

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM053019\
 Data File : BM020599.D
 Acq On : 29 May 2019 14:56
 Operator : JU/SJ
 Sample : K2790-02RE
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SSSI-0509-DH-4RE

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-BM052419.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	5.205	372	377	396	rBV	686341	1136272	36.27%	6.529%
2	6.804	643	649	665	rBV	641588	1202849	38.40%	6.911%
3	7.157	702	709	727	rBV	758860	1333180	42.56%	7.660%
4	7.622	783	788	798	rBV	141989	258270	8.25%	1.484%
5	7.940	835	842	855	rBV	570098	993066	31.70%	5.706%
6	8.798	981	988	1011	rBV	310803	707306	22.58%	4.064%
7	10.416	1256	1263	1275	rBV	165489	313634	10.01%	1.802%
8	12.898	1679	1685	1705	rBV	1107095	1662891	53.09%	9.554%
9	13.751	1824	1830	1849	rBV	109039	172963	5.52%	0.994%
10	14.286	1915	1921	1930	rBV2	326624	499094	15.93%	2.868%
11	15.786	2170	2176	2193	rBV	1182538	1831645	58.47%	10.524%
12	17.039	2383	2389	2404	rBV2	399090	668831	21.35%	3.843%
13	17.933	2535	2541	2555	rBV2	90857	208500	6.66%	1.198%
14	19.110	2736	2741	2747	rBV	41758	61885	1.98%	0.356%
15	19.221	2755	2760	2778	rBV2	174847	360867	11.52%	2.073%
