

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022519\
 Data File : BM018917.D
 Acq On : 25 Feb 2019 17:24
 Operator : JU/SJ
 Sample : K1597-11
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP-22

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	5.287	367	374	388	rBV	4961851	7026144	6.52%	1.344%
2	6.869	633	643	655	rBV	4794797	7650376	7.10%	1.464%
3	7.228	696	704	718	rBV	5011508	7827764	7.27%	1.497%
4	7.693	776	783	789	rBV	863249	1342638	1.25%	0.257%
5	8.010	829	837	846	rBV	3209067	5147499	4.78%	0.985%
6	8.857	973	981	994	rBV	2693950	4483312	4.16%	0.858%
7	10.481	1249	1257	1265	rBV	1029254	1745907	1.62%	0.334%
8	12.957	1671	1678	1693	rBV	5855745	8408003	7.81%	1.608%
9	14.339	1906	1913	1924	rBV2	1400794	2269079	2.11%	0.434%
10	15.839	2162	2168	2176	rBV	5146191	7166920	6.65%	1.371%
11	17.092	2376	2381	2387	rBV2	1797389	2569205	2.39%	0.491%
12	18.027	2521	2540	2550	rBV	26318220	75200155	69.81%	14.386%
13	18.398	2593	2603	2607	rBV	4277885	13483006	12.52%	2.579%
14	18.557	2623	2630	2633	rBV	3963772	9633017	8.94%	1.843%
15	19.139	2724	2729	2730	rBV	1782299	2512404	2.33%	0.481%
16	19.163	2731	2733	2738	rVB	1385406	1820794	1.69%	0.348%
17	19.310	2743	2758	2780	rVB	35023551	78074876	72.48%	14.936%
18	19.733	2825	2830	2835	rVB	9408009	11447333	10.63%	2.190%
19	20.392	2935	2942	2960	rVB3	1349839	6217694	5.77%	1.189%
20	20.845	2996	3019	3031	rVB	30367534	107718865	100.00%	20.607%
21	20.992	3036	3044	3059	rVB	2638670	5649598	5.24%	1.081%
22	21.292	3090	3095	3099	rBV	2141143	2764883	2.57%	0.529%
23	21.427	3114	3118	3125	rVB	3514358	3956942	3.67%	0.757%
24	21.639	3149	3154	3161	rVB	1084136	2179268	2.02%	0.417%
