

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
 Data File : BM018302.D
 Acq On : 19 Dec 2018 18:34
 Operator : JU/SJ
 Sample : J6465-02
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 EB01_0-2

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-BM121518.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	4.681	300	305	310	rBV	66302	89992	2.10%	0.197%
2	5.122	374	380	394	rBV	1574620	2229342	52.05%	4.870%
3	6.687	639	646	662	rBV	1486488	2412852	56.33%	5.271%
4	7.028	697	704	717	rBV	1560488	2446860	57.13%	5.346%
5	7.487	774	782	791	rBV	345428	552335	12.90%	1.207%
6	7.798	828	835	846	rVB	1169081	1809623	42.25%	3.953%
7	8.645	971	979	988	rBV	811009	1387712	32.40%	3.032%
8	10.251	1245	1252	1262	rBV	393243	680882	15.90%	1.488%
9	12.751	1670	1677	1688	rBV	1896166	2772819	64.74%	6.058%
10	13.621	1818	1825	1835	rBV	96335	148451	3.47%	0.324%
11	14.145	1908	1914	1925	rVB2	550963	824088	19.24%	1.800%
12	14.598	1985	1991	1996	rBV4	27187	46399	1.08%	0.101%
13	15.651	2164	2170	2181	rBV	1457341	2162149	50.48%	4.724%
14	16.333	2280	2286	2289	rBV3	54199	92129	2.15%	0.201%
15	16.468	2290	2309	2310	rBV5	159257	586250	13.69%	1.281%
16	16.910	2378	2384	2392	rBV	598427	899639	21.00%	1.965%
17	17.692	2512	2517	2521	rBV5	28722	53366	1.25%	0.117%
18	17.827	2532	2540	2557	rBV	1601253	2474719	57.78%	5.406%
19	18.621	2661	2675	2685	rBV3	490040	1733627	40.48%	3.787%
20	18.692	2685	2687	2695	rVB7	36688	48638	1.14%	0.106%
21	18.968	2730	2734	2736	rBV2	65823	92064	2.15%	0.201%
22	18.998	2736	2739	2748	rVB6	82460	150964	3.52%	0.330%
23	19.115	2754	2759	2775	rBV	774380	1249434	29.17%	2.730%
24	19.562	2830	2835	2844	rVB	2799721	3266255	76.26%	7.136%
25	19.815	2870	2878	2887	rBV2	887059	1913903	44.69%	4.181%
26	20.021	2906	2913	2929	rBV	536381	1493526	34.87%	3.263%