16	19.474	2799	2803	2809	rVB	37194	54504	1.74%	0.313%
17	19.674	2832	2837	2848	rBV	2257244	3132385	100.00%	17.998%
18	20.374	2952	2956	2959	rBV3	52462	84046	2.68%	0.483%
19	20.939	3048	3052	3062	rBV3	159218	257658	8.23%	1.480%
20	21.239	3098	3103	3108	rBV	623403	913838	29.17%	5.251%
21	21.374	3124	3126	3129	rVB3	48577	37520	1.20%	0.216%
22	21.803	3196	3199	3202	rBV	84582	117039	3.74%	0.672%
23	22.256	3273	3276	3280	rBV2	113602	180061	5.75%	1.035%
24	22.756	3358	3361	3365	rVB	119562	145090	4.63%	0.834%
25	23.315	3452	3456	3461	rVB	133862	216640	6.92%	1.245%
26	23.468	3476	3482	3491	rBV	424948	854403	27.28%	4.909%

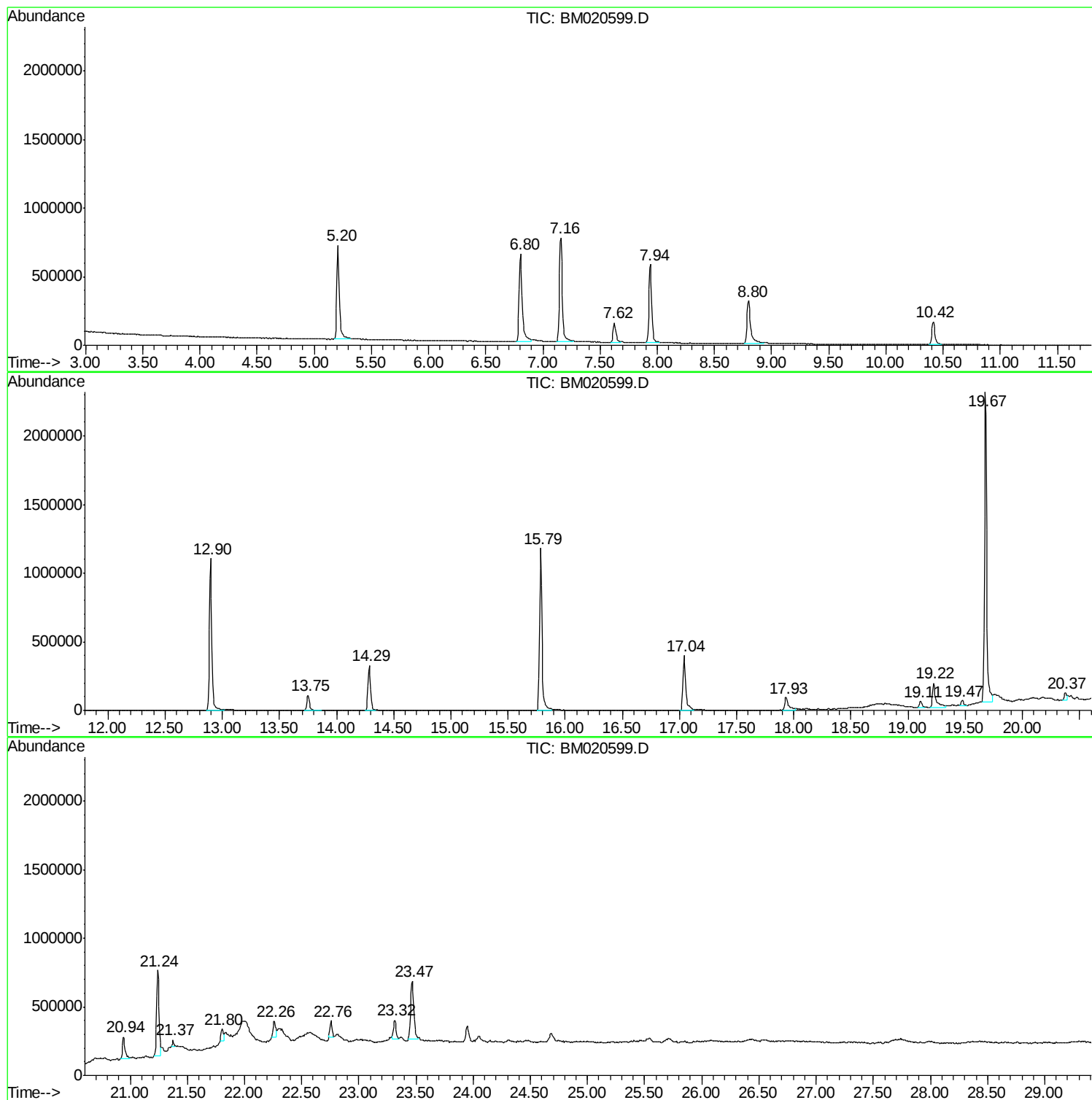
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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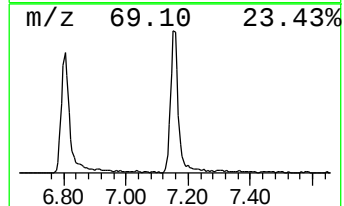
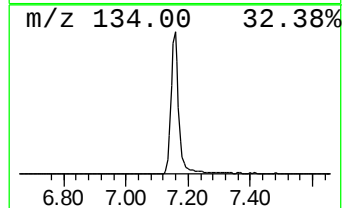
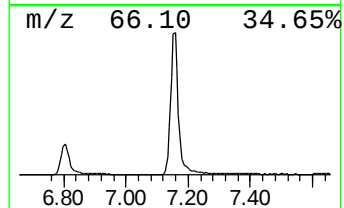
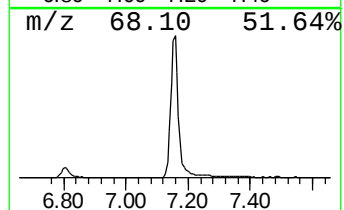
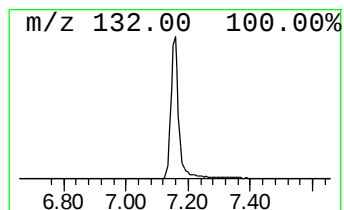
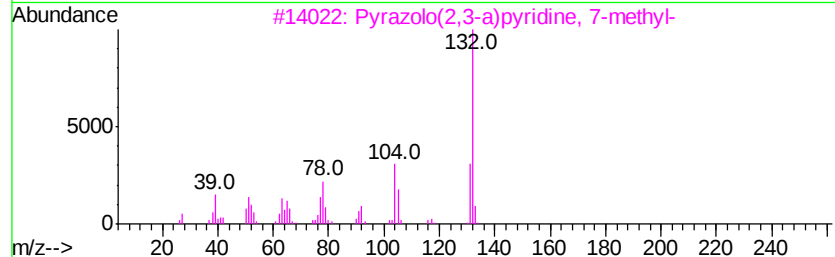
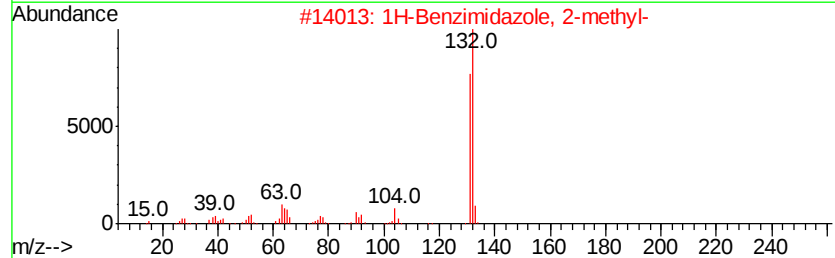
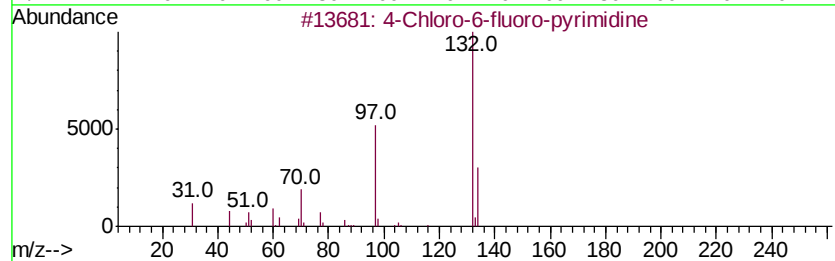
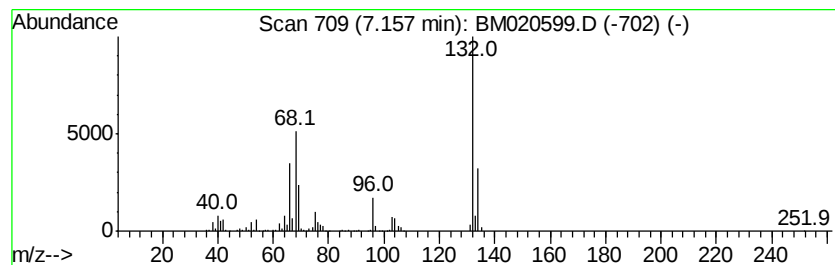