25	21.721	3161	3168	3183	rVB3	4577992	13557959	12.59%	2.594%
26	21.862	3187	3192	3195	rBV	6046751	7371142	6.84%	1.410%
27	22.021	3206	3219	3234	rVB	13340469	42743506	39.68%	8.177%
28	22.321	3265	3270	3284	rVB	8046742	11072988	10.28%	2.118%
29	22.833	3351	3357	3362	rBV	7969206	11218767	10.41%	2.146%
30	23.304	3427	3437	3447	rVV	4955274	17265908	16.03%	3.303%
31	23.398	3447	3453	3467	rVB	7711106	12810792	11.89%	2.451%
32	23.539	3472	3477	3493	rVB	1554776	3524072	3.27%	0.674%
33	24.045	3556	3563	3572	rVB	4848395	9428392	8.75%	1.804%
34	24.798	3682	3691	3708	rVB	5461088	17448100	16.20%	3.338%

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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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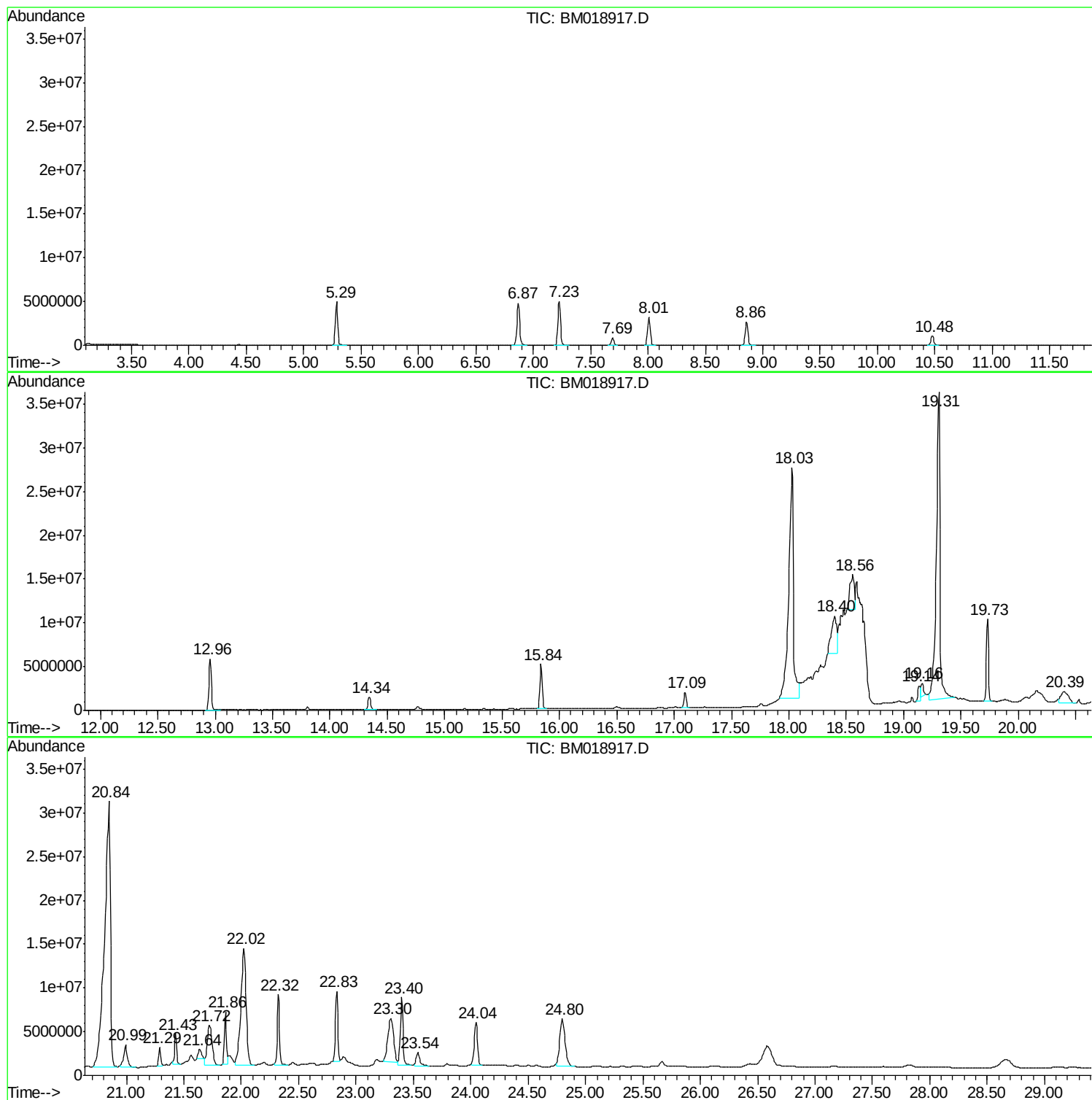
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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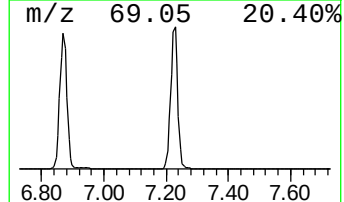
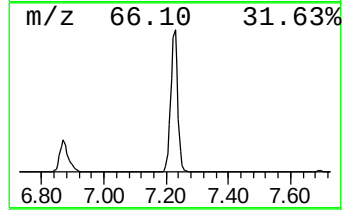
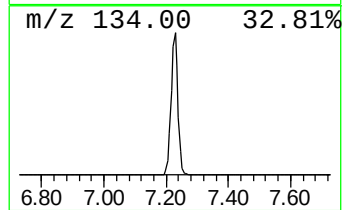
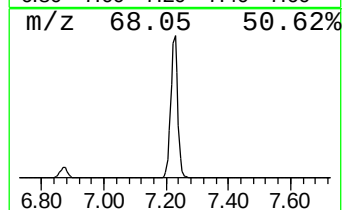
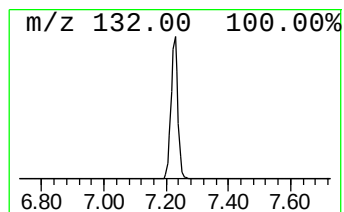
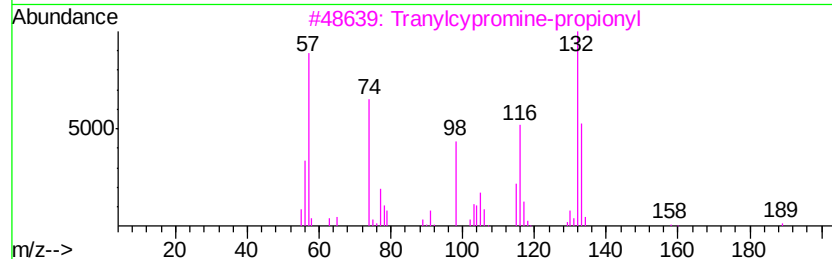
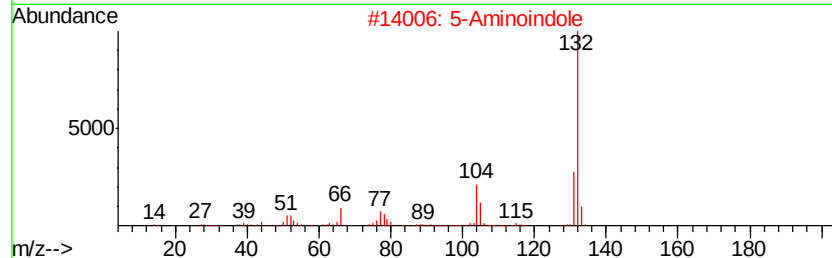
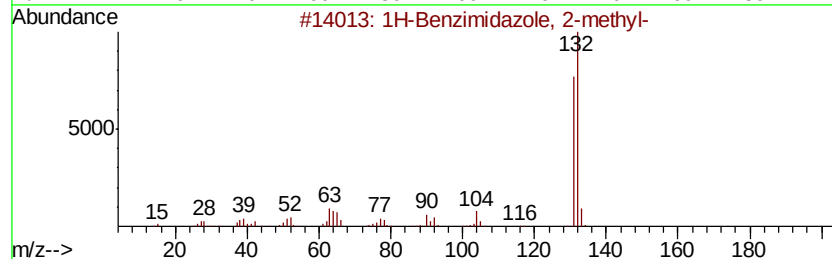
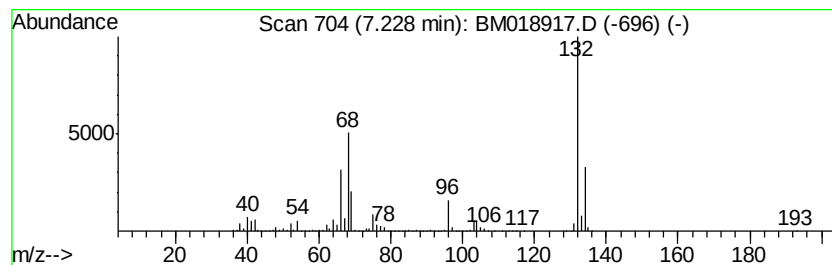
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.23 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	116.60 ng	7827760	1,4-Dichlorobenzene-d4	7.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2		5-Aminoindole	132	C8H8N2	005192-03-0	22
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11



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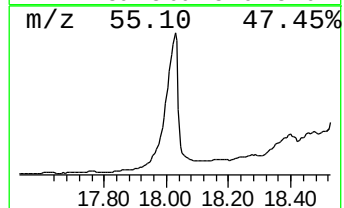