27	20.386	2972	2975	2982	rVB4	53383	94168	2.20%	0.206%
28	20.703	3023	3029	3040	rBV	1033561	2001408	46.73%	4.372%
29	20.856	3051	3055	3065	rVB	303531	398325	9.30%	0.870%
30	21.133	3097	3102	3107	rBV	796370	1101057	25.71%	2.405%
31	21.292	3127	3129	3133	rVB3	65944	64659	1.51%	0.141%
32	21.433	3147	3153	3162	rBV	975511	1795765	41.93%	3.923%
33	21.715	3199	3201	3204	rBV2	73371	76824	1.79%	0.168%
34	22.133	3267	3272	3281	rVB	739106	1376938	32.15%	3.008%

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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-BM121518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	22.280	3292	3297	3304	rVB	3358573	4283049	100.00%	9.357%
36	22.644	3356	3359	3364	rVB	144426	191693	4.48%	0.419%
37	22.909	3399	3404	3412	rVB	354411	736925	17.21%	1.610%
38	23.180	3446	3450	3456	rVB	161337	258811	6.04%	0.565%
39	23.291	3464	3469	3481	rVB	654376	1157142	27.02%	2.528%
40	23.780	3547	3552	3560	rVB2	310615	618335	14.44%	1.351%

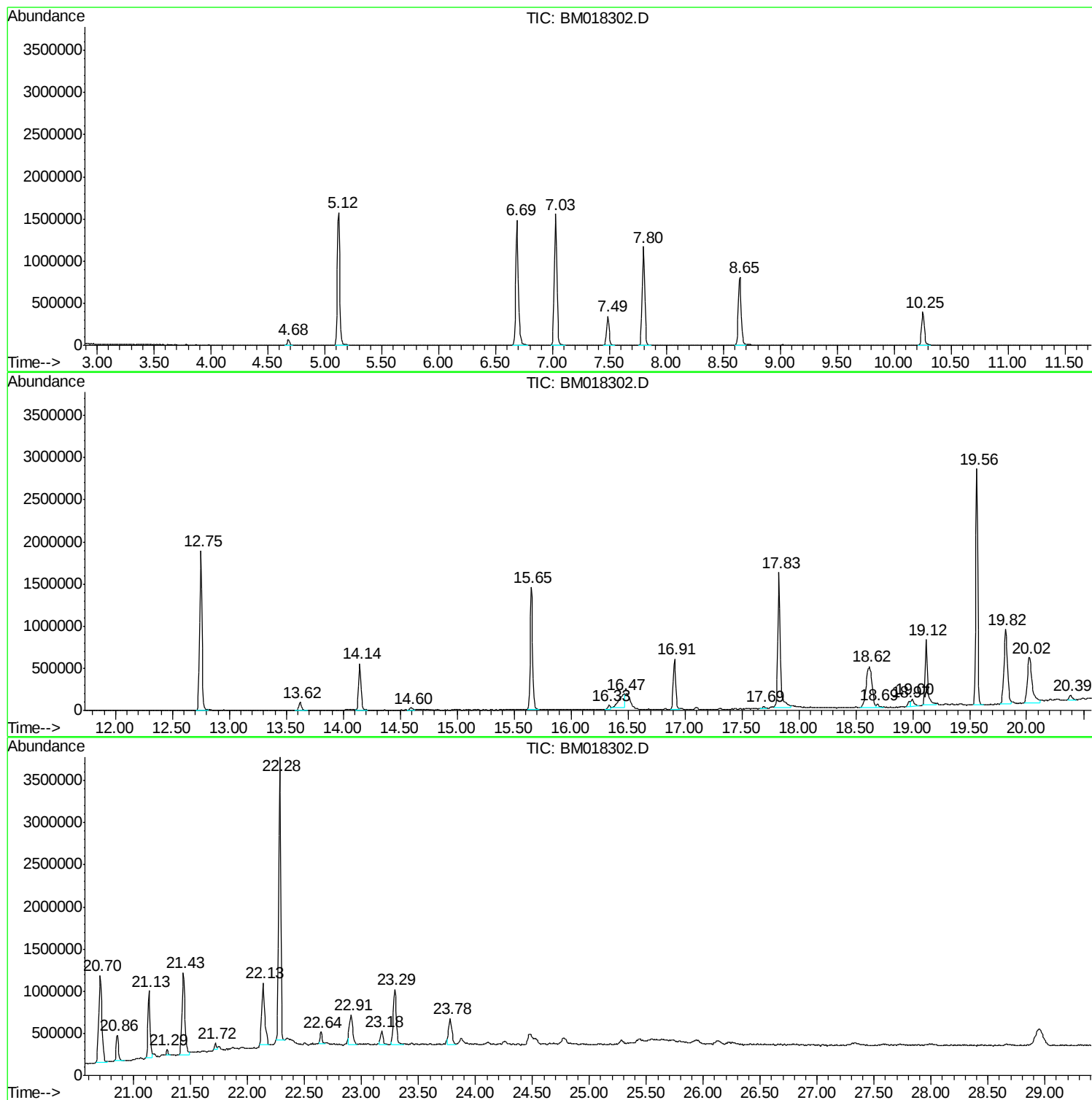
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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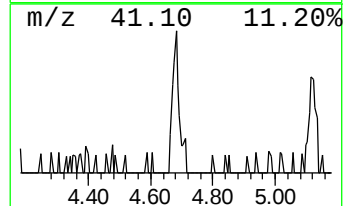
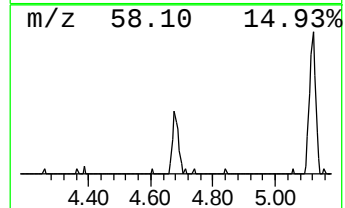
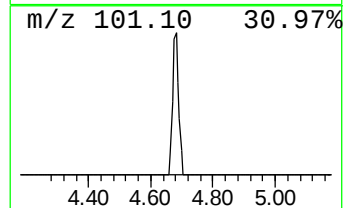
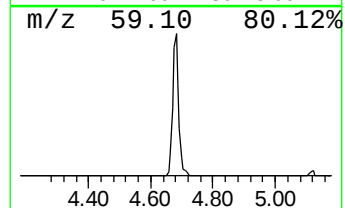
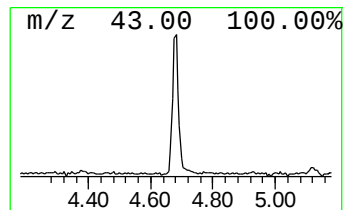
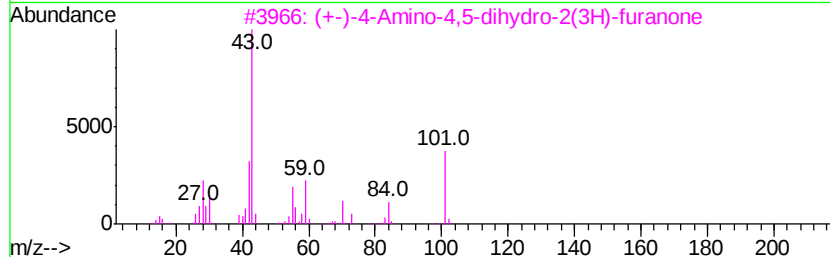
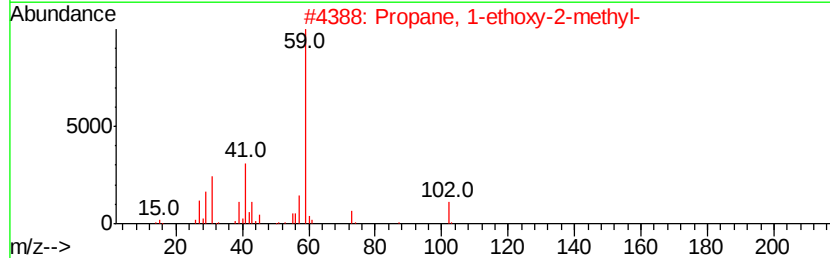
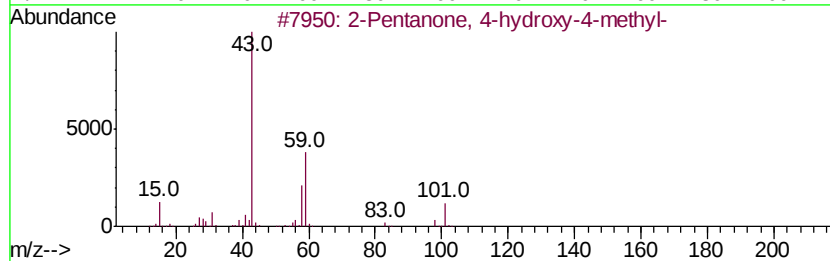
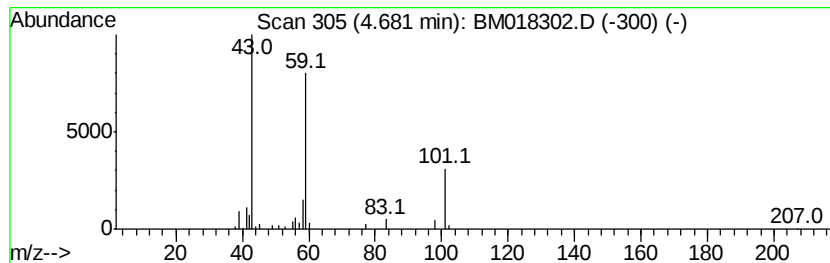
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	3.26 ng	89992	1,4-Dichlorobenzene-d4	7.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	38
3			(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	35
4			3-Pentanol	88	C5H12O	000584-02-1	28
5			t-Butyl ethyl ether	102	C6H14O	1000118-18-4	25