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.16 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	103.24 ng	1333180	1,4-Dichlorobenzene-d4	7.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12



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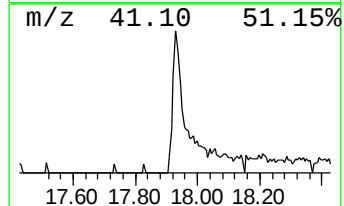
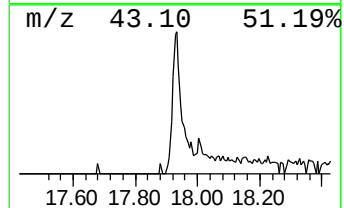
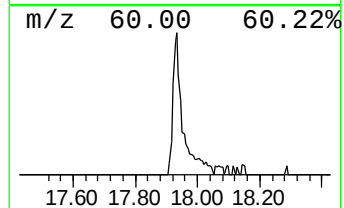
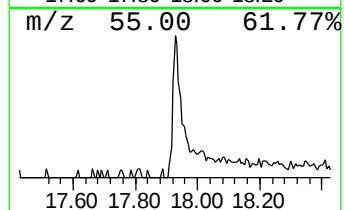
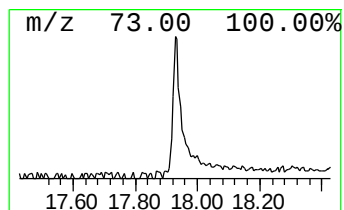
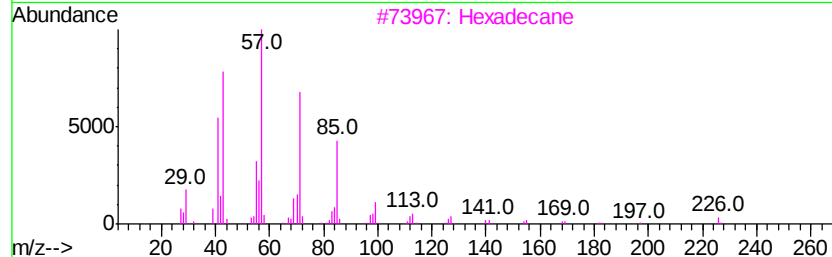
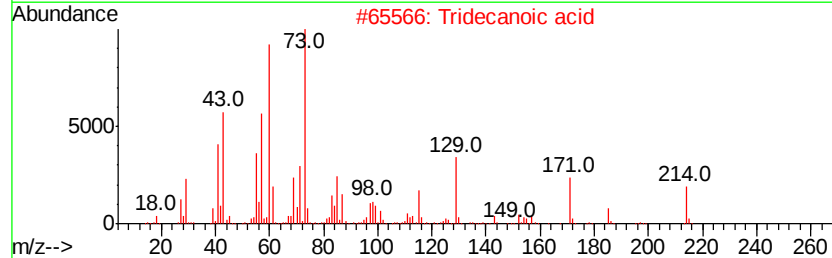
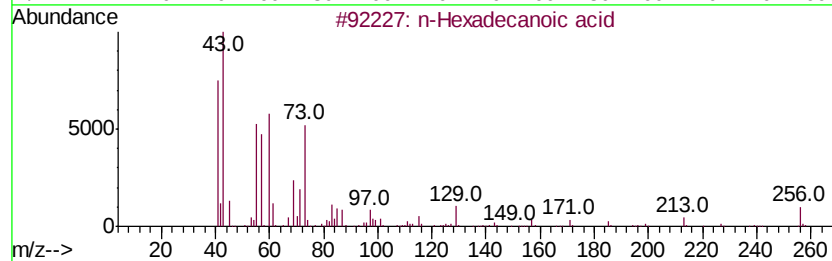
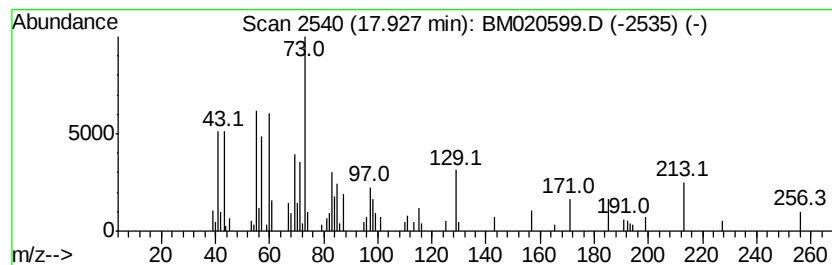
Instrument :
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ClientSampleId :
SSSI-0509-DH-4RE

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.93	6.23 ng	208500	Phenanthrene-d10		17.04
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	38
3	Hexadecane	226	C16H34	000544-76-3	18
4	Tetradecane	198	C14H30	000629-59-4	14
5	1-Nonene, 4,6,8-trimethyl-	168	C12H24	054410-98-9	14



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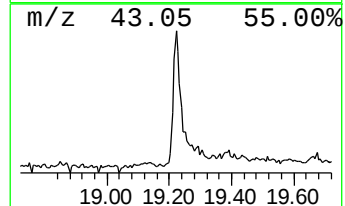
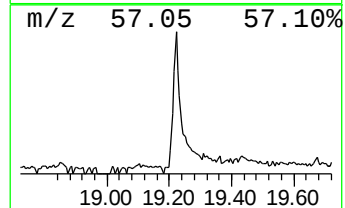