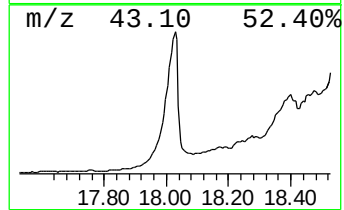
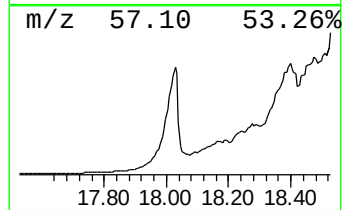
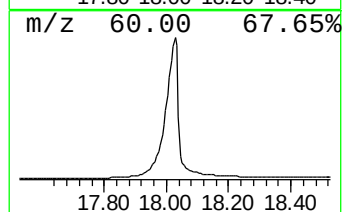
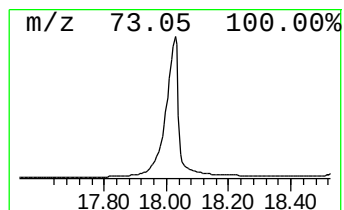
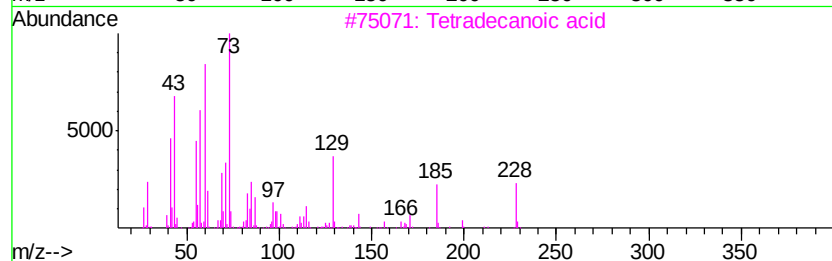
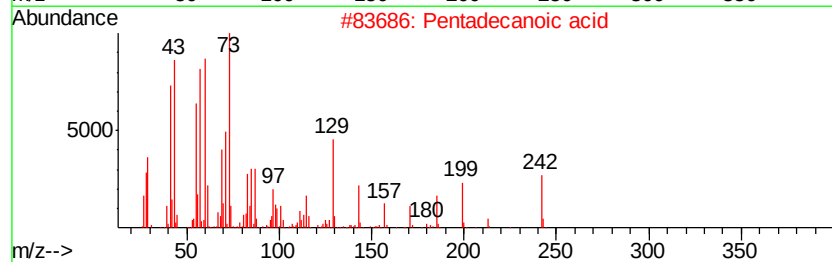
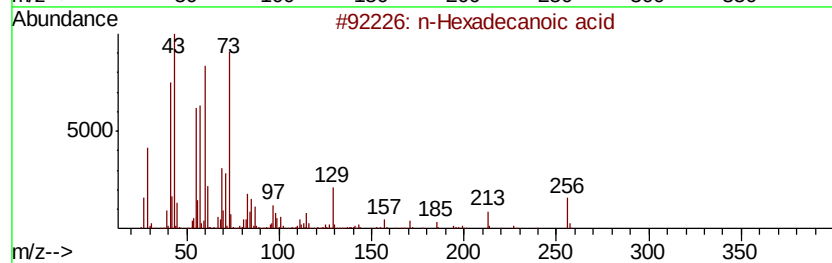
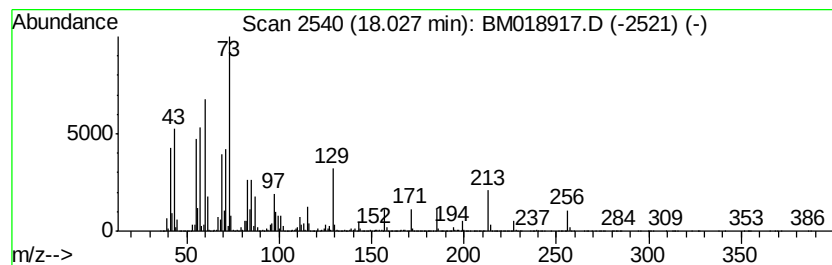
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.03	585.40 ng	75200200	Phenanthrene-d10	17.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	47
4		Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	35
5		Hexadecane	226	C16H34	000544-76-3	18



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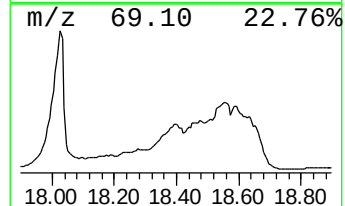
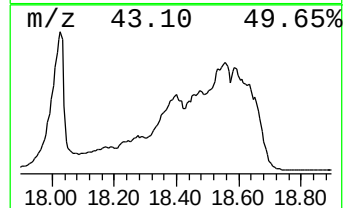
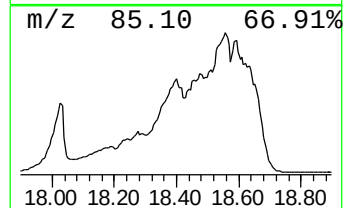
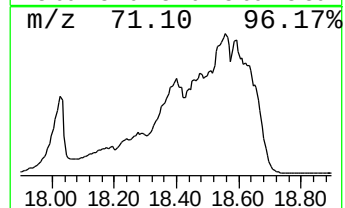
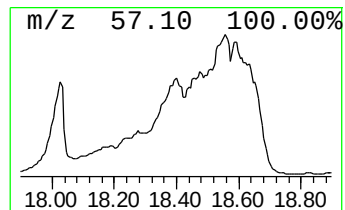
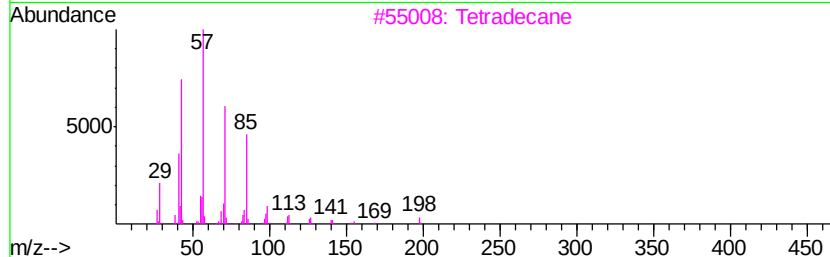
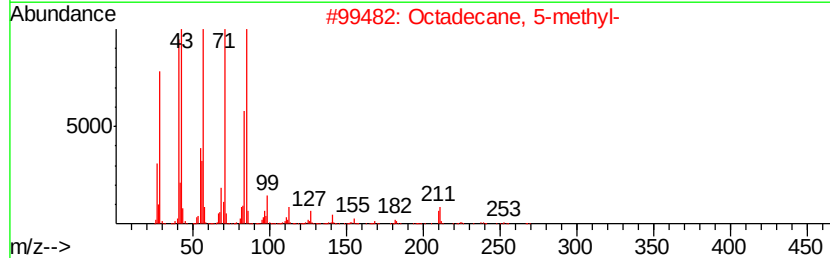
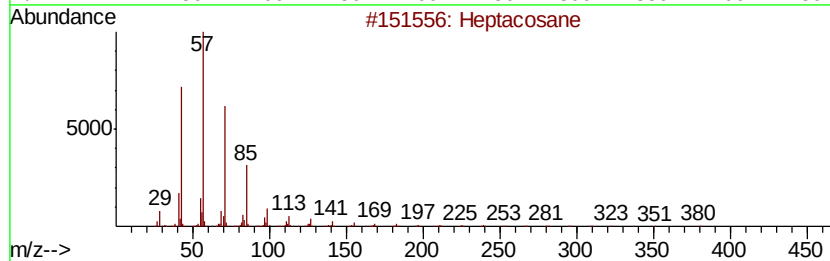
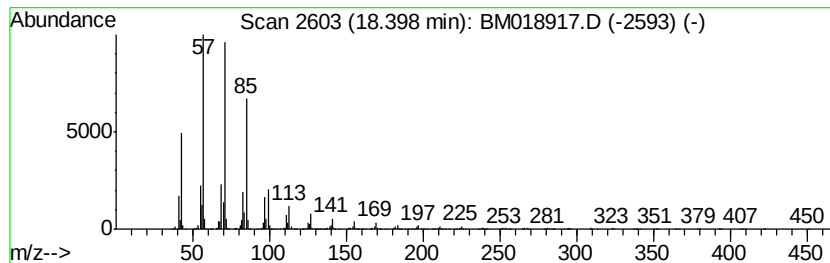
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.40	104.96 ng	13483000	Phenanthrene-d10	17.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Octadecane, 5-methyl-		268	C19H40	025117-35-5	76
3	Tetradecane		198	C14H30	000629-59-4	74
4	Octacosane		394	C28H58	000630-02-4	72
5	Tridecane, 7-hexyl-		268	C19H40	007225-66-3	68



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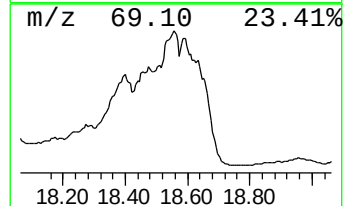
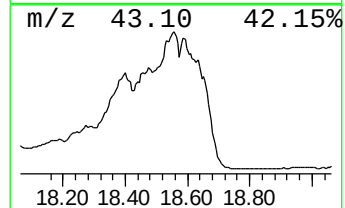
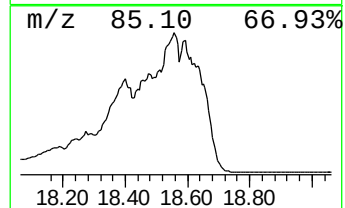
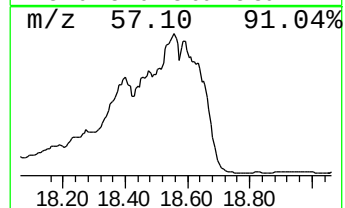
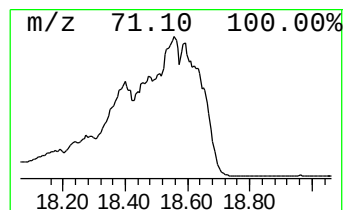
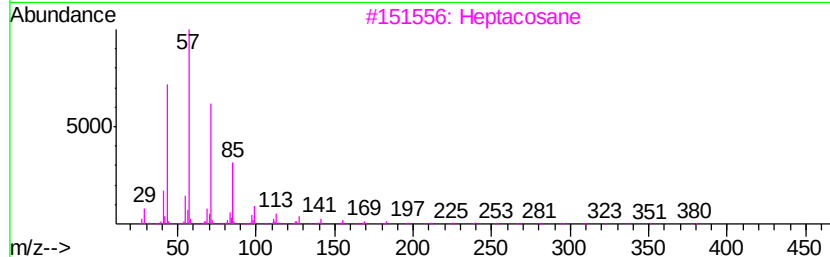
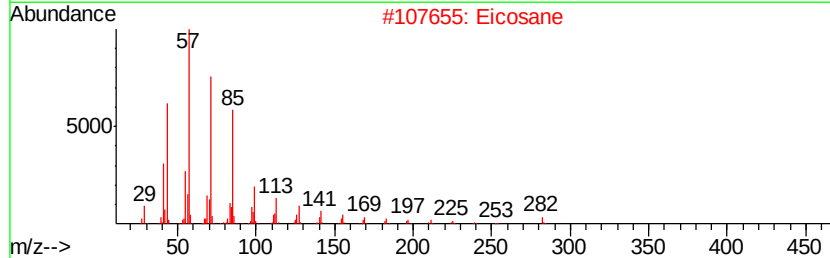