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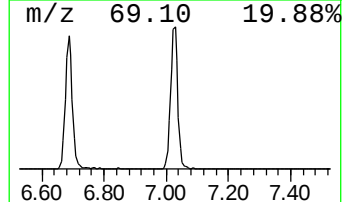
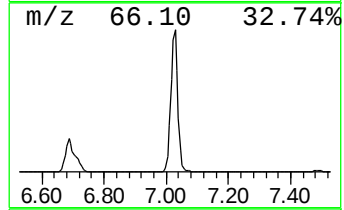
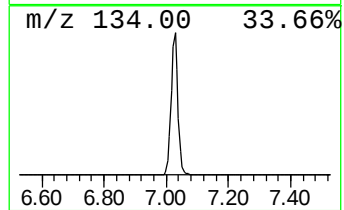
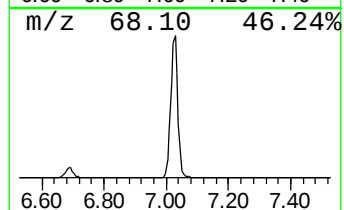
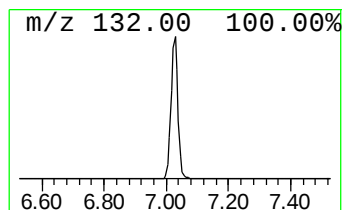
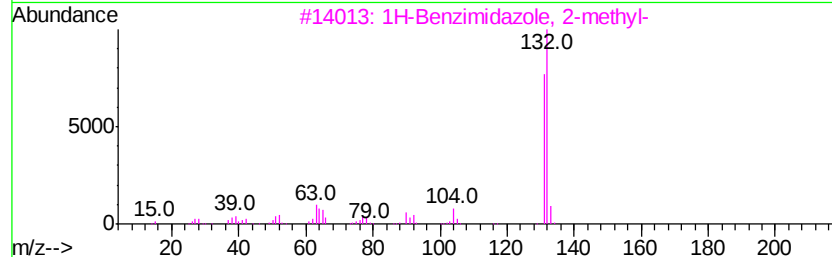
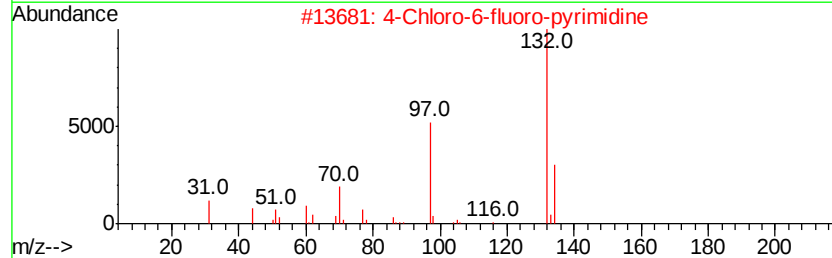
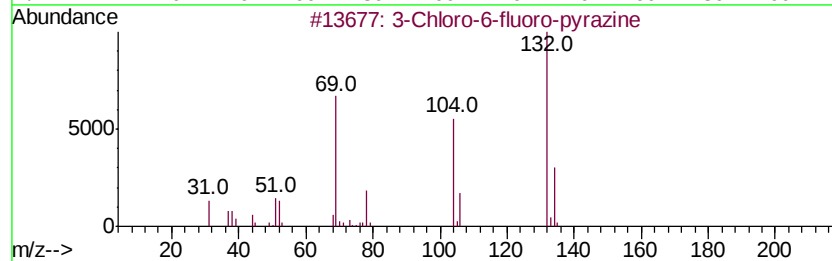
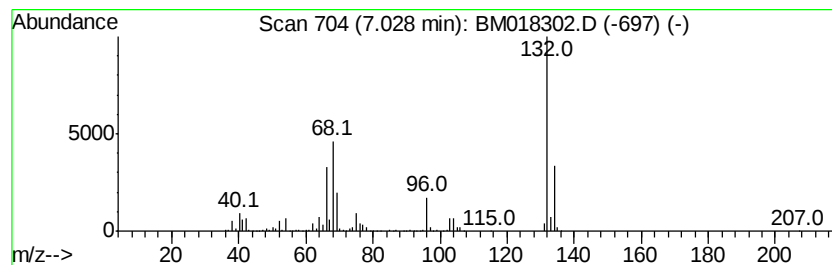
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Peak Number 2 unknown7.03 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	88.60 ng	2446860	1,4-Dichlorobenzene-d4	7.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12



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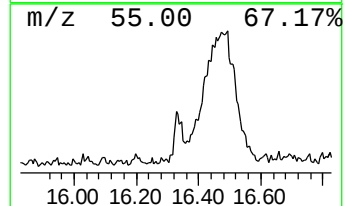
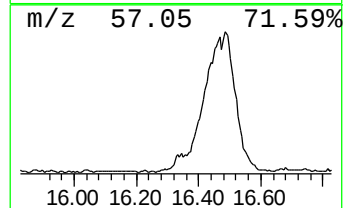
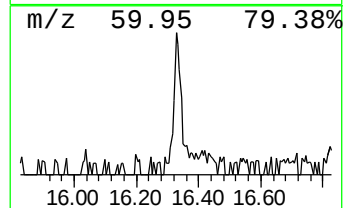
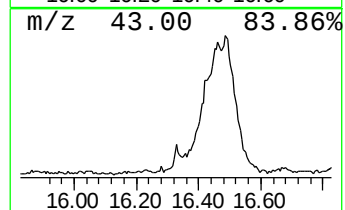
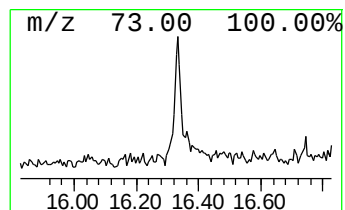
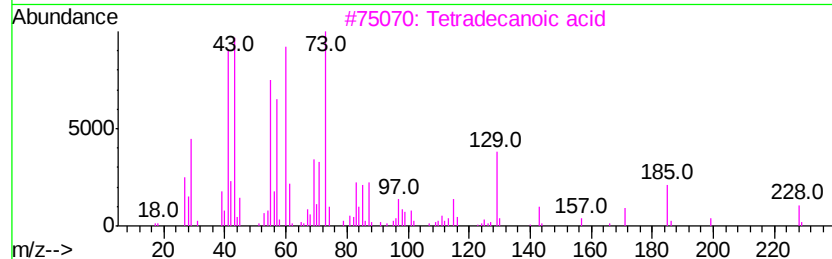
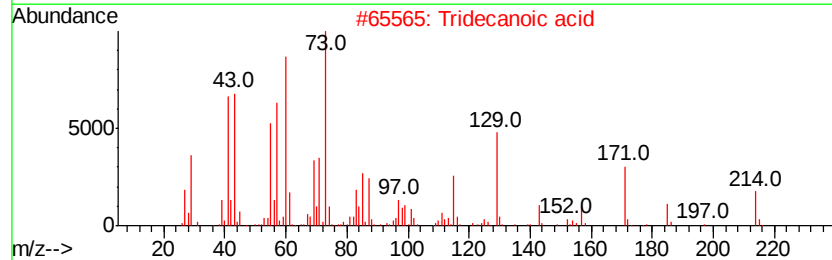
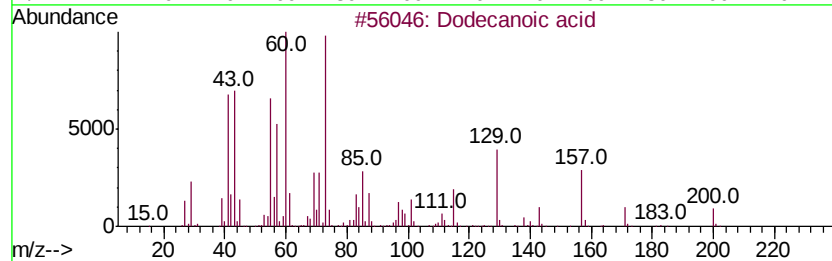
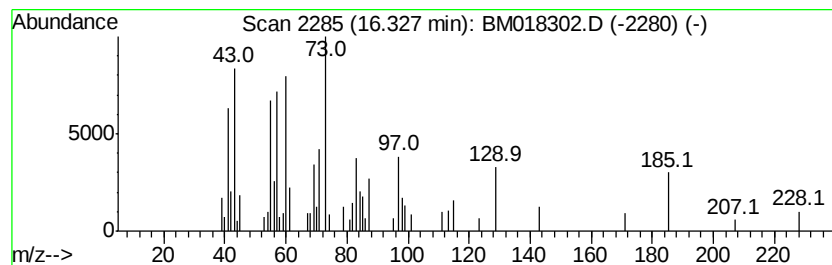
Instrument :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown16.33 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.33	2.05 ng	92129	Phenanthrene-d10		16.91
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	47
2	Tridecanoic acid	214	C13H26O2	000638-53-9	47
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	43
4	n-Decanoic acid	172	C10H20O2	000334-48-5	38
5	Lactose	342	C12H22O11	000063-42-3	35



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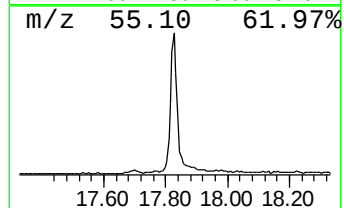
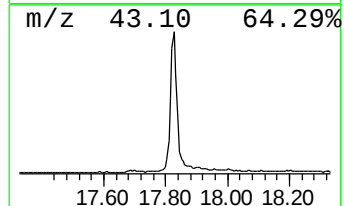
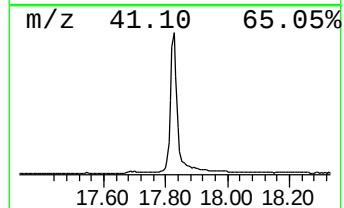
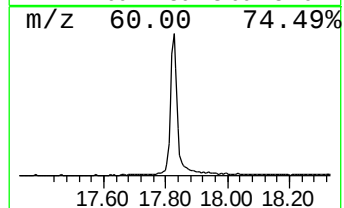
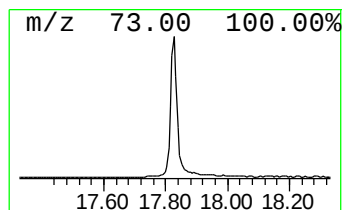
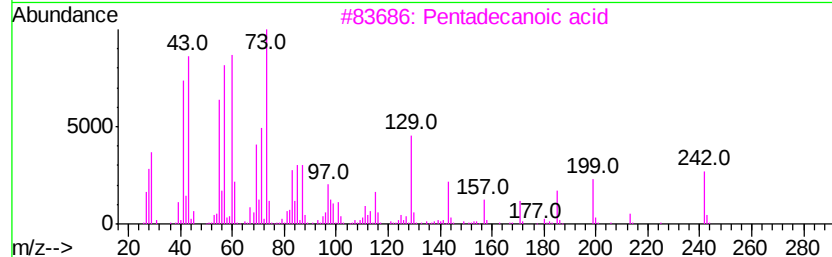