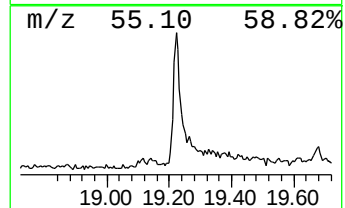
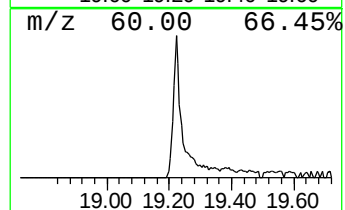
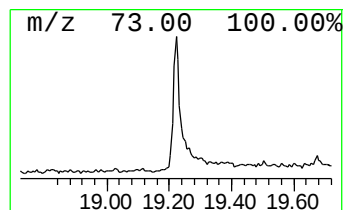
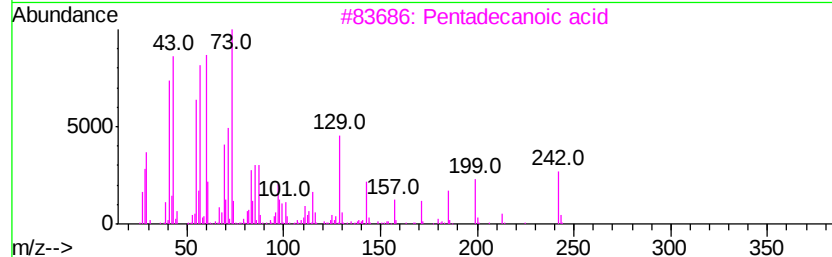
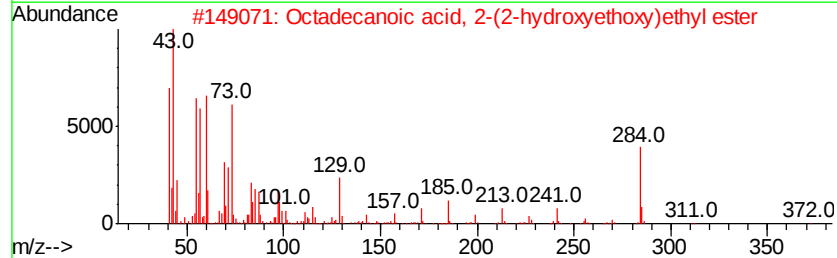
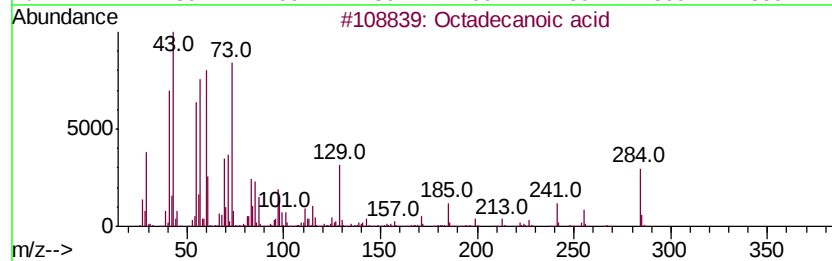
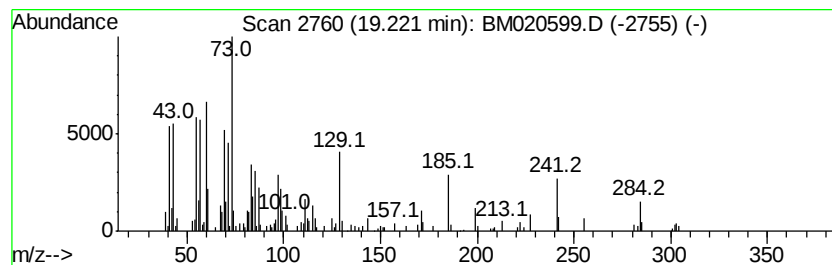
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.22	7.90 ng	360867	Chrysene-d12	21.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	86
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	52
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5		n-Decanoic acid	172	C10H20O2	000334-48-5	49



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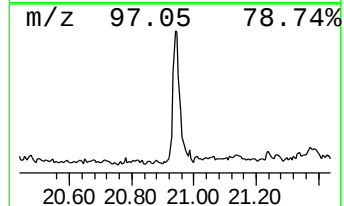
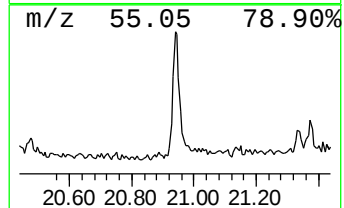
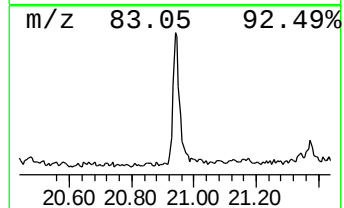
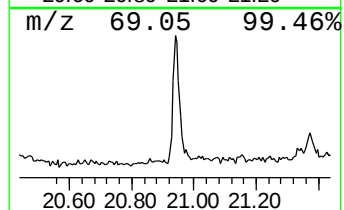
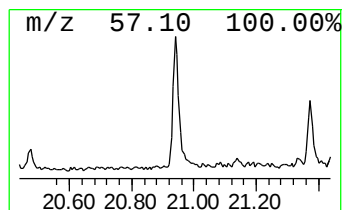
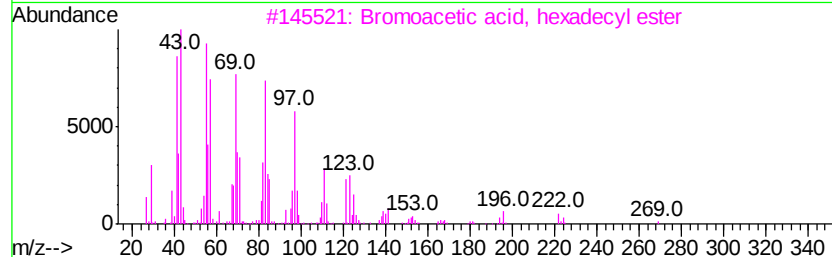
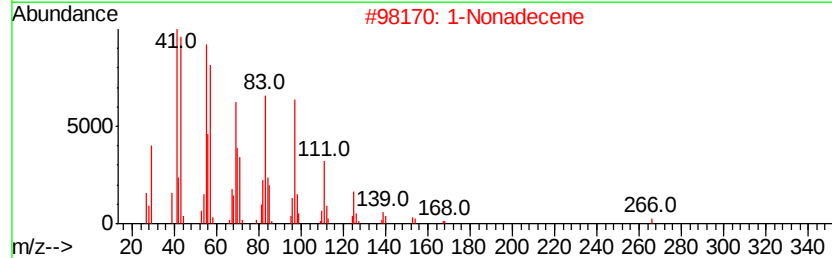
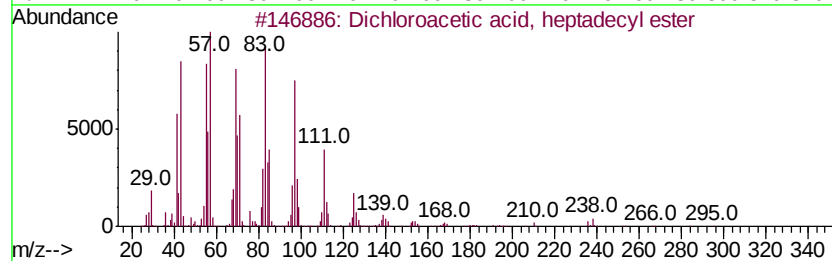
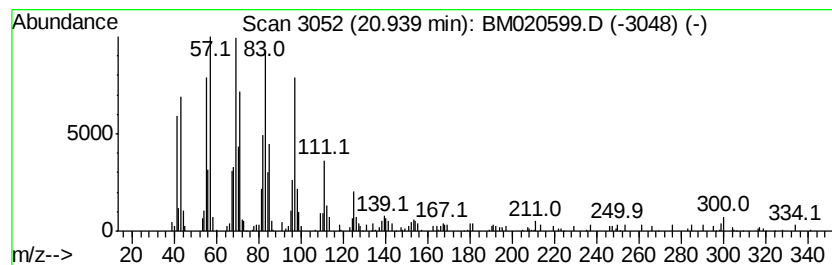
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Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.94	5.64 ng	257658	Chrysene-d12	21.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2		1-Nonadecene	266	C19H38	018435-45-5	92
