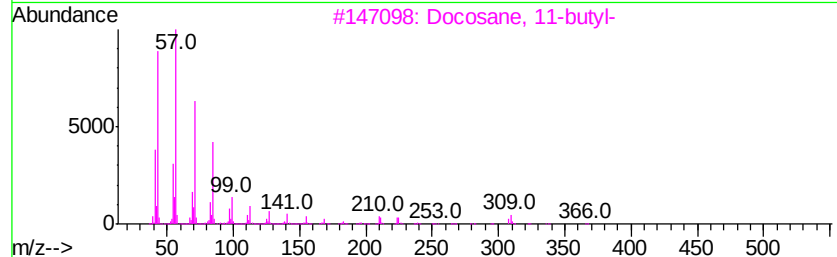
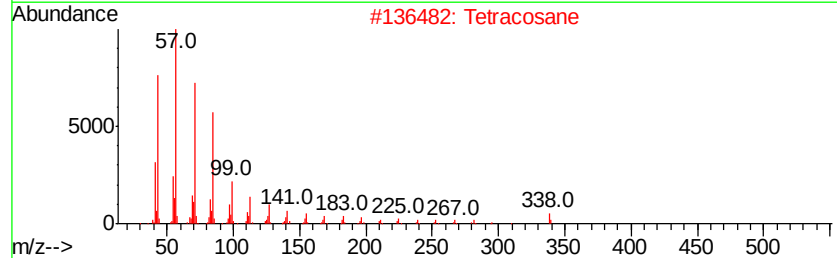
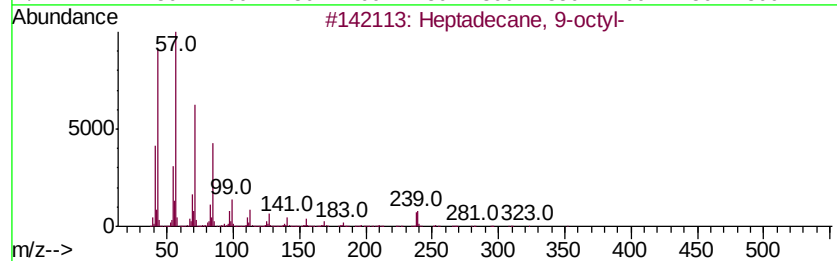
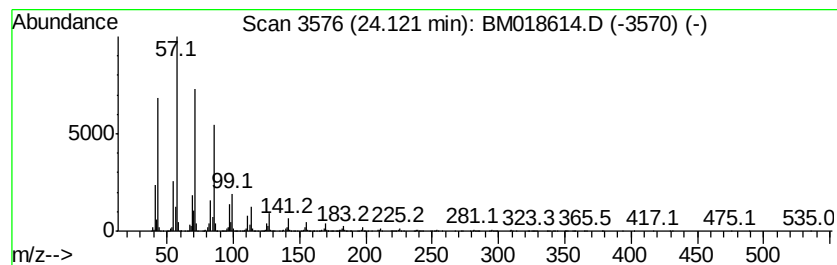
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.12	23.65 ng	3931790	Perylene-d12	23.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
2		Tetracosane	338	C24H50	000646-31-1	94
3		Docosane, 11-butyl-	366	C26H54	013475-76-8	91
4		Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	91
5		Tetratriacontane	479	C34H70	014167-59-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
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Acq On : 17 Jan 2019 15:11
Operator : JU/SJ
Sample : K1139-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-2

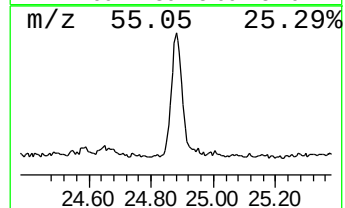
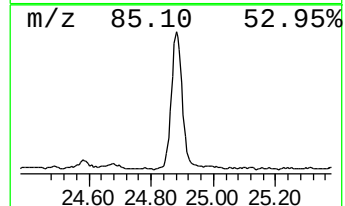
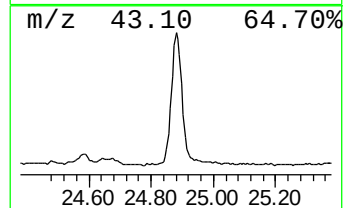
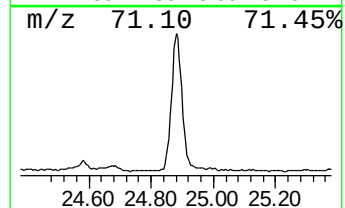
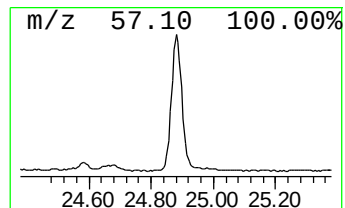
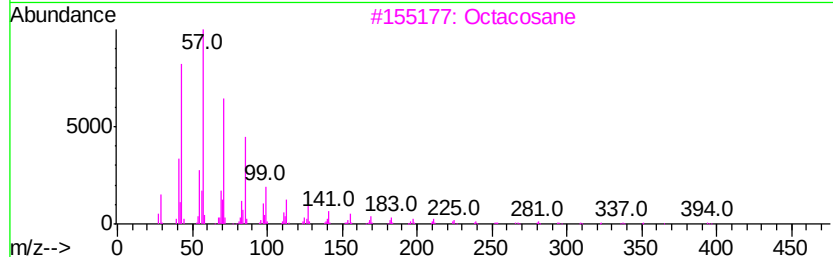
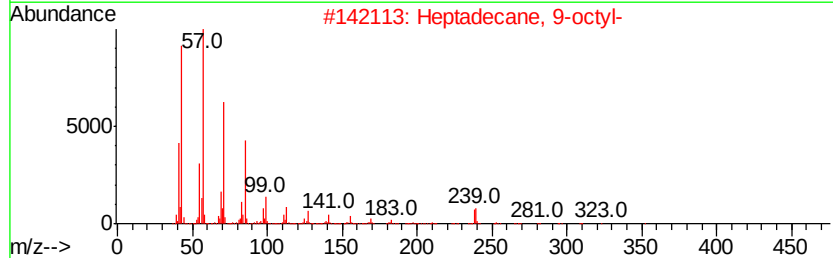
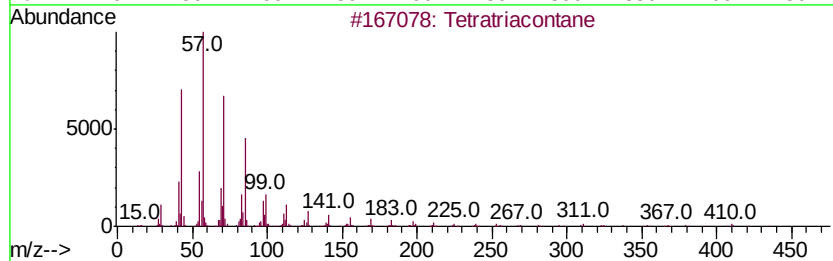
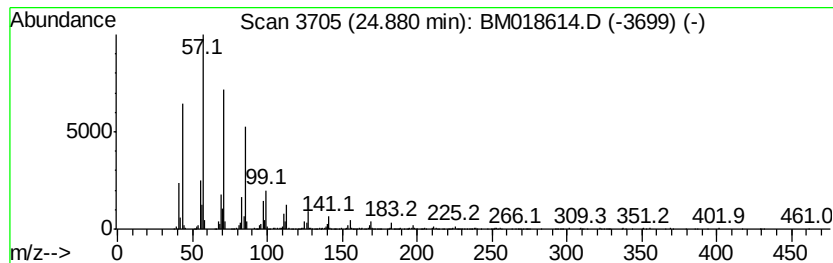