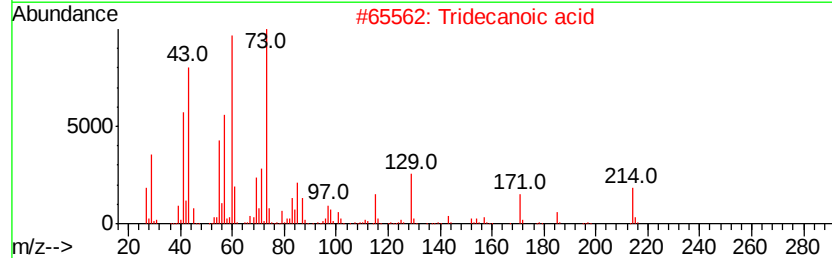
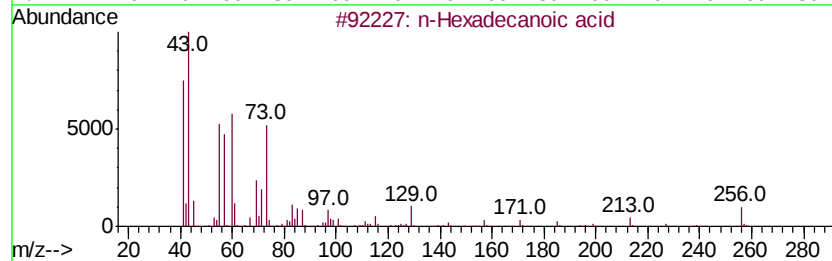
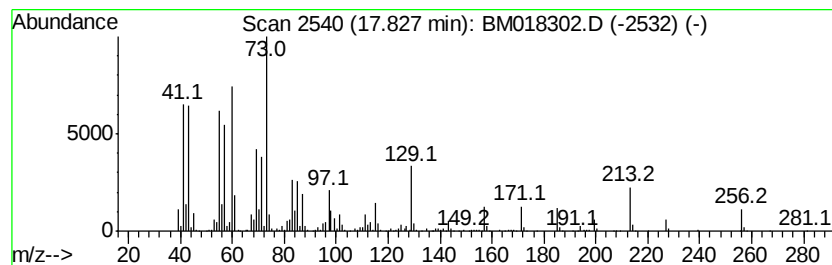
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	55.02 ng	2474720	Phenanthrene-d10	16.91

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	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Estra-1,3,5(10)-trien-17.β.-ol	256	C18H24O	002529-64-8	30
5	Eicosane	282	C20H42	000112-95-8	11



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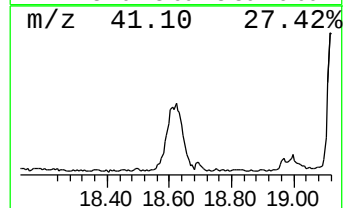
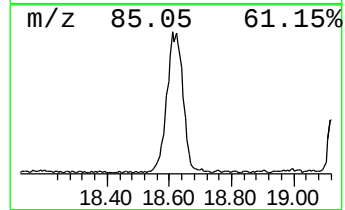
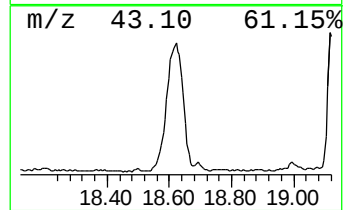
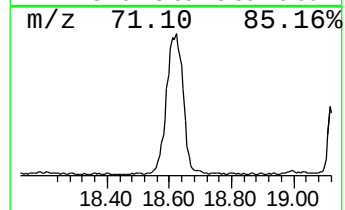
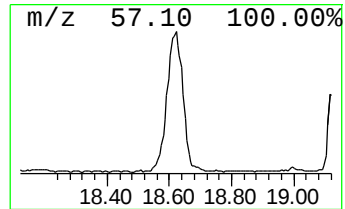
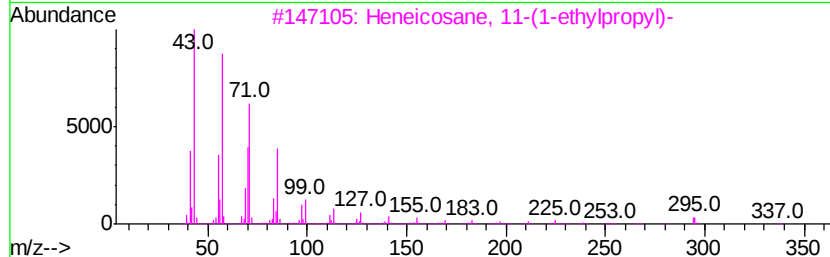
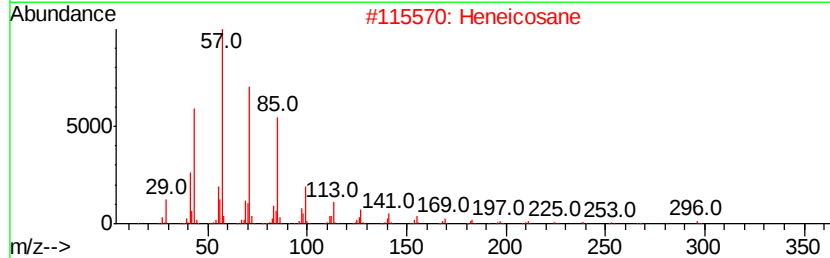
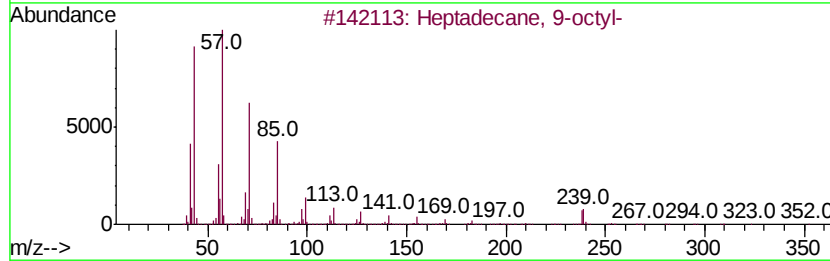
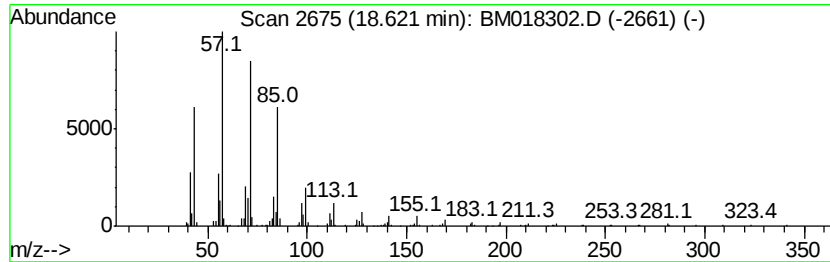
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.62	38.54 ng	1733630	Phenanthrene-d10	16.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4		Heptadecane	240	C17H36	000629-78-7	90
5		Octadecane, 2-methyl-	268	C19H40	001560-88-9	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018302.D
Acq On : 19 Dec 2018 18:34
Operator : JU/SJ
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Misc :
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ClientSampleId :
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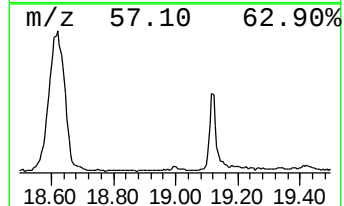
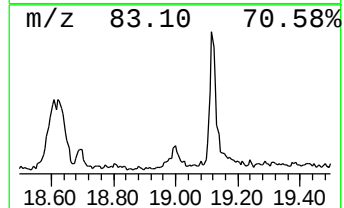
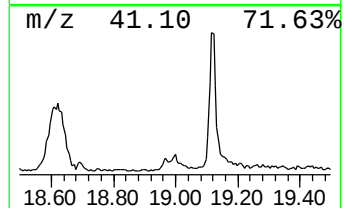
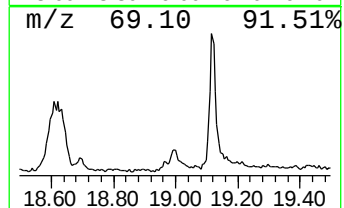
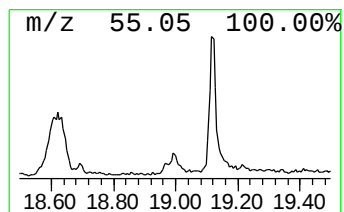
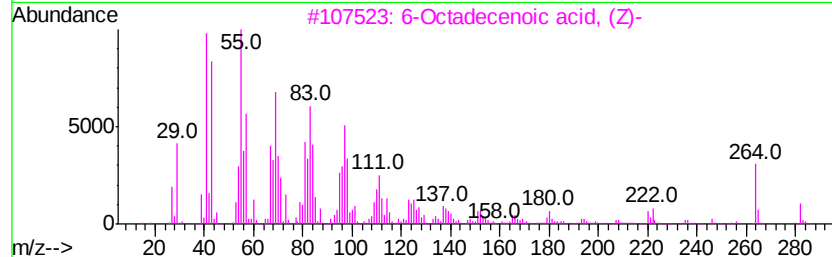
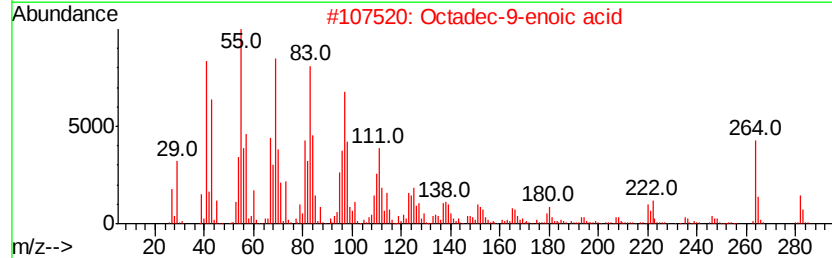
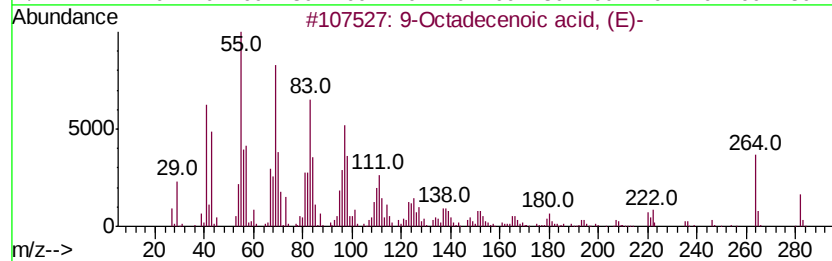
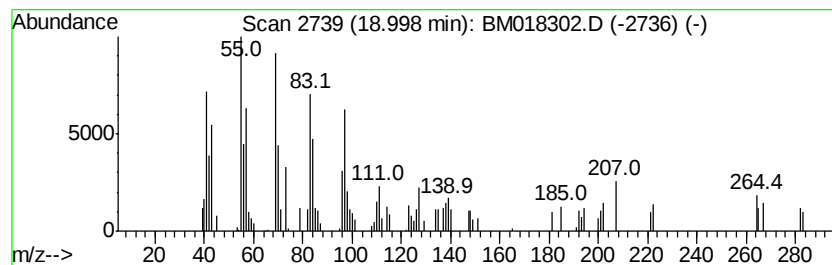