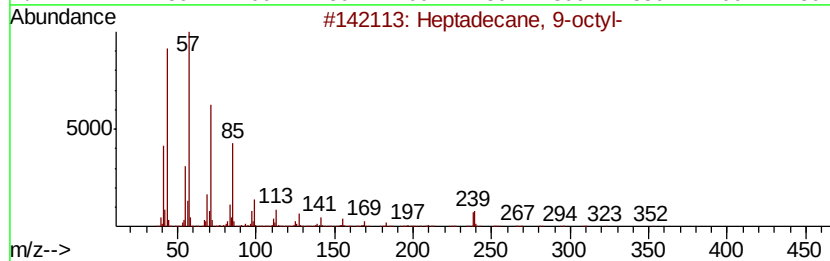
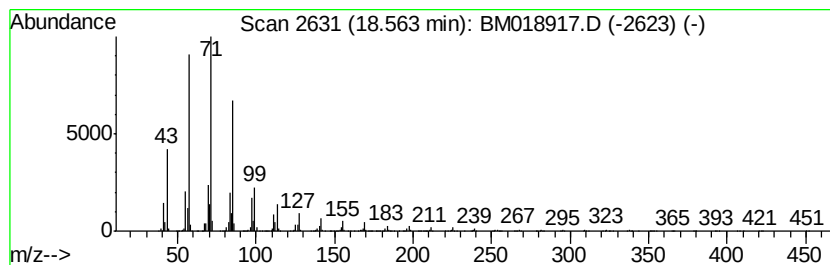
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TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 5 Heptadecane, 9-octyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.56	74.99 ng	9633020	Phenanthrene-d10	17.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
2		Eicosane	282	C20H42	000112-95-8	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Triaccontane	422	C30H62	000638-68-6	90
5		Tetratetracontane	619	C44H90	007098-22-8	87



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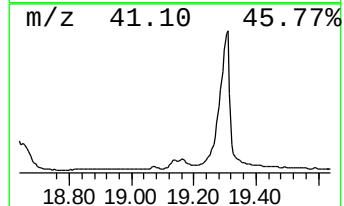
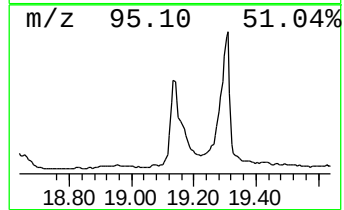
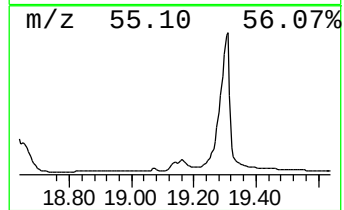
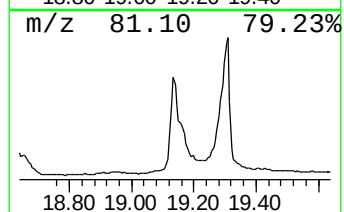
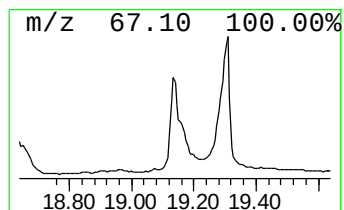
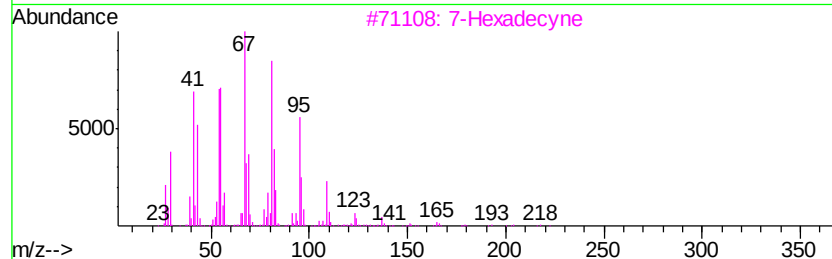
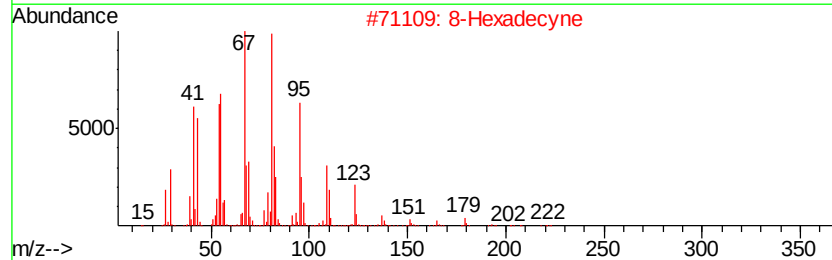
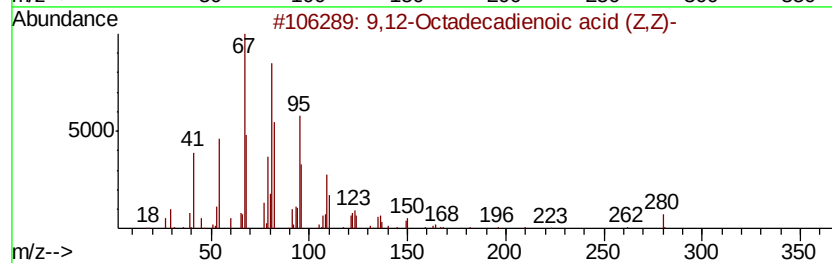
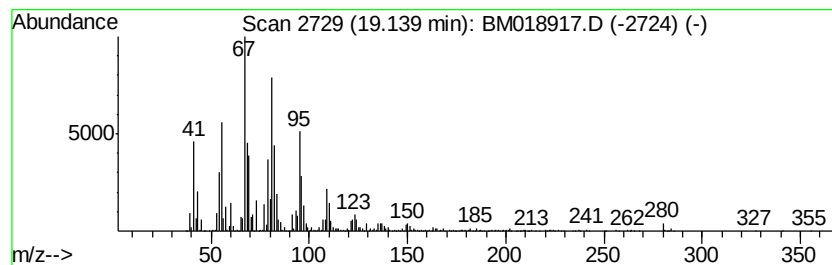
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9,12-Octadecadienoic acid (... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.14	19.56 ng	2512400	Phenanthrene-d10	17.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	98
2		8-Hexadecyne	222	C16H30	019781-86-3	91
3		7-Hexadecyne	222	C16H30	074685-28-2	86
4		3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	81
5		Cycloundecene, 1-methyl-	166	C12H22	088828-82-4	80



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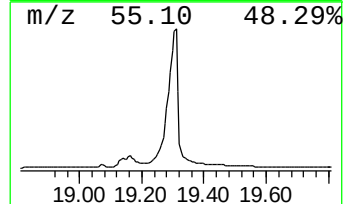
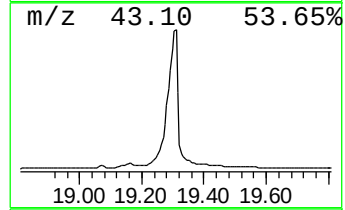
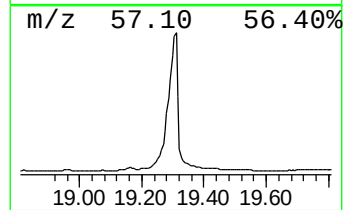
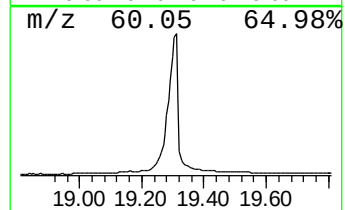
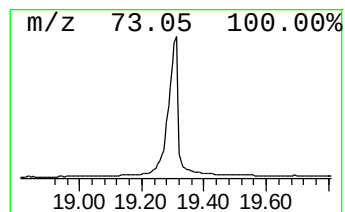
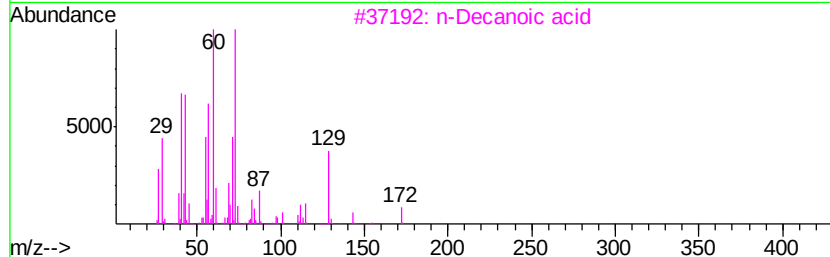