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Tetratriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.88	12.96 ng	2153980	Perylene-d12	23.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratriacontane	479	C34H70	014167-59-0	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Eicosane	282	C20H42	000112-95-8	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM011719\
Data File : BM018614.D
Acq On : 17 Jan 2019 15:11
Operator : JU/SJ
Sample : K1139-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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
2-Pentanone, 4-hy...	4.88	2.3	ng	242766	1	7.74	2114350	20.0
unknown7.27	7.27	47.0	ng	4968860	1	7.74	2114350	20.0
n-Hexadecanoic acid	18.03	10.0	ng	1843280	4	17.14	3681940	20.0
Octadecanoic acid	19.31	5.3	ng	1063400	5	21.33	3982640	20.0
5-Eicosene, (E)-	21.03	3.9	ng	775263	5	21.33	3982640	20.0
Heneicosane	21.47	2.4	ng	476920	5	21.33	3982640	20.0
Pentadecane, 8-he...	21.91	7.7	ng	1529600	5	21.33	3982640	20.0
Tricosane	22.37	16.5	ng	3281890	5	21.33	3982640	20.0
2,6,10,14,18,22-T...	22.51	2.1	ng	343453	6	23.60	3324560	20.0
Tetracosane	22.89	28.8	ng	4792980	6	23.60	3324560	20.0
Docosane, 11-butyl-	23.47	31.2	ng	5181430	6	23.60	3324560	20.0
Heptadecane, 9-oc...	24.12	23.6	ng	3931790	6	23.60	3324560	20.0
Tetratriacontane	24.88	13.0	ng	2153980	6	23.60	3324560	20.0