3		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
4		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	90
5		17-Pentatriacontene	491	C35H70	006971-40-0	90



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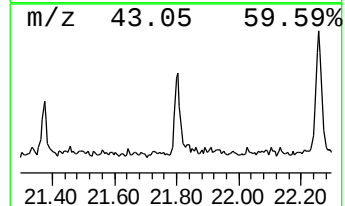
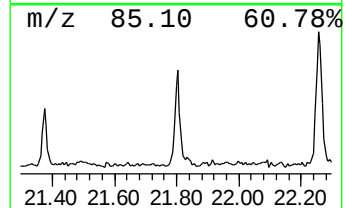
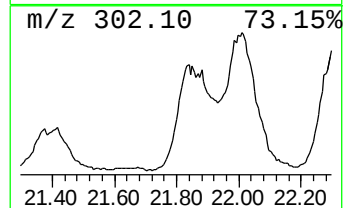
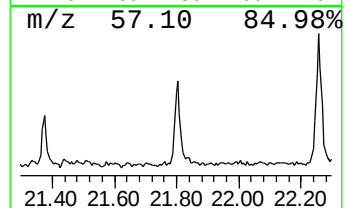
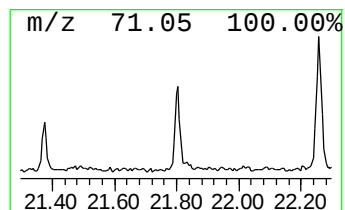
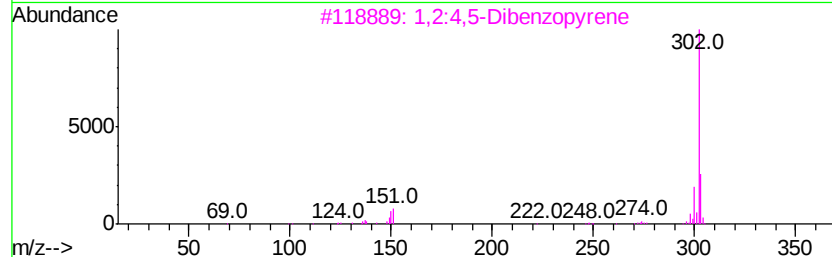
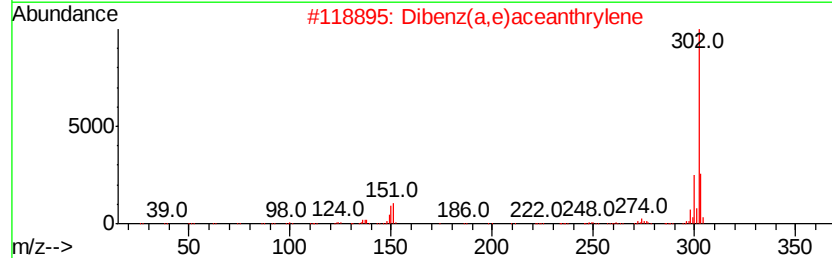
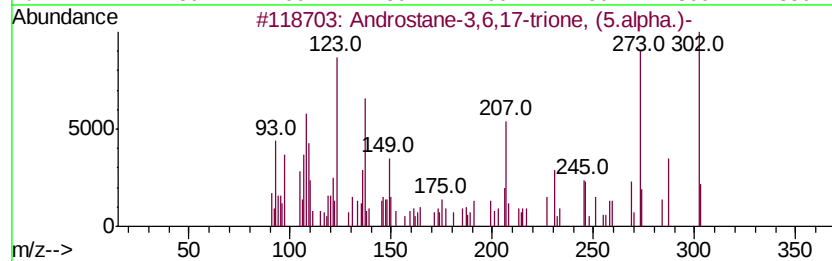
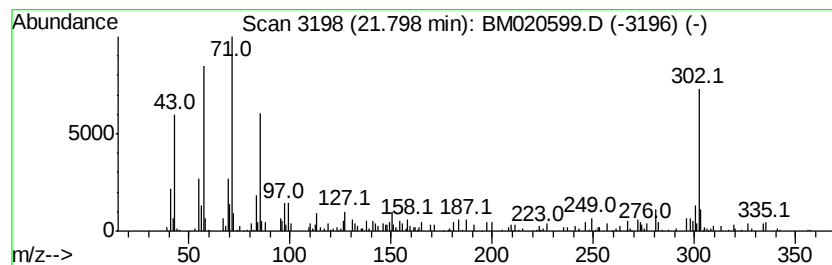
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Peak Number 6 Androstane-3,6,17-trione, (... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.80	2.56 ng	117039	Chrysene-d12	21.24		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Androstane-3,6,17-trione, (5.alpha...	302	C19H26O3	002243-05-2	92
2		Dibenz(a,e)aceanthrylene	302	C24H14	005385-75-1	70
3		1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	70
4		3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	62