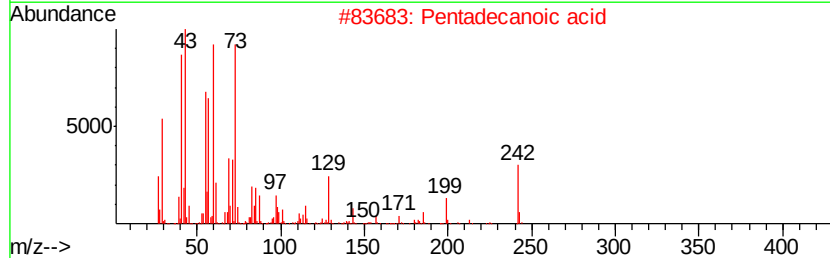
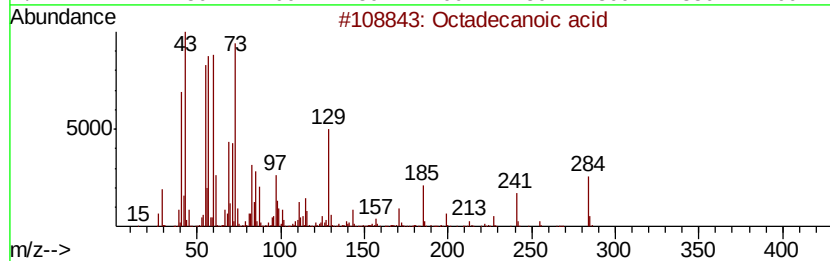
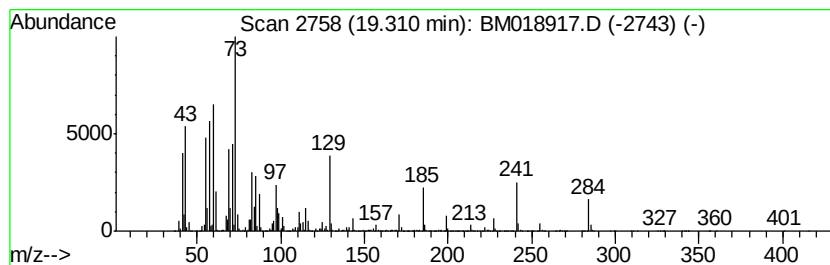
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.31	564.76 ng	78074900	Chrysene-d12	21.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	96
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3		n-Decanoic acid	172	C10H20O2	000334-48-5	58
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022519\
Data File : BM018917.D
Acq On : 25 Feb 2019 17:24
Operator : JU/SJ
Sample : K1597-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

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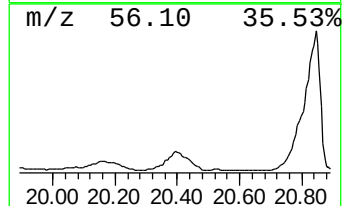
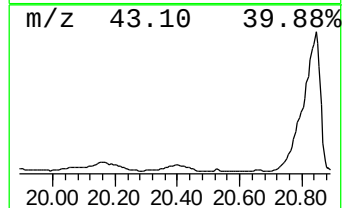
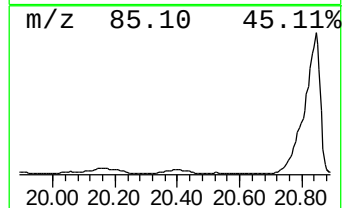
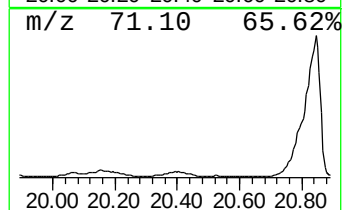
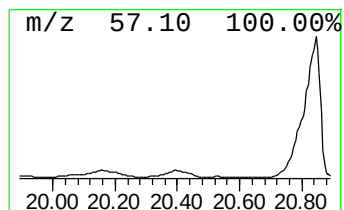
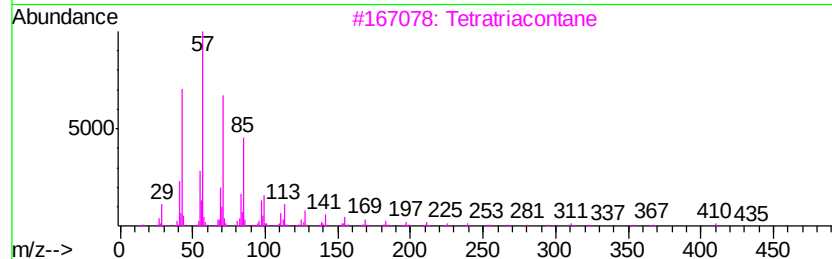
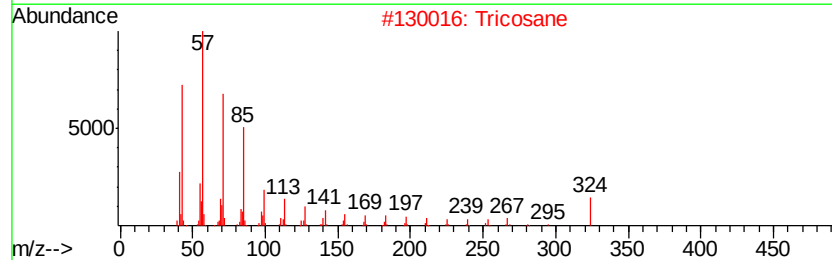
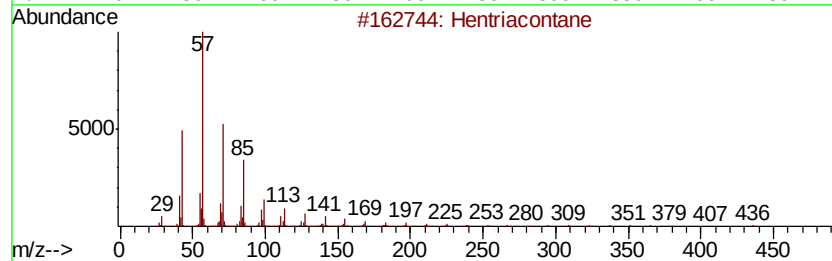
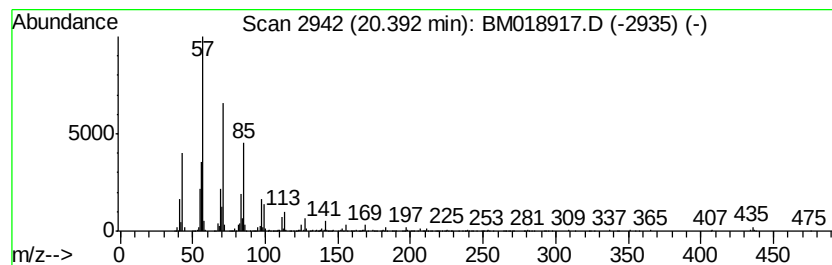
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Hentriacontane Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.39	44.98 ng	6217690	Chrysene-d12	21.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	92
2		Tricosane	324	C23H48	000638-67-5	89
3		Tetratriacontane	479	C34H70	014167-59-0	87
4		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
5		Hexacosane, 9-octyl-	479	C34H70	055429-83-9	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022519\
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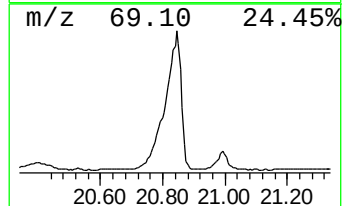
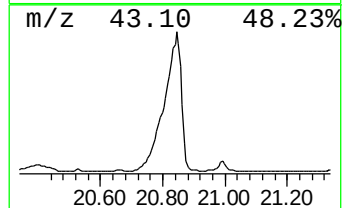
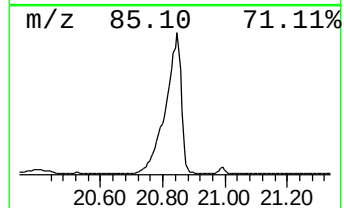
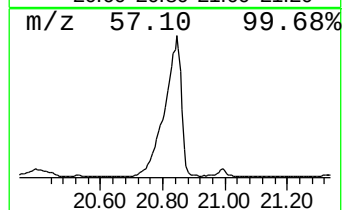