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenoic acid, (E)- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.00	3.36 ng	150964	Phenanthrene-d10	16.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	86
2		Octadec-9-enoic acid	282	C18H34O2	1000190-13-7	74
3		6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	66
4		14-Pentadecenoic acid	240	C15H28O2	017351-34-7	58
5		1-Decene	140	C10H20	000872-05-9	55



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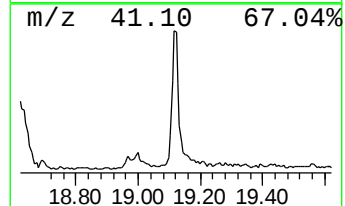
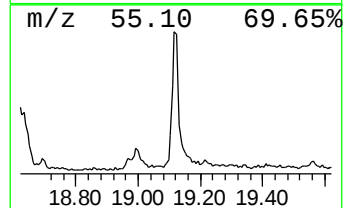
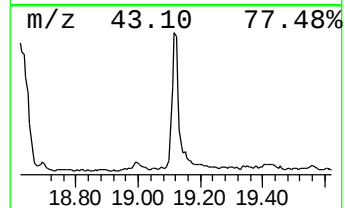
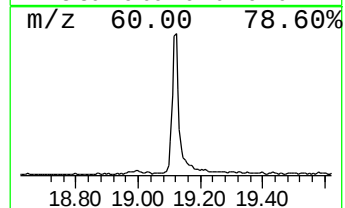
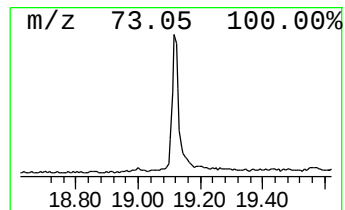
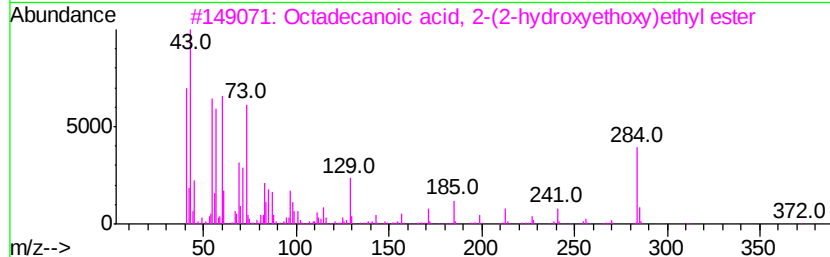
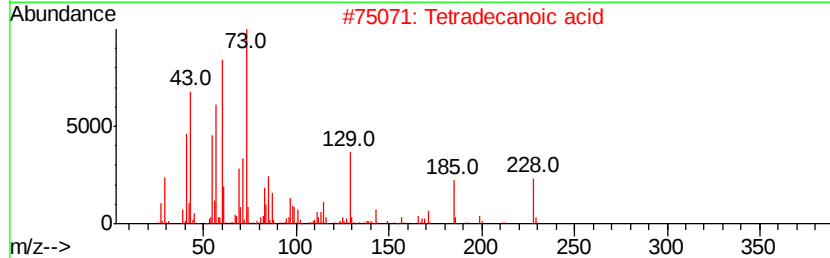
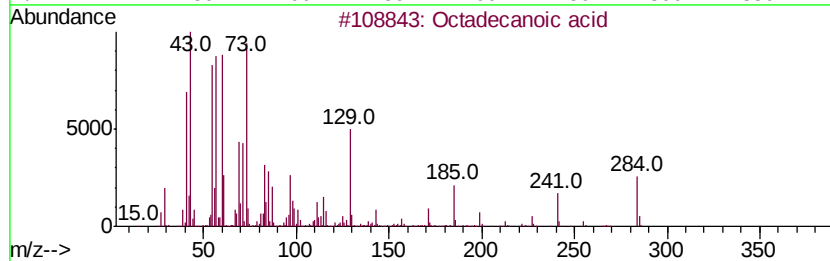
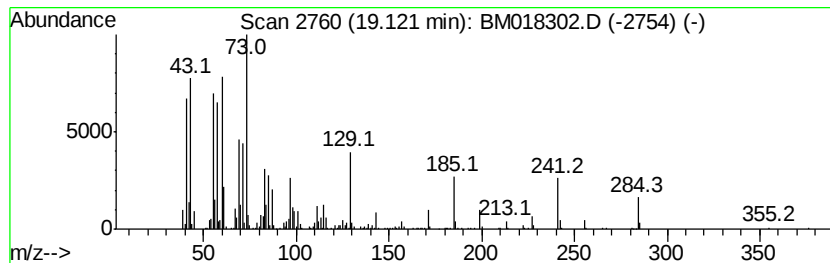
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.12	22.70 ng	1249430	Chrysene-d12	21.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	72
4		Tridecanoic acid	214	C13H26O2	000638-53-9	70
5		n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018302.D
Acq On : 19 Dec 2018 18:34
Operator : JU/SJ
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Misc :
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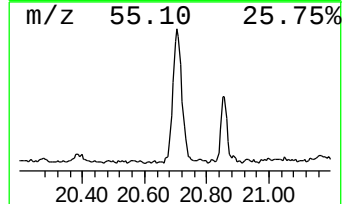
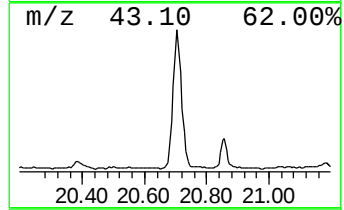
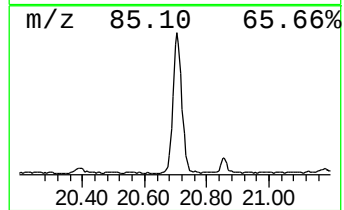
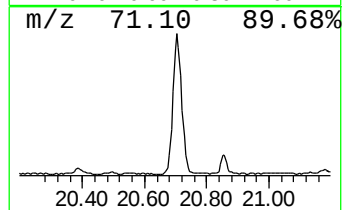
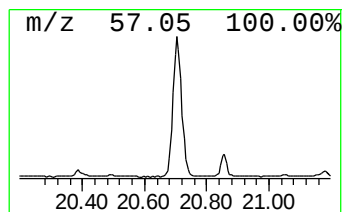
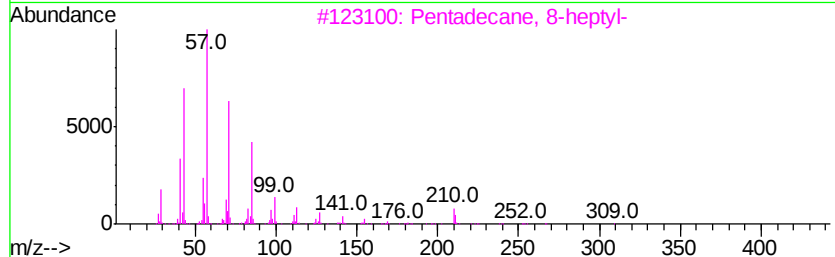
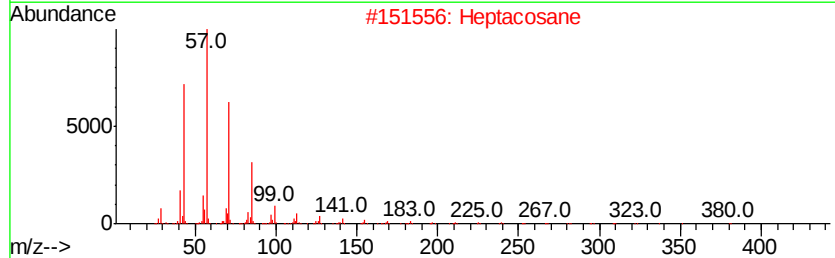
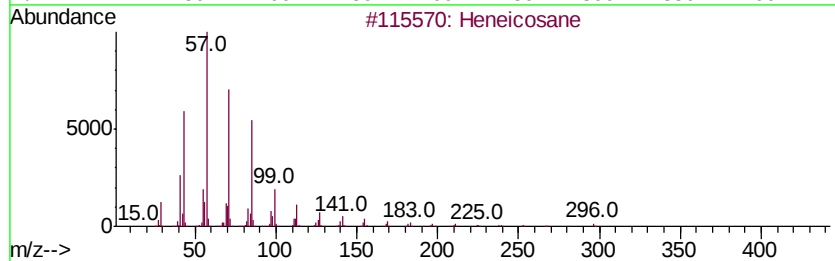
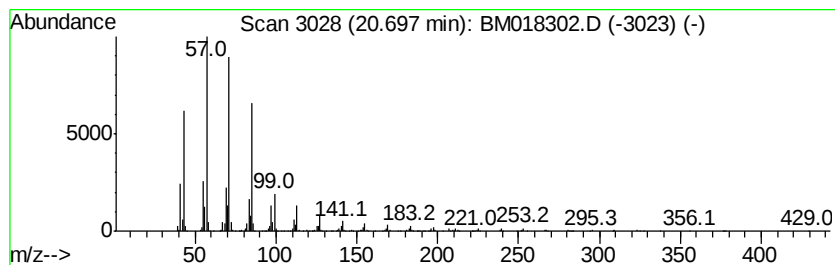
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.70	36.35 ng	2001410	Chrysene-d12	21.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
4		Octacosane	394	C28H58	000630-02-4	87