5		1,2:3,4-Dibenzopyrene	302	C24H14	000191-30-0	58



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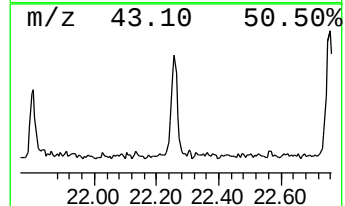
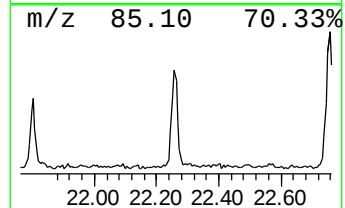
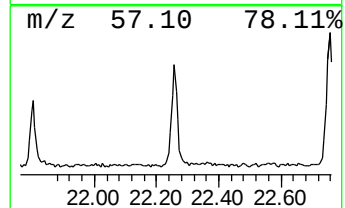
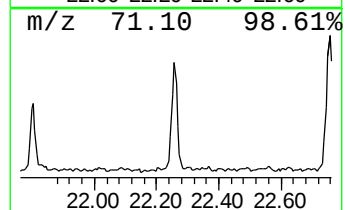
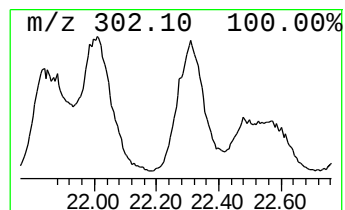
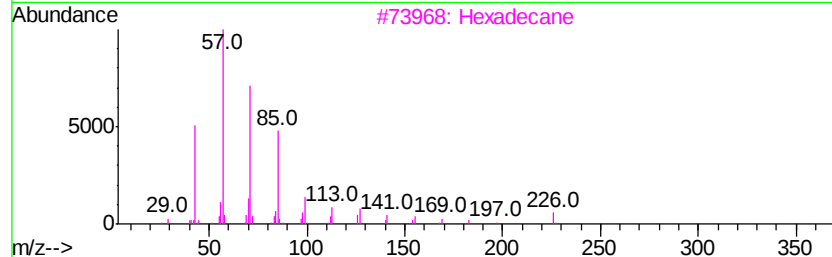
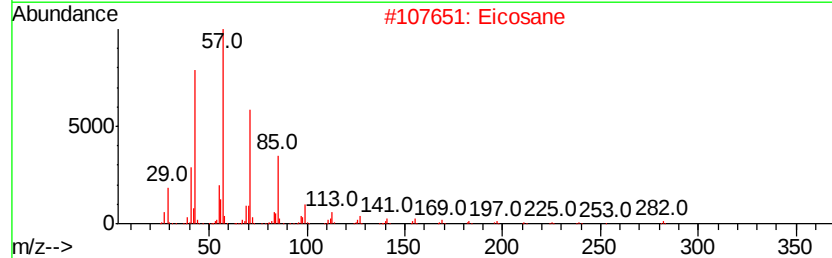
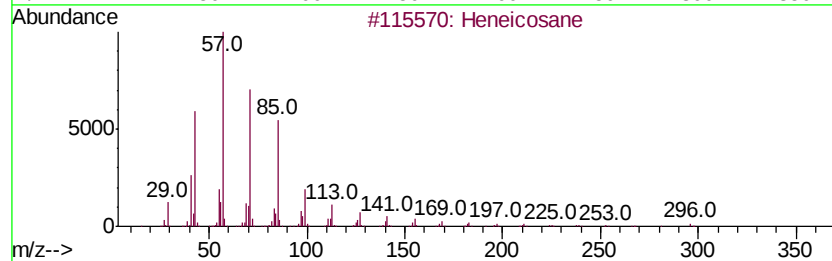
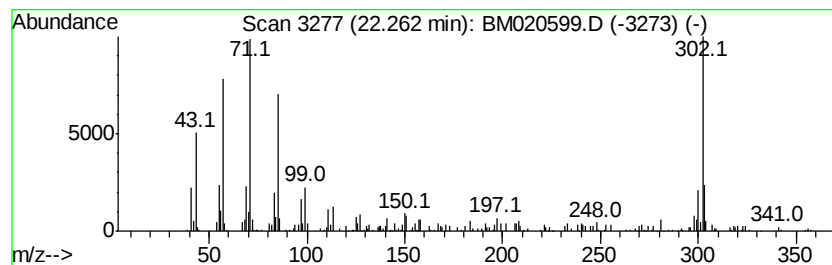
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.26	3.94 ng	180061	Chrysene-d12	21.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	86
2		Eicosane	282	C20H42	000112-95-8	83
3		Hexadecane	226	C16H34	000544-76-3	60
4		Pentadecane	212	C15H32	000629-62-9	60
5		Octacosane	394	C28H58	000630-02-4	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM053019\
Data File : BM020599.D
Acq On : 29 May 2019 14:56
Operator : JU/SJ
Sample : K2790-02RE
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SSSI-0509-DH-4RE

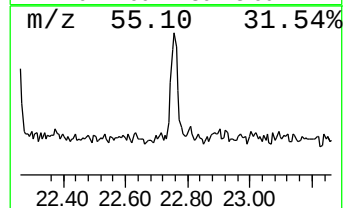
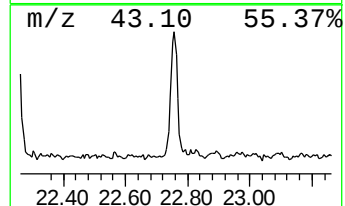
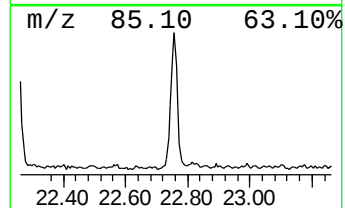
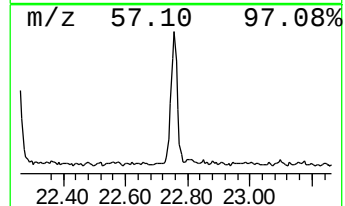