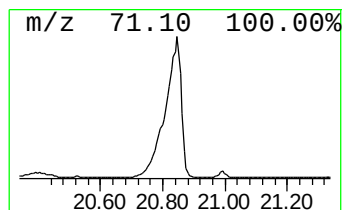
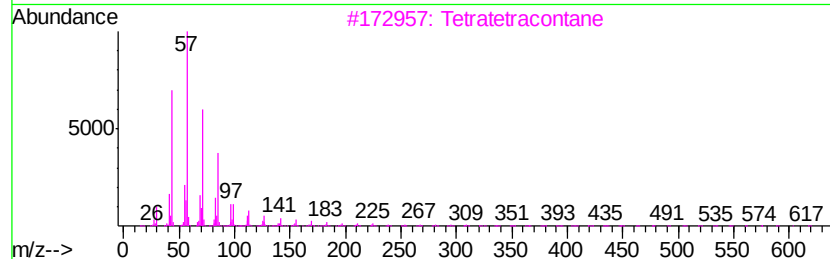
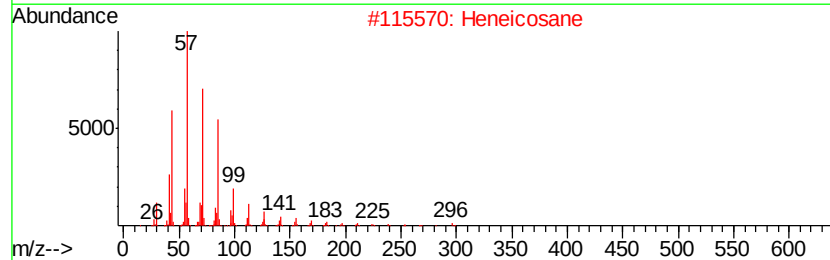
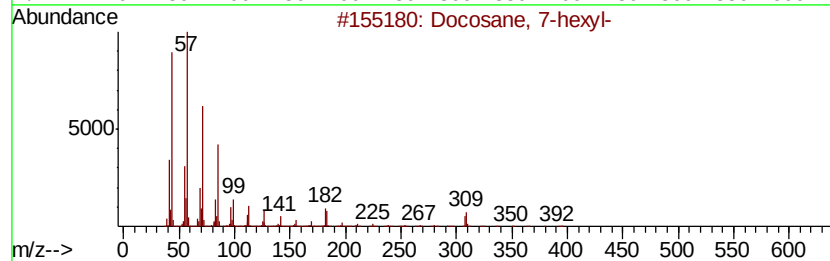
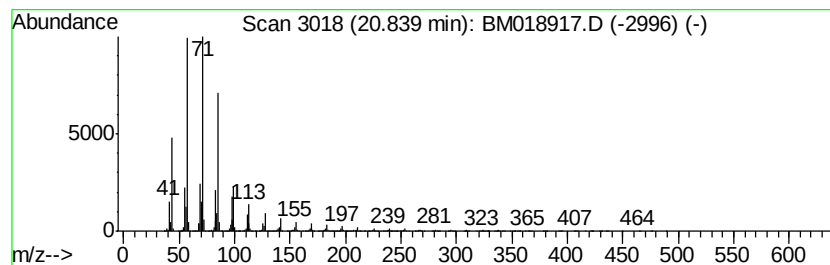
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Docosane, 7-hexyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.84	779.19 ng	107719000	Chrysene-d12	21.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 7-hexyl-	394	C28H58	055373-86-9	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		Tetratetracontane	619	C44H90	007098-22-8	74
4		Hexadecane	226	C16H34	000544-76-3	74
5		Tetracosane	338	C24H50	000646-31-1	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022519\
Data File : BM018917.D
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Sample : K1597-11
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Instrument :
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ClientSampleId :
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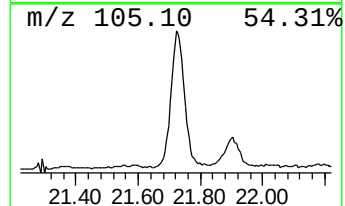
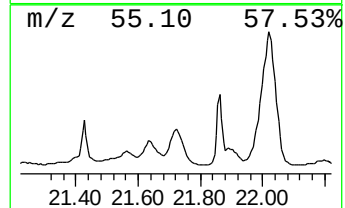
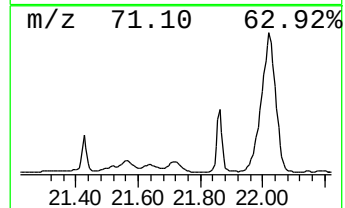
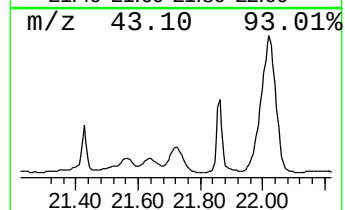
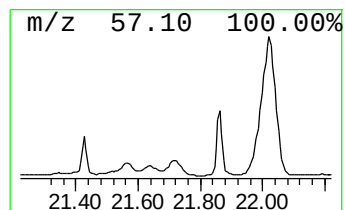
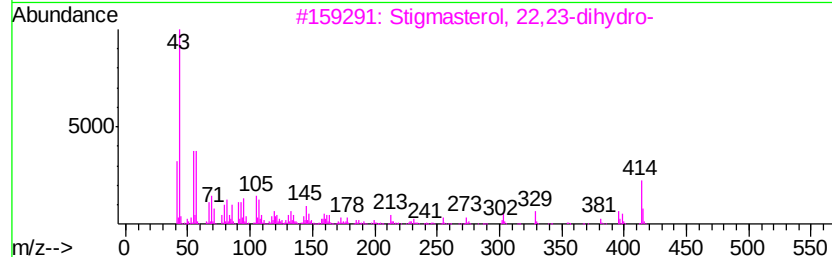
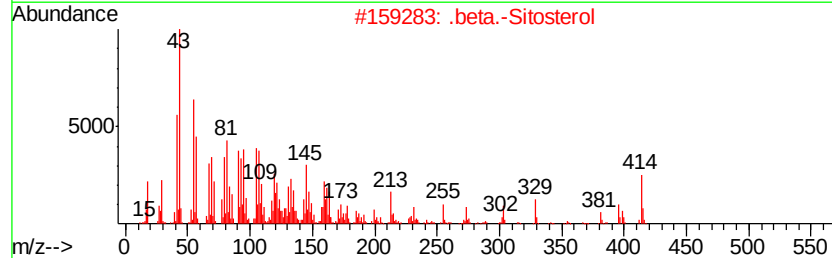
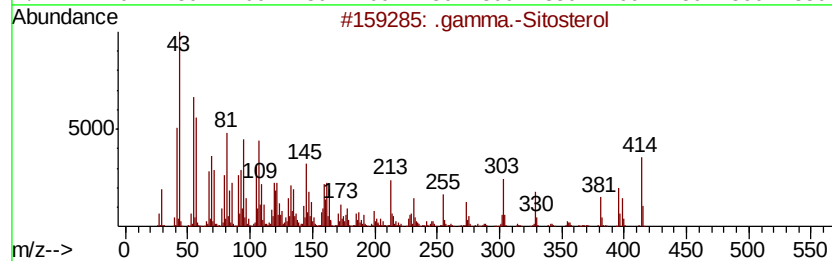
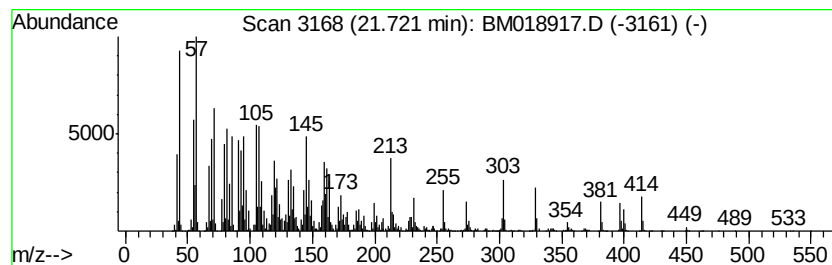
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 .gamma.-Sitosterol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.72	98.07 ng	13558000	Chrysene-d12	21.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2		.beta.-Sitosterol	414	C29H50O	000083-46-5	93
3		Stigmasterol, 22,23-dihydro-	414	C29H50O	1000214-20-7	68