5		Tetracosane	338	C24H50	000646-31-1	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018302.D
Acq On : 19 Dec 2018 18:34
Operator : JU/SJ
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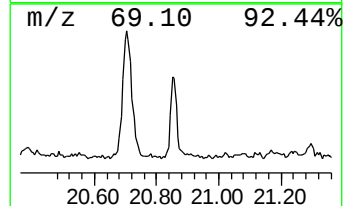
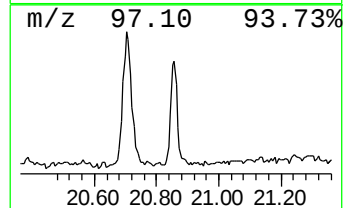
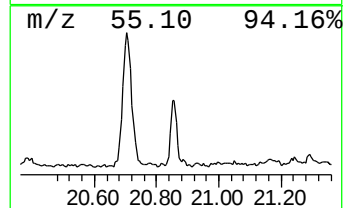
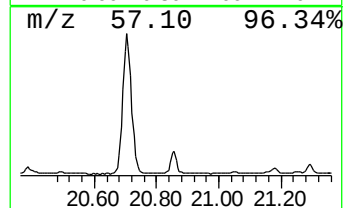
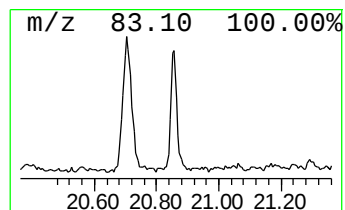
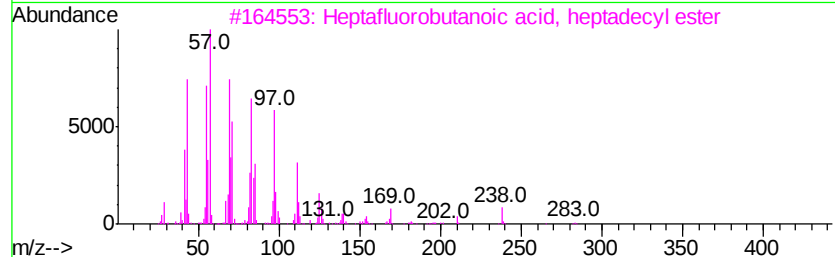
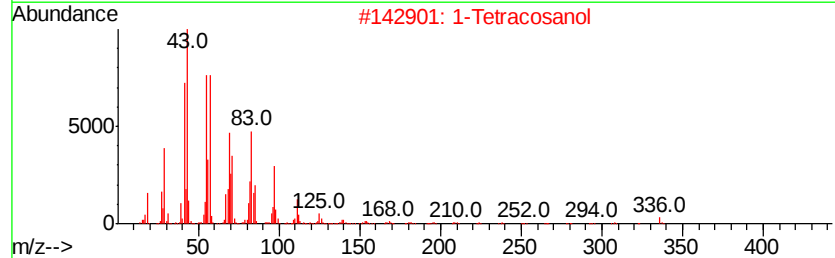
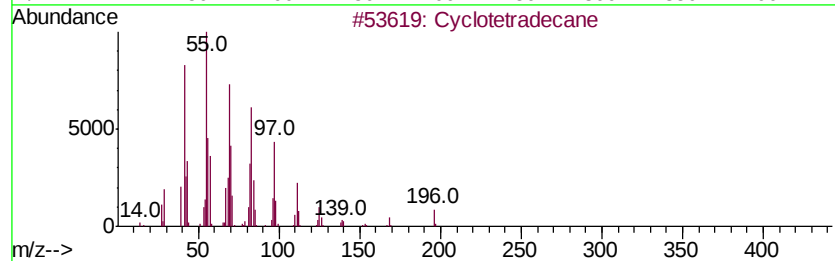
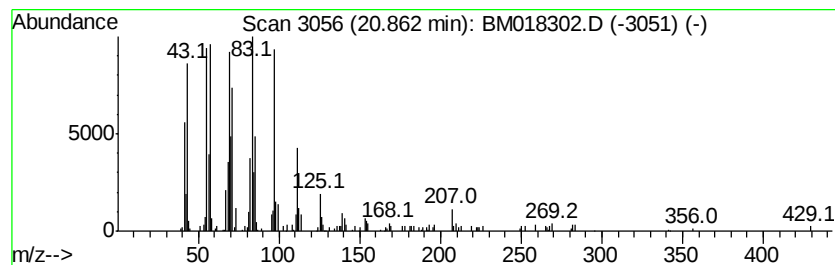
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Cyclotetradecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	7.24 ng	398325	Chrysene-d12	21.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclotetradecane	196	C14H28	000295-17-0	91
2		1-Tetracosanol	354	C24H50O	000506-51-4	90
3		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	87
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87
5		1-Octadecanol	270	C18H38O	000112-92-5	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018302.D
Acq On : 19 Dec 2018 18:34
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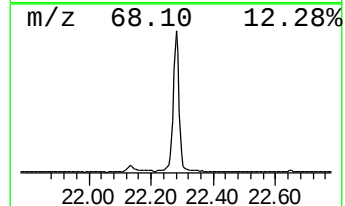
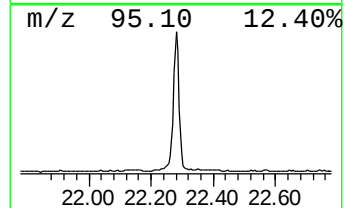
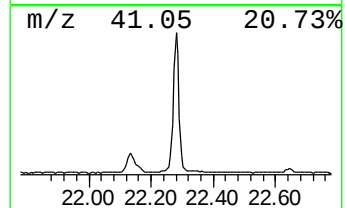
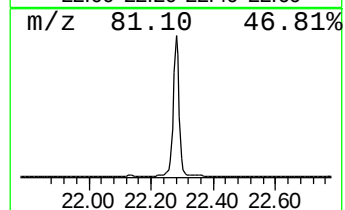
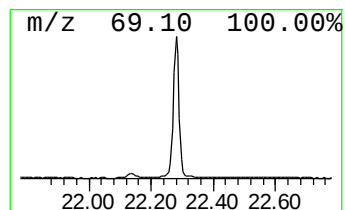
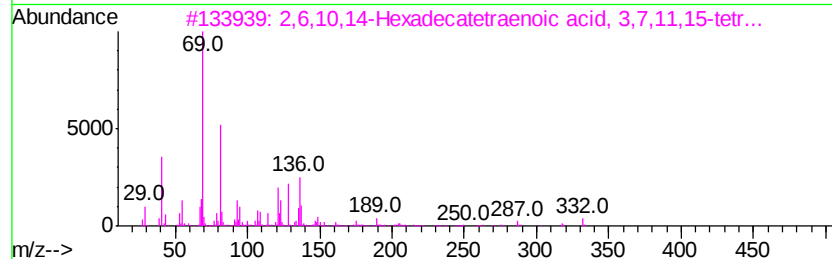
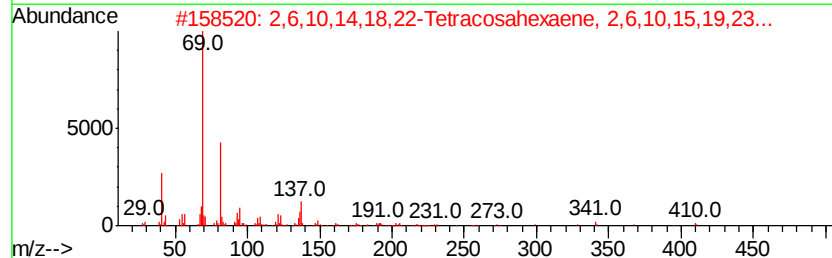
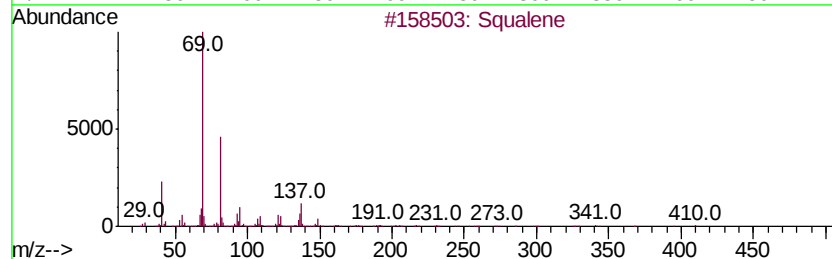
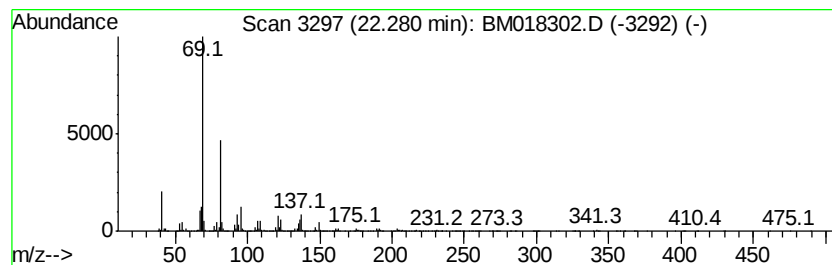
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	74.03 ng	4283050	Perylene-d12	23.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	83
4		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	74
5		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
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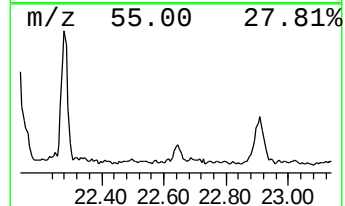