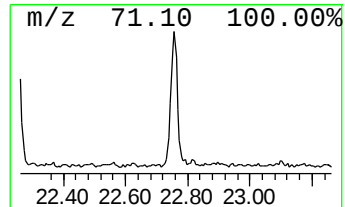
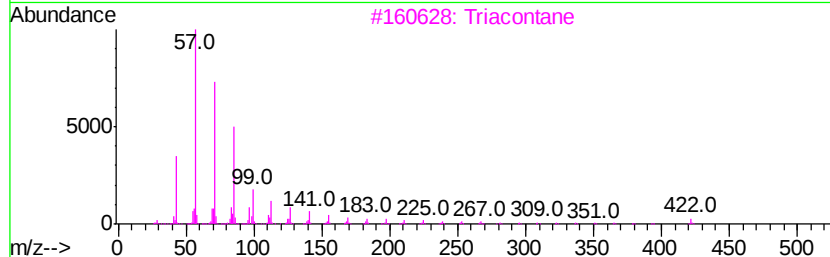
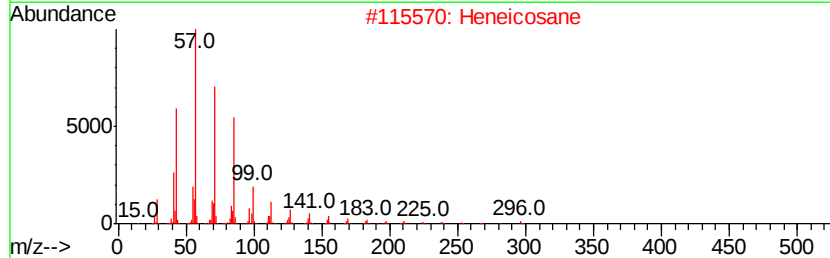
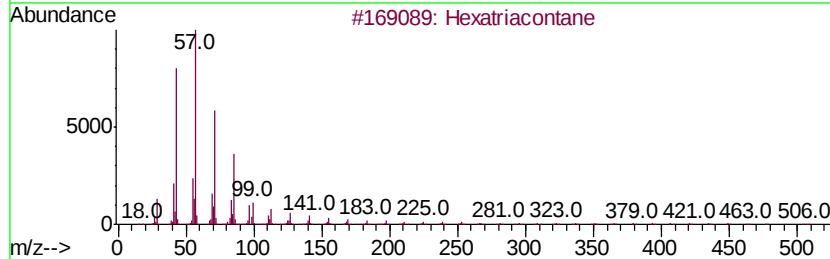
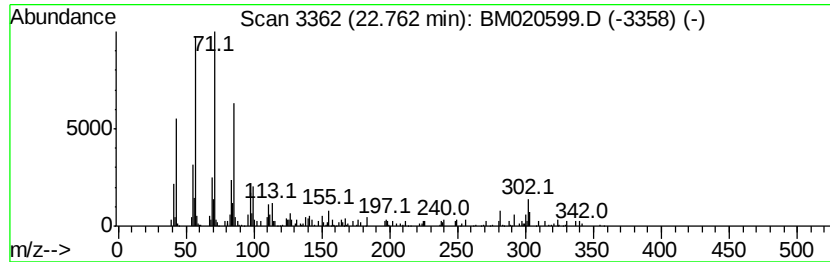
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexatriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.76	3.40 ng	145090	Perylene-d12	23.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexatriacontane	507	C36H74	000630-06-8	86
2		Heneicosane	296	C21H44	000629-94-7	83
3		Triacontane	422	C30H62	000638-68-6	81
4		Tetratriacontane	479	C34H70	014167-59-0	80
5		Tetratetracontane	619	C44H90	007098-22-8	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM053019\
Data File : BM020599.D
Acq On : 29 May 2019 14:56
Operator : JU/SJ
Sample : K2790-02RE
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SSSI-0509-DH-4RE

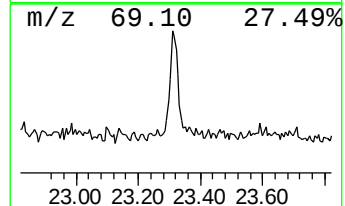
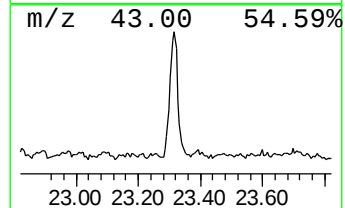
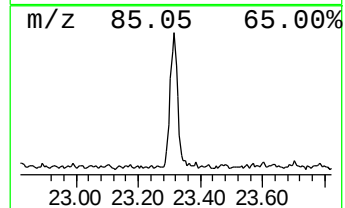
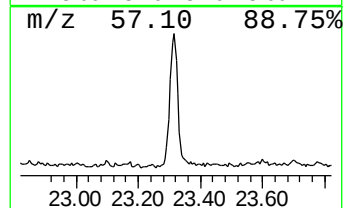
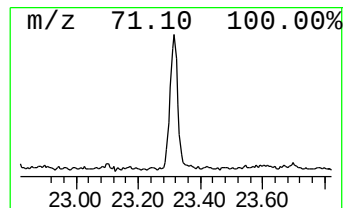
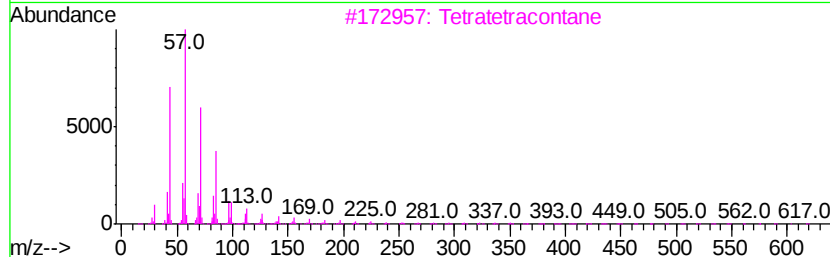
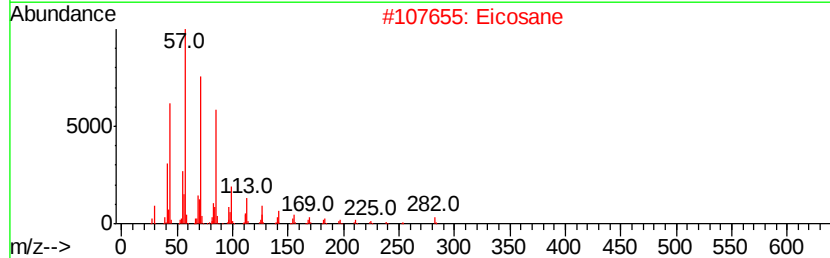
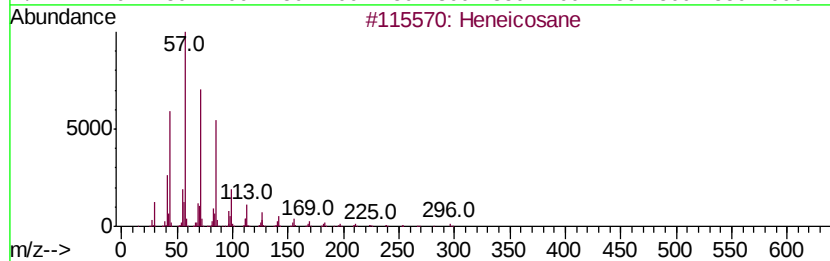