4		Campesterol	400	C28H48O	000474-62-4	43
5		Ergost-7-en-3-ol, (3.beta.)-	400	C28H48O	026047-31-4	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022519\
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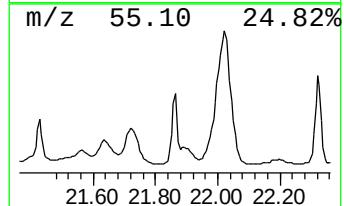
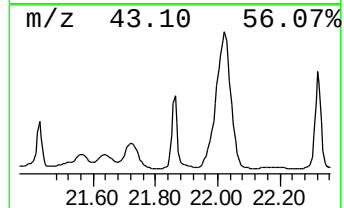
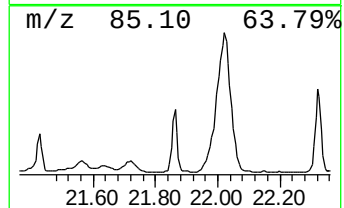
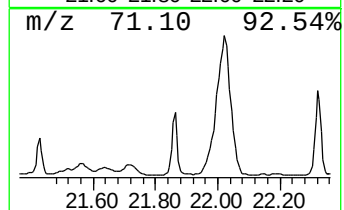
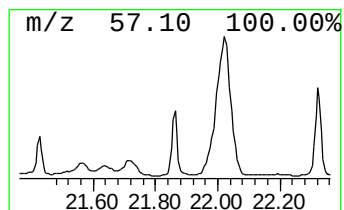
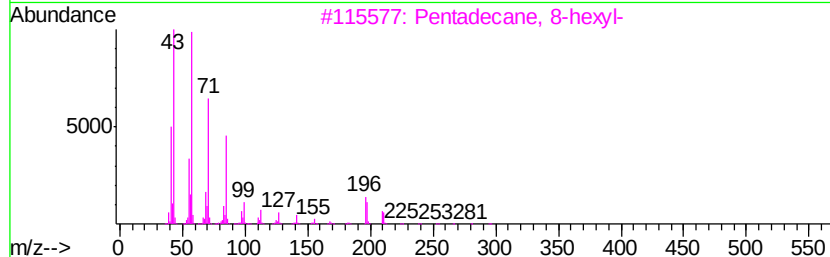
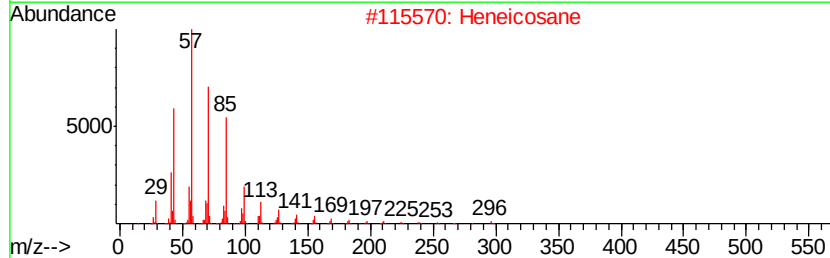
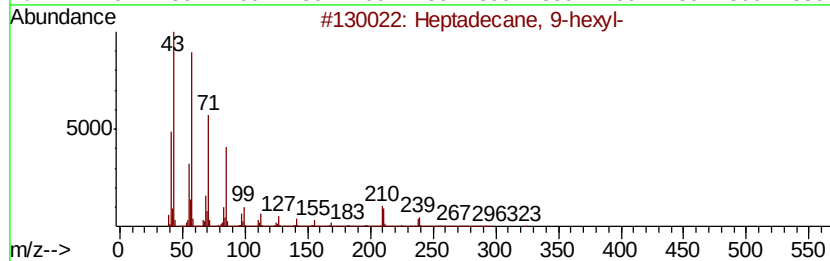
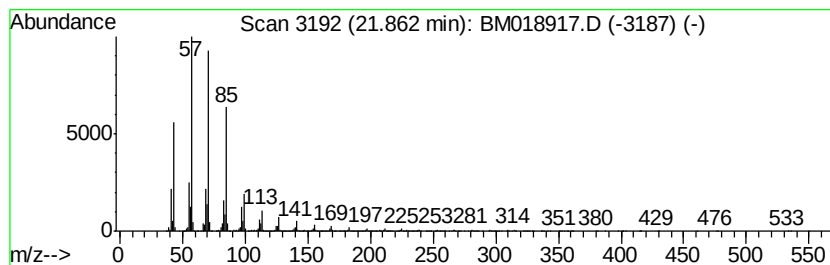
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Heptadecane, 9-hexyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.86	53.32 ng	7371140	Chrysene-d12	21.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
4		Heptacosane	380	C27H56	000593-49-7	90
5		Nonadecane	268	C19H40	000629-92-5	90



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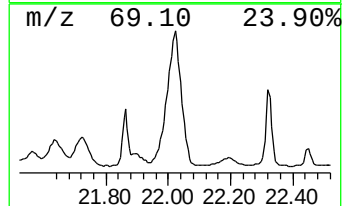
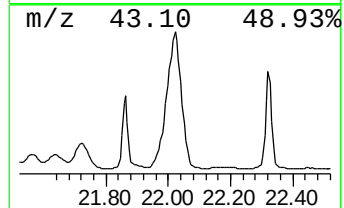
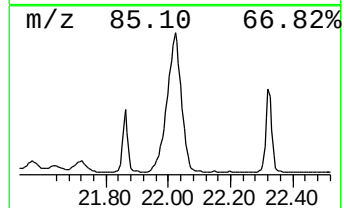
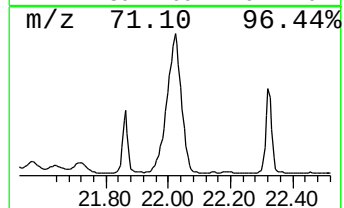
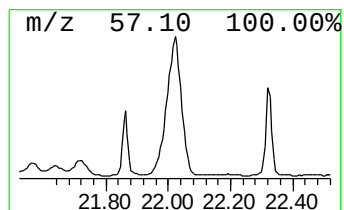
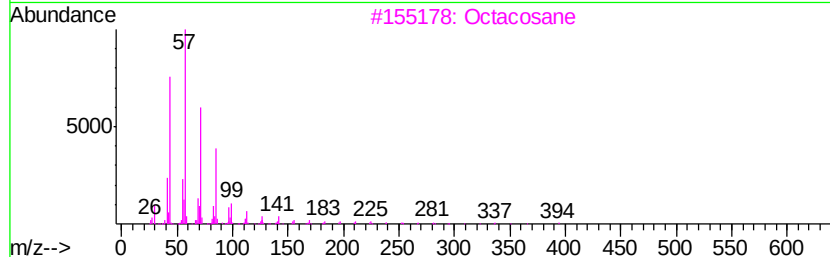
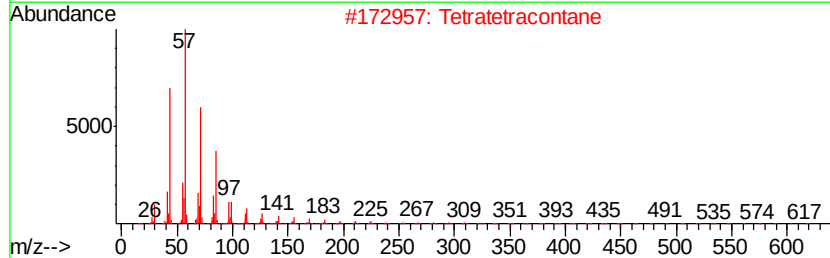
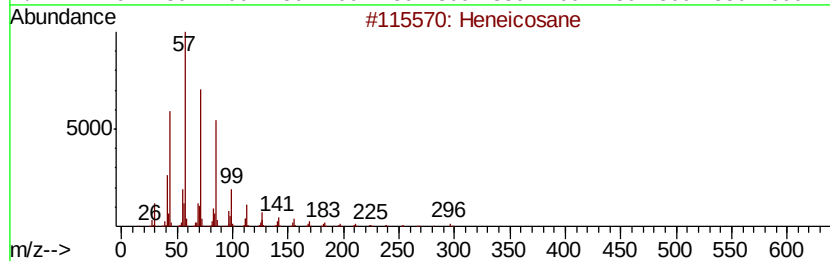
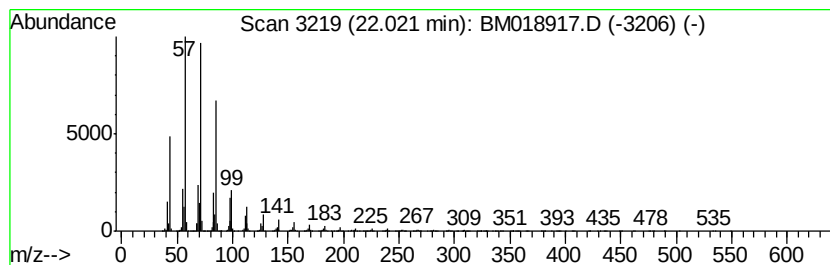
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.02	309.19 ng	42743500	Chrysene-d12	21.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Tetratetracontane	619	C44H90	007098-22-8	87
3		Octacosane	394	C28H58	000630-02-4	87
4		Nonadecane	268	C19H40	000629-92-5	74
5		Tetratriacontane	479	C34H70	014167-59-0	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022519\