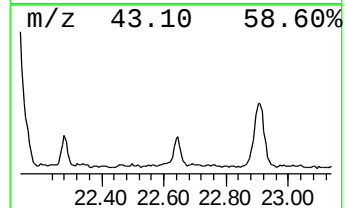
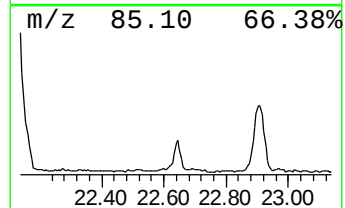
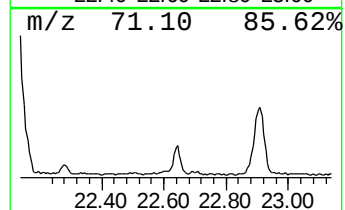
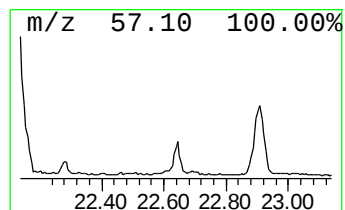
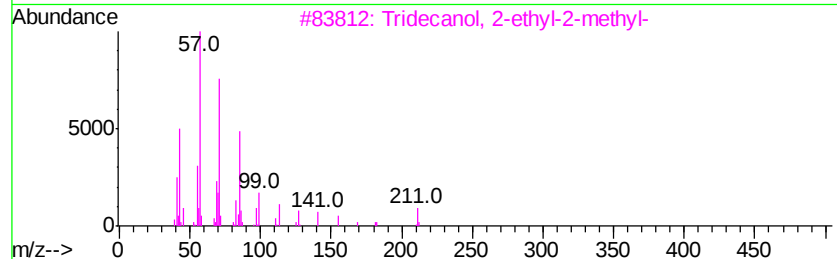
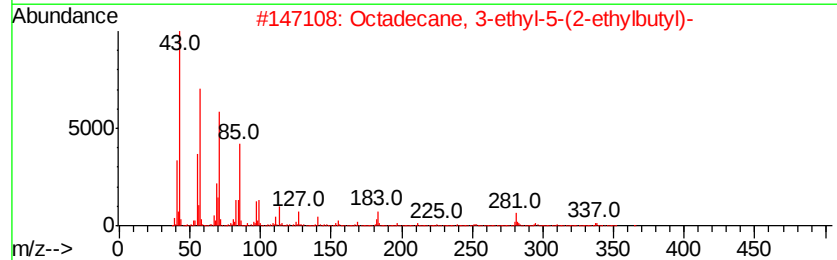
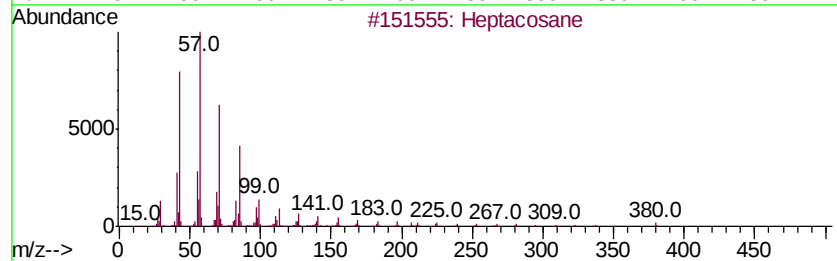
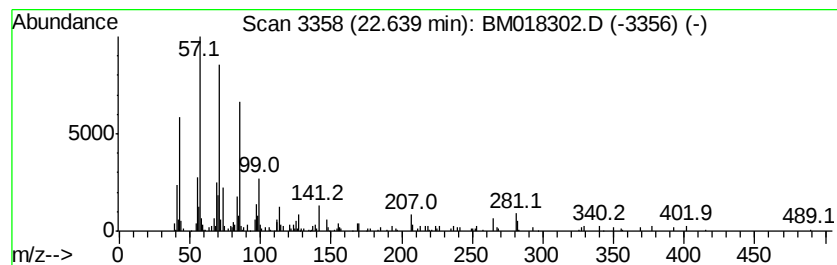
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Heptacosane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.64	3.31 ng	191693	Perylene-d12	23.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	80
2			Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	80
3			Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	74
4			triacontane	422	C30H62	000638-68-6	74
5			Heneicosane	296	C21H44	000629-94-7	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018302.D
Acq On : 19 Dec 2018 18:34
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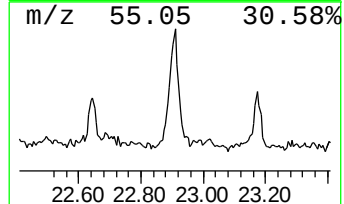
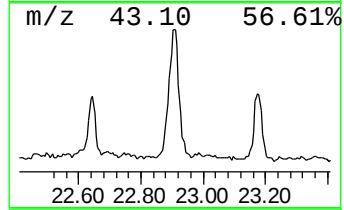
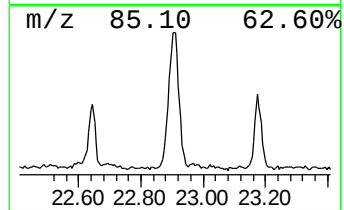
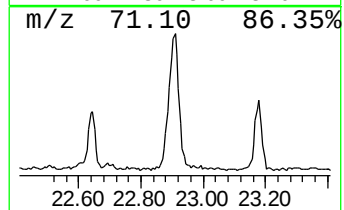
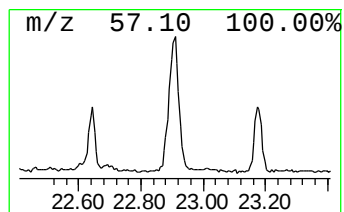
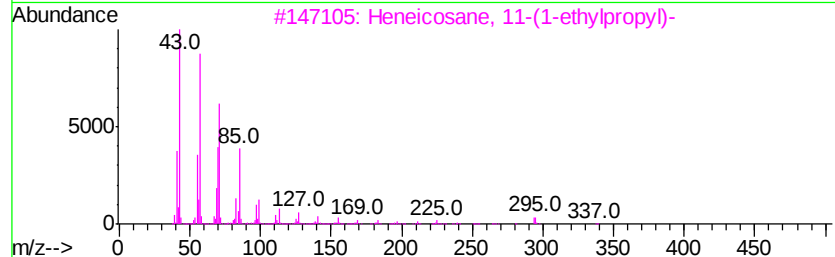
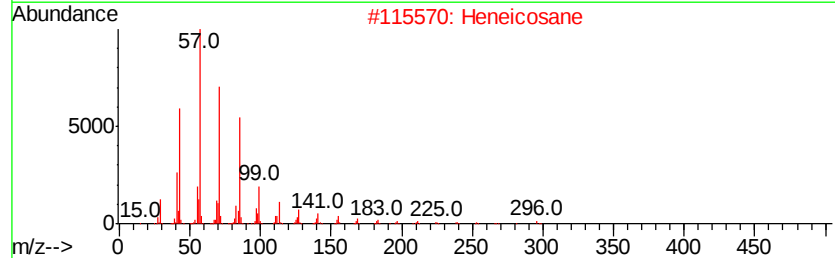
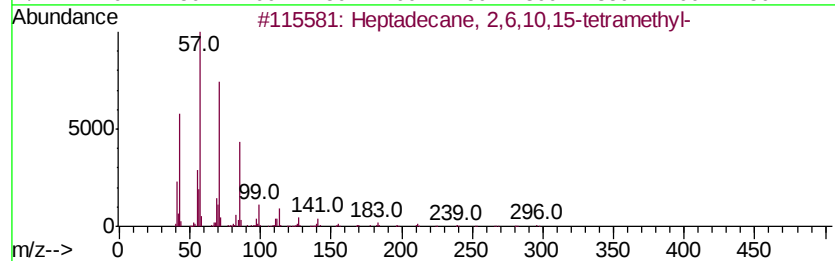
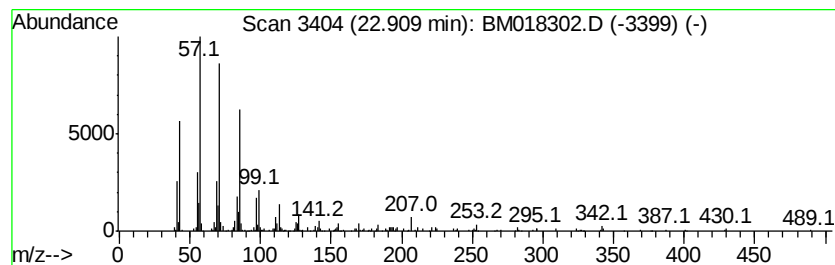
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Heptadecane, 2,6,10,15-tetr... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.91	12.74 ng	736925	Perylene-d12	23.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4		Nonadecane, 2,3-dimethyl-	296	C21H44	075163-99-4	90
5		Eicosane	282	C20H42	000112-95-8	89



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018302.D
Acq On : 19 Dec 2018 18:34
Operator : JU/SJ
Sample : J6465-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EB01_0-2