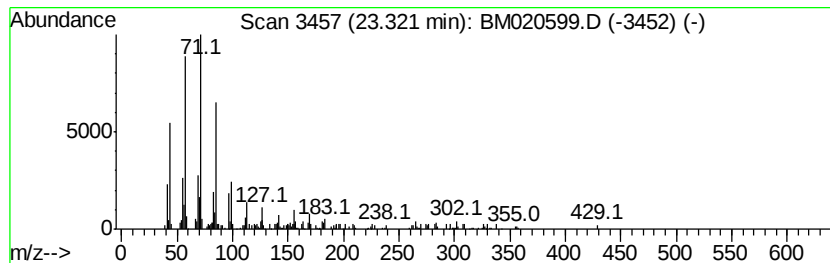
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.32	5.07 ng	216640	Perylene-d12	23.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Eicosane	282	C20H42	000112-95-8	83
3	Tetratetracontane	619	C44H90	007098-22-8	83
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	76
5	Heptacosane	380	C27H56	000593-49-7	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM053019\
Data File : BM020599.D
Acq On : 29 May 2019 14:56
Operator : JU/SJ
Sample : K2790-02RE
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SSSI-0509-DH-4RE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM052419.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
unknown7.16	7.16	103.2	ng	1333180	1	7.62	258270	20.0
n-Hexadecanoic acid	17.93	6.2	ng	208500	4	17.04	668831	20.0
Octadecanoic acid	19.22	7.9	ng	360867	5	21.24	913838	20.0
Dichloroacetic ac...	20.94	5.6	ng	257658	5	21.24	913838	20.0
Androstane-3,6,17...	21.80	2.6	ng	117039	5	21.24	913838	20.0
Eicosane	22.26	3.9	ng	180061	5	21.24	913838	20.0
Hexatriacontane	22.76	3.4	ng	145090	6	23.47	854403	20.0
Heneicosane	23.32	5.1	ng	216640	6	23.47	854403	20.0