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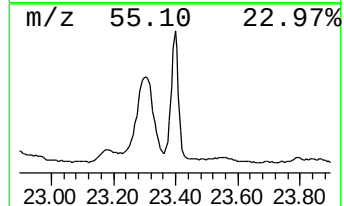
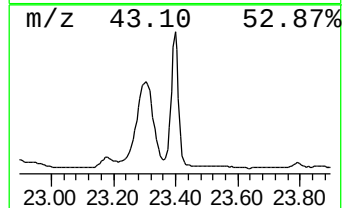
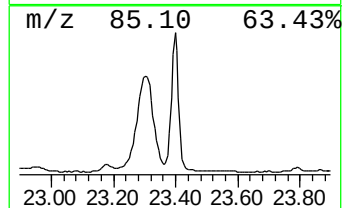
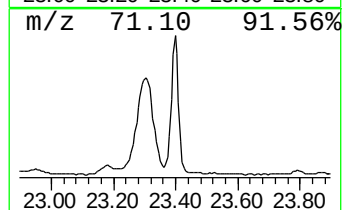
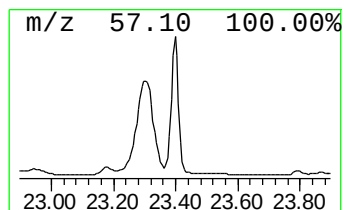
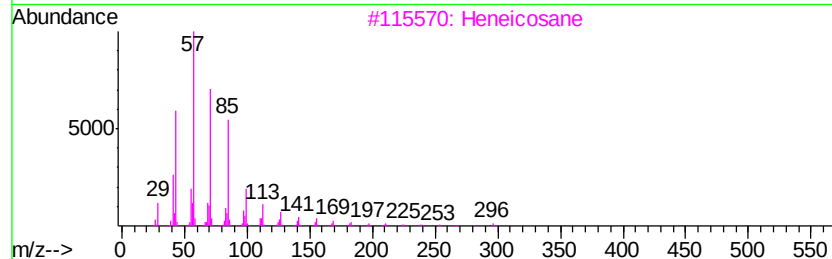
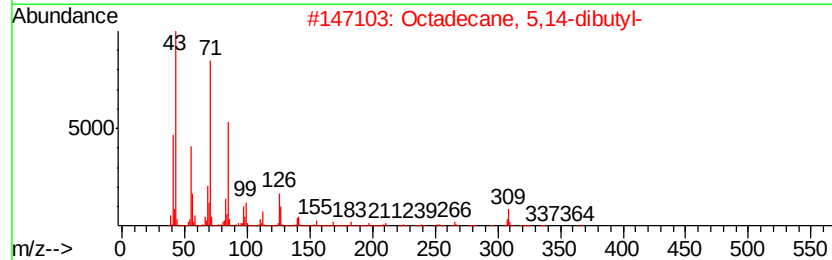
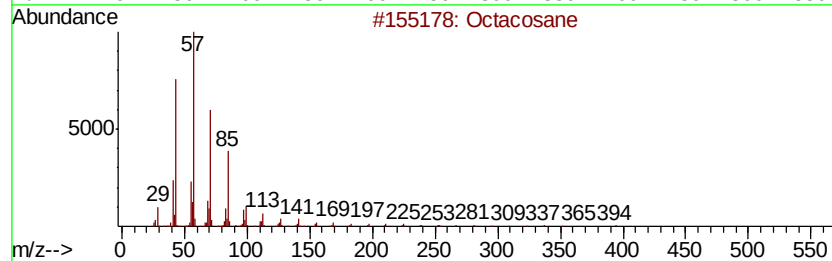
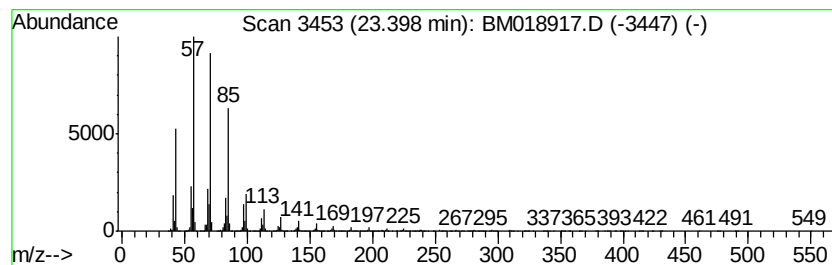
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 Octacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.40	72.70 ng	12810800	Perylene-d12	23.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	95
2		Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	90
5		Heptacosane	380	C27H56	000593-49-7	87



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Sample : K1597-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-22

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
unknown7.23	7.23	116.6	ng	7827760	1	7.69	1342640	20.0
n-Hexadecanoic acid	18.03	585.4	ng	75200200	4	17.09	2569210	20.0
Heptacosane	18.40	105.0	ng	13483000	4	17.09	2569210	20.0
Heptadecane, 9-oc...	18.56	75.0	ng	9633020	4	17.09	2569210	20.0
9,12-Octadecadien...	19.14	19.6	ng	2512400	4	17.09	2569210	20.0
Octadecanoic acid	19.31	564.8	ng	78074900	5	21.29	2764880	20.0
Hentriacontane	20.39	45.0	ng	6217690	5	21.29	2764880	20.0
Docosane, 7-hexyl-	20.84	779.2	ng	107719000	5	21.29	2764880	20.0
.gamma.-Sitosterol	21.72	98.1	ng	13558000	5	21.29	2764880	20.0
Heptadecane, 9-he...	21.86	53.3	ng	7371140	5	21.29	2764880	20.0
Heneicosane	22.02	309.2	ng	42743500	5	21.29	2764880	20.0
Octacosane	23.40	72.7	ng	12810800	6	23.54	3524070	20.0