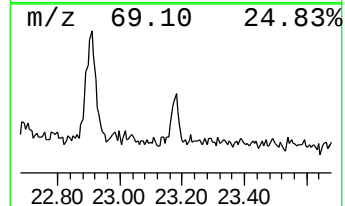
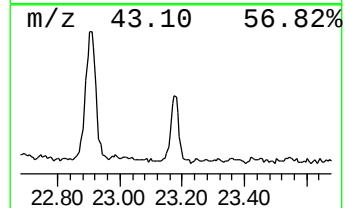
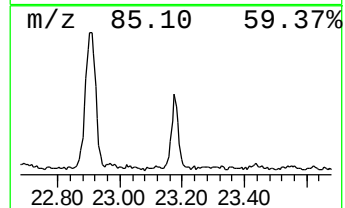
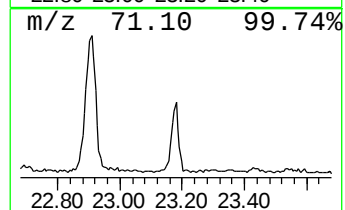
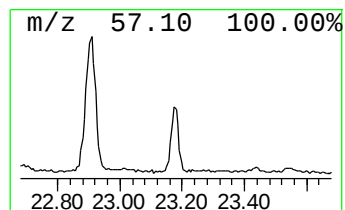
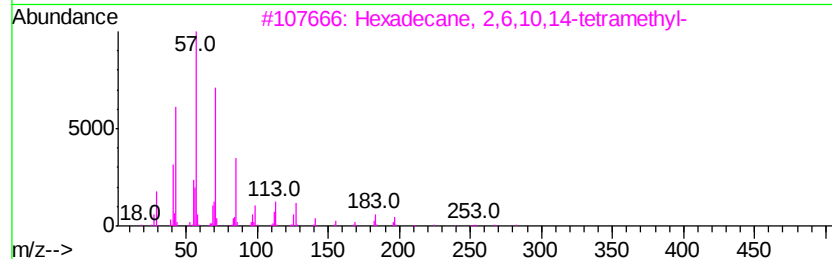
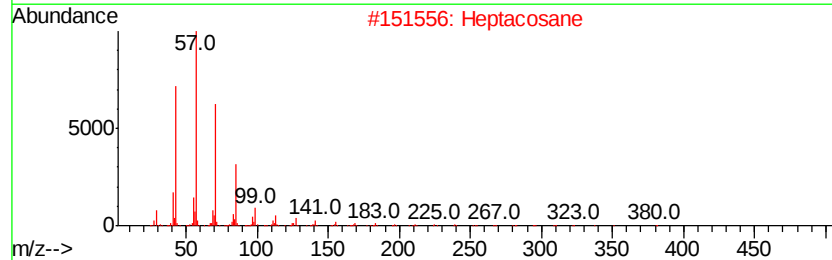
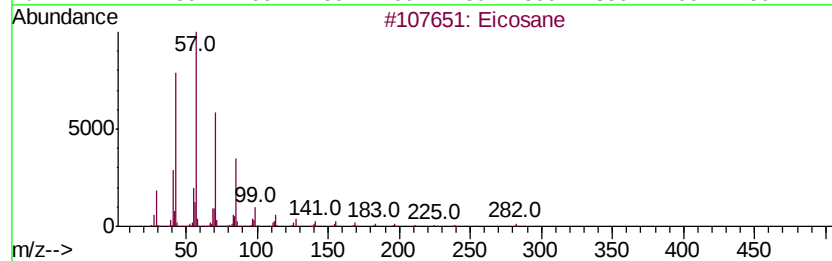
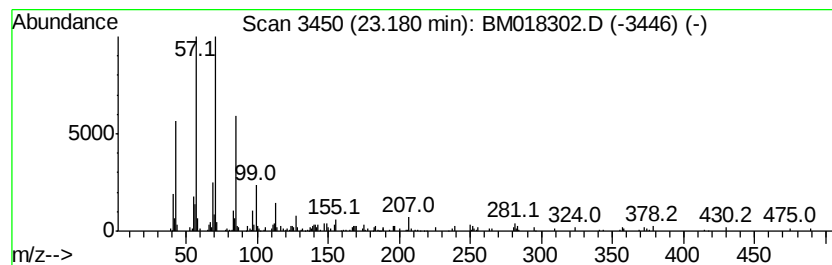
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Eicosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	4.47 ng	258811	Perylene-d12	23.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	90
2			Heptacosane	380	C27H56	000593-49-7	83
3			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	80
4			Nonacosane	408	C29H60	000630-03-5	72
5			Hexadecane	226	C16H34	000544-76-3	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM121918\
Data File : BM018302.D
Acq On : 19 Dec 2018 18:34
Operator : JU/SJ
Sample : J6465-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB01_0-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.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...	4.68	3.3	ng	89992	1	7.49	552335	20.0
unknown7.03	7.03	88.6	ng	2446860	1	7.49	552335	20.0
unknown16.33	16.33	2.0	ng	92129	4	16.91	899639	20.0
n-Hexadecanoic acid	17.83	55.0	ng	2474720	4	16.91	899639	20.0
Heptadecane, 9-oc...	18.62	38.5	ng	1733630	4	16.91	899639	20.0
9-Octadecenoic ac...	19.00	3.4	ng	150964	4	16.91	899639	20.0
Octadecanoic acid	19.12	22.7	ng	1249430	5	21.13	1101060	20.0
Heneicosane	20.70	36.4	ng	2001410	5	21.13	1101060	20.0
Cyclotetradecane	20.86	7.2	ng	398325	5	21.13	1101060	20.0
Squalene	22.28	74.0	ng	4283050	6	23.29	1157140	20.0
Heptacosane	22.64	3.3	ng	191693	6	23.29	1157140	20.0
Heptadecane, 2,6,...	22.91	12.7	ng	736925	6	23.29	1157140	20.0
Eicosane	23.18	4.5	ng	258811	6	23.29	1157140	20.0